Factors Governing Chiral Recognition Phenomena — A Multiple Approach

***

Einflußgrößen für chirale Erkennungsphänomene — ein multipler Ansatz

Dissertation

der Fakultät für Chemie und Pharmazie
der Eberhard-Karls-Universität Tübingen

zur Erlangung des Grades eines Doktors
der Naturwissenschaften

2001

vorgelegt von
Wei Zhou

Tag der mündlichen Prüfung:	27. 02. 2001
Dekan:	Prof. Dr. H. Probst
1. Berichterstatter:	Prof. Dr. B. Koppenhoefer
2. Berichterstatter:	Prof. Dr. G. Häfelinger

This thesis has been prepared under the guidance of Prof. Dr. Bernhard Koppenhoefer between June 1997 and October 2000 at the Institut fuer Organische Chemie der Universitaet Tuebingen.

My cordial thanks are to Prof. Dr. B. Koppenhoefer for proposing the topic, for his ample support and for his interest in this investigation.

Acknowledgements

I would like to acknowledge Mrs. P. T. Nguyen, Mrs. M. Lange and Mr. B. Maier for recording the NMR-spectra, Mr. H. Bartholomä and Mr. R. Müller for MS-spectra, Mr. W. Bock for elemental analyses, and Dr. U. Dettlaff for recording the IR-spectra.

My special thanks are due to Gesellschaft Deutscher Chemiker (GDCh) and to Deutsche Forschungsgemeinschaft (DFG) for grants.

Moreover, I would like to thank to my colleagues, Dr. A. Jakob, Dr. B. Christian, Dipl. Chem. R. Schlunk, Dipl. Chem. S. Wuerthner and Dr. Guo-Sheng Yang for the good atmosphere, for fruitful discussions and helpful suggestions.

To my parents and my husband

Abbreviations and Definitions

α	resolution factor
ACN	acetonitrile
bp	boiling point
CDR	Chiral Derivatizing Reagent
CMP	Chiral Mobile Phase
CPG	Controlled-Porous Glass
CSP	Chiral Stationary Phase
δ	chemical shift
DCM	dichlormethane
de	diastereomer excess
DIBAH	diisobutylaluminiumhydride
DMF	N,N-dimethylformamide
DMSO	dimethylsulfoxide
dr	diastereomer resolution
e	erythro
EA	Elemental Analysis
EI	Electron Impact
er	enantiomer resolution
FID	Flame Ionization Detector
ΔG	free enthalpy difference
g	gauche
ΔH	enthalpy difference
HPLC	High Performance Liquid Chromatography
HTS	High Throughput Screening
IR	Infrared spectroscopy
MBE	(3aR-(2α,3a α,4β,7β,7a α))-Octahydro-7,8,8,trimethyl-4,7-methanobenzofuran-2-yl
MHz	Megahertz
ml	milliliter
mmol	millimol
MO	Molecular Orbital

mp	melting point
MS	Mass Spectroscopy
NMR	Nuclear Magnetic Resonance Spectroscopy
RIFS	Reflectometric Interference Spectroscopy
ΔS	entropy difference
t	threo
THP	tetrahydropyran
TFA	trifluoroacetic acid
TSMR	Thickness Shear-Mode Resonators
ppm	parts per million
p-TsOH	p-toluene sulfonic acid
UV	Ultraviolet Visible
Val	Valine

Contents

Abstract

A multiple approach is desirable to collect an amount of information that is sufficient to analyze the complex phenomenon “chiral recognition”. In this thesis, factors governing three different systems have been studied by applying such a multiple approach.

In chapter 1, an intriguing new methodology is reported. Here, a weak covalent bond is formed between a chiral selector of the acetal type and suitable nucleophiles. Multiple sets of racemic nucleophiles have been used to form an acetal, and the selector has been attached to a multitude of solid supports. Usually, a nonpolar, nonprotic solvent and acid catalysis are favourable conditions. A controlled release of the analyte by lowering the pH allows to effectively separate the enantiomers.

In chapter 2, the multiple approach is applied to a complete search through all possible local minima of a medium sized organic molecule, i.e., N-trifluoroactyl-L-phenylalanine 3'-pentyl ester **S-24**. The concept of chirality enhancement through preferential induction of particular chiral conformations of the flexible 3’-pentyl ester group was scrutinized in an extended search of 4224 permutations of 8 essential single bonds, 2083 of which were found to exist within the limits of the MM2 method applied. Boltzmann analysis at 300 K reveals a uniform twist in the intrinsically prochiral 3’-pentyl group, where $\mathbf{g}^-$ conformations with anti-clockwise orientation of two crucial dipoles are preferred.

In chapter 3, heterocyclic oxiranes are presented that have been varied systematically for the first time, and isolated as pure racemic compounds. These synthons do not only bear a potential for finding new drug candidates by combining this set of 14 reactive compounds with well known and extended sets of classical nucleophilic pharmacophores, but they have also served as a test set for the systematic study of chiral recognition phenomena with a series of 5 structurally related chiral HPLC phases of the DAICEL type. It has turned out that the main rule established to predict enantiomer separation in this family of chiral phases is indeed valid, namely, each of the 11 compounds bearing an aromatic or containing heterocyclic ring could be separated into the enantiomers, while no separation was found for any of the 3 simple (hetero-) aliphatic systems that did not contain such an additional π system.

In conclusion, the multiple approach has proven necessary and valid to establish rules and guidelines for further progress in discovery of chiral recognition phenomena.

Part 1. Diastereoselective Synthesis and Enantiomer Separation through Adduct Formation of Camphorlactol and its Derivates

1.1. Introduction

Stereochemistry (from the Greek '*stereos'*, meaning solid) refers to chemistry in three dimensions. It was not until 1874 that van't Hoff in Utrecht, the Netherlands and Le Bel (1874) in Paris, France independently and almost simultaneously proposed the case for enantiomerism in substance of the type C_{abcd}: the four substituents are arranged tetrahedrally around the central carbon atom to which they are linked. The four linkages to a carbon atom point towards the center of a regular tetrahedron (Figure1-1); thus, two nonsuperposable arrangements (enantiomers) are possible.

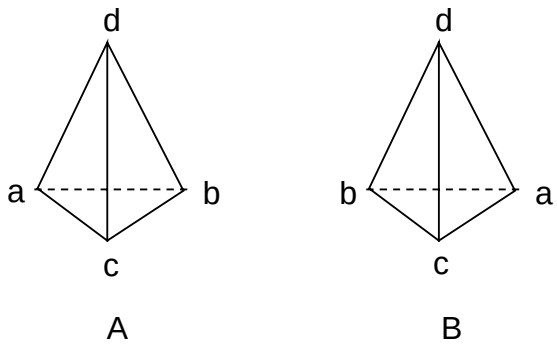


Figure 1-1: Tetrahedral carbon

The model corresponding to a given enantiomer (e.g., Figure 1-1 A), as well as the molecule that it represents, is called "chiral" (meaning hand, Greek '*cheir'*), because, like hands, the molecules are not superposable with their mirror images [1].

A stereoselective synthesis involves introduction of a stereogenic center into a molecule in such a way that one stereoisomer of the product is predominantly formed. The synthesis may be either enantioselective or diastereoselective. Diastereoselective synthesis may either start from a single enantiomer or start from a racemate; indeed, any excess of one enantiomer over the other may be possible between these extremes. In any case, the introduction of a new stereogenic center into a chiral substrate is the crucial step [2].

Typically, the reaction of an achiral precursor with a chiral reagent (or in the presence of a chiral auxiliary, called a chiral adjuvant) will give a chiral reaction product.

Conformational analyses are fundamental to a proper understanding of the structure and reactivity of organic compounds. The introduction of a single oxygen atom into a carbon chain or ring has only a minor effect on its conformation. Hence, the conformational properties of the tetrahydropyran ring resemble those of cyclohexane, as the chair form is preferred.

The chair form preferred by a substituted cyclohexane is generally the one with the higher number of equatorial substituents, thus minimizing the number of gauche interactions and non-bonded repulsions between axial substituents. On the other hand, tetrahydropyran is known for preferring electronegative substituents (e.g., –OH) close to the ring oxygen to be axially oriented (see Figure 1-2); this is called the *anomeric effect* [3]. The reason for the anomeric effect is the stability of the electronic interaction between the σ* orbital of the axially oriented C-OH group and the electron lone pair of the ring oxygen atom.

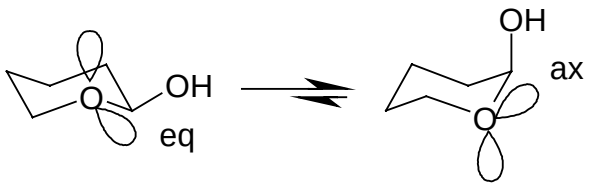
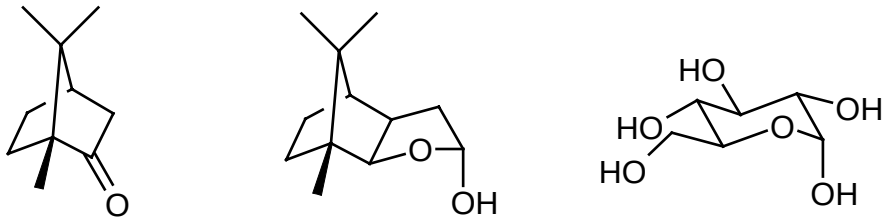


Figure 1-2: The axial position of an electronegative substituent is preferred in the THP system

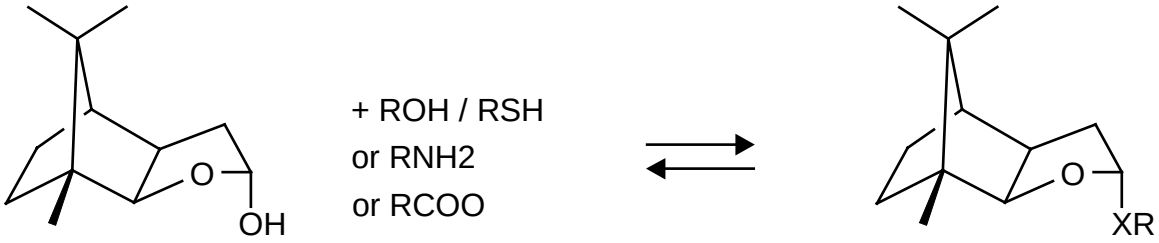
If there are several substituents, the steric effect is predominant, such as in β-D-Glucose [3]. As depicted in Figure 1-3, the rigid structure (1R,4R)-(+)-camphor may be fused to a furanol ring. Through this, a steric fixation is achieved, similar in effect to the steric preference for hydroxy substituents in carbohydrate compounds. Therefore, a racemic alcohol can only approach from one side in an electrophilic attack [4], [5], [6]. Through the chiral surroundings of the reaction centre, the preference for one enantiomer of the nucleophile is mediated.



1 **2** **3**

Figure 1-3: Structures of (1R,4R)-(+)-camphor (**1**), exo-lactol (**2**) and α-L-glucose (**3**)

The enantiomerically pure lactol (**2**) is a very versatile anomer-selective protective group and chiral auxiliary; it was used for establishing or enhancing the enantiomeric purity of alcohols, thiols, acids and amines [4] (see Figure 1-4).



2 **4** **5 + 6**

Figure 1-4: Chiral lactols (**2**) are used to separate various racemic compounds (**4**) by forming diastereomers (**5**) and (**6**)

Auxiliaries like camphorlactol react with the enantiomers of alcohols to form diastereomeric compounds or at least adducts which may be distinguished due to their different chemical and physical properties. A useful and versatile class of chiral alcohols is based on the b-pl-H type [7], where “pl” is an aromatic or π-system group, “b” denotes a more or less bulky aliphatic group, and H means hydrogen.

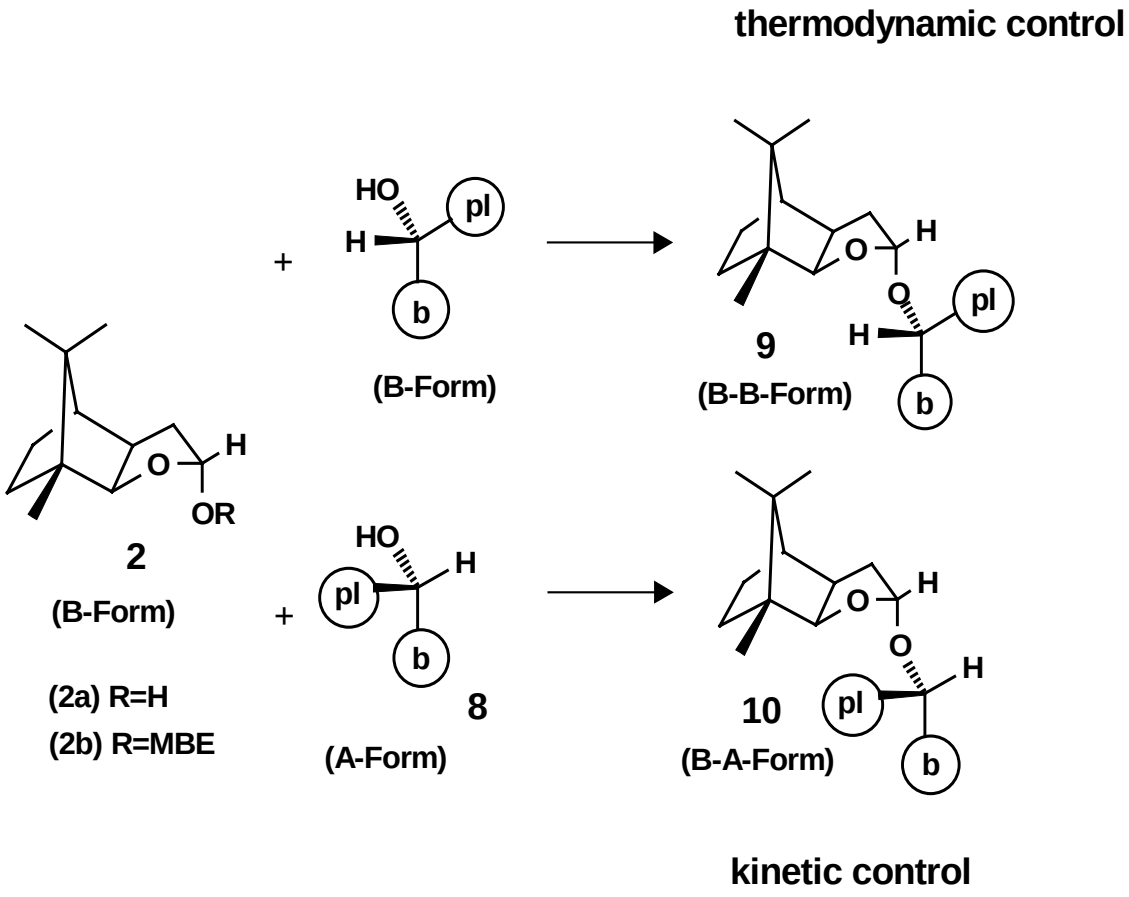


Figure 1-5: Thermodynamic and kinetic control in the enantiomer separation of a b-pl-H type analyte

In Figure 1-5, the reaction of lactol (**2a**) and its condensation product (**2b**) (R=MBE), respectively, with a racemic alcohol is shown. The term 'A-form' is used to describe a clockwise arrangement of the substitutes b, pl, H, while in the 'B-form' the substitutes b, pl, H are arranged in an anti-clockwise manner. The lactol (**2**), as depicted, can react with a racemic alcohol under either thermodynamic or kinetic control; thus, the enantiomer selectivity may be triggered by suitable reaction conditions.

Since enantiomeric drugs, such as (+)- and (-)-sotalol [8], [44] frequently differ in their pharmacodynamic effect, and in many other cases exhibit differences in their pharmacokinetic parameters, there is an ongoing interest in the synthesis and investigation of enantiomers of pharmacologically active compounds. Thus, the chirality of drugs is generally an important issue from pharmacological, toxicological and regulatory points of view, and the development of methods to determine their optical purity is likewise important. Enantiomer separations by

chromatography may be performed after derivatization with optically pure reagents to diastereomers [9], [10], or by the direct separation on chiral stationary phases (CSPs) [11].

The usage of chiral stationary phases (CSPs), chiral mobile phases (CMPs), and pre-column chiral derivatization (also called the indirect resolution mode) are the three major techniques that have frequently been applied to the separation of chiral alcohols by HPLC [12]. In recent years, considerable attention has been directed to the study of the application of CSP and CMP systems, respectively. However, the indirect resolution mode is still of great importance, especially for the biomedical analysis of alcohol drugs, because it has several advantages over the CSP and CMP methods:

(a) Better detectability of alcohols after derivatization.

(b) Employment of conventional LC systems.

(c) Prevention of certain hydroxyl groups from decomposition during chromatography and detection of alcohol drugs.

Lactol 2 reacts with the enantiomers of a given alcohol, thus separation of the diastereomers with HPLC is possible. The main purpose in the current study was to optimize the selectivity and the depletion of enantiomers. The impact of the amounts of solvents and various catalysts on the kinetic behaviour of the enantiomers of a triazol, a cyanohydrin and a simple carbinol was of particular interest. Derivatives of the lactol, including sulfochlorides, were also used to investigate and optimize the selectivity and the preferential depletion of one enantiomer during the course of the reaction.

1.2. Fundamentals

1.2.1. General

Chiral alcohols and their derivatives are ubiquitous, with numerous examples occurring as natural products, as well as in intermediates for the synthesis of other chiral molecules. Chiral alcohols, being found in a variety of biogenic compounds and drugs such as the terpenoid family, steroids and insect pheromones, are often of great significance in the field of biomedical research. Therefore, the development of techniques for effective separation, sensitive detection and accurate determination of chiral alcohols is pressingly required in many areas of biomedical research on

these compounds.

The selectivity of diastereomer formation depends on the structure of the chiral moiety of the CDR and on the type of chemical bond formed in the reaction. The aims to instruct the application of a particular chiral reagent and the technical approach to be used should be beneficial to the development of an indirect resolution method for enantiomeric alcohols as well as to the biomedical investigation of the differences between the antipodes of chiral alcohols [12].

Approximately fifty chiral derivatization reagents have been developed thus far. Based on their functional groups, reaction conditions, resolution systems and applications along with the corresponding references, seven types of chiral compounds are discerned: acids, activated acids, chloroformates, isocyanates, carbonyl nitriles, oxazolidin-2-ones and lactones [12]; these reagents react with alcohols to form diastereomeric esters, carbamates and carbonates.

The chiral lactol (**2**) was introduced by Noe et al. in 1982 [13]. The diastereoselectivity for the derivatives formed from this lactol and racemic alcohols is exceptionally high.

Underivatized camphorlactol (**2**) reacts with a variety of substances, rendering it a valuable tool for the enantiopure hydroxyl protection [13], for the separation of racemic alcohols, and for the determination of enantiomeric purity and the absolute configuration of secondary alcohols [14]. The thermodynamically controlled preferential formation of one diastereoisomer can be explained by a simple conformational analysis of the two possible structures by considering steric and stereoelectronic effects for bulky and planar substituents, respectively. It has been described in detail elsewhere [15], [16] (see also Figure 1-5), and is supported by the anomeric effect (see also Figure 1-2).

The analysis of the diastereoselectivity under thermodynamic control, the influence of the stereoelectronic effect as compared to the steric hindrance, and last not least the effect of different solvents, are of particular interest. The focus of our work was aimed at studying the enantioselectivity in the reaction of enantiopure lactol with an excess of racemic alcohols of the b-pl-H type under thermodynamic conditions.

1.2.2. Reversible Adduct Formation with Immobilized Camphorlactol (2)

As stated above, camphorlactol (**2**) and its derivates are useful tools for enantiomer resolution, and they allow the determination of the absolute configuration and enantiomeric purity of alcohols, cyanohydrins, thiols, acids and amines [17]. Immobilization on a solid support i.e., polymers, kieselgel, glass, quarz and membranes, respectively, is supported to facilitate the separation of enantiomers. This principle is the subject of the following part of this thesis.

The possible positions for attachment of suitable anchor groups on camphor (**1**), camphorlacton (**11**) and camphorlactol (**2**) are shown in Figure 1-6.

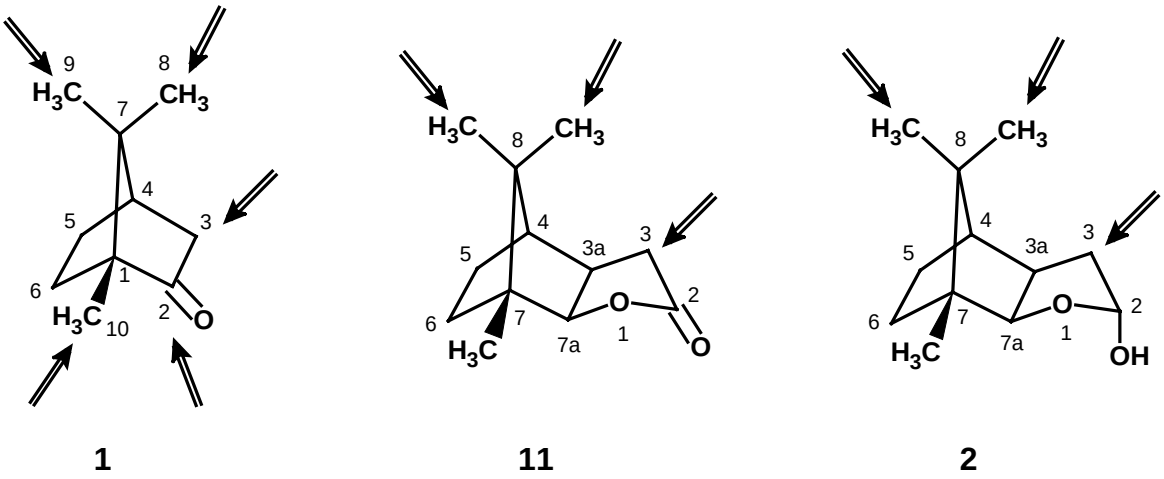


Figure 1-6. The possible positions for derivatization of the target structure

The most convenient position for binding camphorlacton (**11**) and camphorlactol (**2**) to a polymer and kieselgel support, respectiviely, is the 7-methyl group. The purpose of this work is to investigate the synthesis of such derivatives.

1.3. Enantiomer Separation through Adduct Formation with Camphorlactol

1.3.1. Distribution of Enantiomers between Two Liquid Phases

As stated above, enantiomeric drugs exhibit characteristic differences in their pharmacodymic and pharamacokinetic parameters. Distribution of the two enantiomers in a racemate between two liquid phases offers on out of the many possibilties to obtain the pure enantiomeric forms [17], [18], [19]. For an example of medical interest, racemic INN proxyphyllin (**12**) was reacted with the chiral lactol (**2**) (see Figure 1-7)

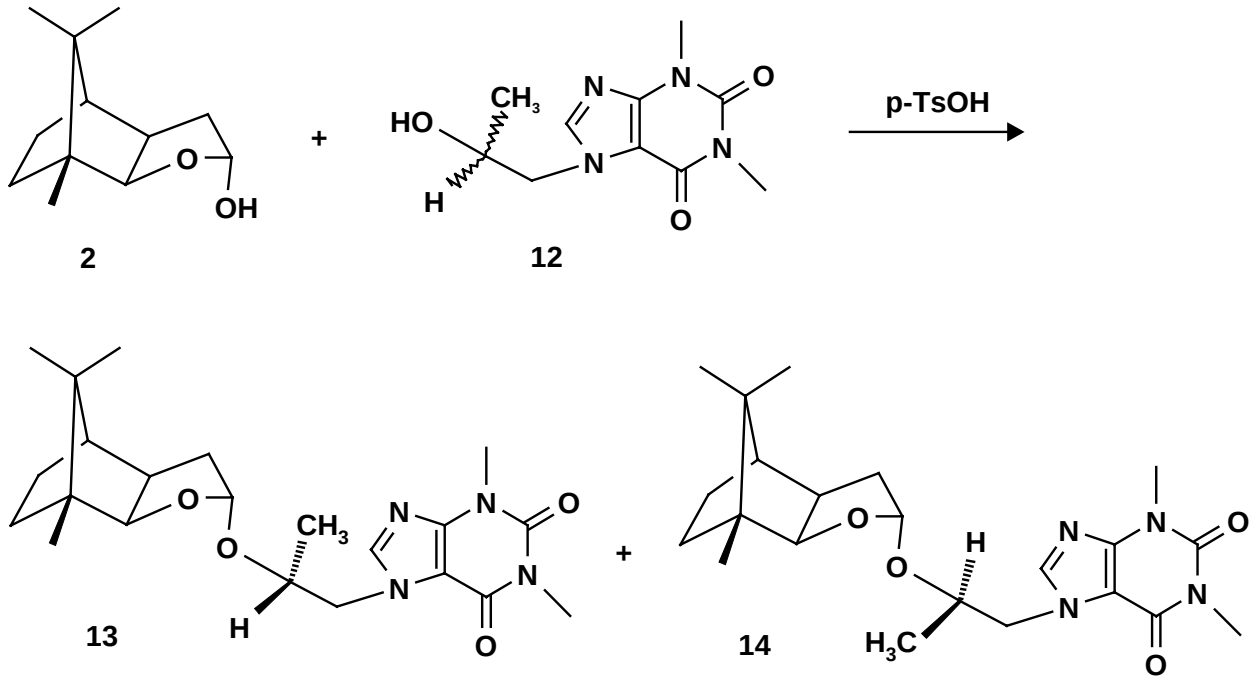
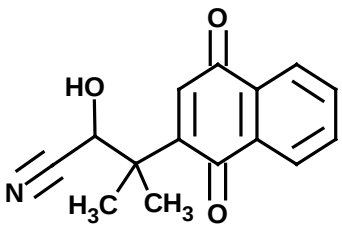
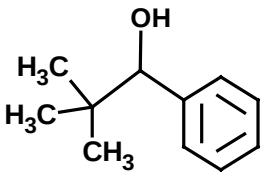
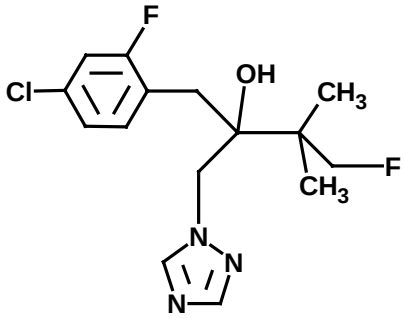


Figure 1-7: Diastereomer formation with racemic drug INN proxyphllin (**12**)

In analogy to the literature [20], lactol (**2**) and racemic proxyphyllin (**12**) (molar ration 1:1) were stirred in dried dichloromethane with p-toluene sulfonic acid (p-TsOH) at room temperature for two hours. After passing a chromatography column filled with triethylamine-impregnated kieselgel, with ethyl acetate as the mobile phase, evaporation of the solvent afforded white crystals.







Cyanhydrin (Nr. 01) ***Carbinol (Nr. 07)*** ***Triazol (Nr.08)***

15 **16** **17**

Figure 1-8: Three test compounds from an unpublished screening study
(*Old nubering as in an unpublished study)

The modified camphorlactol selector reacted in an enantioselective manner with the analyte to form a weak colvalent bond. The two diastereomers **13** and **14** are formed in a ratio of 10:7, and the two diastereomers formed with carbinol (**16**) (see Figure 1-8) and 2 are 73:27, the two diastereomers of cyanohydrin (**15**) (see Figure 1-8) with **2** are 3:2.

We have shown that the native lactol (**2**) is suitable for forming adduct with a large range of chiral molecules; it is not only successful in the transformation with carbinol (**16**) and cyanhydrin (**15**) of the b-pl-H type, but also with previously unpromising basic compounds, as the triazole (**17**) was reacted with good success.

The crucial steps in extractive enantiomer separation (see Figure 1-9) include the formation of adduct, in two diastereomeric forms, the separation of the adduct from unreacted analyte part, separation of the adduct diastereomers by distribution in a Craig apparatus, splitting off the analyte, and recycling the lactol (**2**) auxiliary.

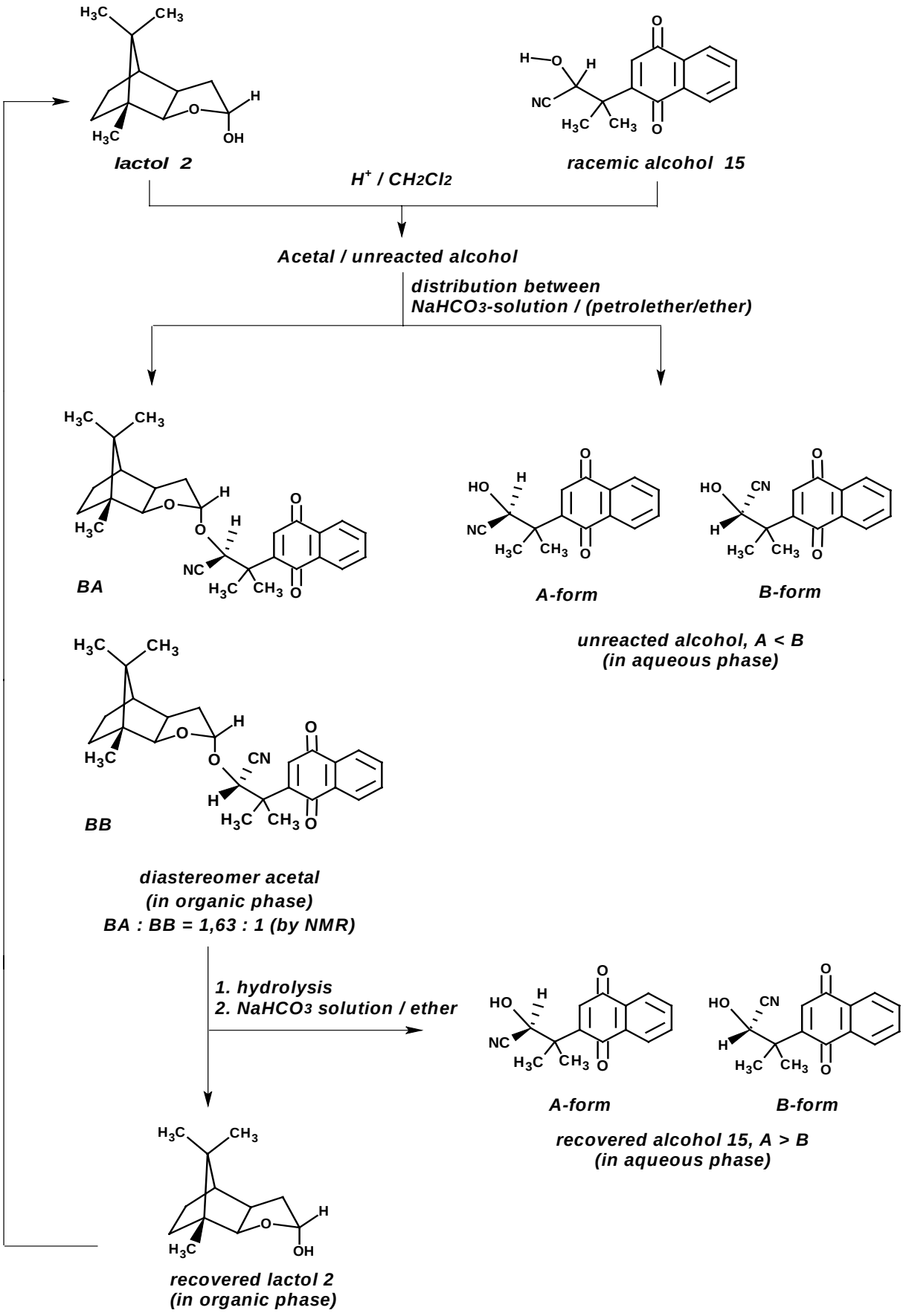
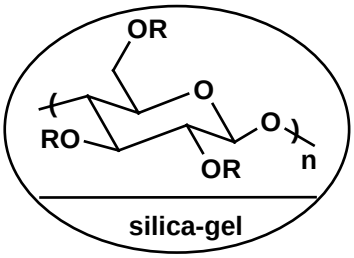
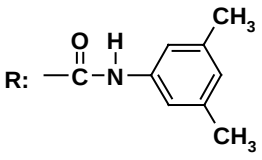
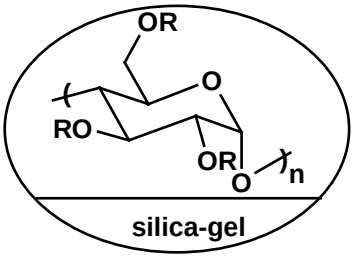
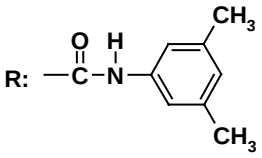
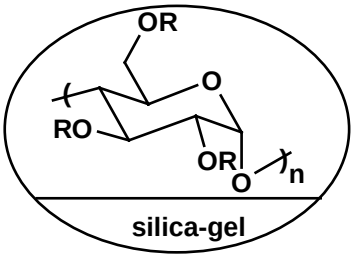
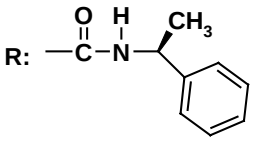
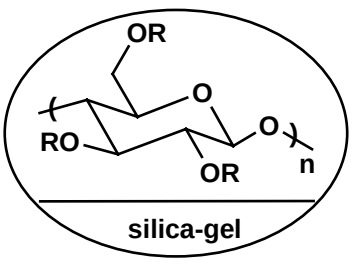
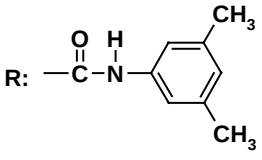


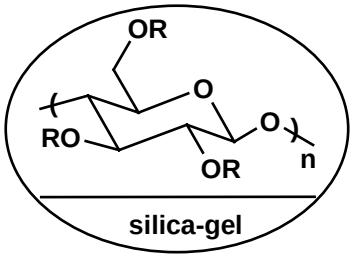
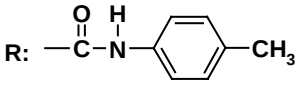
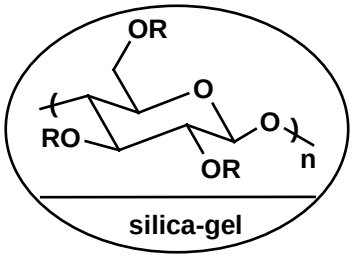
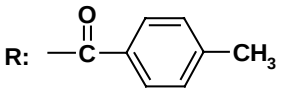
Figure 1-9: Extractive enantiomeric separation with camphorlactol (**2**), e.g., for cyanhydrin (**15**)

1.3.2. Reactivity and Selectivity of Acetal Formation Studied by HPLC

The following study on the reactivity and selectivity of acetal formation was carried out in microscale. The characterization of the reaction product was performed with HPLC on several chiral Daicel phases (see Table 1-1).

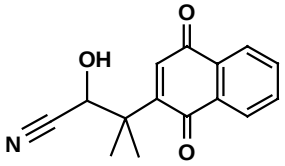
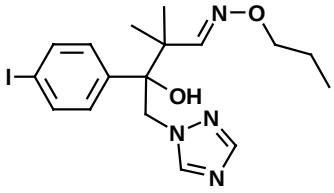
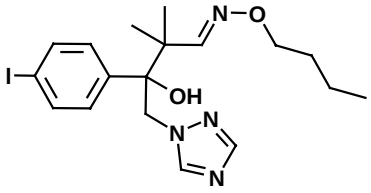
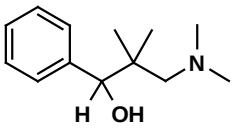
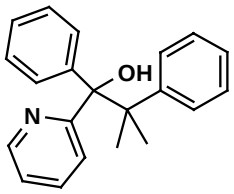
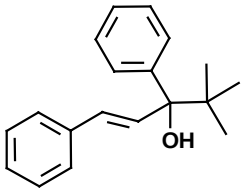
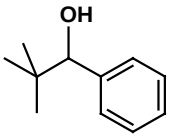
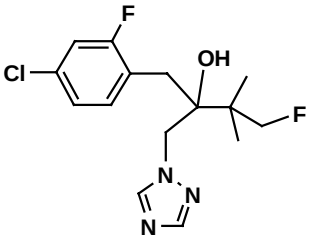
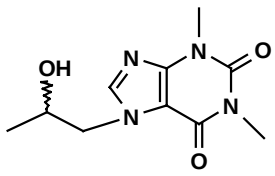
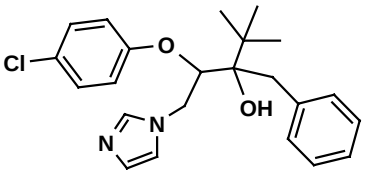
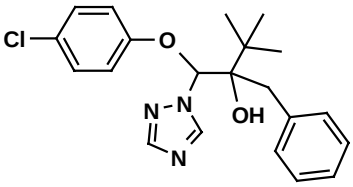
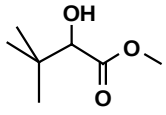
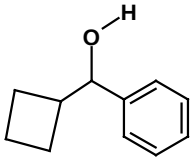
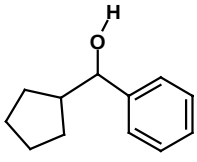
Tabelle 1-1: Stationary Phase for HPLC (Daicel-Phase)

Name	Structure
Chiral OD-H	 Cellulose tris(3,5-dimethylphenyl carbamate) on a 5 µm silica-gel substrate 
Chiral AD	 Amylose tris(3,5-dimethylphenyl carbamate) coated on a 10 µm silica-gel substrate 
Chiral AS	 Amylose tris[(S)-α-methylbenzyl carbamate] coated on a 10 µm silica-gel substrate 
Chiral OD	 Cellulose tris(3,5-dimethylphenyl carbamate) on a 10 µm silica-gel substrate 

Name	Structure
Chiral OG	 Cellulose tris(4-methylphenyl carbamate) on a 10 μm silica-gel substrate 
Chiral OJ	 Cellulose tris(4-methylbenzoate) on a 10 μm silica-gel substrate 

The conversion of substances Nr.01* to Nr.07* and Nr.20* to Nr.24* (structures were shown in Table 1-2, * old numbers as in an unpublished studies) with camphorlactol (**2**) was performed in each case at mole ratio of racemic analyte to lactol 2:1.

Table 1-2: Structures of reactants that form acetals with **2** in an enantioselective manner
(*Old numbers as in two previous unpublished studies)

		
15 (Nr. 01*, 6*)	(Nr. 02*, 8*)	(Nr. 03*, 9*)
		
(Nr. 04*, 10*)	(Nr. 05*, 11*)	(Nr. 06*, 12*)
		
16 (Nr. 07*, 5*) phenyl-*tert*-butylcarbinol	**17** (Nr. 08*, 13*)	(Nr. 18*, 7*) INN proxyphyllin
		
(Nr. 20*, 14*)	(Nr. 21*, 15*)	(Nr. 22*, 16*)
		
(Nr. 23,* 17*) phenyl-*cyclo*-butylcarbinol	(Nr. 24*, 18*) phenyl-*cyclo*-pentylcarbinol	

TFA as catalyst was added at 0.1 mole %, and $CDCl_3$ served as a solvent in this reaction. For substance **16**, ^{t}Bu-OMe was also added, and acetonitrile was used as a solvent, again with 0.1 mole % TFA as a catalyst. All reactions were carried out in 1 ml reactive vials at room temperature for 5 hours.

After reaction, the solvent was blown off by N_2 gas, then two portions of 30 µl absolute toluene were added and evaporated each to completely remove the catalyst TFA. The residue was dissolved in $CDCl_3$ for recording the NMR spectrum. From this solution, 5 µl was pipetted and dried by blowing off with N_2 gas, the residue was dissolved in 500 µl of a mixture of n-heptane / ethanol (9:1, v/v) and analyzed by HPLC. The analysis results and separation conditions are shown in Table 1-3.

Table 1-3: Separation condition and enantioselectivity of product-acetal by HPLC
(* Old numbers as in two previous unpublished studies,
** reaction series and names altered, *cf*. unpublished screening study)

Reaction series	Separation conditions	File name
Bay06-1** (Nr.01*, 6*)	90/10 heptane/EtOH (1% diethylamine) 0.2 ml/min OD-H not well separated, five products (including some impurities) more conditions: [98/2 heptane/EtOH 0.2]; [90/10 heptane/iso-propanol 0.2]; [60/40 heptane/EtOH 0.2]; [30/70 heptane/EtOH 0.4 AD]; [gradient step 100/0-60/40(25-27)-0/100(30-31)-100/0(35-45)]	B-6-1b1**
Bay06-2** (Nr.02*, 8*)	90/10 heptane/EtOH 0.4 ml/min OD-H only one product by different conditions more conditions: [70/30 heptane/2-propanol 0.2]; [80/20 heptane/EtOH 0.4, 0.2]; [gradient step 100/0-60/40(25-27)-0/100(30-31)-100/0(35-45)]	B-6-2**
Bay06-3** (Nr.03*, 9*)	98/2 heptane/EtOH 0.2 ml/min OD-H only one product by different conditions more conditions: [90/10 heptane/iso-propanol 0.4]; [60/40 heptane/EtOH 0.2]	B-6-3**

Reaction series	Separation condition	File name
Bay06-4** (Nr.04*, 10*)	98/2 heptane/EtOH (1% diethylamine) 0.2 ml/min OD-H no reaction, reactant: α=1.344; Rs=1.015 ratio ≈ 1:1.27 more conditions: [90/10 heptane/iso-propanol 0.4]; [gradient step 100/0-60/40(25-27)-0/100(30-31)-100/0(35-45)]	B-6-4b**
Bay06-5** (Nr.05*, 11*)	90/10 heptane/EtOH 0.4 ml/min OD-H only one main product, by gradient step two products visible more conditions: [80/20 heptane/EtOH 0.4, 0.2]; [60/40 heptane/EtOH 0.2] [gradient step 100/0-60/40(25-27)-0/100(30-31)-100/0(35-45)]	B-6-5a**
Bay06-6** (Nr.06*, 12*)	98/2 heptane/EtOH 0.2 ml/min OD-H two products, diastereomers α=1.123; Rs=0.898 ratio ≈ 1:1 reactant, enantiomers α=1.249; Rs=1.080 ratio ≈ 1:1 more conditions: [90/10 heptane/iso-propanol 0.4]	B-6-6**
Bay06-7** (Nr.07*, 5*)	90/10 heptane/EtOH 0.4 ml/min OD-H mainly one product, small amounts of second product more conditions: [95/5 heptane/EtOH 0.2]; [60/40 Heptane/EtOH 0.2]	B-6-7b**
Bay06-8** (Nr.08*, 13*)	9o/10 heptane/EtOH 0.2 ml/min OD-H mainly one product, small amounts of second product more conditions: [95/5 heptane/EtOH 0.2]; [60/40 heptane/EtOH 0.2]	B-6-7c**
Bay06-18** (Nr.18*, 7*)	90/10 heptane/EtOH 0.4 ml/min OD-H two products α=6.589; Rs=4.671 ratio ≈ 1:1 Nr. 18 achiral	B-6-18**
Bay06-19** (Nr.19*)	90/10 heptane/EtOH 0.4 ml/min OD-H two products α=1.286; Rs=0.787 ratio ≈ 1.5:1 Nr. 19 achiral	B-6-19**

Reaction series	Separation condition File name
Bay06-20** (Nr.20*, 14*)	90/10 heptane/EtOH 0.4 ml/min OD-H B-6-20** two products, diastereomers: α=1.258; Rs=1.139 ratio ≈ 1:1 (small amount) reactant, enantiomers: α=2.247; Rs=2.690 ratio ≈ 1:1 more conditions: [60/40 heptane/EtOH 0.2]
Bay06-21** (Nr.21*, 15*)	98/2 heptane/EtOH 0.2 ml/min OD-H B-06-21** two products, diastereomers α=3.736; Rs=4.029 ratio ≈ 1:2 more conditions: [90/10heptane/EtOH(1%dietnylamine) 0.4 α=1.294; Rs=0.495 ratio ≈ 1:1]; [90/10 heptane/iso-propanol 0.4]; [80/20 heptane/EtOH 0.2]; [gradient step 100/0-60/40(25-27)-0/100(30-31)-100/0(35-45)]
Bay06-22** (Nr.22*, 16*)	noUV absorbance
Bay06-CBu** (Nr.23*, 17*)	98/2 heptane/EtOH 0.2 ml/min OD-H B-6-CBu** two products, diastereomers α=1.500; Rs=0.988 ratio ≈ 1:3 (small amount) reactant, enantiomers α=1.068; Rs=0.238 ratio ≈ 1:1,5 more conditions: [98/2heptane/EtOH(1%dietnylamine)]; 0.2]; [90/10 heptane/EtOH 0.2]; [95/5 heptane/EtOH 0.2]
Bay06-CPn** (Nr.24*, 18*)	98/2 heptane/EtOH 0.2 ml/min OD-H B-6-CPnd** one product cannot be separated with reactant Rt=4.834 more conditions: [90/10heptane/EtOH 0.4; 0.2]; [90/10 heptane/iso-propanol 0.4]; [95/5 heptane/EtOH 0.2]

1.3.3. Influence of Structure, Solvent, Catalyst and Reaction Time on the Reactivity and Diastereoselectivity of Acetal Formation

In this section, the optimization of the yield and selectivity of the acetal formation is described, in particular studying the influence of reaction parameters like reactant structure, solvent, catalyst and reaction time. The following analytes were chosen: cyanhydrin (**15**) (Nr.01*), triazol (**17**) (Nr.08*), carbinol (**16**) (Nr.07*), "CPN" (Nr.24*) and "CBU" (Nr.23*); they were all conversed into acetal with camphorlactol (**2**).

First, the influence of the molecular structure of analytes on the conversion result with camphorlactol (**2)** were studied for three carbinols (Nr.07*, Nr.23* and Nr24*); these substrates are all of the b-pl-H type, where the substituents are b = "bulky" (alkyl), pl = "planar" (aryl, carbonyl, π-system) and H (hydrogen).

Conditions:	Solvent:	CH_2Cl_2
	Temperature:	293K
	Reaction time:	5 hours
	Catalyst:	TFA
	Mole ratio:	$n_{Reactant} / n_{Lactol} = 2:1$
		$n_{TFA} / n_{Reactant} = 5 \cdot 10^{-4}:1$ (acc. to R. Schlunk [unpublished])

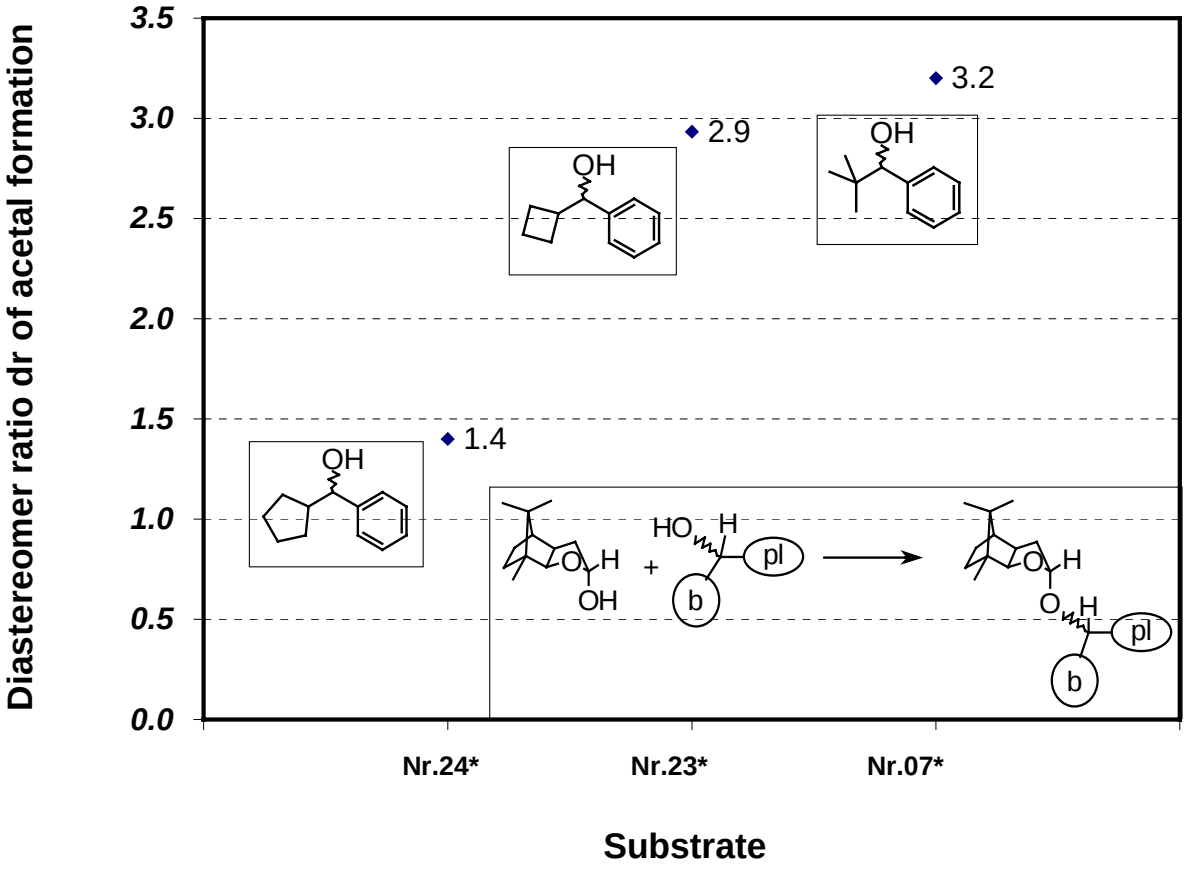


Figure 1-10: Influence of different substituents b of the carbinols on the diastereoselectivity (dr), as determined by HPLC on a Daicel Chiralcel OD-H column (mobile phase: 90/10 n-heptane / ethanol (0.1% diethylamine); flow rate: 0.4 ml/min; UV detector 254 nm)

The highest diastereoselectivity (see Figure 1-10) in these b-pl-H-type carbinols was found for phenyl-tert-butylcarbinol (Nr.07*) with the very rigid and spacious tert-butyl group. The larger but more flexible cyclopentyl group in phenyl-cyclopentylcarbinol (Nr.24*) produces a much lower diastereoselectivity, while the cyclobutyl analogon (Nr.23*) lies in-between.

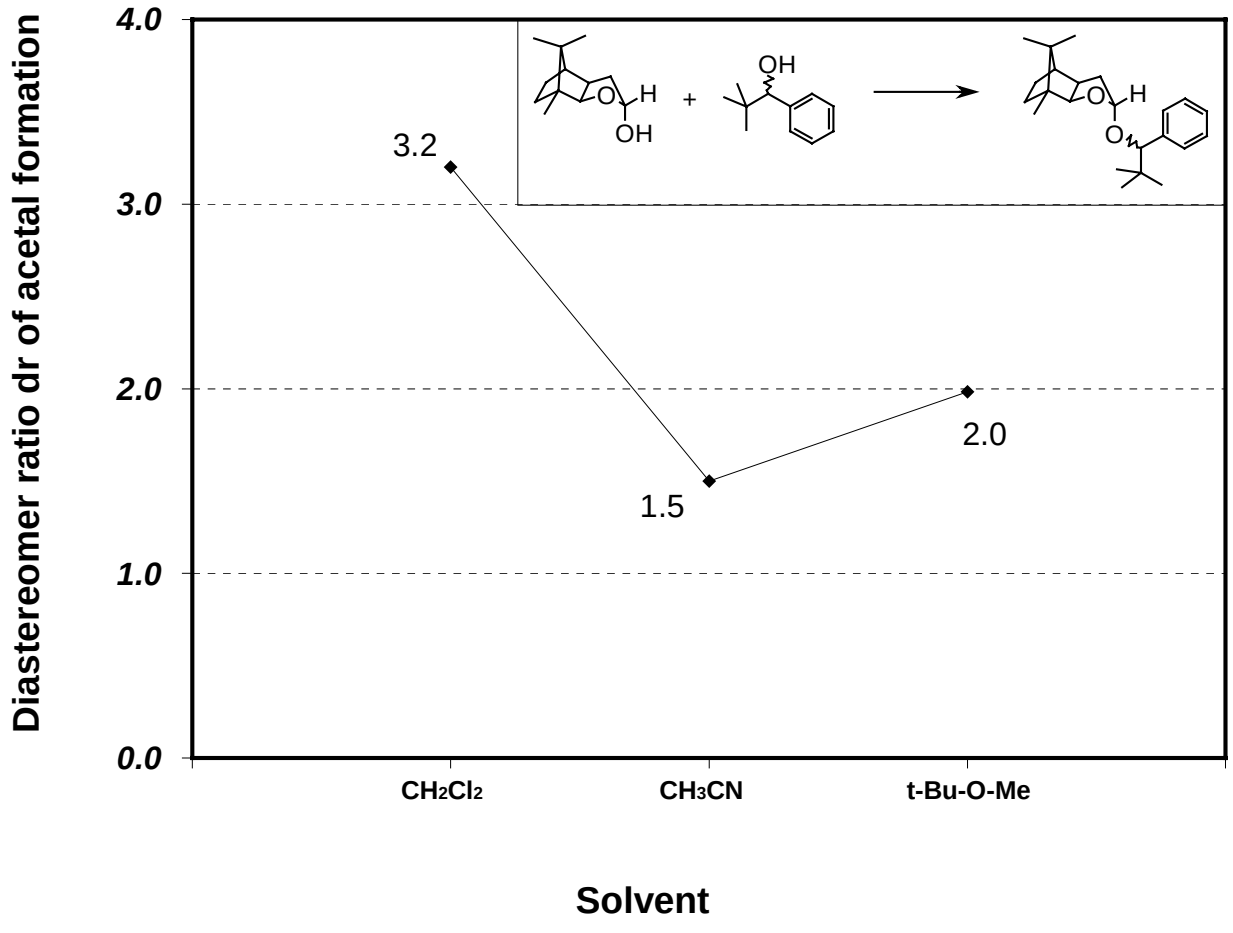


Figure 1-11: Influence of the solvent of reaction on the diastereomer ratio (dr) of the acetal formation, as determined with a Daicel Chiralcel OD-H column (mobile phase: 90/10 n-heptane / ethanol (0.1% diethylamine); flow rate 0.4 ml/min; UV detector 254 nm)

The influence of different polar solvents on the diastereomer ratio (dr) of the carbinol (**16**) is shown in Figure 1-11. It is evident that, the formation of the glycosidic bond is controlled by dipole interactions via the anomer effect; hence, a solvent of low polarity should be preferred. To our experience, dichlormethane is one of the best solvents for achieving high diastereoselectivities.

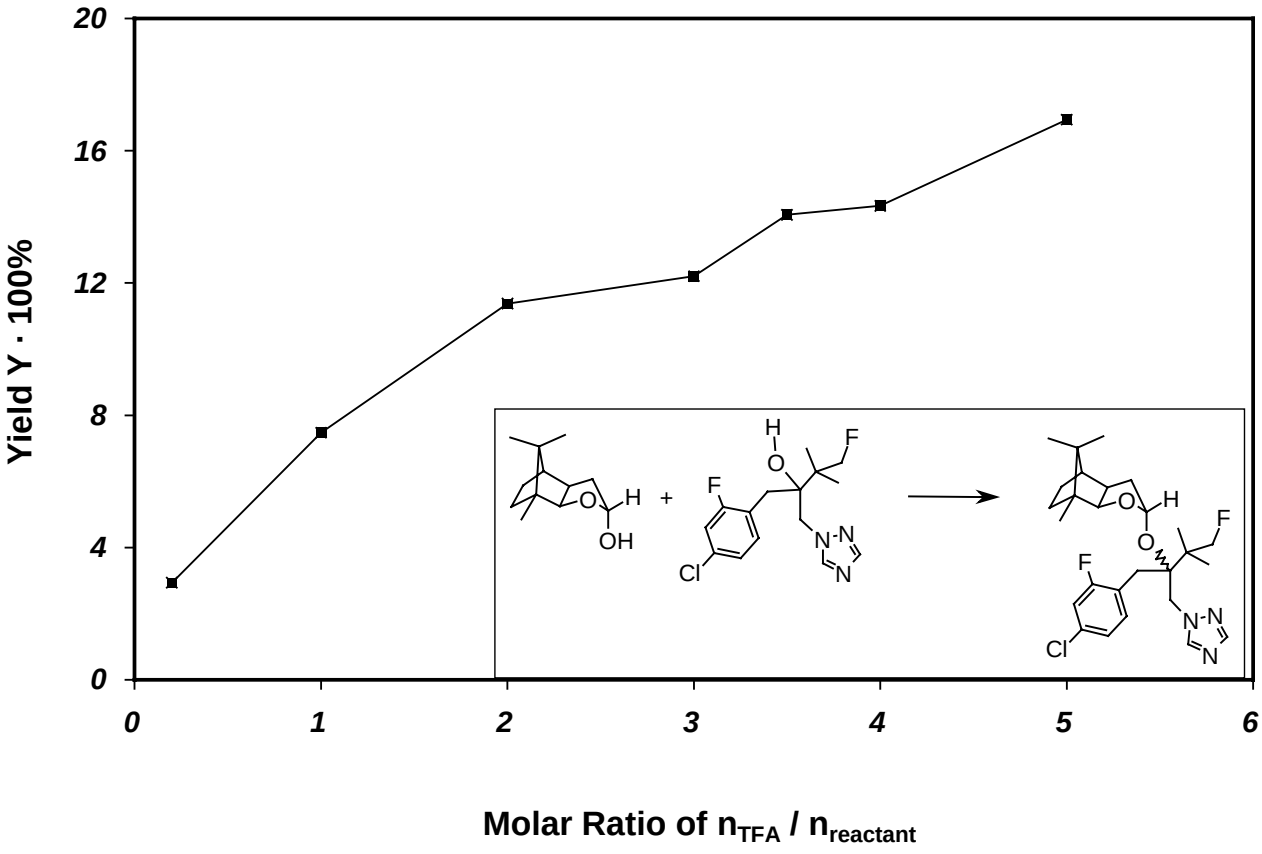


Figure 1-12: Influence of the amount of acid catalyst on the yield of the acetal formation from **17**, as determined by HPLC on a Daicel Chiralcel OD-H column (mobile phase: 90/10 n-heptane / ethanol (0.1% diethylamine); flow rate 0.4 ml/min; UV detector 254 nm)

The influence of the amount of acid catalyst on the yield of the acetal formation of campherlactol (**2**) with reactant triazol (**17**) is shown in Figure 1-12. This triazol type reactant represents a special challenge in two different respects. On one hand, it is not clearly following the b-pl-H-type, which may result in a lower diastereoselectivity. On the other hand, triazol is a strong basic group that may cause trouble in acetal formation.

Indeed, no conversion was observed after addition of 0.1 – 1 mole % acid catalyst (related to the amount of reactant), but a further increase to higher molar amounts of the catalyst appeared successful (see Figure 1-12), although the yields were still low.

Reaction conditions:	Solvent:	CH_2Cl_2
	Temperature:	293K
	Catalyst:	TFA
	$n_{Reactant}$ / n_{Lactol}:	2:1
	n_{TFA} / $n_{Reactant}$:	4:1

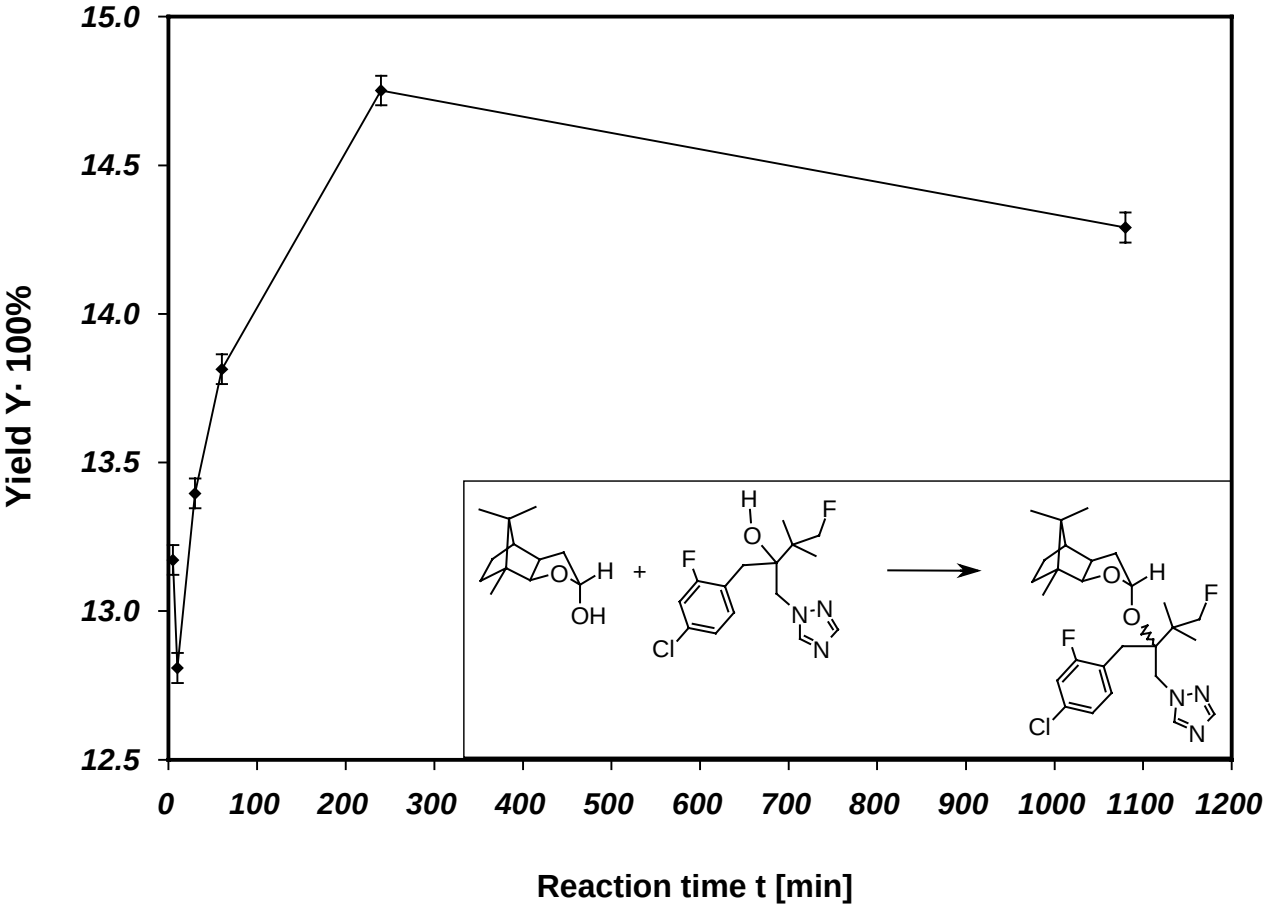


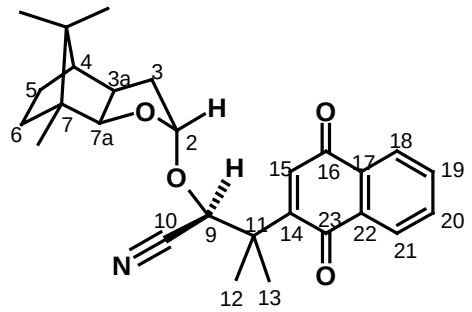
Figure 1-13: Influence of the reaction time on the yield of the acetal formation from triazol (**17**), as determined by HPLC on a Daicel Chiralcel OD-H column (mobile phase: 90/10 n-heptane / ethanol (0.1% diethylamine); flow rate 0.4 ml/min; UV detector 254 nm)

At a ratio of catalyst / reactant of 4:1 (400 mole % TFA related to **17**), a series of experiments revealed the influence of the reaction time on the reaction yield. As shown in Figure 1-13, the chemical yield has an optimum for a reaction time of 5 hours.

For the acetal formation from camphorlactol (**2**) and the cyanohydrin (**15**) as the reactant, the amount of acid catalyst is also 1 mole % relative to the reactant, similar to the conditions used for phenyl-tert-butylcarbinol (**16**).

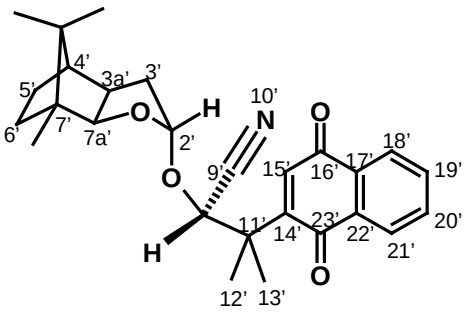
Reaction conditions:	Solvent:	CH_2Cl_2
	Temperature:	293K
	Catalyst:	TFA
	$n_{Reactant}$ / n_{Lactol}:	2:1
	n_{TFA} / $n_{Reactant}$:	$1 \cdot 10^{-2}$:1

The interplay between yield and selectivity for the cyanohydrin (**15**) as the reactant is puzzling. The relationship between yield, reaction time and diastereomer excess (de) is shown in Figure 1-14. At short reaction time, the B-A-form **18**, as depicted below (see Figure 1-5), is preferred, but the yield remains low, while in the long course of the reaction, the selectivity is decreased, and after 2 – 2.5 hours, there is a crossover to the B-B form **19** (see Figure 1-14).



O,O-Acetal from R-"Nr.01" B-A-form

18



O,O-Acetal from S-"Nr.01" B-B-form

19

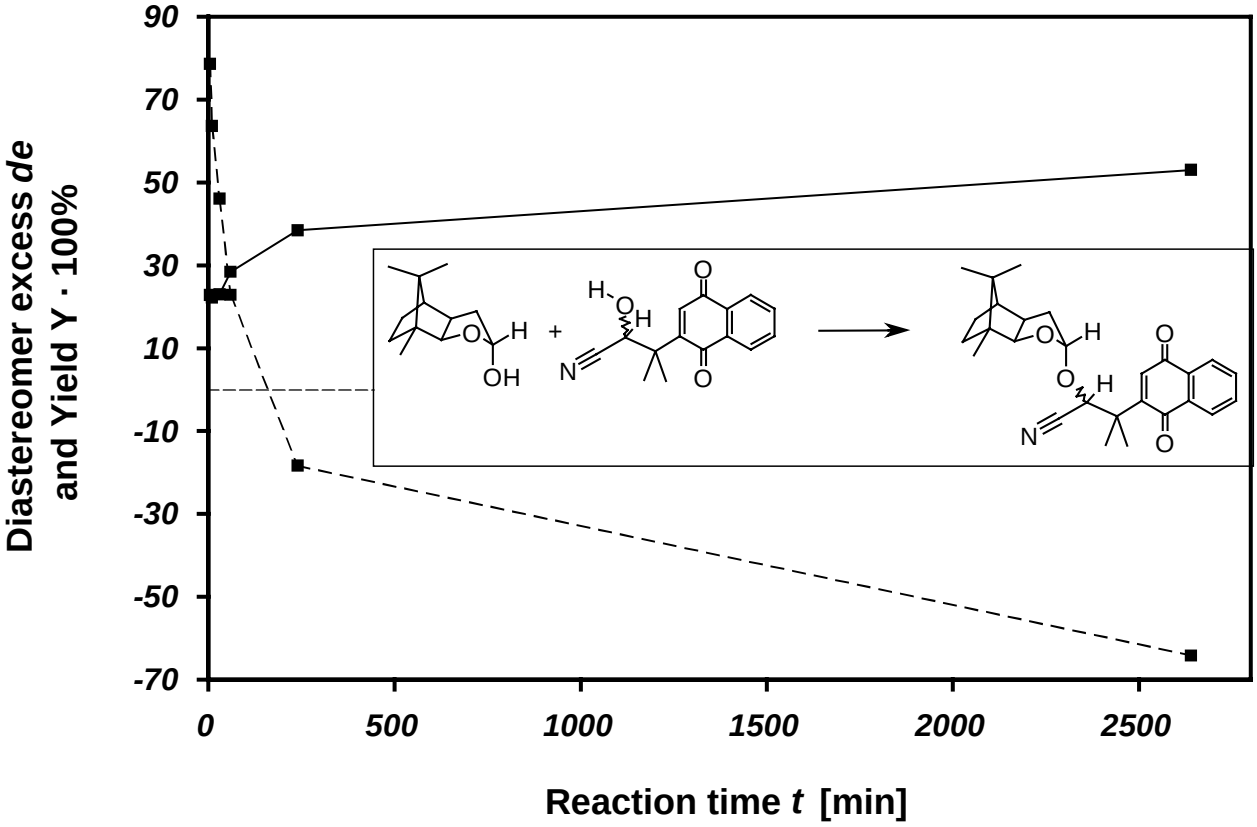


Figure 1-14: Influence of the reaction time on the yield (——) and de (------) of the acetal formation from cyanhydrin (**15**), as determined by HPLC on a Daicel Chiralcel OD-H column (mobile phase, 90/10 n-Heptane / Ethanol (0.1% Diethylamine); flow rate 0.4 ml/min; UV Detector 254 nm).

1.3.4. Binding of the Lactol to a Solid Support (Polymer, Silicagel, Glass)

The chiral lactol could be bound to a solid support (polystyrene, silicagel or porous glass, respectively), see Figure 1-15. To this end, [2S-(2α,3aα,4β,7β,7aα)]-2,2'-oxy-bis-[octahydro-8,8-dimethyl-4,7-methanobenzofuran-7-methanesulfonyl chloride] was reacted with polystyrene resin, silicagel, and controlled-porous glass (CPG). The materials obtained can be used to separate enantiomers via suitable nucleophiles, that tend to form adducts in a more or less diastereoselective manner. After hydrolysis of the acetal bond, the solid support can be recycled and reused.

For the conversion of a set of analytes, the selectivities and yields were determined dependent on the reaction parameters. By suitable choice of the reaction conditions, the selectivity and yield can be optimized through the variation of the solid support, the anchor group, the coupling conditions, and also the solvent used for acetal formation. The reaction can be either conducted batch-wise or by chromatography on a reactive column.

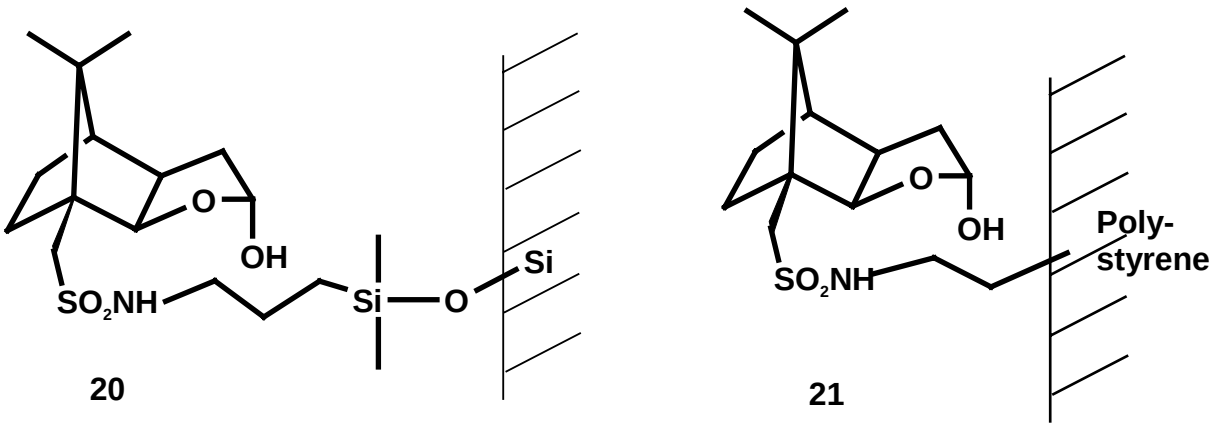


Figure 1-15: Binding of Noe-lactol via a sulfonamide spacer to silicagel and porous glass, respectively, to give the reagent 20, and to amino fuctionalized polystyrene, to give the polymeric reagent 21 („PS-lactol").

As outlined in Figure 1-16, the lactone 1 was sulfonated at the 7-methyl group and then reacted with phosphorous pentachloride to give the sulfonyl chloride (**22**) [18], which after reduction with isobutylaluminium hydride afforded the lactol (**23**) [19]. In the following step, the sulfonyl chloride (**23**) was coupled to the amino functionalized solid support to give the final reagent (**20**).

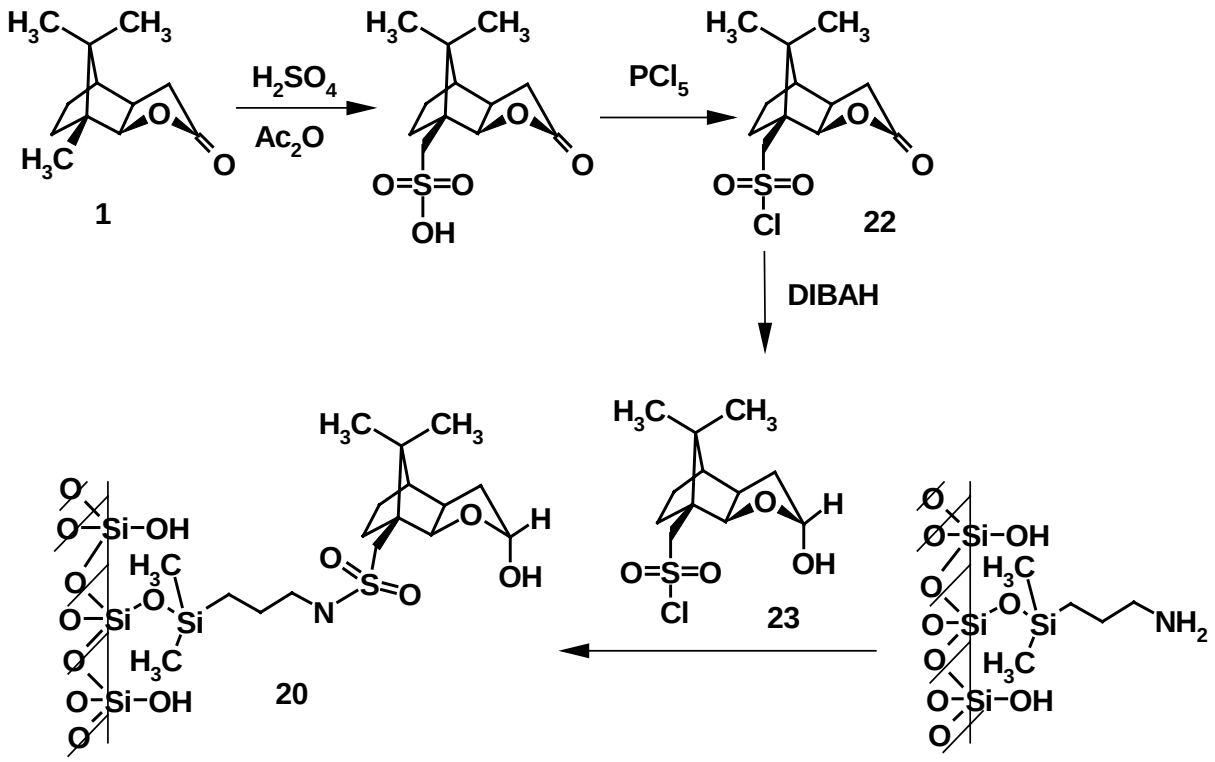


Figure 1-16: Synthesis of the sulfonamide bound lactol (**20**) with silicagel as the solid support

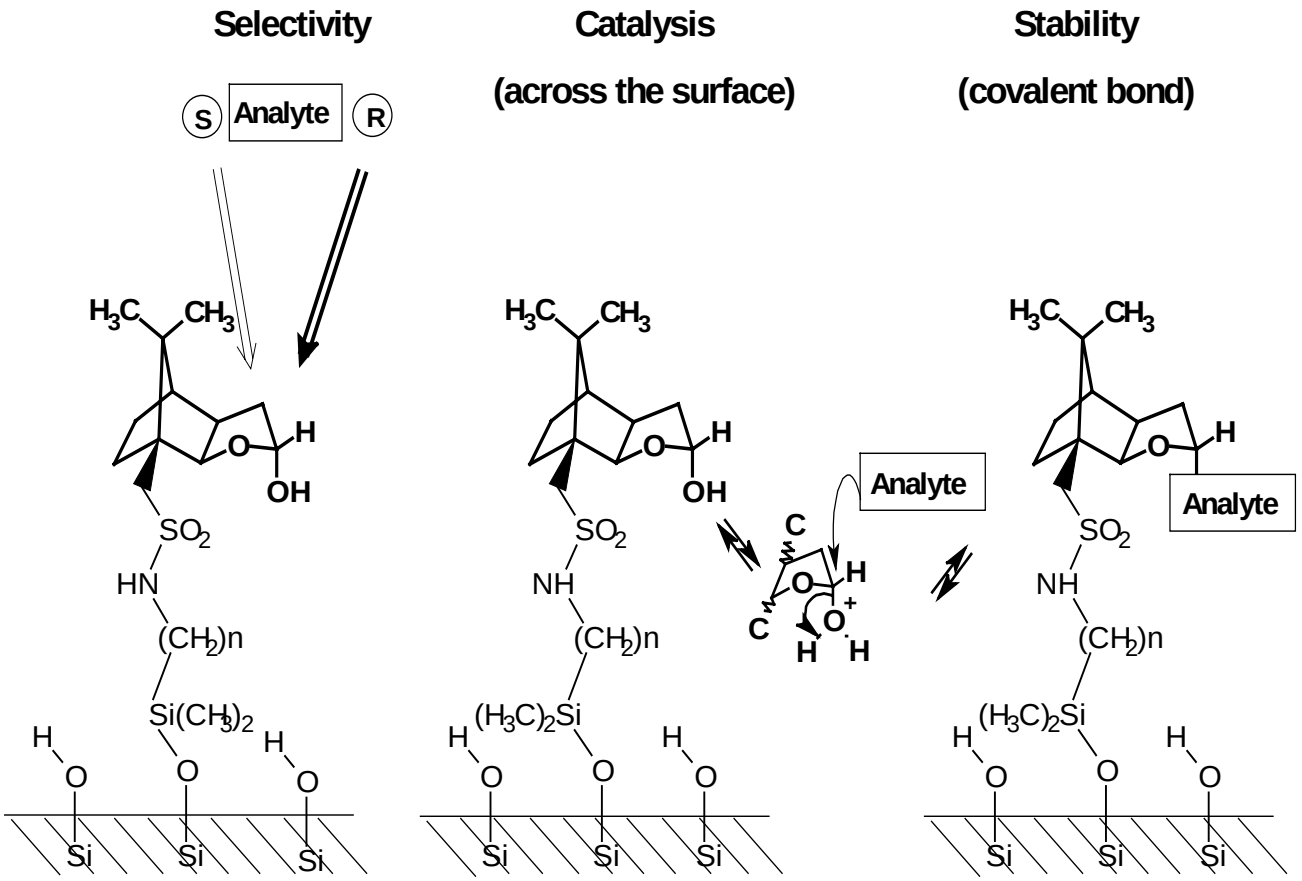


Figure 1-17: Possible catalysis on the modified silicagel phase

The behaviour of the reagent may be affected either by a shift to lower pH in the solution (weak acid) or by an acidic silanol group on the surface of the support (see Figure 1-17). This reagent should be especially suitable for chromatography as it can act as a “chiral sponge” that binds one enantiomer preferentially from the solution. After hydrolysis of the acetal bond, the analyte is released into the solution. In this way, the two enantiomers of the analyte are finally separated.

1.4. Summary

1.4.1. Separation of Enantiomers by Distribution Between Two Liquid Phases via Diastereomeric Acetals

The acetals were formed from racemic nucleophiles, in particular alcohols, with the chiral lactol (**2**), and also with derivatives of **2**. The diastereomers formed were separated by means of a Craig-apparatus; after splitting the acetal bond, the two enantiomers of the reactant were recovered separately.

In an early stage of the reaction, the diastereomer ratio (dr) is determined by kinetic control, in a later stage by thermodynamic control. Lactols functionalized in 10-position show an increased enantiomer selectivity, possibly due to steric hindrance. Usually, a nonpolar, nonprotic solvent (for example CH_2Cl_2) and acid catalysis are favourable conditions.

However, for water-soluble salts, e.g., of basic drugs, these conditions may not be applicable, due to their low solubility in an nonpolar solvent. By means of a Craig-apparatus, the diastereomers formed under thermodynamic control can be separated by distribution between two immiscible organic phases. Furthermore, the diastereomers formed under kinetic control can be separated from the reactant, and subsequently hydrolyzed. By these means, both enantiomers of the reactant are readily accessible.

The reaction of the two enantiomers with the lactol can be followed by HPLC, allowing to optimize the selectivity and the depletion of one enantiomer. We have investigated the influence of solvent and catalyst used for three different substrates, of the type of a triazol, a cyanohydrin and a more simple carbinol. A sulfonyl chloride of the lactol is also used, and the selectivity and the depletion of one enantiomer are shown in a similar fashion.

1.4.2. Binding of the Lactol to a Solid Support (Polymer, Silicagel, Glass)

The chiral lactol could be bound to a solid support (polymer, silicagel, porous glass, respectively) through a suitable spacer; the modified support should be useful for enantiomer separation. For now, we have applied this approach to polystyrene (“PS-Lactol”), to silicagel, and also to controlled porous glass (CPG, “Bioran”).

The experiments reported in this thesis show that the selectivity is influenced by the conditions of the coupling reaction. Residual cosolvents and side products of the coupling, which we attempted to remove by rinsing the lactol-modified solid support with suitable solvents, may still influence the selectivity and reactivity. The highest selectivity was obtained in nonpolar solvents, and the selectivity increases with growing reactant proportion.

The immobilized agent can be compared to a “chiral sponge” or “chiral glue”, as it is supposed to preferentially bind to one enantiomer of a substrate that can lateron be released “on demand” by acid catalysis. It seems feasible to have an additional acidic group at the solid support in such a way that the adduct formed is split easily by catalysis, thus opening up a new route to rapid, straightforward enantiomer separation.

1.5. Experimental Section

1.5.1. Instrumentation

1.5.1.1 HPLC

Spectra Physics SP8800 HPLC Pump, Spectra Physics SP8880 Autosampler, Spectra Physics Spectra 100 Detector, Spectra Physics Chromjet Integrator, Computer 486DX2, 16MB, Software PC1000 Version 3.0, Mobile phases: heptane / isopropanol and 0.1 % diethylamine, HPLC-grade (Merck). Chemical reagent: diethylamine (Fluka) >= 99.7 %. Sample volume: 10µl

1.5.1.2 IR-Spectrometer

Perkin-Elmer 281 B. All wave numbers in cm^{-1}.

1.5.1.3 NMR-Spectrometer

Bruker AC 250 (250 MHz) and Bruker WM 400 (400 MHz). Chemical shift δ in ppm (TMS and TSP, respectively, as standard)

1.5.1.4 Elemental Analysis

C, H, N: Carlo Erba Elemental Analyzer Mod. 1106, Mikroanalytisches Labor der Universitaet Tuebingen.

1.5.1.5 MS-Spectrometer

Double Physical Focus Sector Field-MS (AMD Intectra), and Tri-Stage-Quadrupol-MS TSQ 70 (Finnigan-MAT).

1.5.2. Chemicals

Basic chemicals were purchased from ABCR, Aldrich, Fluka, Merck, and Schuetz & Co.

TLC Plates: Silica gel 60 F_{254} (E. Merck, Darmstadt). UV detection, staining with $Ce(SO_4)_2$ / H_2SO_4 / $(NH_4)_6Mo_7O_{24}.4H_2O$

LC column filling: Silica gel 60 (0.032-0.063 mm) (E. Merck, Darmstadt); this silica gel was impregnated with triethylamine and suspended in petrolether (30 - 50 ^oC) / diethyl ether / triethylamin (9 / 3 / 7), filtered, and finally dried in vacuo at 50°C.

Acetanhydride was purified by addition of dry sodium acetate, refluxing for 5 h, and fractional distillation.

Acetone was dried over water-free potassium carbonate for 3 h, filtered and distilled.

Acetonitrile was dried over $Ca(OH)_2$ and stored over 3 Å molecular sieve.

Dichloromethane was stirred with water-free $CaCl_2$ over night and then distilled.

Diethyl ether was refluxed over sodium in the presence of benzophenone until a blueviolet colour was persistent, and then distilled.

Toluene was refluxed over sodium in the presence of benzophenone until a blueviolet colour was persistent, and then distilled.

Triethylamine was refluxed over sodium in the presence of benzophenone until a blueviolet colour was persistent, and then distilled.

Chloroform was shaken with concentrated sulfuric acid, washed twice with water, then dried over $CaCl_2$ and distilled, finally stored over 4 Å molecular sieve.

Tetrahydrofuran was permeated through a basic Al_2O_3 column to remove peroxides, then it was refluxed with sodium in the presence of benzophenone under N_2 gas until the blueviolet colour persisted, distilled under N_2 gas, and finally stored over CaH_2.

1.5.3. Syntheses

1.5.3.1 [2R-(2α,3aα,4β,7β,7aα)]-2,3,3a,4,5,6,7,7a-Octahydro-7,8,8-trimethyl-4,7-methano-benzofuran-2-ol

According to literature [23], [3aR-(3aα,4β,7β,7aα)]-3a,4,5,6,7,7a-hexahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2(3H)-one (3.0 g, 15.8 mMol) was dissolved in abs. toluene (12.6 ml). The reaction was stirred at -40°C, and a 1 molar solution of diisobutylaluminiumhydride (DIBAH) in n-hexane (16.9 ml) was added drop by drop at -40 °C. After 3 hours stirring at -40 °C, the reaction was stirred overnight at room temperature, and then diethyl ether (18 ml) and water (9 ml) were added at -40 °C, then the dry ice bath (liquid CO_2) was removed. At room temperature, 2N NaOH (about 70 ml) were added to the reaction mixture until the precipitate of $Al(OH)_3$ was dissolved. The organic phase was separated, and the aqueous phase was extracted twice with diethyl ether, the combined organic phase was washed with water until pH=7. The organic phase was dried over Na_2SO_4. The solvent was removed in vacuo as far as possible. The product was dried in high vacuo.

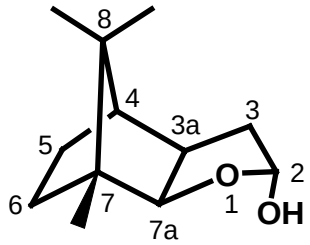
Yield: 1.8 g (59 %) (partial losses due to accidental breaking of the flask)

Colourless liquid; $[\alpha]_D^{20} = -67.7^o$ (c = 0.84 in diethyl ether)

EI-MS: m/e (rel. intensity) = 197 (2), 196 (19), 179 (4), 153 (4), 149 (12), 137 (10), 135 (6), 125 (5), 121 (5), 114 (23), 112 (12), 111 (18), 110 (14), 109 (13), 108 (35), 107 (10), 96 (22), 95 (100), 86 (33), 83 (14), 69 (16), 55 (21), 41 (24)

IR (film): 1/λ = 3400 (O-H), 2960/2880 (C-H), 1040/1020 (C-O) cm^{-1}

^{1}H-NMR ($CDCl_3$): δ = 0.77/0.89 (2s, 9H, 3 CH_3), 1.0-2.4 (m, 8H, aliphatic-H), 4.01 (d, ^{3}J = 7.6 Hz, 1H, H-7a), 5.52 (t, ^{3}J = 2.1 Hz, 1H, OCHO) ppm



^{13}C-NMR ($CDCl_3$): δ = 11.5 (7-CH_3), 20.5 (CH_3), 22.9 (CH_3), 28.9 (C-5), 32.3 (C-6), 39.2 (C-3), 45.8 (C-3a), 47.0 (C-8), 47.6 (C-7), 48.5 (C-4), 91.4 (C-7a), 99.8 (C-2) ppm

$C_{12}H_{20}O_2$ (196.29): Calculated C 73.43, H 10.27

Found C 74.42, H 9.35

1.5.3.2 [3aR-(3aα, 4β, 7β, 7aα)]-8, 8-Dimethyl-octahydro-2-oxo-4,7-methanobenzofuran-7-yl-methanesulphonic acid

According to literature [24], concentrated sulphuric acid (26.0 ml, 0.155 Mol) was dripped into acetanhydride (29.0 ml, 0.309 Mol) under cooling, while the temperature should not exceed 20°C. Then [3aR-(3aα,4β,7β,7aα)]-3a,4,5,6,7,7a-hexahedron-7,8,8-trimethyl-4,7-methanobenzofuran-2(3H)-one (30.0 g, 0.155 Mol) was dissolved in the reaction mixture, and it was left to stand at room temperature for 7 days. The precipitate was filtered off by sucking with a water pump, and washed with small amounts of dry diethyl ether, affording colourless crystals. The product was dried in high vacuo.

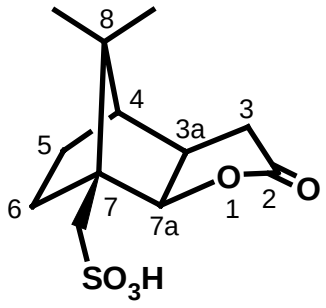
Yield: 20.1 g (47%)

White crystals (a little bit brown), mp.: 201°C

EI-MS: m/e (rel. intensity) = 278 (1), 257 (3), 256 (2), 231 (3), 228 (4), 195 (3), 194 (5), 193 (10) 192 (10), 178 (5), 177 (7), 176 (11), 161 (4), 151 (13), 149 (34), 148 (22), 147 (10), 133 (51), 107 (22), 95 (20), 81 (100), 80 (34), 79 (18), 64 (11), 55 (8), 43 (18)

IR (KBr): $1/\lambda$ = 2950 (C-H), 1170 (C=O), 1180 (SO_2O), 1085/1030 (C-O) cm^{-1}

^{1}H-NMR (DMSO-d_6): δ = 4.82 (d, ^{3}J = 7,8 Hz, 1H, H-7a), 1.0-3.0 (m, 10H, aliphatic-H), 0.81 (s, 6H, $2CH_3$) ppm



^{13}C-NMR (DMSO-d_6): δ = 178.6 (C-2), 87.8 (C-7a), 48.0/48.7/48.8 (7-CH_2SO_3H/C-7/C-8/C-4), 42.1 (C-3a), 34.5 (C-3), 28.0/27.9 (C-5/C-6), 19.9/23.0 (8-CH_3) ppm

$C_{12}H_{18}O_5S$ (274.34): Calculated C 52.54, H 6.61, S 11.69

Found C 51.01, H 6.74, S 11.57

1.5.3.3 [3aR-(3aα,4β,7β,7aα)]-8,8-Dimethyl-3a,4,5,67,7a-hexahydro-2-oxo-4,7-methano-benzofuran-7-yl-methanesulfonyl chloride

According to literature [24], dry [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methanobenzofuran-7-yl-methanesulfonic acid (20.1 g, 73.3 mMol) was stirred with phosphorous pentachloride (20.1 g, 96.4 mMol) under cooling in an ice bath until liquidified. After stirring at room temperature for 8 h, ice water was added into the reaction mixture, a colourless precipitate was formed that was filtered off and washed with ice water until pH = 7, to afford colourless crystals. The product was dried in high vacuo.

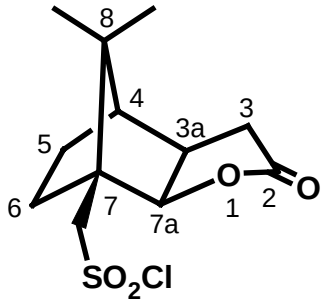
Yield: 17.0 g (79%)

White crystals, mp.: 122°C

EI-MS: m/e (rel. intensity) = 295 (1), 293 (2), 229 (5), 194 (6), 193 (55), 170 (13), 151 (21), 133 (100), 128 (44), 108 (40), 95 (79), 81 (33), 64 (29), 41 (18)

IR (KBr): $1/\lambda$ = 2950 (C-H), 1770 (C-O), 1370 (SO_2), 1170/1040 (C-O) cm^{-1}

^{1}H-NMR ($CDCl_3$): δ = 4.8-4.9 (d, ^3J = 7.6 Hz, 1H, H-7a), 3.71/3.76/4.22/4.27 (AB-system, 2H, J_{AB} = 13.7 Hz, CH_2SO_2), 1.1-2.9 (m, 8H, aliphatic-H), 0.97/1.00 (2s, 6H, $2CH_3$) ppm



^{13}C-NMR ($CDCl_3$): δ = 177.8 (C-2), 87.0 (C-7a), 65.8 (7-CH_2SO_2), 50.2/50.2 (C-7/C-8), 48.6 (C-4), 43.0 (C-3a), 34.6 (C-3), 28.4/28.6 (C-5/C-6), 20.4/23.3 (8-CH_3) ppm

$C_{12}H_{17}ClO_4S$ (292.78): Calculated C 49.23, H 5.85, Cl 12.11, S 10.95

Found C 48.01, H 6.10, Cl 12.70, S 10.77

1.5.3.4 [2S-(2α,3aα,4β,7β,7aα)]-2,2'-Oxy-bis-[octahydro-8,8-dimethyl-4,7-methanobenzofuran-7-methanesulfonyl chloride]

According to literature [22], [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methanobenzofuran-7-yl-methanesulfonyl chloride (8.64 g, 29.5 mMol) was dissolved in dry dichloromethane (135 ml) and cooled at -70°C under an atomsphere of N_2, then 1.0 molar DIBAH-solution in n-hexane (37 ml, 37 mMol) was dripped slowly under stirring at -70°C for 4 h, eventually the reaction was stirred overnight at room temperature. Dichloromethane (400 ml) and 2N hydrochloric acid (420 ml) were added to the reaction mixture that was then stirred as far as possible until the two phases became clear. The two phases were separated, the aqueous phase was extracted twice with dichloromethane, to the combined organic phase toluene (10 ml) was added, and it was dried over sodium sulfate, filtered and the solvent was evaporated. The product was dried in high vacuo.

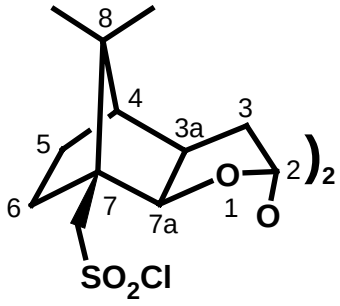
Yield: 7.34 g (87%)

Light yellow crystals, mp. : 145°C

FD-MS: m/e (rel. intensity) = 573 (6), 510 (6), 474 (14); 472 (32), 409 (7), 407 (29), 295 (15), 293 (30), 279 (44), 277 (91), 229 (45), 213 (100), 193 (14)

IR (KBr): $1/\lambda$ = 2940 (C-H), 1760 (C-O), 1360 (SO_2), 1170/1090 (C-O) cm^{-1}

^{1}H-NMR ($CDCl_3$): δ = 5.41 (d, ^3J = 2.5 Hz, 1H, H-2), 4.26 (d, ^3J = 7.5 Hz, 1H, H-7a), 3.64/3.69/4.30/4.35 (AB-system, J_{AB} = 13.5 Hz, 2H, CH_2SO_2), 2.34 (m, 1H, H-3a), 0.9-2.5 (m, 7H, aliphatic-H), 0.87/1.01 (2s, 6H, $2CH_3$) ppm



^{13}C-NMR ($CDCl_3$): δ = 99.7 (d, C-2), 86.5 (d, C-7a), 67.0 (t, CH_2SO_2), 50.5 (s, C-7), 49.6 (s, C-8), 47.6 (d, C-4), 46.4 (d, C-3a), 38.2 (t, C-3), 28.6/28.9 (2t, C-5/C-6), 20.5/23.1 (2d, $2CH_3$) ppm

$C_{24}H_{36}Cl_2O_7S_2$ (571.58):	Calculated	C 50.43, H 6.35, Cl 12.06, S 11.22
	Found	C 50.94, H 7.03, Cl 12.00, S 10.73

1.5.3.5 [3aS-(3aα,4β,7α,7aα)]-N,N-Di(phenylmethyl)-(octahydro-8,8-dimethyl-2-oxo-4,7-methano-benzofuran-7-yl)-methanesulfonamide

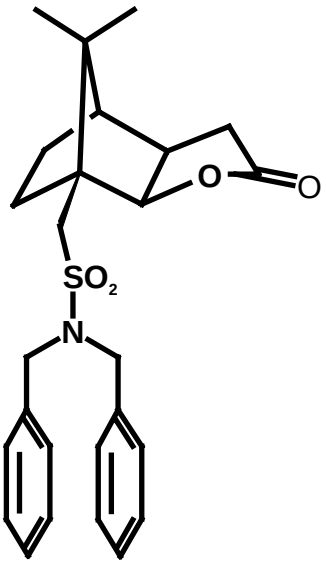
2.9 g (10.0 mMol) [3aS-(3aα,4β,7α,7aα)]-N-[(octahydro-8,8-dimethyl-2-oxo-4,7-methano-benzo-furan-7-yl)methylsulfonyl]-N-(phenylmethyl)-glycine ethylester was added to 6.0 g (30.0 mMol) dibenzylamine, then 2.5 equivalents of base were added, and the mixture was stirred overnight. The colourless precipitate was filtered off, the reaction solvent was removed by silica gel filtration (solvent: ether), the permeate was washed with H_2O, the organic phase was dried over Na_2SO_4 and the solvent was evaporated. The residue was recrystallized from n-hexane/toluene.

Yield: 2.2 g (48%)

White crystals, mp.: 115 ^{o} - 118 ^{o}C

EI-MS: m/e (rel. intensity) = 454 (m+1, 0.3), 362 (14), 196 (83), 194 (22), 147 (8), 133 (9), 106 (47), 91 (100), 79 (7), 55 (6)

^{1}H-NMR ($CDCl_3$): δ = 7.45 (m; 10H, aromatic-H), 4.99 (m, 1H, H-7a), 4.35 (s; 4H, N-CH_2), 3.10 (d; 1H, CH-SO_2), 2.65 (d; 1H, CH-SO_2), 2.8-1.0 (m; 8H, aliphatic-H), 0.8 (2s; 6H, 2CH_3) ppm



^{13}C-NMR ($CDCl_3$): δ = 178.4 (d; C-2), 135.6 (s; C(Ph)-1), 129.0 (d; C(Ph)-2, C(Ph)-6), 128.8 (d; C(Ph)-3, C(Ph)-5), 128.1 (d; C(Ph)-4), 89.0 (d; C-7a), 50.7 (t; CH_2SO_2), 50.0 (t-NCH_2), 49.1 (s; C-7), 48.6 (s; C-8), 47.3 (d; C-4), 42.9 (d; C-3a), 35.0 (t; C-3), 28.6 (t; C-5), 28.3 (t; C-6) 23.2/20.3 (2q; 2 x CH_3) ppm

$C_{26}H_{31}NO_4S$ (453.60): Calculated C 68.85, H 6.89, N 3.09, S 7.05
Found C 68.42, H 6.72, N 3.03, S 6.96

1.5.3.6 [2S-(2α,3aα,4β,7α,7aα)]-N,N-Di(phenylmethyl)-(octahydro-2-hydroxy-8,8-dimethyl-4,7-methanobenzofuran-7-yl)-methanesulfonamide

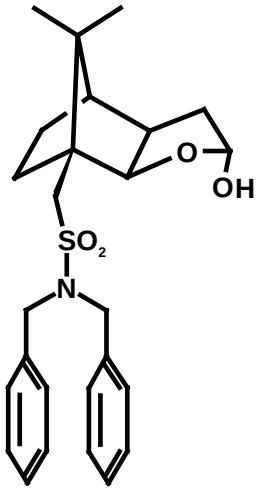
According to literature [22], [3aS-(3aα,4β,7α,7aα)]-N,N-di(phenylmethyl)-(octahydro-8,8-dimethyl-2-oxo-4,7-methano-benzofuran-7-yl)-methanesulfonamide (2.1 g, 4.62 mMol) was dissolved in dry dichloromethane (50 ml), and cooled to -60°C under an atmosphere of N_2 gas. A 1.6 equivalent of a 2.5 molar solution of DIBAH in n-hexane (9.8 ml, 9.8 mMol) was dropped slowly into it and stirred at -60°C for 3h, then the mixture was stirred overnight at room temperature. Dichloromethane (100 ml) and 2N hydrochloric acid (100 ml) were added to the reaction mixture and stirred as far as possible until the two phases were clear. The two phases were separated, the aqueous phase was extracted twice with dichloromethane, the combined organic phase was washed with saturated sodium hydrogen carbonate solution until pH=7, and then it was dried over sodium sulfate. The solvent was evaporated. The product was dried in high vacuo.

Yield: 2.01 g (93%)

White crystals, mp.: 103 ^{o} - 105 ^{o}C

EI-MS: m/e (rel. intensity) = 437 (0.6), 362 (0.1), 355 (0.8), 354 (4), 304 (5), 226 (4), 196 (85), 177 (7), 135 (5), 133 (17), 106 (100), 91 (91), 69 (12)

^{1}H-NMR ($CDCl_3$): δ = 7.26 (m; 10H, aromatic-H), 5.47 (m, 1H, H-2), 4.53 (d, 1H H-7a), 4.38-4.28 (s; 4H, N-CH_2), 3.20 (d; 1H, CH-SO_2), 2.95 (bs; 1H, OH), 2.50 (d; 1H, CH-SO_2), 2.28-1.0 (m; 8H, aliphatic-H), 0.84/0.70 (2s; 6H, 2CH_3) ppm



^{13}C-NMR ($CDCl_3$): δ = 135.9 (s; C(Ph)-1), 129.0 (d; C(Ph)-2, C(Ph)-6), 128.8 (d; C(Ph)-3, C(Ph)-5), 127.9 (d; C(Ph)-4), 99.7 (d C-2), 87.5 (d; C-7a), 52.6 (t; CH_2SO_2), 50.0 (t-NCH_2), 49.4 (t; CH_2-Ph), 49.1 (s; C-7), 48.4 (s; C-8), 47.6 (d; C-4), 46.1 (d; C-3a), 39.2 (t; C-3), 28.9 (t; C-5), 28.5 (t; C-6) 23.1/20.3 (2q; 2 x CH_3) ppm

$C_{26}H_{33}NO_4S$ (455.62): Calculated C 68.54, H 7.30, N 3.07, S 7.02
Found C 67.99, H 7.55, N 2.96, S 6.95

1.5.3.7 [3aR-(3aα,4β,7β,7aα)]-7-(Bromomethyl)-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-4,7-methanobenzofuran-2(3H)-one

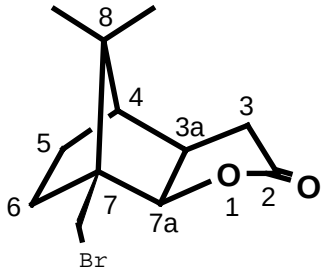
According to literature [25], [3aR-(3aα,4β,7β,7aα)]-hexahydro-7,8,8-trimethyl-4,7-methanobenzofuran-2(3H)-one (Noe-lacton) (1.94 g, 10.0 mMol) was dissolved in nitrobenzene (2.5 ml), and bromine (0.55 ml, 10 mMol) was added. The reaction was stirred under reflux at 90°C. After 5 h, the reaction mixture was cooled to room temperature, and diethyl ether (ca. 10 ml) was added. The organic layer was washed with a saturate solution of sodium hydrogen sulfite ($NaHSO_3$) (300 ml) until colourless, and the aqueous layer was extracted with diethyl ether (200 ml). The combined organic layer was dried over magnesium sulfate ($MgSO_4$). The solvent was removed in vacuo as far as possible. Liquid chromatography on silica gel with dichloromethane furnished colourless crystals.

Yield: 1.44 g (44%)

White solid; mp.: 96 °C

TLC: R_f-value: 0.55 (CH_2Cl_2)

^{1}H-NMR ($CDCl_3$): δ = 4.63 (d; ^3J = 7.7 Hz, 1H, C7a-H), 3.66/3.62/3.36/3.33 (AB-system, 2H, J_{AB} = 10.0 Hz, CH_2Br), 2.8 - 2.3 (m; 3H, C_3-H, C_{3a}-H), 2.0 - 1.0 (m; 5H, aliphatic-H), 0.94/0.91 (2s, 6H, 2 CH_3) ppm



^{13}C-NMR ($CDCl_3$): δ = 178.5 (C-2), 88.2 (C-7a), 52.6 (C-7), 51.1 (C-4), 48.2 (C-8), 42.3 (C-3a), 34.7 (C-3), 32.9 (7-CH_2Br), 30.2 (C-6), 28.1 (C-5), 23.5/20.6 (8-2CH_3) ppm

1.5.3.8 Binding of camphorlactol on an aminosilicagel support

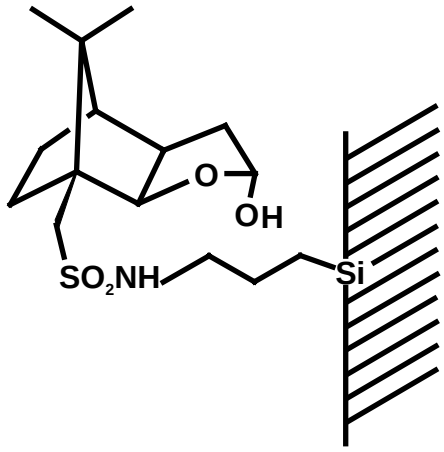
Ingredients:

1 g	GROM-SIL 300 Amino-5 ST (GROM, Herrenberg-Kayh, Germany), 5 µm bead size, Part-No. GSNH50530, Batch 3012 (0.21 mMol NH_2)
244 mg	[3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methano-benzofuran-7-yl-methanesulfonyl chloride (0.42 mMol)
25 ml	Dichloromethane, abs.
0.09 ml	Triethylamine, abs. (0.63 mMol)

Procedure:

1 g Aminosilicagel and 244 mg [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methanobenzofuran-7-yl-methanesulfonyl chloride were placed in a flask, and 25 ml of dichloromethane was added. After 1 h, 0.09 ml triethylamine was added, and the slurry was stirred at room temperature while keeping dry with a $CaCl_2$-tube for 48 h. The solid was isolated and cleaned through a G4 filter, rinsed with dichloromethane, acetone, water, acetone, and eventually with dichloromethane. The product was dried in high vacuo.

Yield: 0.96 g



EA:

Calculated (aminosilicagel)	C 1.772, H 3.428, N 0.254
Found (modif. aminosilicagel)	C 3.899, H 1.082, N 0.325, S 0.647, Cl 0.09

^{13}C-CP-MAS-NMR: δ = 8.7, 20.6, 27.8, 48.1, 87.9, 98.0 ppm

1.5.3.9 Binding of camphorlactol on an aminopolystyrene support in CCl_4

Ingredients:

10.92 g Polystyrene A NH_2 (Rapp Polymere, Tuebingen, Germany), HA1 400 02, 200-400 mesh, capacity 0.89 mMol/g (9.72mMol)

4.99 g [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methano-benzofuran-7-yl-methanesulfonyl chloride (8.59 mMol)

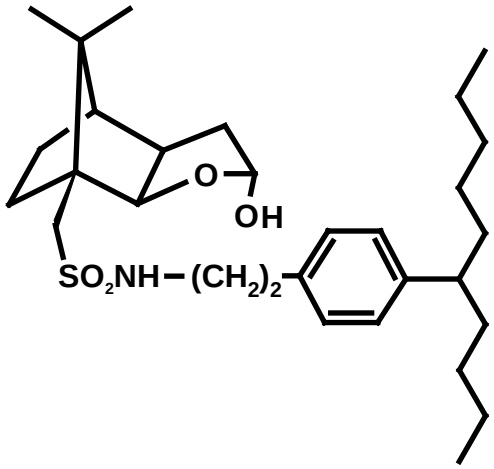
100 ml Carbontetrachloride, abs.

1.5 ml Triethylamine, abs.

Procedure:

10.92 g Aminopolystyrene and 4.99 g [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexa-hydro-2-oxo-4,7-methanobenzofuran-7-yl-methanesulfonyl chloride were placed in a flask, and 100 ml CCl_4 was added. After 2 h, 1.5 ml triethylamine was added and the slurry was stirred at room temperature while keeping dry by a $CaCl_2$-tube for 48 h. The solid was isolated and cleaned through a G4 filter, and rinsed with CCl_4. The solvent should not be discarded, as there is some unreacted lactol in it, that may be recovered from the filtrate by evaporating in vacuo. The polymer bound lactol was dried in high vacuo at 50°C.

Yield: 14.29 g



^{13}C-CP-MAS-NMR (13C DSX 200 Rf 1000Hz): δ = 145.7, 127.9, 86.7, 40.1, 29.0, 20.8 ppm

EA:

Calculated (aminopolystyrene) C 87.87, H 5.806, N 1.351

Found (modif. aminopolystyrene) C 82.73, H 7.316, N 1.263, S 1.448, Cl 1.24

1.5.3.10 Binding of camphorlactol on an aminopolystyrene support in DMF

Ingredients:

1.05 g Polystyrene A NH_2 (Rapp Polymere, Tuebingen, Germany), HA1 400 02, 200-400 mesh, capacity 1,08 mMol/g) (1.14 mMol)

0.42 g [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methano-benzofuran-7-yl-methanesulfonyl chloride (0.73 mMol)

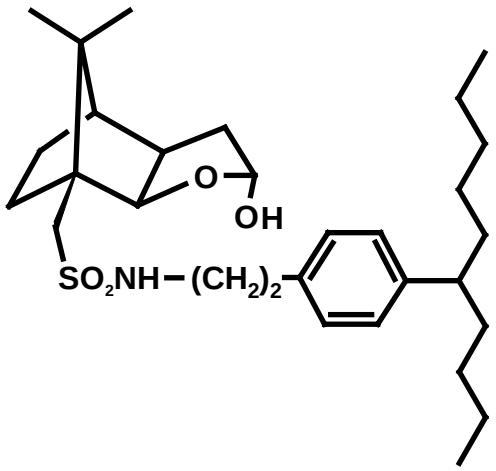
10 ml DMF (N,N-dimethylformamide), abs.

100 mg Triethylamine, abs.

Procedure:

1.05 g Aminopolystyrene and 0.42 g [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexa-hydro-2-oxo-4,7-methanobenzofuran-7-yl-methanesulfonyl chloride were placed in a flask, and 10 ml DMF was added. After 2 h, 100 mg triethylamine was added and the slurry was stirred at room temperature while keeping dry by a $CaCl_2$-tube for 48 h. The solid was isolated and cleaned through a G4 filter, rinsed with DMF (8 ml), and eventually rinsed with DCM (4 x 10 ml). The product was dried in high vacuo at 50°C.

Yield: 1.26 g



^{13}C-CP-MAS-NMR (^{13}C DSX 200 Rf 1000Hz): δ = 145.8, 129.9, 97.0, 47.8, 40.1, 28.8, 23.3 ppm

EA:

Calculated (aminopolystyrol) C 87.87, H 5.806, N 1.351

Found (modif. aminopolystyrol) C 74.98, H 7.224, N 1.720, S 1.481, Cl 8.39

1.5.3.11 Binding of camphorlactol on an aminomethylated polystyrene support in DCM

Ingredients:

1.00 g Aminomethylated polystyrene resin (**nova**biochem) 01-64-0010, capacity 1,08 mMol/g (1.08 mMol)

1.13 g [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methano-benzofuran-7-yl-methanesulfonyl chloride (1.98 mMol)

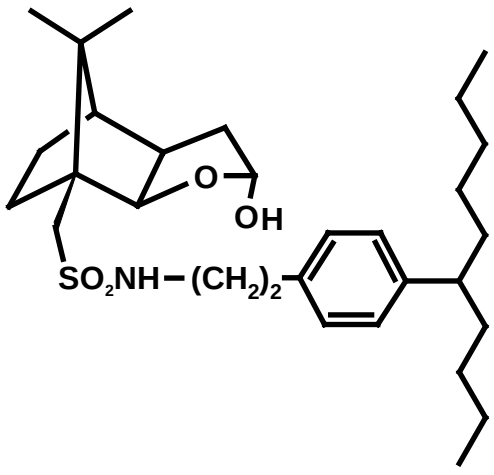
25 ml DCM (Dichloromethane), abs.

0.41 ml Triethylamine, abs. (2.97 mMol)

Procedure:

1.00 g Aminopolystyrene and 1.13 g [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexa-hydro-2-oxo-4,7-methanobenzofuran-7-yl-methanesulfonyl chloride were placed in a flask, and 25 ml DMF was added. After 2 h, 0.41 ml triethylamine was added and the slurry was stirred at room temperature while keeping dry by a $CaCl_2$-tube for 48 h. The solid was isolated and cleaned through a G4 filter, rinsed with DMF, actone, water, actone, and eventually with DCM (4 x 10 ml). The product was dried in high vacuo at 50°C.

Yield: 1.30 g



^{13}C-CP-MAS-NMR (^{13}C DSX 200 Rf 1000Hz): δ = 145.8, 129.9, 97.0, 47.8, 40.1, 28.8, 23.3 ppm

EA:

Calculated (aminopolystyrol)	C 87.87, H 5.806, N 1.351
Found (modif. aminopolystyrol)	C 74.98, H 7.224, N 1.720, S 1.481, Cl 8.39

1.5.3.12 Binding of camphorlactol on an amino modified porous glass support in DCM

Ingredients:

1 g BIORAN G001/030/C/060 (SCHOTT, Mainz, Germany), grain size 30 - 60 µm, pore diameter 15.1 nm, surface modif. NH_2, Lot #G0131

0.82 g [3aR-(3aα,4β,7β,7aα)]-8,8-dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methano-benzofuran-7-yl-methanesulfonyl chloride (1.41 mMol)

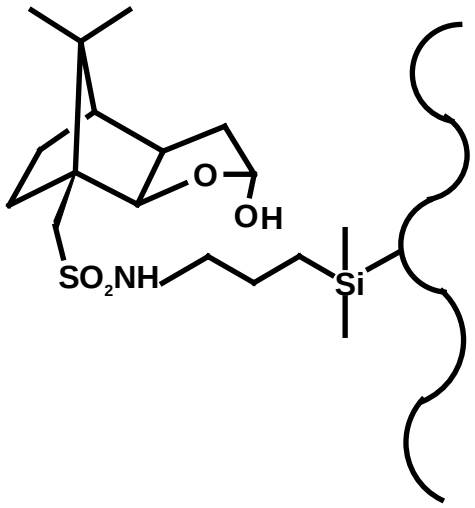
25 ml DCM (Dichloromethane), abs.

0.3 ml Triethylamine, abs. (2.16 mMol)

Procedure:

0.82 g [3aR-(3aα,4β,7β,7aα)]-8,8-Dimethyl-3a,4,5,6,7,7a-hexahydro-2-oxo-4,7-methanobenzo-furan-7-yl-methanesulfonyl chloride were placed in a flask with 25 ml DCM, and 0.3 ml tri-ethylamine was added, then 1 g bioran glass was added and the slurry was stirred at room temperature while keeping dry by a $CaCl_2$-tube for 48 h. The solid was isolated and cleaned through a G4 filter, rinsed with DMF, actone, water, actone, and eventually with DCM (4 x 10 ml). The product was dried in high vacuo at 50°C.

Yield: 0.965 g



^{13}C-CP-MAS-NMR: δ = 9.2, 20.8, 27.8, 42.4, 48.2, 87.3, 98.1 ppm

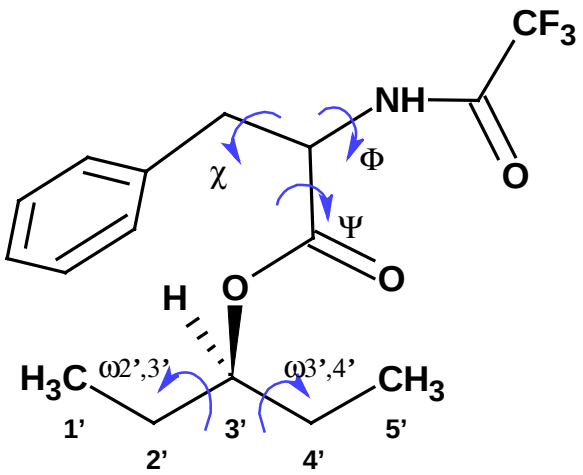
EA: Found (modif. aminopolystyrol): C 4.486, H 1.035, N 0.897, S 0.475

Part 2. Analysis of the Complete Conformational Space of N-TFA-Phenylalanine 3'-Pentyl Ester for Contribution to Chiral Recognition Enhancement

2.1. Introduction

In recent years, the focus of numerous studies in life sciences was on quantitative analysis of the chemical and enantiomeric composition of biologically as well as pharmaceutically relevant substances using synthetic chiral model receptors. Chiral recognition phenomena operating with artificial receptor models have attracted heightened interest [26], [27], [28]. In particular, the thermodynamic factor of interaction of enantiomeric guests, for example, N-TFA amino acid esters [29], with the chirally modified polysiloxane Chirasil-Val [30] and derivatives [26] reveal characteristic differences.

In recognition studies with Chirasil-Val, 3'-pentyl esters gave particularly large differences in interaction energies, as compared to other esters of amino acids [29] and hydroxy acids [31], respectively. Following the hypothesis that the 3'-pentyl group might contribute to the magnitude of these differences by preferentially adopting a set of chiral conformations, N-acyl amino acid-3'-pentyl esters should be of particular interest within this class of compounds. N-trifluoroacetyl-phenylalanine-3'-pentyl ester (**24**) seemed a most promising candidate, in view



24

of the expected steric repulsion between the benzyl group and parts of the 3'-pentyl moiety in particular conformations of the title compound **24**. The results of an attempt to completely search for all stable minima including the global minimum are outlined in the following.

However, it is very difficult to model these interactions with empirical and semi-empirical calculation methods, because of the large number of possible conformations and relative orientations of host and guest. In order to better understand the recognition processes involved, thermodynamics of the gas chromatographic separation of a variety of N-TFA-amino acid ester enantiomers on Chirasil-Val [32] were studied. We concluded from the experimental facts that systematic investigations on the conformational space of guest's molecular structure may help to elucidate the complex recognition process.

2.2. Foundation

2.2.1. Chiral Recognition in Sensor Science by the Model Receptor Octyl-Chirasil-Val

Odour perception in humans can sometimes discriminate different enantiomers of a chiral compound, such as limonene [33], [34]. Chiral discrimination represents one of the greatest challenges in attempts to devise selective and sensitive gas sensors. Natural odour receptors are proteins that use only one enantiomeric form (the L form) of the amino acid building blocks. In a cooperation of our group with Goepel, Gauglitz et al. [35], the chiral model receptor Octyl-Chirasil-Val (Figure 2-1) was used that is derived from the well-know chiral gas chromatography stationary phase Chirasil-Val [30]. It contains chiral peptide residues for enantiomer recognition and non-chiral lipophilic side chains [36].

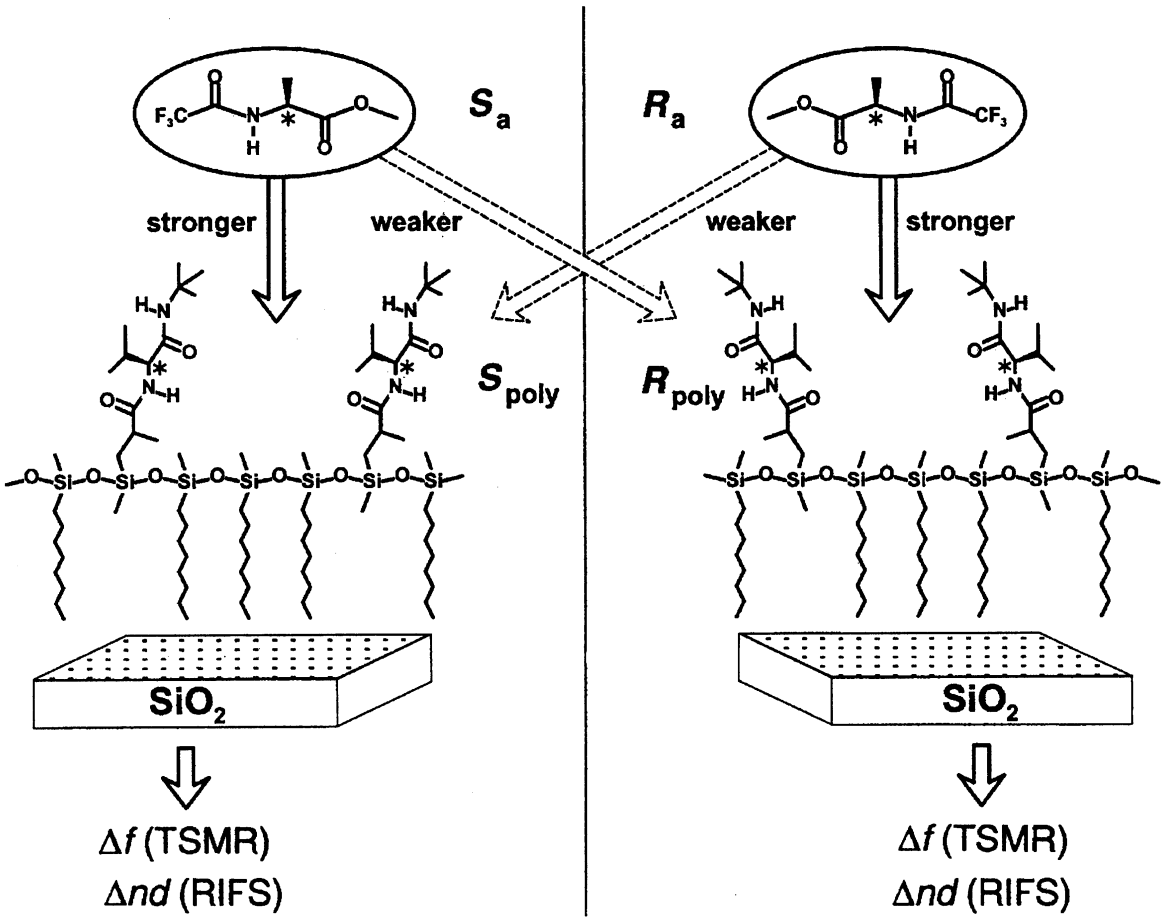


Figure 2-1. Principle of chiral recognition by gas sensors: chiral discrimination by preferential sorption of the enantiomers of N-TFA-Ala-OMe into enantioselective (R)- and (S)-Octyl-Chirasil-Val polymers [35].

The stationary phase will sorb the analyte, the sorption strength depends on the interaction mechanisms (H-bond, dispersion force) between matrix and analyte molecules. $\Delta\Delta G^o$ is the enantiomeric difference in Gibbs free energy of sorption, where the acid group is protected by esterification and the amino group by a trifluoroacetyl group. In comparative GC experiments, it has been established that the interactions between (S)-analyte and (S)-polymer as well as (R)-analyte and (R)-polymer are stronger than between the pairs (R)/(S) and (S)/(R), respectively. A detailed analysis of the conformational space of similar substrates, as presented in this thesis, may serve a better understanding of the underlying discrimination mechanisms.

2.2.2. Packing Phenomena in Chiral Liquids: Binary Mixtures of Enantiomers

In a cooperation of our group with Lepori [37], the work has been guided by the experimental facts to believe that systematic investigations on the conformational space of the guest's molecular structure may help to elucidate the complex recognition process.

Extending preceeding experiments, we here report on the volume changes upon mixing the enantiomeric pair of three amino acid derivatives, *i.e.*, the N-trifluoroacetyl methyl esters of alanine (N-TFA-Ala-OMe 1), valine (N-TFA-Val-OMe 2), and leucine (N-TFA-Leu-OMe 3). The liquid mixtures to be studied were made up by adding successively weighed amounts of a pure enantiomer to a given amount of the other. For each mixture, the excess molar volume, V^E, was determined through equation 2-1.

$$V^E = M\left(1/\rho - \chi_1/\rho_1 - \chi_2/\rho_2 \right) \qquad (2\text{-}1)$$

Here, ρ is the density of the mixture, M is the average molecular weight of the two components, χ_1 and χ_2 are their mole fractions, ρ_1 and ρ_1 are the densities of the pure liquids of two components, respectively.

As illustrated in Figure 2-2, different amounts of enantiomeric pairs of amino acid derivates were mixed, the excess molar volumes V^E at 25°C appeared symmetrical around χ = 0.5. The V^E data were fitted by a least-squares method to equation 2-2,

$$V^E = \alpha\chi(1-\chi) \qquad (2\text{-}2)$$

χ being the mole fraction of (S)-enantiomer, the value of parameter α/4 is equal to the excess volumes at equimolar composition $V^E\chi=0.5$, that means there are packing phenomena in chiral liquids. The volumetric effects for the valine derivative (N-TFA-Val-OMe) and (N-TFA-Ala-OMe) are of opposite direction: whereas the (R)- and (S)- enantiomers of (N-TFA-Val-OMe) are packed together more tightly in racemic mixture than in the scalemic (enantiomerically enriched) liquid, the opposite holds true for (N-TFA-Ala-OMe). It was one of the goals of the thesis presented to understand these phenomena better by studying the conformations of such molecules.

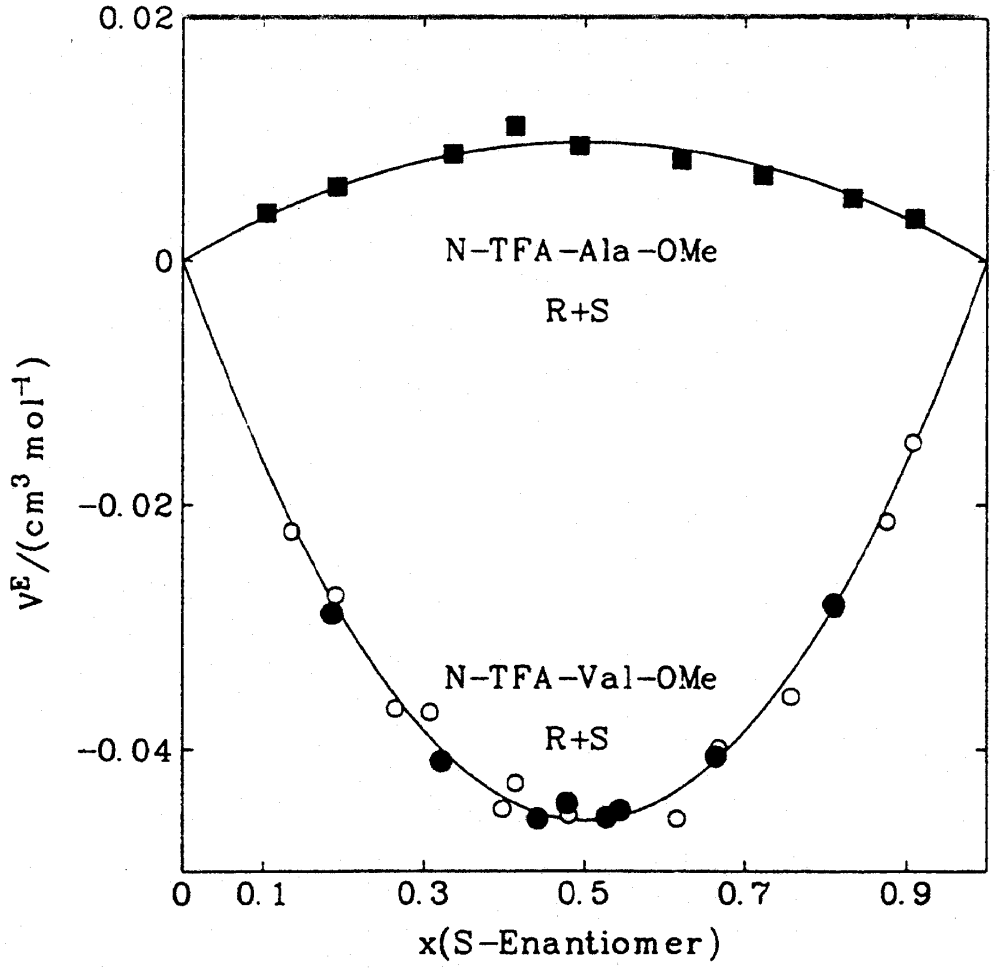


Figure 2-2. Excess molar volumes V^E at 25°C for (R)-1+(S)-1(■), (R)-2+(S)-2 pure (●), and contaminated (o) enantiomer samples {(R)-2: chemical purity 99%, ρ=1.22860 gcm^{-3}; (S)-2: chemical purity 98.5%, ρ=1.23088 gcm^{-3}} [37].

2.2.3. Possible Chirality Enhancement in 3'-Pentyl Esters

The thermodynamic parameters of interaction of enantiomeric guests, such as N-TFA amino acid esters, with the chirally modified polysiloxane Chirasil-Val and derivatives show characteric differences [29]. Especially 3'-pentyl esters gave large differences in interaction energies, as compared to other esters of amino acids and hydroxy acids, respectively. The resolution factor (α) of the enantiomers of a particular 3'-pentyl amino acid ester at a given temperature is usually higher than that of any other ester investigated (see Table 2-1). This suggests that the 3'-pentyl group may adopt a particular set of chiral conformations where one enantiomorph may be preferentially induced by the presence of the stereogenic center at the α-

carbon of the amino acid. The systematic investigation of the conformation space of the guest's molecular structure may help to elucidate the complex recognition process.

Table 2-1: Thermodynamic parameters of enantiomer separation of N-TFA-Phenylalanine esters at L-Chirasil-Val (acc. to M. Hummel [29])

Ester group	$-\Delta\Delta H$ [cal/mol]	$\Delta\Delta S$ [cal/grd mol]	$-\Delta\Delta G_{298}$ [cal/mol]	α T=298K
Methyl	452.3 ±21.1	0.955 ±0.005	167.5 ±6.3	1.327 ±0.014
Ethyl	528.2 ±22.3	1.126 ±0.055	192.6 ±6.4	1.384 ±0.002
Isobutyl	504.4 ±12.4	1.076 ±0.031	183.5 ±3.7	1.363 ±0.008
3'-Pentyl	703.0 ±34.8	1.514 ±0.009	251.7 ±10.1	1.529 ±0.026
Cyclopentyl	601.3 ±50.1	1.279 ±0.124	219.7 ±14.4	1.449 ±0.035

From Table 2-1, we see that the 3'-pentyl ester shows the best resolution factor ($\alpha = 1.529$), while the methyl, ethyl, and isobutyl esters of N-TFA-phenylalanine are typically in the range 1.327 - 1.363. As a preliminary working hypothesis, this was attributed to the formation of pseudo-diastereomeric conformations, since the flexible 3'-pentyl moiety is not necessarily in the symmetric state that is usually drawn in the molecular structure.

The proposed induction of a certain enantiomorph of the ester group seems to depend on the steric repulsion between the benzyl group and part of the 3'-pentyl moiety in particular conformations of the title compound. Also in α-hydroxy acid esters, the 3'-pentyl esters show the best enantiomer separation. It has been pointed out that the separation factor is closely related to structural features, therefore, it is not surprising that a relatively high specificity was observed in the retention behaviour [38]. From all these observations it seems important to study all possible conformations of this compound.

2.3. Theoretical Basis of the Computational Method

Advances in computing, and particularly the ready availability of high-resolution graphics, has greatly increased the interest in computer-based molecular modeling. It is now widely used as an aid of the interpretation of experimental results and in the design of new materials with desirable properties.

2.3.1. Molecular Modeling and Molecular Mechanics

The basis of molecular modeling is that all important molecular properties, i.e., stabilities, reactivies and electronic properties, are related to the molecular structure [39]. There are many different approaches and related computer programs, including *ab initio* calculations, various semi-empirical molecular orbital (MO) methods, ligand field calculations, molecular mechanics, purely geometrical approaches, and neural networks, that can calculate structures and one or more additional molecular properties [40].

Before any computational study on molecular properties can be carried out, a molecular model needs to be established. Molecular mechanics is one such technique and, primarily for reasons of computational simplicity and efficiency, molecular mechanics can be considered to arise from the Born-Oppenheimer approximation, which assumes that the motion of nuclei of a molecule are independent of the motions of the electrons. In molecular mechanics calculations, the arrangement of the electrons is assumed to be fixed and the positions of the nuclei are calculated. Molecular mechanics is a valuable tool enabling chemist to predict molecular structures and energies [41].

The basis of the molecular mechanics method is that a good estimate of the geometry of a molecule can be obtained by taking into account all the forces between the atoms, calculated by using a mechanical approach.

A simple force field is shown below and the various terms are described:

$$E_{total} = E_{stretch} + E_{bend} + E_{torsion} + E_{nonbonded} \tag{2-3}$$

$$E_{stretch} = k_{stretch} \frac{(r - r_o)^2}{2} \tag{2-4}$$

$$E_{bend} = k_{bend} \frac{(\theta - \theta_o)^2}{2} \tag{2-5}$$

$$E_{torsion} = k_{torsion} \frac{(1 + \cos(m(\phi_{ijkl} + \phi_{offset})))}{2} \tag{2-6}$$

$$E_{nonbonded} = \varepsilon \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^{6} \right] \tag{2-7}$$

The force fields described above is not meant to represent any one of the many existing force field available to today's researchers [42]. It is meant, rather, to give some appreciation of the complexities of the problem and to suggest a general format. The force field defines the mechanical model to be used in computing a molecular structure and its relative energy. The input can be done by means of a computer graphical drawing program; once an input structure has been entered into the program, a set of parameters describing the molecular geometry is computed, i.e., bond lengths, and torsion angles. These values are then fed into the terms of the force field equation and a steric energy is calculated.

The next step in the process is to alter the structure in a systematic way to minimize the steric energy. This process will carry the molecule to an energy minimum somewhere on the molecular potential energy surface.

In a word, a molecular mechanics calculation will take the input structure and modify it into the direction of the nearest local minimum on the potential energy surface.

2.3.2. Geometry Optimization and Conformational Analysis

Molecular mechanics has become a valuable tool enabling chemists to predict structures of molecules and their energies. In many applications of molecular mechanics, it is important that the lowest energy structure, i.e., the global energy minimum, is found. In using molecular mechanics, we typically introduce an approximate, trial structure into a computer program which adjusts it so as to decrease the (theoretical) energy, halting when a minimum energy structure is obtained. Optimization methods used proceed downhill from the starting structure toward a “local minimum“ or conformation [43]. As stated previously, the energy minimization routines employed by molecular mechanics programs usually refine the starting geometry leading to a local minimum, which is not necessarily the global minimum [40]. The aim of a conformational search is to find as many low-energy minima as possible, which hopefully include the global minimum. A geometry optimization must be performed subsequently, in the course of minimization procedure the molecular structure will be relaxed.

A basic problem of molecular mechanics calculations [40] is that the energy minimization must be done on a complex hypersurface with many local minima. Therefore, optimized structures can depend heavily on the chosen starting geometries. Due to local minima, there is a danger that direct optimization methods stop far away from the global minimum. In order to get the global minimum, it is better to find all local minima. Clearly, if one could set up and evaluate all possible conformations, then one could arrive at the global minimum.

A good conformational search requires a method for generating starting geometries that cover all of the potential energy surface. If only part of the surface is covered, one cannot be sure that the global minimum will be found. The most reliable method for finding the global energy minimum is by systematically scanning the entire potential energy surface. It is well known that the bond lengths and bond angles do not change much between different conformations of a molecule and that the major variations are in torsion angles [45]. For this reason, the searches systematically vary all torsional angles in a molecule.

At first glance, it appears very easy to obtain the most stable conformation, however, in practice the energy barriers between the local minima prevent changes from one conformation to the other during geometry optimization. This problem can only be overcome by a complete search for all stable conformations.

In principle, a systematic conformational search may be performed in both internal (torsion angle) and external (Cartesian) coordinate frames [46]. Most currently used conformation searches operate as follows. First, a crude starting geometry is proposed, and its structure is optimized by molecular mechanics energy minimization. The resulting minimum energy conformer is then compared with previously found conformers to test for possible duplication. If the conformer thus generated is a previously undiscovered one, it is added to an accumulating list of unique conformers. The cycle is then repeated by obtaining a new crude starting geometry, energy minimization, etc.. After all given starting geometries have been used, in other words, when new minima are no longer being found, the search is terminated. Since the energy minimization part of the process simply refines starting geometries to a nearby local minimum, it is the starting geometry generation algorithm which most directly controls the overall effectiveness of the search in reaching convergence.

The methods used to generate starting geometries can be divided into two broad categories: deterministic searches which cover all areas of conformational space systematically and stochastic methods which use a random element in exploring space. The systematic or grid searches are typically conducted by altering torsion angles and operate by generating all combinations of selected values for some or all rotatable torsion angles to produce starting geometries distributed throughout the conformational space [46]. For searching the conformational space of molecules, we therefore use one of the well-known properties of conformers (i.e., that they differ primarily in torsion angles) to confine our searches to torsion space alone. Thus, internal coordinates in general and torsion angles in particular would seem to provide the most appropriate angles in coordinate frame in which to conduct conformational searches.

2.3.3. Building a Tree of Molecular Structures for Comprehensive Search of all Stable Conformations

In the first stage, the torsion angles of the "starting structure" are randomly chosen within torsion angle bounds, then they are changed systematically. It is very important to find a method getting all conformers of a molecule. We therefore developed a method for searching the torsional space of molecules by using a tree-search which efficiently and uniformly generates starting geometries throughout the entire conformational space; a similar approach

was discussed in the literature but not used [47], [48]. The torsion angles are arranged in a graph as a tree of molecular structure. The structure generation phase begins with selection of a series of possible values (e.g., 0^o, 60^o, 120^o, 150^o, ...) for each torsion angle and then formation of all possible combinations of the values to generate starting geometries which are compatible with nonbonded contact and ring closure constraints. Starting conformers are generated selectively by using geometrical restrictions, such as allowable dihedral angles, ring closure distance, and transannular distances.

At the lowest level of the tree, the leaves stand for each of the possible products (conformations) of the generation process and each edge stands for a torsional rotation. Intermediate nodes in the tree represent partially completed structures. Nonbonded distance tests provide one of the most efficient ways to eliminate unstable structures.

Torsion angle tree-searching provides a rapid method for generating molecular geometries approximating the various conformers.

Thus, searching the torsional space of molecules by using a tree-search will efficiently and uniformly generate starting geometries throughout the whole conformational space.

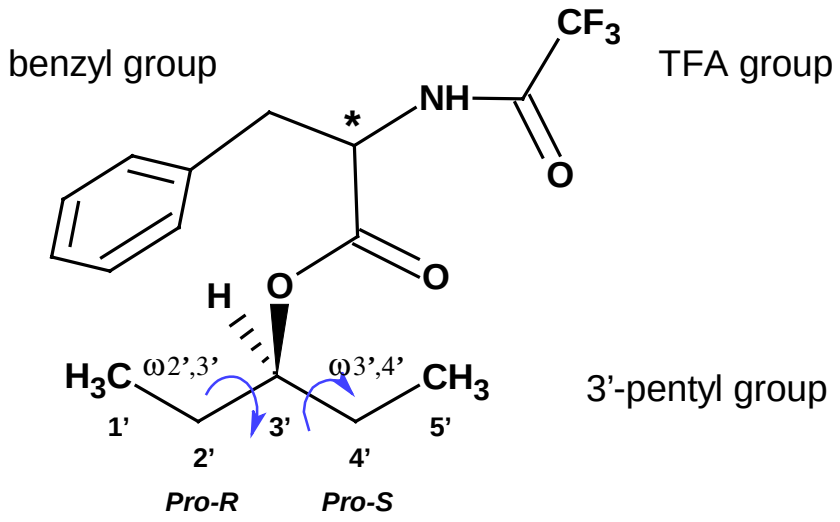
2.3.4. Computational Method

MMX force field calculations were carried out with the program PCMODEL (version 4.0 for DOS) [49]. PCMODEL is a full molecular modeling program and uses the MMX force field developed by J. J. Gajewski and K. E. Gilbert [50]. The force field implemented in this program is derived from Allinger's MM2 force field [51] without Pi electrons, with extensions and modifications as described [49].

2.4. Results and Discussion

2.4.1. MMX Structures and Energies of N-TFA-L-Phe-O-3'-Pentyl (24)

The molecular geometries and relative energies of N-trifluoroactyL-phenylalanine-3'-pentyl ester (**24**), as calculated by MMX (without Pi electrons), are compiled in **Appendix I**. In total, 2083 stable conformations were obtained. In Figure 2-3, the three bulky groups are shown, along with the two crucial torsions within the (locally prochiral) 3'-pentyl group. The two (locally enantiotopic) methylen groups 2' and 4', denoted "*Pro-R*" and "*Pro-S*", respectively [1], are diastereotopic due to the presence of the stereogenic center (marked *) [52].



24

Figure 2-3: Three bulky groups of N-TFA-L-Phe-O-3'-pentyl (**S-24**), and the two crucial torsions within the 3'-pentyl group, where both arrows describe a movement in positive direction

According to these MMX force field calculations, the most stable conformation, in other words the global minimum of N-TFA-L-Phe-O-3'-pentyl, shows a *pseudo meso* conformation (symmetric coplanar situation) of the (locally prochiral) 3'-pentyl group (see Figure 2-4). Here, the two crucial torsion angles $\omega_{2',3'}$ (178.7°) and $\omega_{3',4'}$ (175.0°) both take a trans conformation (tt). This molecular geometry is in good agreement with an ideal all-trans conformation where the two torsion angles are at 180°.

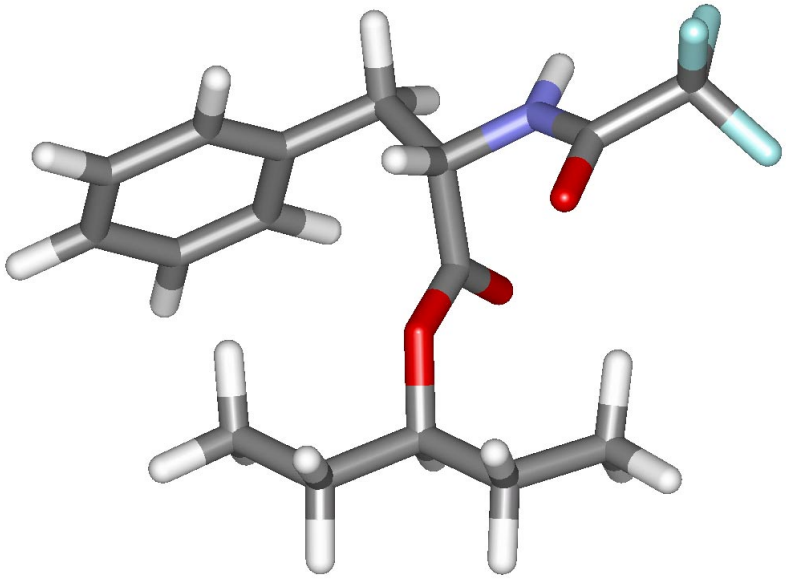
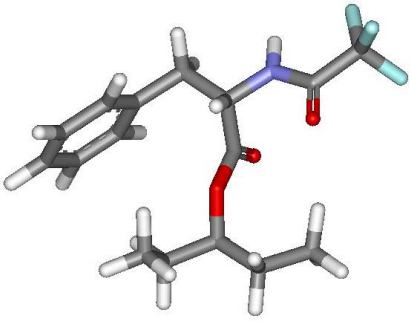


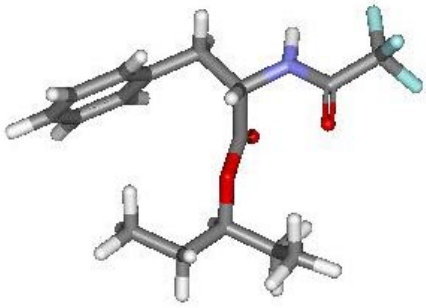
Figure 2-4: Global minimum of N-TFA-L-Phe-O-3'-pentyl, MMXE = 38.05 kcal/mol, $\omega_{2',3'}$ = 178.7°, $\omega_{3',4'}$ = 175.0° (**tt**)

The global minimum shows a balanced orientation of the three most bulky groups: benzyl, trifluoroacetyl and 3'-pentyl ester. As illustrated in Figure 2-3, the two crucial torsion angles in the 3'-pentyl group are $\omega_{2',3'}$ and $\omega_{3',4'}$. Torsion around these bonds will lead to gauche conformations (either g^+ or g^-) of higher (less favourable) energy. Since the methylen groups 2' (*Pro-R*) and 4' (*Pro-S*) are diastereotopic due to the chirality of the L-phenylalanine residue, the energy difference between the global minimum and corresponding local minima is not exactly the same. This will be illustrated in the following examples, where both the benzyl group and the TFA group still take extended, balanced conformations that do not differ significantly from the global minimum, *cf.* Figure 2-4 and Figures 2-5 to 2-7.



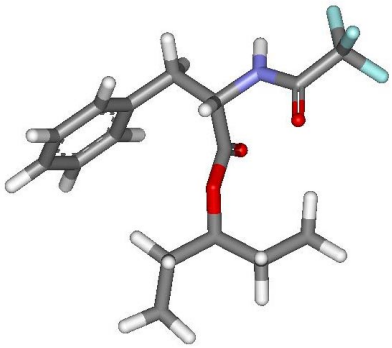
(**g**$^{+}$**t**) MMXE = 38.70 kcal/mol

$\omega_{2',3'}$ = 59.1°, $\omega_{3',4'}$ = 173.7°



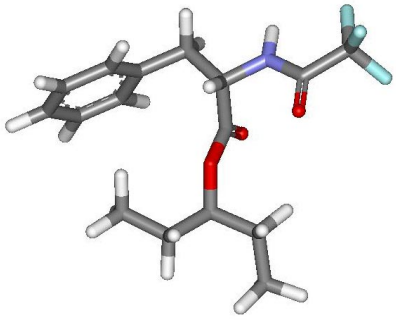
(**tg**$^{-}$) MMXE = 38.83 kcal/mol

$\omega_{2',3'}$ = -170.0°, $\omega_{3',4'}$ = -65.0°



(**g**$^{-}$**t**) MMXE = 39.03 kcal/mol

$\omega_{2',3'}$ = -64.4°, $\omega_{3',4'}$ = 176.8°

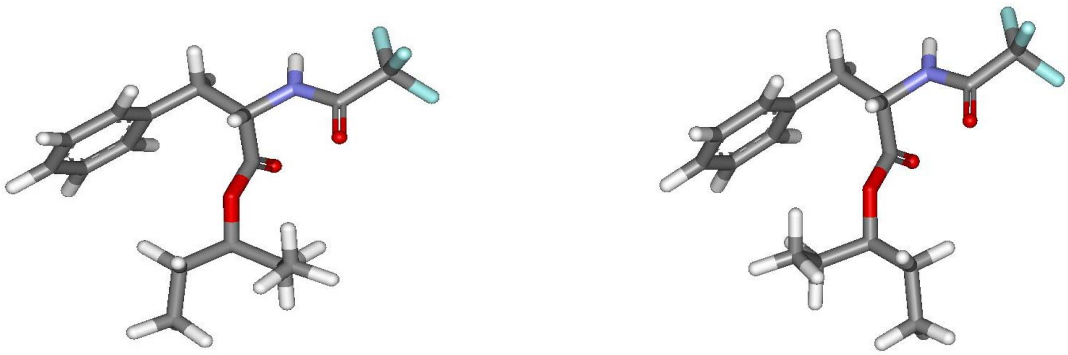


(**tg**$^{+}$) MMXE = 38.94 kcal/mol

$\omega_{2',3'}$ = 176.0°, $\omega_{3',4'}$ = 66.1°

Figure 2-5: Four local minima conformations after torsion of either one of the two diastereotopic methylen groups of the (**tt**)-conformation of 3'-pentyl around the C-C bonds at C-3', by appr. – or +120°; the denotation (**g**$^{+}$**t**) means: $\omega_{2',3'} \cong 60°$(**g**$^{+}$), $\omega_{3',4'} \cong 180°$(**t**), etc.

For the torsion of either one of the two diastereotopic methylen groups from (**tt**) to either (**g**$^{+}$**t**) and (**g**$^{-}$**t**) for the *Pro-R* group or (**tg**$^{-}$) and (**tg**$^{+}$) for the *Pro-S* group, the average increase in MMX energy was appr. 0.83 kcal/mol. In Figure 2-5, the lowest energy minima of these clusters are shown for each conformer. The diastereomorphic conformations (**g**$^{+}$**t**) and (**tg**$^{-}$) differ in MMX energy by 0.13 kcal/mol, while (**g**$^{-}$**t**) and (**tg**$^{+}$) differ by 0.11 kcal/mol.



($\mathbf{g}^{-}\mathbf{g}^{-}$) MMXE = 39.48 kcal/mol

$\omega_{2',3'}$ = -60.9°, $\omega_{3',4'}$ = -57.0°

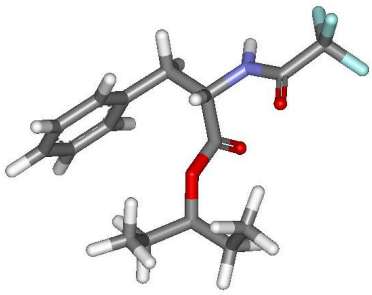
($\mathbf{g}^{+}\mathbf{g}^{+}$) MMXE = 39.50 kcal/mol

$\omega_{2',3'}$ = 56.8°, $\omega_{3',4'}$ = 60.8°

Figure 2-6: Two local minima conformations after conrotatory movement of both diastereotopic methylen groups of the (**tt**)-conformation of 3'-pentyl around the C-C bonds at C-3', by appr. + or –120°; the denotation ($\mathbf{g}^{-}\mathbf{g}^{-}$) means: $\omega_{2',3'} \cong$ -60°($\mathbf{g}^{-}$), $\omega_{3',4'} \cong$ -60°($\mathbf{g}^{-}$), etc.

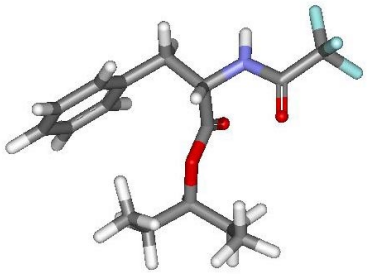
In Figure 2-6, two local minima (lowest energy conformers) after conrotatory movement of both diastereotopic methylen groups of the (**tt**)-conformation to either ($\mathbf{g}^{-}\mathbf{g}^{-}$) or ($\mathbf{g}^{+}\mathbf{g}^{+}$) are shown; the average increase in MMX energy was appr. 1.44 kcal/mol. This energy difference can be estimated by addition of the two increments of appr. 0.7 – 0.8 kcal/mol for each torsion. The difference between the two diastereomorphs is negligible (0.02 kcal/mol).

After disrotatory torsions of the two crucial bonds in the (**tt**)-conformation, four local minima (lowest energy conformers) were obtained, see Figure 2-7. The average increase in MMX energy from (**tt**) to either ($\mathbf{g}^{+}\mathbf{g}^{\ominus}$), ($\mathbf{g}^{\oplus}\mathbf{g}^{-}$), ($\mathbf{g}^{-}\mathbf{g}^{\oplus}$), and ($\mathbf{g}^{\ominus}\mathbf{g}^{+}$) was appr. 3.42 kcal/mol. The sum of the two torsion angles must not be zero degrees, because of strong nonbonded (repulsive) H-H interactions. Hence, the system tends to flip out of plane with either one of the two methyl groups, thereby widening the sum of torsion angles to appr. ±30°. Another consequence is the existence of a closely related pair of similar conformations ("Entartung").



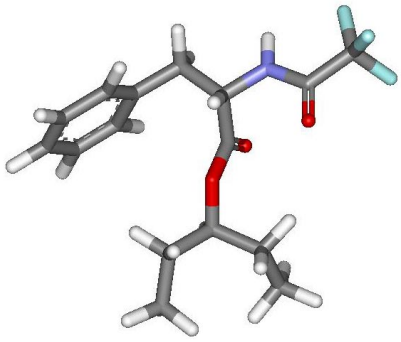
($\mathbf{g}^{+}\mathbf{g}^{\ominus}$) MMXE = 41.22 kcal/mol

$\omega_{2',3'}$ = 59.4°, $\omega_{3',4'}$ = -91.1°



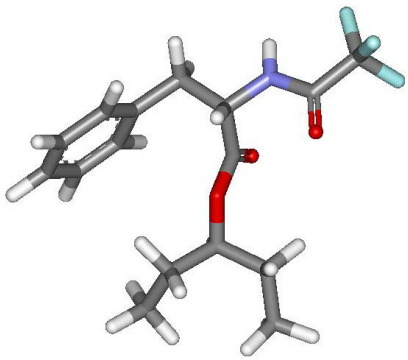
($\mathbf{g}^{\oplus}\mathbf{g}^{-}$) MMXE = 41.61 kcal/mol

$\omega_{2',3'}$ = 93.3°, $\omega_{3',4'}$ = -62.0°



($\mathbf{g}^{-}\mathbf{g}^{\oplus}$) MMXE = 41.55 kcal/mol

$\omega_{2',3'}$ = -61.5°, $\omega_{3',4'}$ = 94.2°



($\mathbf{g}^{\ominus}\mathbf{g}^{+}$) MMXE = 41.48 kcal/mol

$\omega_{2',3'}$ = -97.2°, $\omega_{3',4'}$ = 62.7°

Figure 2-7: Four local minima conformations after disrotatory movement of both diastereotopic methylen groups of the (**tt**)-conformation of 3'-pentyl around the C-C bonds at C-3', by either (-120° and +90°) or (-90° and +120°); the denotation ($\mathbf{g}^{+}\mathbf{g}^{\ominus}$) means: $\omega_{2',3'} \cong 60°(\mathbf{g}^{+})$, $\omega_{3',4'} \cong -90°(\mathbf{g}^{\ominus})$ where the circle indicates a widening of the torsion angle due to nonbonded (repulsive) H-H interactions

Up to here, we have only dealt with the most stable arrangement of the other residues. A systematic variations of all important torsion angles will be discussed in the following.

2.4.2. Systematic Variation of the Torsion Angles in S-24 and Model Compounds 25, 26

In N-TFA-L-phenylalanine 3'-pentyl ester (**S-24**), the three bulky groups benzyl, trifluoroacetyl and 3'-pentyl will dominate the preferred conformations, in other words, the set of torsion angles in relation to the MMX energy. In order to investigate the complete conformational space, it seemed a reasonable approach to simplify this structure by two model compounds, pentane (**25**) and 3'-pentyl formiate (**26**) (see Figure 2-8). These prestudies guided us to organize the conformations of (**S-24**) in a tree structure.

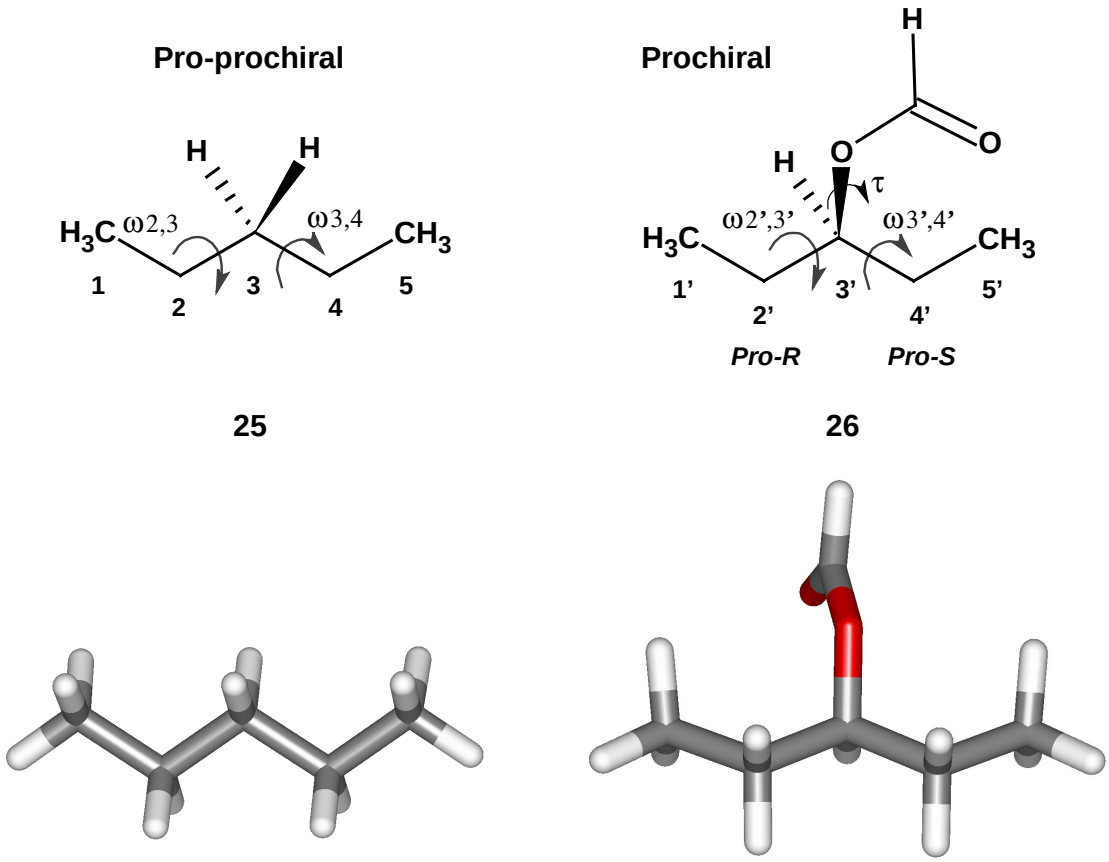


Figure 2-8: Top: Denotation of **25** and **26**, positive torsion angles shown. Bottom: Global minimum of pentane (**25**), MMXE = 2.82 kcal/mol, $\omega_{2,3}$ = 179.9°, $\omega_{3,4}$ = 178.0° (**tt**); double global minima of 3'-pentyl formiate (**26**), MMXE = 2.91 kcal/mol, $\omega_{2',3'}$ = -177.0°, $\omega_{3',4'}$ = 178.5° (**tt**), τ = 12.3° and $\omega_{2',3'}$ = 178.0°, $\omega_{3',4'}$ = -177.5° (**tt**), τ = -13.4°, racemate of two (chiral) atropic isomers (τ = $HC^{3'}OC$)

A systematic variation of the two torsion angles of pentane led to 10 more (altogether 11) combinations, that are shown in the following Figures.

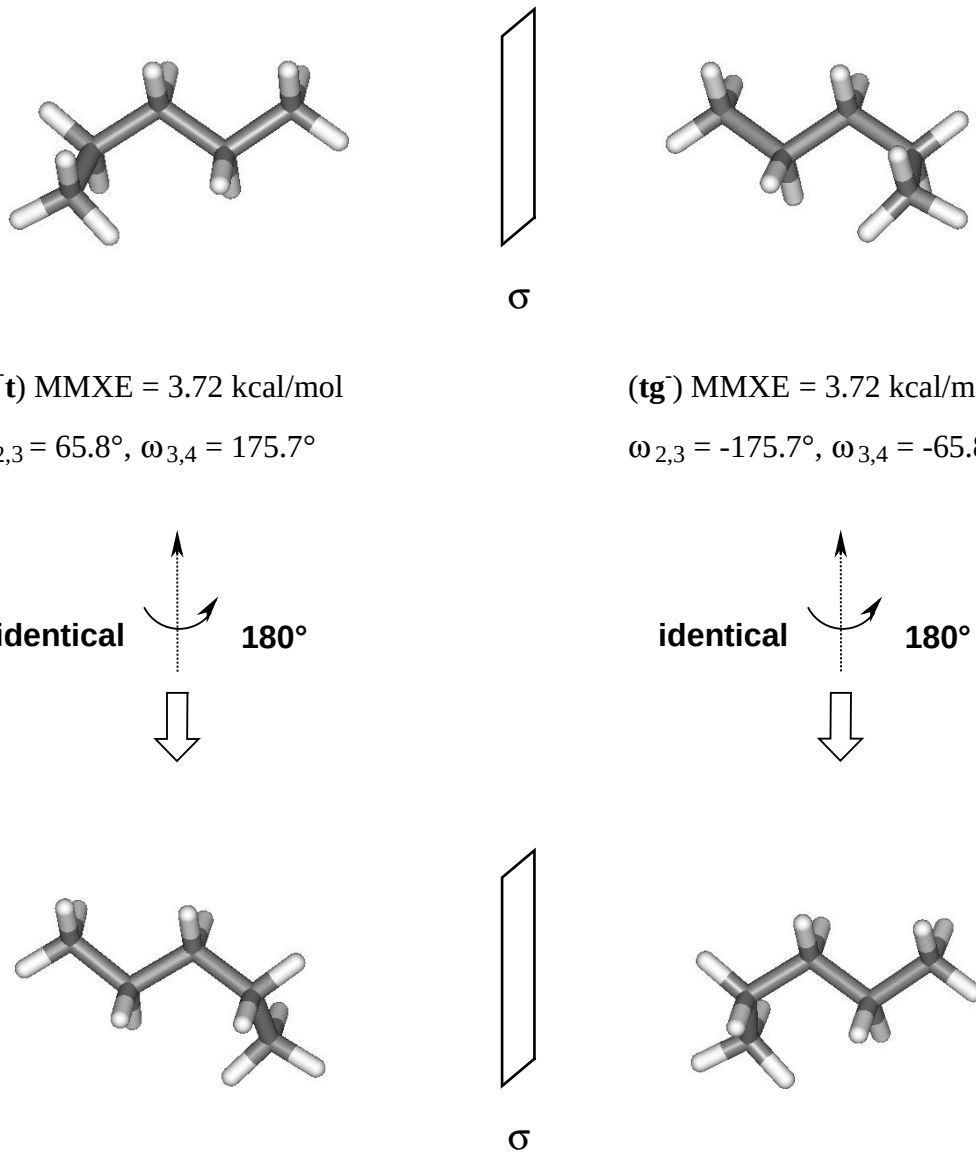
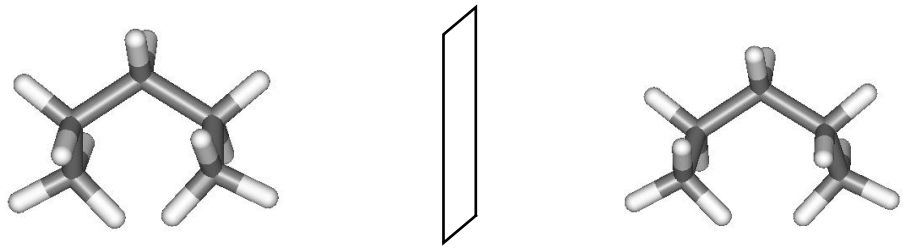


Figure 2-9: Two local minima conformations (one mirror image pair) of pentane after torsion around either one of the two C-C bonds of the (**tt**)-conformation by appr. – or +120°; apart from the sign, $\omega_{2,3}$ and $\omega_{3,4}$ are similar for all four combinations

For pentane, torsion of $\omega_{2,3}$ from (**tt**) to (**g$^+$t**) (upper left in Figure 2-9) by appr. –120° has the same effect as torsion of $\omega_{3,4}$ from (**tt**) to (**tg$^+$**) (bottom left) by appr. –120°; identity can be shown by superposition after rotation by 180°. (**tg$^-$**) and (**g$^-$t**) (upper and bottom right) represent the mirror image of (**g$^+$t**) and (**tg$^+$**). The increase in MMX energy was again 0.9 kcal/mol. Due to the high symmetry, all four combinations have the same MMX energy.



σ

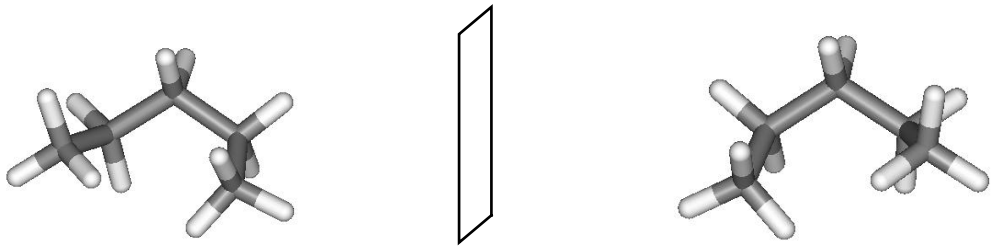
($\mathbf{g}^{-}\mathbf{g}^{-}$) MMXE = 4.45 kcal/mol
$\omega_{2,3}$ = -59.9°, $\omega_{3',4'}$ = -59.9°

($\mathbf{g}^{+}\mathbf{g}^{+}$) MMXE = 4.45 kcal/mol
$\omega_{2,3}$ = 59.9°, $\omega_{3,4}$ = 59.9°

Figure 2-10: Two local minima conformations (one mirror image pair) of pentane after conrotatory movement of both C-C bonds of the (**tt**)-conformation by appr. – or +120°; apart from the sign, all values of $\omega_{2,3}$ and $\omega_{3,4}$ are similar

In Figure 2-10, two local minima after conrotatory movement of both C-C bonds of the (**tt**)-conformation to either ($\mathbf{g}^{-}\mathbf{g}^{-}$) or ($\mathbf{g}^{+}\mathbf{g}^{+}$) are shown; the increase in MMX energy was 1.63 kcal/mol in both cases, that again reflect a mirror image situation..

After disrotatory torsion of the two crucial bonds in the (**tt**)-conformation, two local minima conformations (one mirror image pair) were obtained, see Figure 2-11. The increase in MMX energy from (**tt**) to either ($\mathbf{g}^{+}\mathbf{g}^{\ominus}$), ($\mathbf{g}^{\oplus}\mathbf{g}^{-}$), ($\mathbf{g}^{-}\mathbf{g}^{\oplus}$), and ($\mathbf{g}^{\ominus}\mathbf{g}^{+}$) was always 3.22 kcal/mol. For pentane, torsion of $\omega_{2,3}$ and $\omega_{3,4}$ from (**tt**) to ($\mathbf{g}^{+}\mathbf{g}^{\ominus}$) (upper left in Figure 2-11) by appr. –120° has the same effect as torsion of $\omega_{2,3}$ and $\omega_{3,4}$ from (**tt**) to ($\mathbf{g}^{-}\mathbf{g}^{\oplus}$) (bottom left) by appr. –120°; identity can be shown by superposition after rotation by 180°. ($\mathbf{g}^{\oplus}\mathbf{g}^{-}$) and ($\mathbf{g}^{\ominus}\mathbf{g}^{+}$) (upper and bottom right) again represent the mirror image of ($\mathbf{g}^{+}\mathbf{g}^{\ominus}$) and ($\mathbf{g}^{-}\mathbf{g}^{\oplus}$). Like in **24**, the sum of the two torsion angles must not be zero degrees, because of strong nonbonded (repulsive) H-H interactions, causing the system to flip out of plane with either one of the two methyl groups, thereby widening the sum of torsion angles to appr. ±30°.



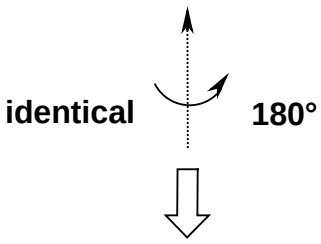
σ

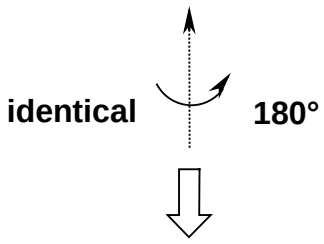
($\mathbf{g}^{+}\mathbf{g}^{\ominus}$) MMXE = 6.04 kcal/mol

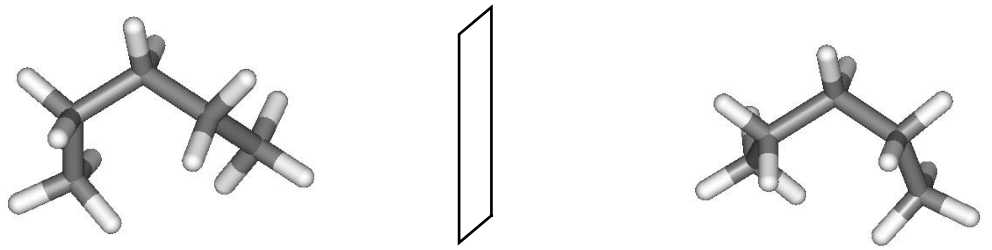
$\omega_{2,3}$ = 62.6°, $\omega_{3,4}$ = -95.0°

($\mathbf{g}^{\oplus}\mathbf{g}^{-}$) MMXE = 6.04 kcal/mol

$\omega_{2,3}$ = 95.0°, $\omega_{3,4}$ = -62.6°







σ

($\mathbf{g}^{-}\mathbf{g}^{\oplus}$) MMXE = 6.04 kcal/mol

$\omega_{2,3}$ = -62.6°, $\omega_{3,4}$ = 95.0°

($\mathbf{g}^{\ominus}\mathbf{g}^{+}$) MMXE = 6.04 kcal/mol

$\omega_{2,3}$ = -95.0°, $\omega_{3,4}$ = 62.6°

Figure 2-11: Two local minima conformations (one mirror image pair) of pentane after disrotatory torsion around both C-C bonds of the (**tt**)-conformation by either (-120° and +90°) or (-90° and +120°); as in Figure 2-7, the circle indicates a widening of the torsion angle from appr. 60° to appr. 90°; apart from the sign, the four combinations of $\omega_{2,3}$ and $\omega_{3,4}$ gave always the same set of values

These 11 combinations of torsion angles $\omega_{2,3}$ and $\omega_{3,4}$ of pentane are shown in Figure 2-12.

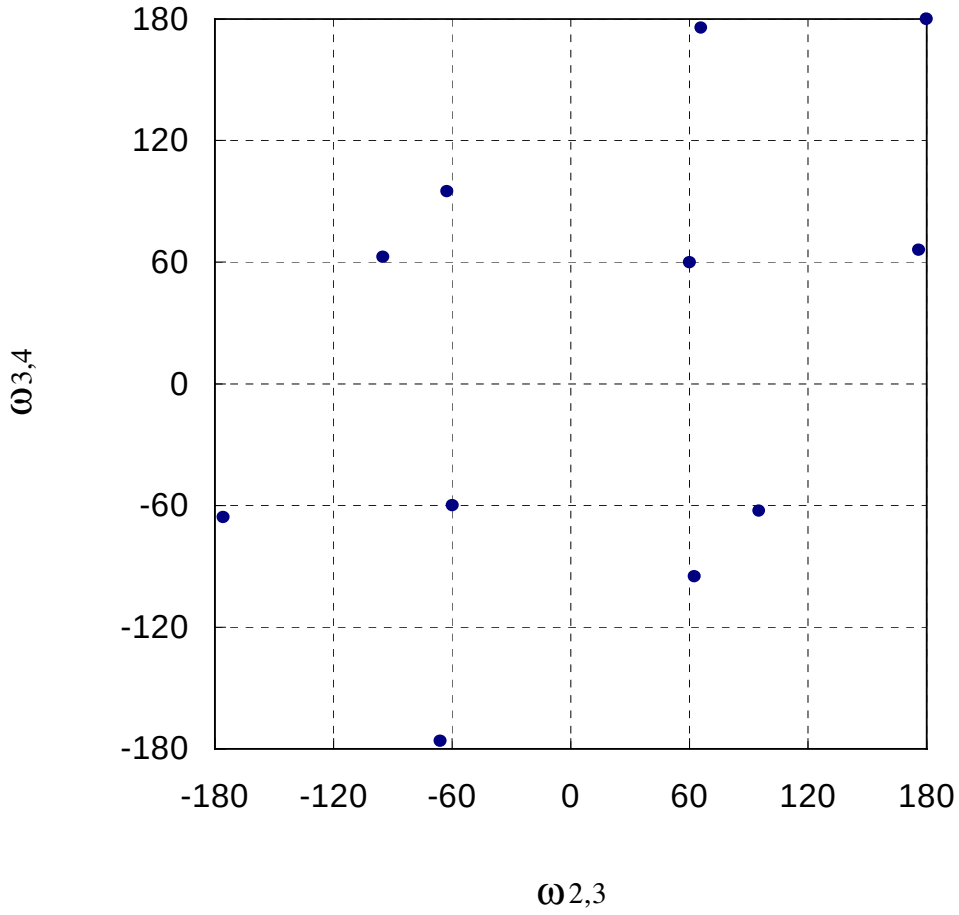
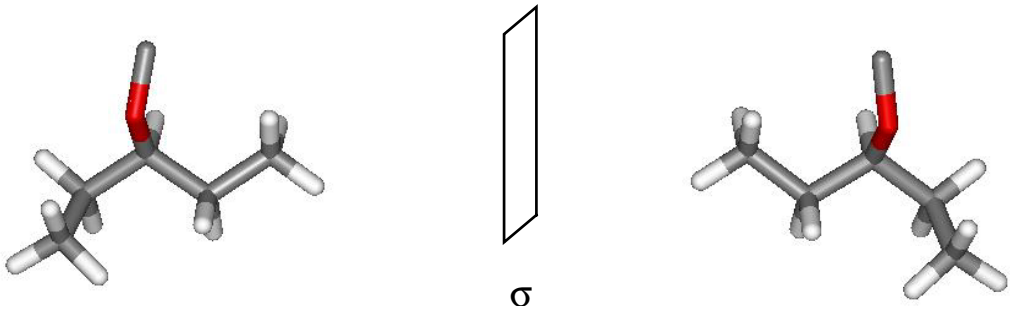


Figure 2-12: Eleven low energy combinations of torsion angles $\omega_{2,3}$ and $\omega_{3,4}$ for pentane **25**

Because of the high symmetry of this Pro-prochiral molecule, the 11 low energy combinations of torsion angles recorded in Figure 2-12 correspond to 1 global and only 6 local minima (that are 3 enantiomeric pairs). Thus, there are 9 different conformations.

A systematic variation of the two torsion angles of 3'-pentyl formiate (**26**) from the global minimum with a (**tt**)-conformation of the 3'-pentyl group (see Figure 2-8) led to 10 more (altogether 11) combinations, that are shown in the following figures.

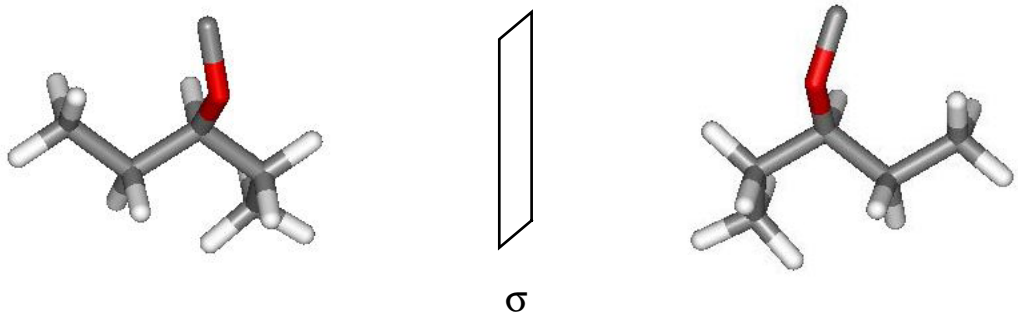


(**g**$^{+}$**t**) MMXE = 3.71 kcal/mol

$\omega_{2',3'}$ = 64.2°, $\omega_{3',4'}$ = 173.9°

(**tg**$^{-}$) MMXE = 3.71 kcal/mol

$\omega_{2',3'}$ = -174.0°, $\omega_{3',4'}$ = -63.4°



(**tg**$^{+}$) MMXE = 3.55 kcal/mol

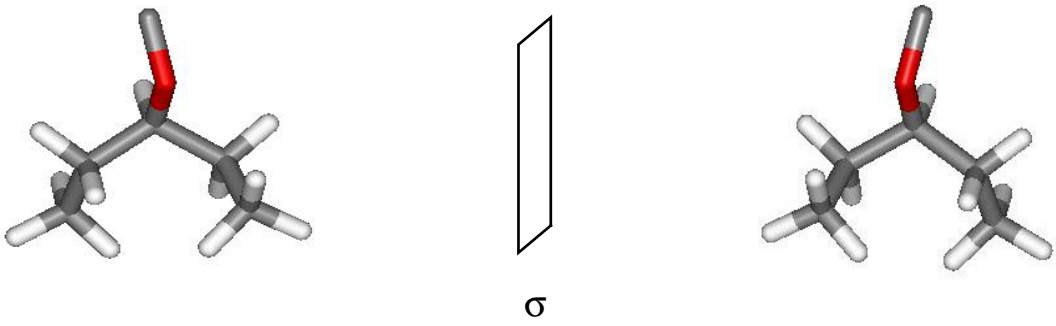
$\omega_{2',3'}$ = 178.7°, $\omega_{3',4'}$ = 67.1°

(**g**$^{-}$**t**) MMXE = 3.56 kcal/mol

$\omega_{2',3'}$ = -67.3°, $\omega_{3',4'}$ = -179.0°

Figure 2-13: Four local minima conformations (two mirror image pairs) of 3'-pentyl formiate after torsion around either one of the two C-C bonds at C-3' of the (**tt**)-conformation by appr. –120° or +120°, the formiate group is truncated (only the carbonyl carbon is shown)

For the torsion of either one of the two diastereotopic methylen groups from (**tt**) to either (**g**$^{+}$**t**) and (**g**$^{-}$**t**) for the *Pro-R* group or (**tg**$^{-}$) and (**tg**$^{+}$) for the *Pro-S* group, the average increase in MMX energy was again appr. 0.80 kcal/mol, for the *syn*-orientation of formiate and methyl (upper pair of enantiomers), but only 0.65 kcal/mol for the *anti*-orientation (bottom pair). While in Figure 2-5, the diastereomorphic conformations (**g**$^{+}$**t**) and (**tg**$^{-}$) of the chiral molecule **S-24** differ in MMX energy by 0.13 kcal/mol and (**g**$^{-}$**t**) and (**tg**$^{+}$) differ by 0.11 kcal/mol, there should not be such differences for the corresponding enantiomeric conformations of the prochiral molecule **26**. In fact, the differences between enantiomers found were negligible, coming from incomplete convergence. Despite the fact that the formiate **26** appeared to be a tricky residue in test calculations with Hyperchem, the similarity of enantiomers obtained with PCMODEL was quite satisfactory.



($\mathbf{g}^{-}\mathbf{g}^{-}$) MMXE = 4.26 kcal/mol

$\omega_{2',3'}$ = -60.4°, $\omega_{3',4'}$ = -58.6°

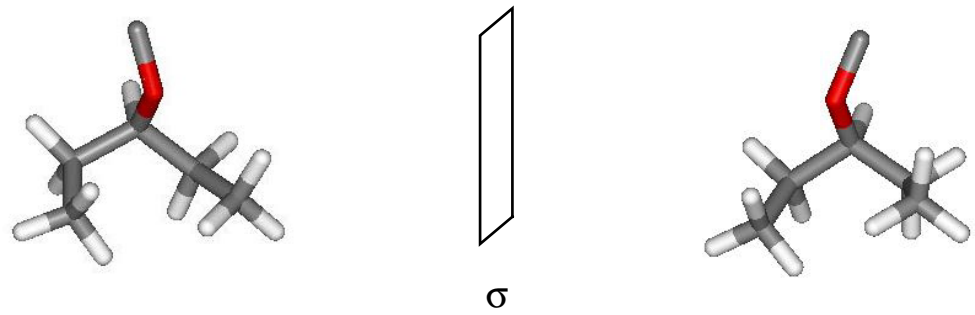
($\mathbf{g}^{+}\mathbf{g}^{+}$) MMXE = 4.26 kcal/mol

$\omega_{2',3'}$ = 58.9°, $\omega_{3',4'}$ = 60.3°

Figure 2-14: Two local minima conformations (one mirror image pair) of 3'-pentyl formiate after conrotatory movement of both C-C bonds of the (**tt**)-conformation by appr. – or +120° (formiate truncated)

In Figure 2-14, a mirror image pair of conformations after conrotatory movement of both enantiotopic methylen groups of the (**tt**)-conformation to either ($\mathbf{g}^{-}\mathbf{g}^{-}$) or ($\mathbf{g}^{+}\mathbf{g}^{+}$) is shown; the average increase in MMX energy was appr. 1.35 kcal/mol. The MMX energies and corresponding torsion angles should be similar, the small deviations found in geometry are due to incomplete geometry optimization.

After disrotatory torsions of the two crucial bonds in the (**tt**)-conformation, four local minima (two enantiomeric pairs) were obtained, see Figure 2-15. The average increase in MMX energy from (**tt**) to either ($\mathbf{g}^{+}\mathbf{g}^{\ominus}$), ($\mathbf{g}^{\oplus}\mathbf{g}^{-}$), ($\mathbf{g}^{-}\mathbf{g}^{\oplus}$), and ($\mathbf{g}^{\ominus}\mathbf{g}^{+}$) was appr. 3.34 kcal/mol for the *syn-syn*-orientation of formiate and the two methyl groups (upper pair of enantiomers), but only 2.67 kcal/mol for the *anti-anti*-orientation (bottom pair). Here, the energies and structures are very similar for each enantiomeric pair. As discussed previously, the sum of the two torsion angles is close to ± 30° instead of 0°, because of strong nonbonded (repulsive) H-H interactions in the latter case, forcing the system to flip out of plane with either one of the two methyl groups.

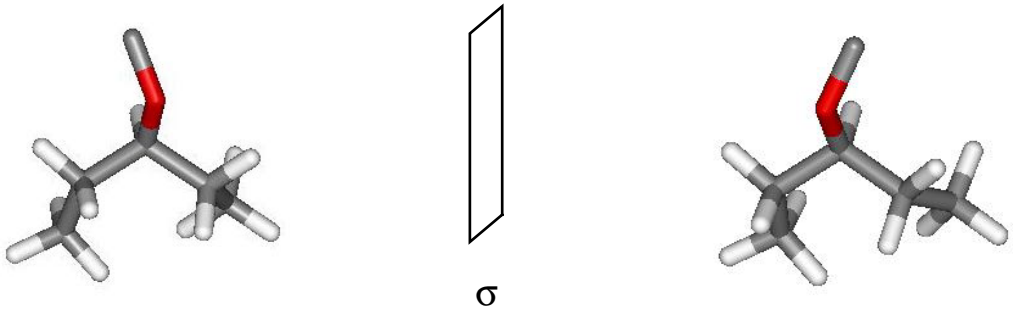


($\mathbf{g}^{+}\mathbf{g}^{\ominus}$) MMXE = 6.25 kcal/mol

$\omega_{2',3'}$ = 58.8°, $\omega_{3',4'}$ = -91.8°

($\mathbf{g}^{\oplus}\mathbf{g}^{-}$) MMXE = 6.25 kcal/mol

$\omega_{2',3'}$ = 91.8°, $\omega_{3',4'}$ = -58.8°



($\mathbf{g}^{-}\mathbf{g}^{\oplus}$) MMXE = 5.58 kcal/mol

$\omega_{2',3'}$ = -63.2°, $\omega_{3',4'}$ = 98.0°

($\mathbf{g}^{\ominus}\mathbf{g}^{+}$) MMXE = 5.58 kcal/mol

$\omega_{2',3'}$ = -98.0°, $\omega_{3',4'}$ = 63.2°

Figure 2-15: Four local minima conformations (two mirror image pairs) of 3'-pentyl formiate after disrotatory torsion around both C-C bonds at C-3' of the (**tt**)-conformation by either (-120° and +90°) or (-90° and +120°); as in Figure 2-7, the circle indicates a widening of the torsion angle from appr. 60° to appr. 90° due to nonbonded (repulsive) H-H interactions (formiate truncated)

In total, there exist 11 combinations of $\omega_{2',3'}$ - $\omega_{3',4'}$ for 3'-pentyl formiate that are shown in Figure 2-16 and Figure 2-17. In the former, the formiate group is truncated (only the carbonyl carbon is shown), in the latter, it is abbreviated by X.

The different combinations of the two crucial torsion angles are summarized in Figure 2-18. The geometries and relative energies of 3'-pentyl formiate, as calculated by MMX (without Pi electrons), are presented in **Appendix II**.

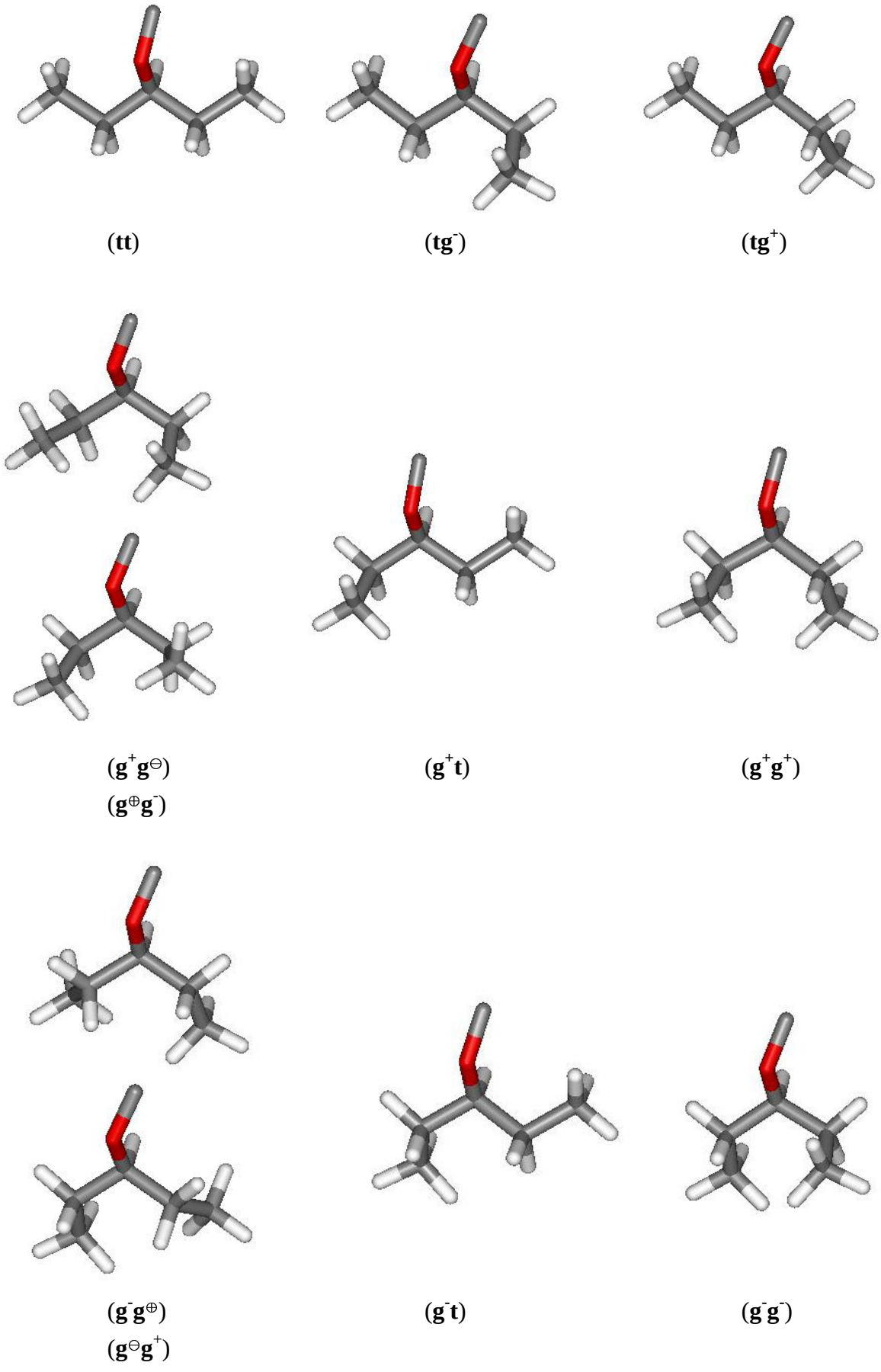
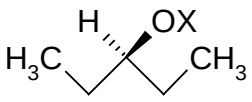
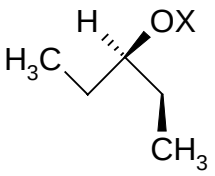


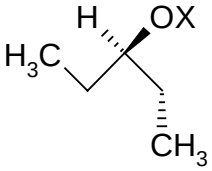
Figure 2-16: Scheme of the 11 combinations of $\omega_{2',3'}$ and $\omega_{3',4'}$ in **26** (formiate truncated)



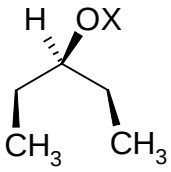
(**tt**)

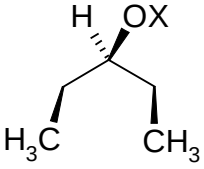


(**tg**$^{-}$)

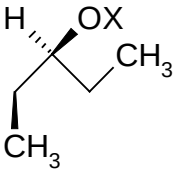


(**tg**$^{+}$)

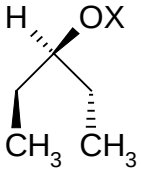




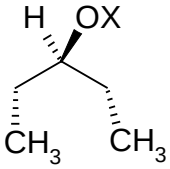
(**g**$^{+}$**g**$^{\ominus}$)
(**g**$^{\oplus}$**g**$^{-}$)

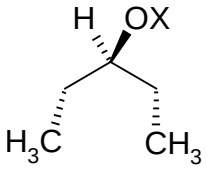


(**g**$^{+}$**t**)

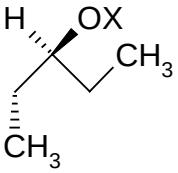


(**g**$^{+}$**g**$^{+}$)

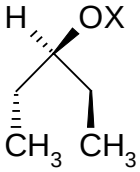




(**g**$^{-}$**g**$^{\oplus}$)
(**g**$^{\ominus}$**g**$^{+}$)



(**g**$^{-}$**t**)



(**g**$^{-}$**g**$^{-}$)

Figure 2-17: Sketch corresponding to the molecular models of Figure 2-16, X is C(=O)H

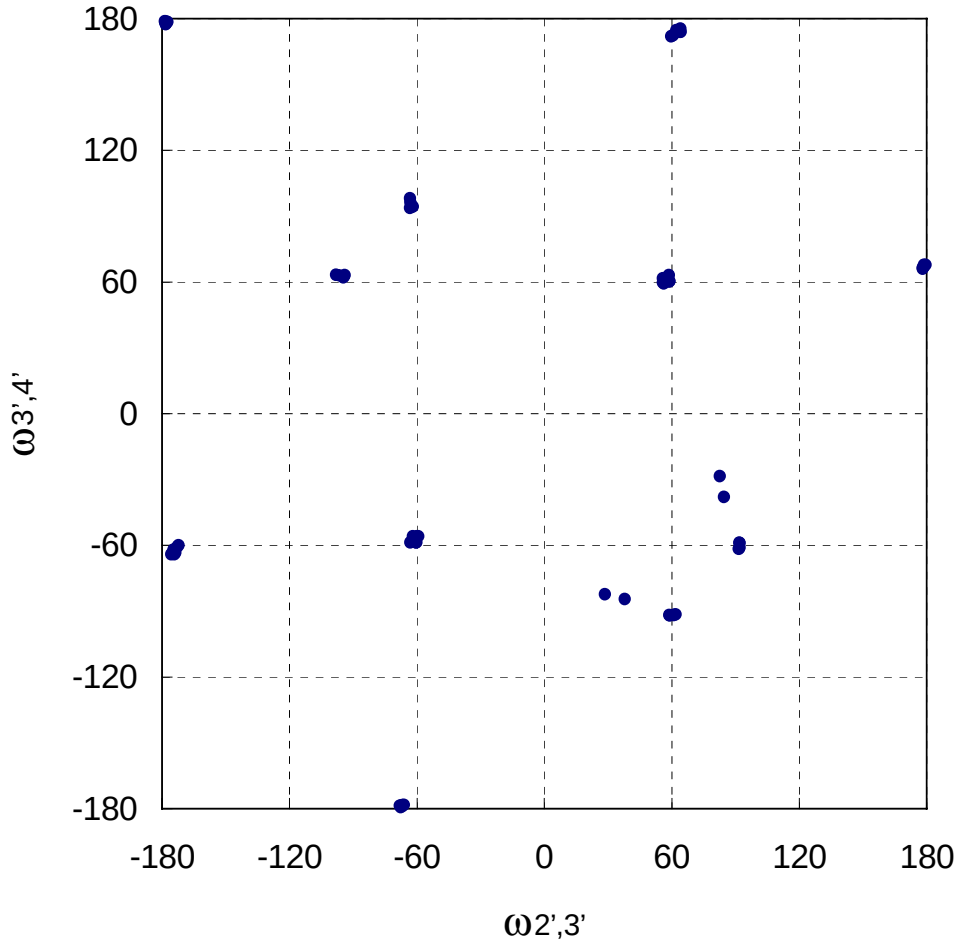


Figure 2-18: Global and local minima of 3'-pentyl formiate (**26**) in the $\omega_{2',3'}$ - $\omega_{3',4'}$ space

As shown before and summarized in Figure 2-19, the conformations of the 3'-pentyl group in N-trifluoroacetyl-L-phenylalanine 3'-pentyl ester (**S-24**) show lower symmetry than those of 3'-pentyl formiate, and the other bulky groups, i.e., benzyl and trifluoroacetyl, will also influence the conformations of this molecule, giving rise to a much higher number of local minima.

The global and local minima of N-trifluoroacetyl-L-phenylalanine 3'-pentyl ester (**S-24**) in the $\omega_{2',3'}$ - $\omega_{3',4'}$ space are displayed in Figure 2-19.

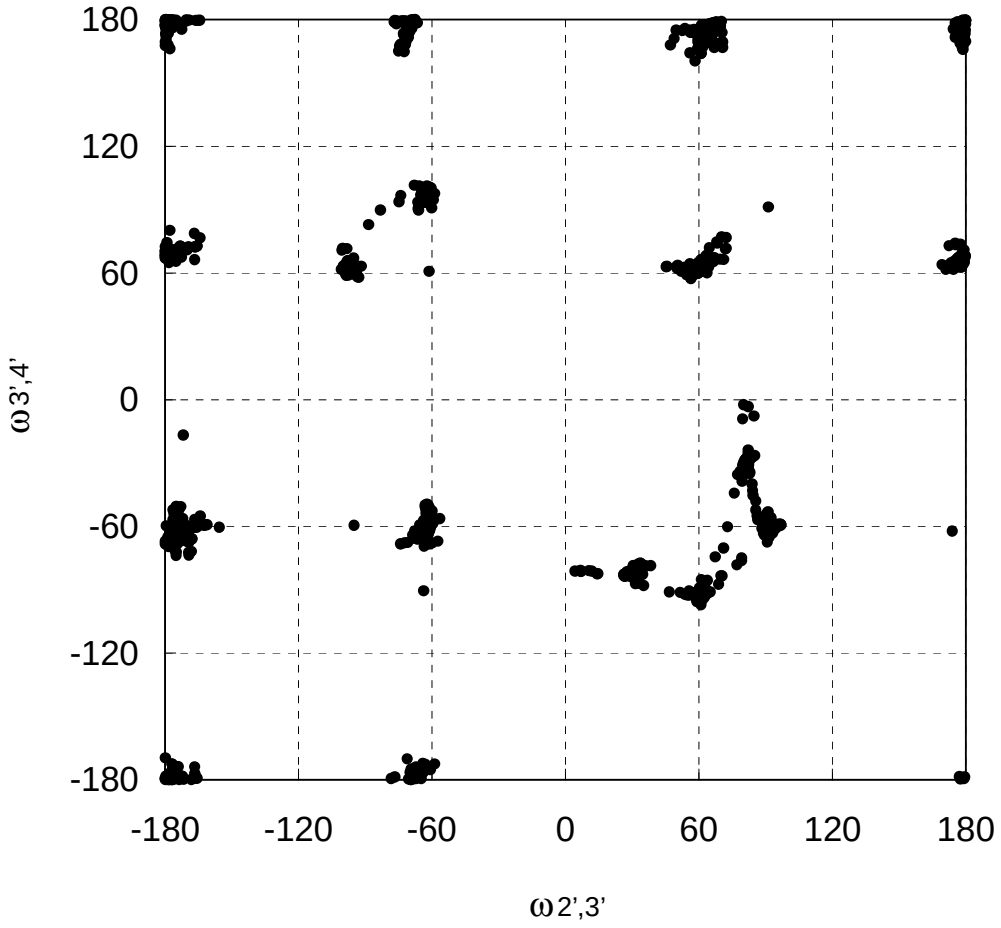


Figure 2-19: Minima of N-TFA-L-Phe-O-3'-pentyl (**S-24**) in the $\omega_{2',3'}$ - $\omega_{3',4'}$ space

An analysis of the torsion angles $\omega_{2',3'}$ and $\omega_{3',4'}$ in the 3'-pentyl group reveals that (**tt**) is the most stable conformation. There is a set of combinations of staggered conformations, characterized by $\pm 60^{o}$ (gauche, $g^{\pm}$) and 180^{o} (trans, t), while (**g^{-}t**), (**tg^{+}**) and (**g^{+}t**), (**tg^{-}**) are preferred. The purpose of this study is a comprehensive search for all minima of this molecule, in order to evaluate their possible impact on an induced chirality of the 3'-pentyl group. Such a comprehensive search can be guided by building up a search tree, as outlined in the following.

2.4.3. Building a Tree of Molecular Structures for a Complete Search of All Stable Conformations of S-24

Nonbonded interactions play an important role in determining the three-dimensional structure and reactivity of organic molecules [48]. In amino acid esters, the main chain N-C*, C*-C(O) and C*-C bonds are relatively free in rotation. These rotations are represented by the torsion angles Φ, Ψ, χ, respectively (as described in Figure 2-21). We constructed the conformational maps in increments of 60° to 120° for Φ, Ψ and χ, the side-chain torsion angles being considered as selected parameters. The torsion angles are a key factor for describing molecular conformations. Hence, they must be imagined and described as three variables in three dimensions at the same time; moreover, this high dimensional space is quite difficult to comprehend. So it is better to design a tree for exploring the complete manifold of stable conformations. Here we describe a method to explore the torsional space of molecule **S-24** by using a tree search which efficiently and uniformly generates starting geometries throughout the entire conformational space. Torsion angle tree-searching provides a rapid method for generating molecular geometries that approximate the various conformers.

Structure generation starts with selection of a series of possible values (e.g. 0^o, $\pm 60^o$, $\pm 120^o$, 180^o, ...) for each torsion angle, followed by creation of all possible combinations to generate starting geometries which are compatible with nonbonded contacts and ring closure constraints. Establishing a hierarchy of torsion angles is a prerequisite for structuring the complete conformer generation process in a tree graph. At the lowest level of the tree, the leaves stand for each of the possible products (conformations) of the generation process and each edge stands for a torsional rotation. Intermediate nodes in the tree represent partially completed structures. For N-trifluoroacetyl-L-phenylalanine 3'-pentyl ester (**S-24**), sections of the tree of conformations are shown in Figure 2-20 and Figure 2-21. The details of the structure tree are presented in **Appendix III.**

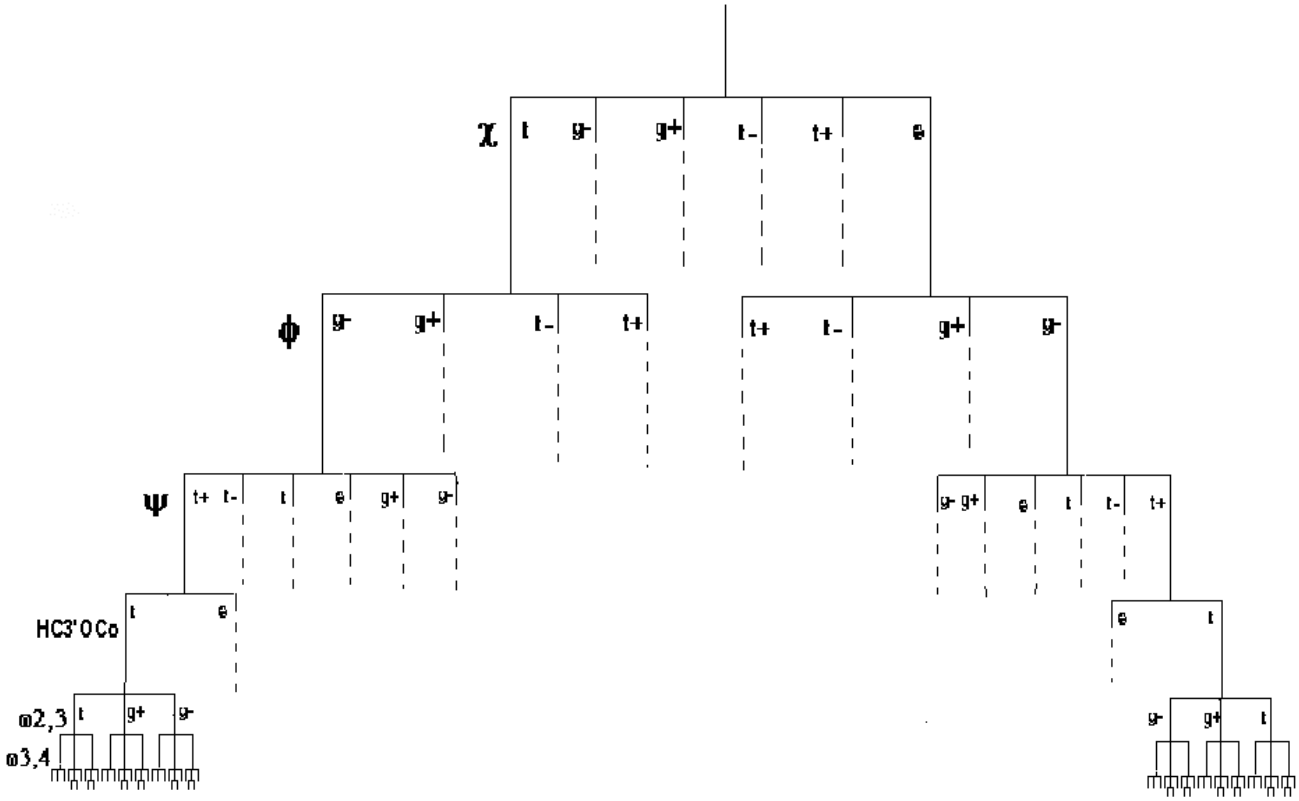
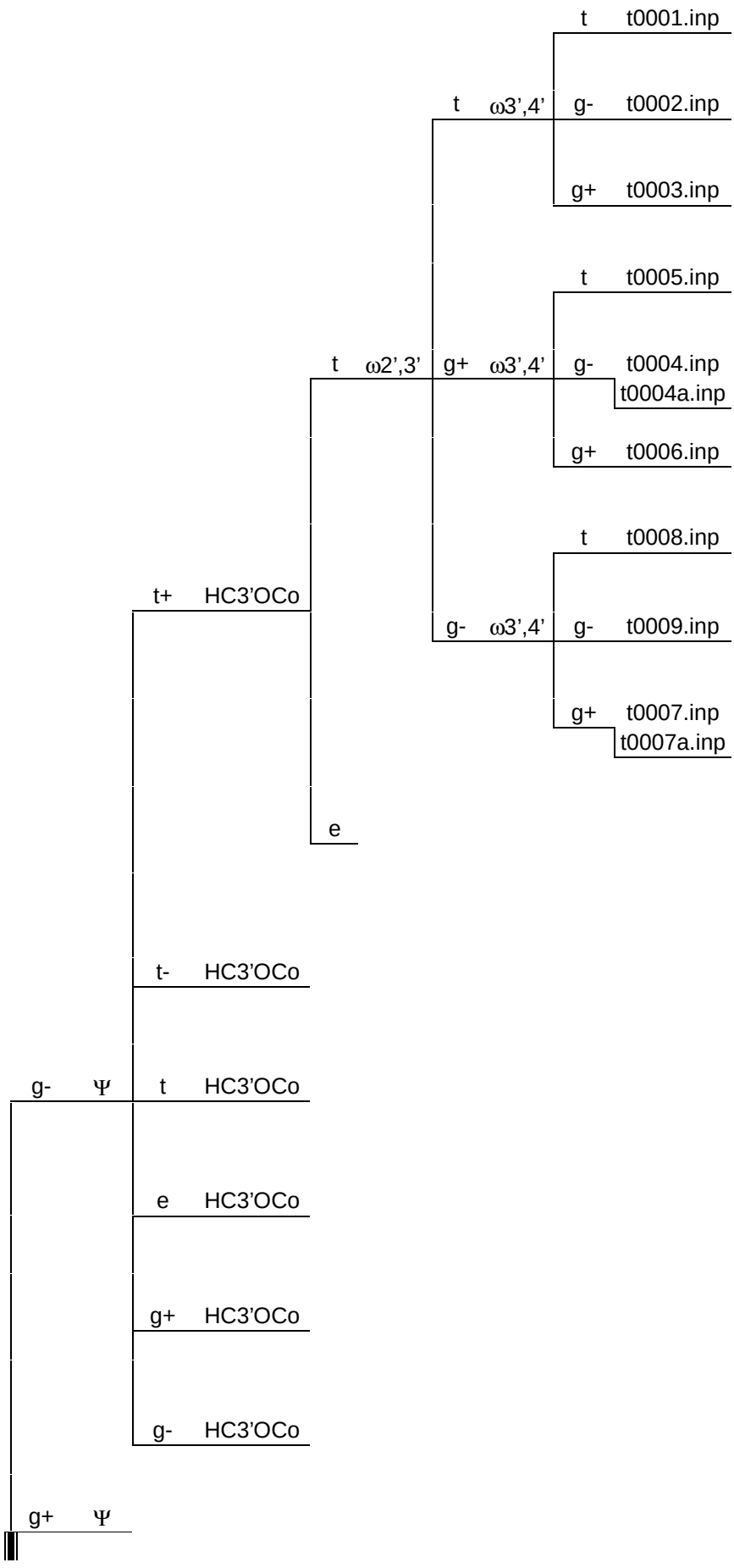
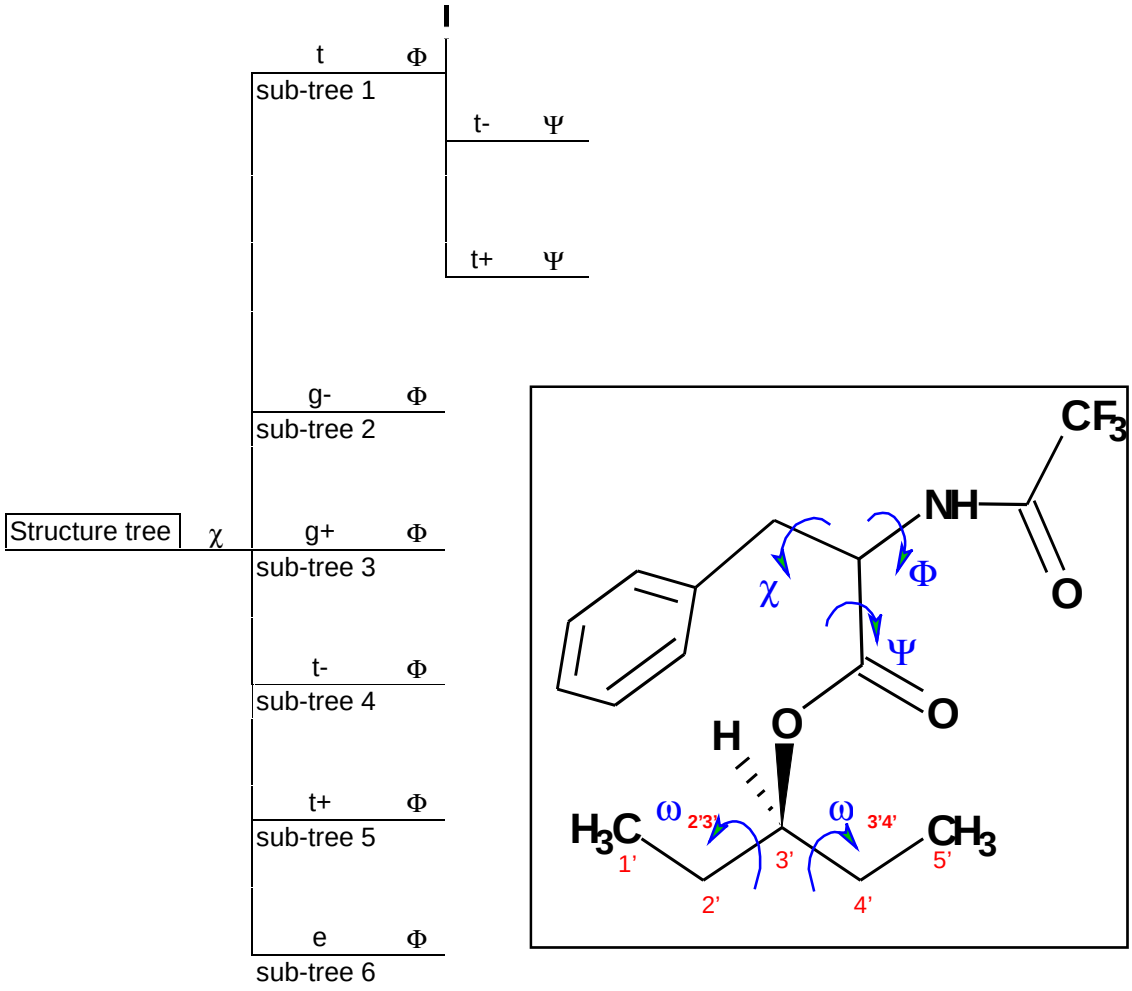


Figure 2-20: Sketch map for the whole tree

In Figure 2-20, the possible torsion angles are shown that are useful for building up this tree of molecular conformations of **S-24**. One branch (sub-tree) will be shown in Figure 2-21.


t t0001.inp
t ω3',4' g- t0002.inp
g+ t0003.inp
t t0005.inp
t ω2',3' g+ ω3',4' g- t0004.inp
t0004a.inp
g+ t0006.inp
t t0008.inp
t+ HC3'OCo
g- ω3',4' g- t0009.inp
g+ t0007.inp
t0007a.inp
e
t- HC3'OCo
g- Ψ t HC3'OCo
e HC3'OCo
g+ HC3'OCo
g- HC3'OCo
g+ Ψ



Note: Torsion angle χ = NC*CC_{Ph}; Φ = CNC*C_O; Ψ = NC*C_OO

Figure 2-21: The structure sub-tree of N-trifluoroacetyl-L-phenylalanine 3'-pentyl ester (**S-24**)

Nonbonded distance tests provide one of the most efficient ways to eliminate chemically unreasonable structures from those generated, as these tests are applied early in the structure generation process. This approach is highly effective for pruning the structure tree (see **Appendix III**). By applying constraint tests to these newly fixed substructures of the molecule, we can eliminate in a single operation all structures which would arise from a partially defined structure that have undesirable components. This elimination corresponds to pruning an entire branch from the structure generation tree. For these reasons, three tree is indispensable for getting all stable conformations.

At first, we have analyzed the situation in a simplified model compound, 3'-pentyl formiate (**26**) (the N-TFA-L-phenylalanine residue was replaced by H). Here, three independent variables exist, and the number of stable conformers obtained was: 66 = 3 (COC_3C_2) * 2

($HCOC_3$) * 11 ($\omega_{2,3}$, $\omega_{3,4}$). The geometry and energy of each conformer is compiled in **Appendix II**.

For N-TFA-L-phenylalanine 3'-pentyl ester (**S-24**), six independent variables have a major effect on the energy and geometry of this molecule. For the torsion of each of the three bulky groups, *i.e.*, trifluoracetyl, benzyl and 3'-pentyl group, three torsion angles are to be considered in the structure tree that is on display in Figure 2-21. From a preliminary estimation, we expect a total of 4224 = 4 (Φ) * 6 (χ) * 8 (Ψ, $C_FC_ONC^*$, $C^*C_OOC_3$) * 11 ($\omega_{2,3}$, $\omega_{3,4}$) * 2 (HC_3OC_O) low energy conformations; however, some of these conformations are not stable, hence, the actual number will always be smaller than the theoretical number of minima expected.

For several combinations of torsion angles, too many high-energy non-bonded interactions are involved and a stable local minimum could not be found, despite manifold attempts. By these constraints, the number of stable solutions is reduced dramatically. Actually, only 2083 conformations were found. From the complete structure tree (see **Appendix III**), we can calculate the number of unstable combinations as 4224 - 2083 = 2141, and all stable combinations are located in the sub-trees 1 to 6. From this we can estimate the average number of solutions for each of the 11 different classes ("clusters") of conformations in the $\omega_{2',3'}$ - $\omega_{3',4'}$ space at appr. 190 data points. For each cluster, the average MMX energy and the number of stable minima are complied in Table 2-2. The tree structure is also helpful in developing rules that determine the relative stability of the conformations obtained. Such rules proved useful during the extended search of all stable conformations.

Table 2-2: Average MMX energy and number of minima, for each of the 11 clusters of 3'-pentyl conformers of **S-24**

3'-Pentyl conformer	$MMXE_{average}$ [kcal/mol]	Number of minima
tt	44.542	198
tg^-	45.915	193
g^+t	45.894	191
g^-t	44.966	191
tg^+	45.016	196
g^-g^-	46.308	192
g^+g^+	46.705	195
$g^{\ominus}g^+$	46.991	190
$g^-g^{\oplus}$	47.022	191
$g^+g^{\ominus}$	49.530	172
$g^{\oplus}g^-$	48.930	174

2.4.4 Boltzmann Analysis of the Conformational Space of S-24

What is the criterion to decide which of the enantiomorphic combinations of $\omega_{2',3'}$ - $\omega_{3',4'}$, such as (**g$^-$t**) compared to (**tg$^+$**), is preferred? In Table 2-2 (see previous chapter), the average MMX energy of clusters of diastereomorphic structures of **S-24** (enantiomorphic regarding 3'-pentyl) did not show a uniform pattern, and it is not necessarily a valid criterion to decide on the preference of either one of the conformers over the other. Only Boltzmann analysis [41] can reveal which conformations contribute predominantly to the conformation state of N-TFA-L-phenylalanine 3'-pentyl ester (**S-24**). This Boltzmann analysis yields sums of probability for the different 3'-pentyl conformations, as displayed in Figure 2-22 for a temperature of 300 K. The underlying number of minima per cluster of similar 3'-pentyl conformations varied between 172 and 198 (see Table 2-3), and the total number of minima was 2083.

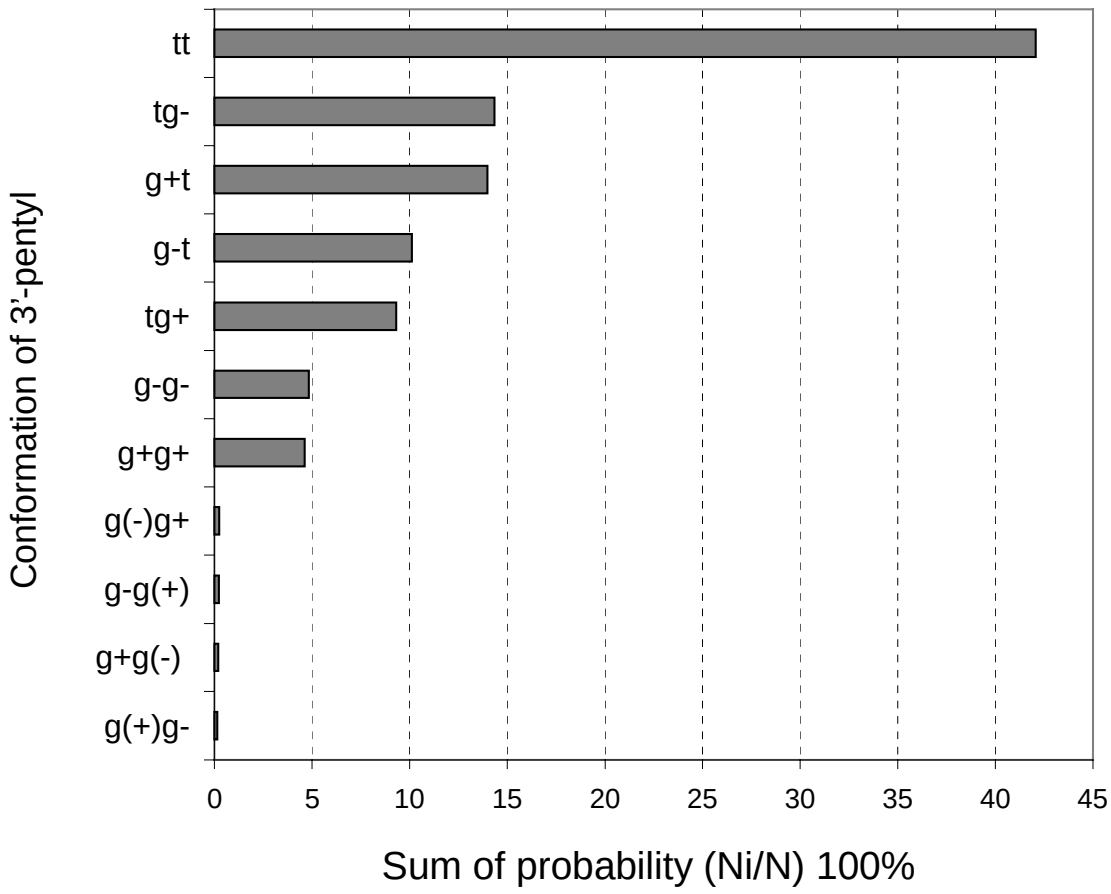


Figure 2-22: Total geometric probability of 3'-pentyl in **S-24** acc. to Boltzmann analysis (at 300 K), based on 172 to 198 minima per cluster, 2083 in total

Table 2-3: Relative average MMX energy (*cf.* Table 2-2 for absolute values), relative MMX energy for lowest minimum per cluster, number of minima and sum of probability (acc. to Boltzmann analysis at 300 K) for each of the 11 clusters of 3'-pentyl conformers of **S-24**

3'-Pentyl conformer	Rel. $MMXE_{av}$ [kcal/mol]	Rel. $MMXE_{min}$ [kcal/mol]	Number of minima	Sum of probability
tt	0.00	0.00	198	0.4203
tg^-	1.37	0.78	193	0.1433
g^+t	1.35	0.65	191	0.1398
g^-t	0.42	0.98	191	0.1010
tg^+	0.47	0.89	196	0.0930
g^-g^-	1.77	1.43	192	0.0483
g^+g^+	2.16	1.45	195	0.0461
$g^{\ominus}g^+$	2.45	3.43	190	0.0024
$g^-g^{\oplus}$	2.48	3.50	191	0.0023
$g^+g^{\ominus}$	4.99	3.17	172	0.0020
$g^{\oplus}g^-$	4.39	3.56	174	0.0015
in total			**2083**	**1.0000**

From these statistical results it is clear that the most stable conformer of the 3'-pentyl group is (**tt**) which has locally the highest symmetry. As preliminarily discussed in chapter 2.4.1, the next higher energy minima are chiral conformations of 3'-pentyl where one C-C bond is rotated by ±120° ($\mathbf{g^+t} \parallel \mathbf{tg^-}$ and $\mathbf{g^-t} \parallel \mathbf{tg^+}$, see Figure 2-5), and then there are conformations where both C-C bonds are rotated ($\mathbf{g^+g^+} \parallel \mathbf{g^-g^-}$, see Figure 2-6). The least stable ones are "pesudo-symmetric" conformers ($\mathbf{g^+g^-}$ and $\mathbf{g^-g^+}$), but as discussed in Figure 2-7, nonbonded (repulsive) interactions between the two methyl groups cause a twist into four chiral conformations ($\mathbf{g^{\oplus}g^-} \parallel \mathbf{g^+g^{\ominus}}$ and $\mathbf{g^{\ominus}g^+} \parallel \mathbf{g^-g^{\oplus}}$).

Intriguingly, all these conformations are “chiral”, however, the differences in the most populated conformers contribute most significantly.

$$\Delta\left(\frac{N_i}{N}\right)_{Chiral} =$$

$$+\left[\sum_i\left(\frac{N_i}{N}\right)_{tg^-}+\sum_i\left(\frac{N_i}{N}\right)_{g^-t}+\sum_i\left(\frac{N_i}{N}\right)_{g^-g^-}+\sum_i\left(\frac{N_i}{N}\right)_{g^{(-)}g^+}+\sum_i\left(\frac{N_i}{N}\right)_{g^+g^{(-)}}\right]$$

$$-\left[\sum_i\left(\frac{N_i}{N}\right)_{g^+t}+\sum_i\left(\frac{N_i}{N}\right)_{tg^+}+\sum_i\left(\frac{N_i}{N}\right)_{g^+g^+}+\sum_i\left(\frac{N_i}{N}\right)_{g^-g^{(+)}}+\sum_i\left(\frac{N_i}{N}\right)_{g^{(+)}g^-}\right]$$

(2-8)

Here, the positive terms all contain a $\mathbf{g}^-$ sub-conformation and the negative terms all contain a corresponding $\mathbf{g}^+$ sub-conformation in the 3’-pentyl group. In other words, in all “chiral” 3’-pentyl conformers, the terms containing $\mathbf{g}^-$ or $\mathbf{g}^{\ominus}$ are higher in sum of probability (N_i/N) than their (local) mirror image. Hence, a uniform twist in the same direction causes an overall degree of asymmetry in this intrinsically symmetric group. In Table 2-4, the differences Δ in the sums of probability (acc. to Boltzmann analysis at 300 K) have been multiplied with –1 and are thus uniformly negative, in order to allow a comparison with the predominantly negative differences in both, relative average and relative minimum MMX energies.

Table 2-4: Differences in rel. MMX energies and sums of probability (at 300 K) for each of the (locally) enantiomeric pairs of 3’-pentyl conformers of **S-24**

3’-Pentyl conformer	Δ Rel. $MMXE_{min}$ [kcal/mol]	Δ Rel. $MMXE_{av}$ [kcal/mol]	- Δ Sum of probability	3’-Pentyl conformer
tt	0	-	-	-
g^-t	+0.09	-0.05	-0.004	tg^+
tg^-	+0.13	+0.02	-0.008	g^+t
g^-g^-	-0.02	-0.39	-0.002	g^+g^+
$g^{\ominus}g^+$	-0.07	-0.03	-0.001	$g^-g^{\oplus}$
$g^+g^{\ominus}$	-0.39	+0.60	-0.005	$g^{\oplus}g^-$

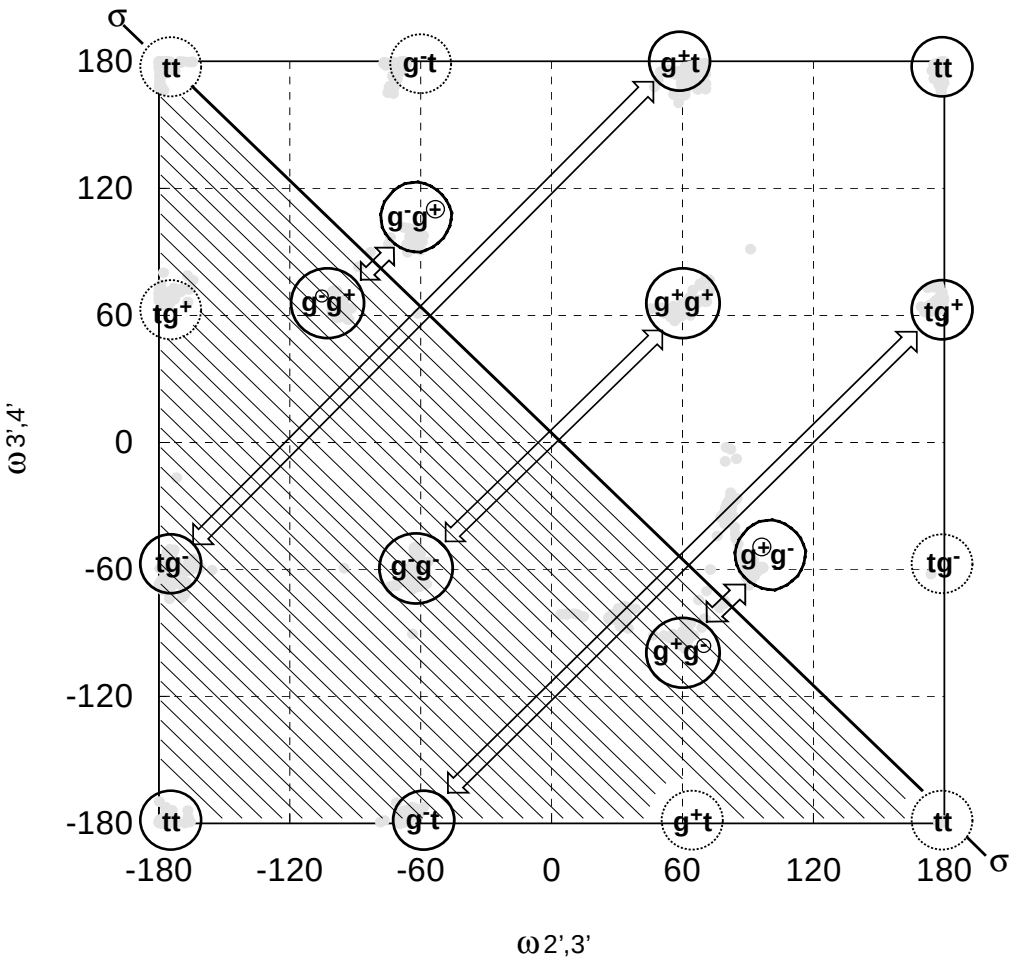


Figure 2-23: Denotation of clusters of minima of **S-24** in the $\omega_{2',3'}$ - $\omega_{3',4'}$ space; sums of probabilities (by Boltzmann analysis) of conformations are higher in the shaded area, compared to their (local) mirror images, as indicated by the arrows perpendicular to the diagonal σ

This distribution of clusters of minima in the $\omega_{2',3'}$ - $\omega_{3',4'}$ space was shown in Figure 2-19. This picture was then illustrated with the denotation of 3'-pentyl conformers of Table 2-4 (multiple occurrence of clusters, depicted in dotted circles at the edge of the unfolded torus topology cannot be avoided, but must not be considered here). For each of the chiral combinations of $\omega_{2',3'}$ - $\omega_{3',4'}$, a mirror image combination is possible. These pairs are connected with broad arrows in Figure 2-23. According to Boltzmann analysis at 300 K, all clusters in the striped area (lower left of the diagonal σ) are more densely populated than the corresponding mirror images (upper right of the diagonal σ). The generality of this phenomenon is striking.

These results open up a new perspective on the phenomenon “chirality” in general. There are a couple of theories on the chirality of molecules [1]. The helical arrangement of dipoles is a fundamental basis for establishing rules on ORD- and CD-effects[53]. We have pointed out that the quadrupole arrangement of two positive and two negative charges on the edges of a distorted tetrahedron may be viewed as a short helix of two perpendicular dipoles that form a quadrupole electric field [54], [55], [56]. Apparently, the four groups around the stereogenic center of L-phenylalanine, *i.e.*, benzyl, TFA-amide, ester and hydrogen, create a chiral electric field in which the distorsion of the 3’-pentyl group uniformly prefers an anti-clockwise direction. This is certainly the most important result of this thesis.

It still remains an open question, however, whether this “chirality enhancement” by induced chirality of the 3’-pentyl group is the main reason for the unique properties of 3’-pentyl esters in intermolecular interactions [26], [35].

2.4.5. Ramachandran Plot of Torsion Angles Φ and Ψ for 24

The Ramachandran plot [57] of pairs of torsion angles Φ and Ψ in the L-phenylalanine residue (Figure 2-24) reveals certain restrictions on these parameters. The torsion angles Φ and Ψ are used to characterize the backbone conformation of amino acids. Most stable conformations are usually found in the ß-plated sheet domain and in the α-helix region that allow efficient hydrogen bonding. For N-TFA-L-phenylalanine 3'-pentyl ester (**S-24**), the most stable conformation occurs at $\Phi = -60^{O}$ (g^{-}) and $\Psi = 120^{O}$ (t^{+}) which is very close to the β-region of peptides; however, intramolecular hydrogen bonding did not yield the lowest energy. Instead, the anti-parallel alignment of the two dipoles, the ester C=O(δ-) and the amide C-N(δ+) bond, are supposed to play an important role. Last not least, Figure 2-24 may serve to understand the packing phenomena of N-TFA amino acid ester enantiomers (*cf.* chapter 2.2.2).

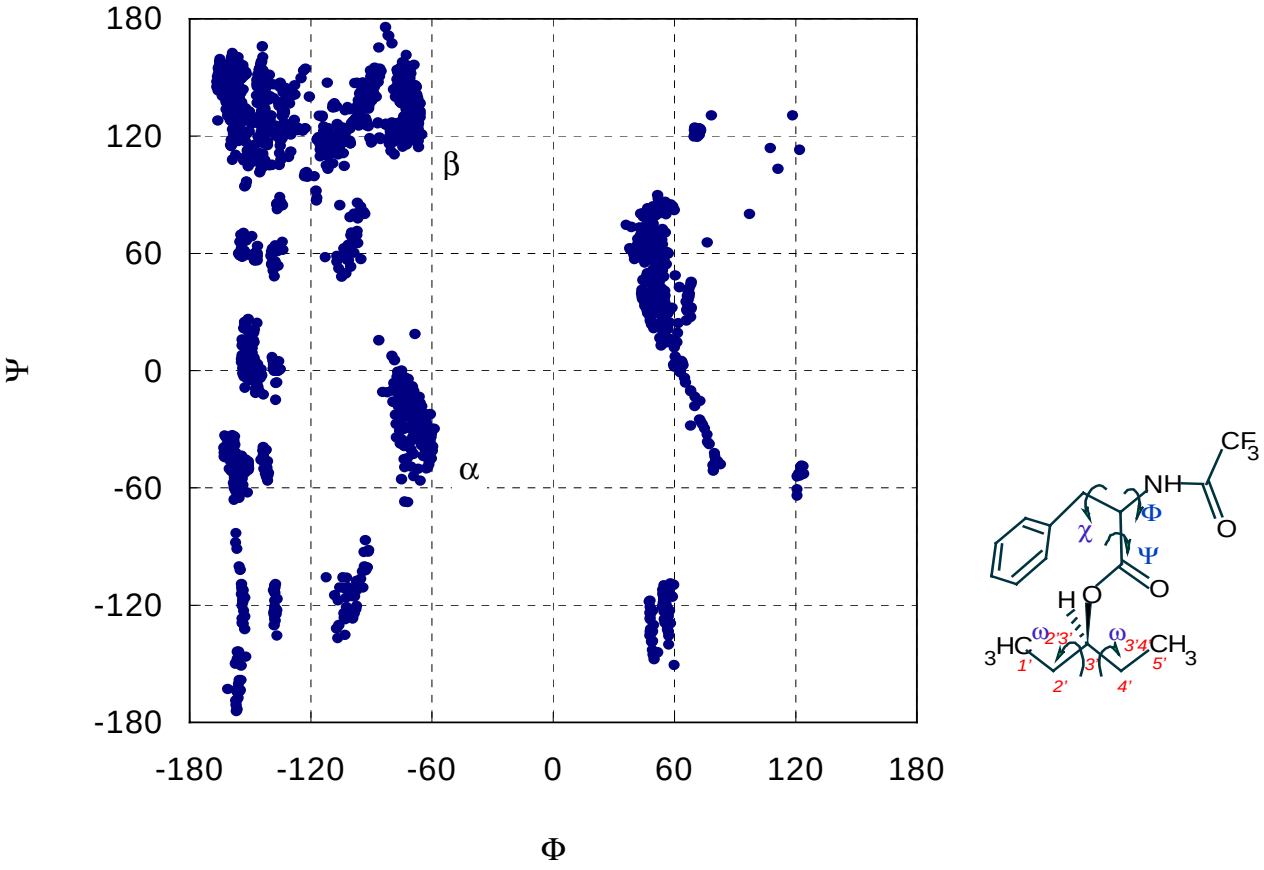


Figure 2-24: Ramachandran plot of **S-24**

2.4.6. Electronic Publishing of Multiminima Problems

The great number of stable conformations obtained for N-TFA-L-phenylalanine 3'-pentyl ester (**S-24**) cannot be shown in an ordinary printed publication. Even for 8 pictures per page, the printed pictures alone would require 260 pages. This raises the question, how this large amount of information should be published. Apparently, the only method that allows a reader to inspect all conformations of such a molecule is an on-line publication.

On-line publication is a perfect medium for presenting results of scientific research produced in the computer, and offers the unique possibility of applying all the daily tools of computational chemistry to the world of scientific publishing, to the benefit of both authors and readers.The electronic version of publishing has a couple of advantages.

A large amount of data can be included in the article. An electronic publication can display much more information than a normal publication. While it is impossible to show all 2083 conformations of **S-24** in a printed version, for an electronic version, all 2083 conformations can be stored on a host computer and opened on reader's request, *e.g.*, by clicking on a certain point in the structure tree. As the material presented here cannot be shown in detail in the thesis printed on paper, we intend to publish the complete material in the electronic journal *J. Molecular Modelling*, published by Springer Verlag, Heidelberg, Germany.

In general, the readers of an electronic publication are able to review visual as well as text information, for their own purpose. This involves colour graphics at no extra costs, and 3D data files and pictures that may be viewed by various computer graphics stereo techniques. An electronic publication has also a significantly shorter publishing time of one to two weeks, while a printed article takes several months to be published.

Electronic publishing in chemistry, in particular, makes best usage of 3-dimensional molecular structures. Even one may allow the reader to manipulate the information interactively, rotate the molecular structure and inspect technical details, *e.g.*, internal coordinates (bond lengths, bond angles and torsion angles), measure certain intra- or intermolecular distances, etc., to the benefit of further scientific progress.

2.5. Summary

The molecular geometries and energies of 2083 stable conformations of N-trifluoroacetyl-L-phenylalanine 3'-pentyl ester (**S-24**) were calculated by the molecular mechanics program PCMODEL, based on the MMX (without P_i electrons) method. The global minimum of **S-24** shows a highly symmetric, zick-zack conformation (**tt**) of the 3'-pentyl group. There is a set of combinations of staggered conformations, characterized by $\pm 60^o$ (gauche, $g^{\pm}$) and 180^o (trans, t), while (**g$^-$t**), (**tg$^+$**) and (**g$^+$t**), (**tg$^-$**) are preferred.

In order to search through 4224 combinations of six crucial torsion angles of **S-24,** these were arranged in a structure tree that allowed a systematic search, eventually ruling out 4224 – 2083 = 2141 combinations that were unstable, because of nonbonded interactions. Prestudies with pentane (**25**) and 3'-pentyl formiate (**26**) proved useful in exploring the entire conformation space of **24**.

Boltzmann analysis at 300 K revealed that the most stable conformer of the 3'-pentyl group in **S-24** is (**tt**) which has locally the highest symmetry. The next higher energy minima are chiral conformations of 3'-pentyl where one C-C bond is rotated by ±120° (**g$^+$t** ‖ **tg$^-$** and **g$^-$t** ‖ **tg$^+$**), and then there are conformations where both C-C bonds are rotated (**g$^+$g$^+$** ‖ **g$^-$g$^-$**). The least stable ones are "pesudo-symmetric" conformers (**g$^+$g$^-$** and **g$^-$g$^+$**), that are twisted by nonbonded (repulsive) interactions into four chiral conformations (**g$^{\oplus}$g$^-$** ‖ **g$^+$g$^{\ominus}$** and **g$^{\ominus}$g$^+$** ‖ **g$^-$g$^{\oplus}$**). Conformers with **g$^-$** or **g$^{\ominus}$** are more densely populated (at 300 K) than the corresponding mirror images. The generality of this phenomenon is striking.

The Ramachandran plot of torsion angles Φ and Ψ in the L-phenylalanine residue shows extended clusters of stable conformations in the β-plated sheet domain and in the α-helix region, mainly due to antiparallel alignment of dipoles. This result may also serve to understand the packing phenomena of N-TFA amino acid ester enantiomers.

Only electronic publishing can display the complete information on the structure tree of 4224 combinations of torsion angles and on the 2083 stable minima found, including full colour 3-D molecular graphics of all these minima. Here, the reader can review the data visually and interactively, to the benefit of further scientific progress.

Part 3. Racemic Oxiranes as Synthons for Drug Candidates in High Throughput Screening

3.1. Introduction

High-throughput screening (HTS) represents one of the most important technologies currently in place within the pharmaceutical industry for the identification of biologically active molecules as potential drug candidates [58]. Today, it is widely anticipated not only in pharmaceutical science but also in analytical chemistry. Recent developments in high-throughput screening have enabled large numbers of single compounds to be evaluated rapidly for biological activity, thus facilitating the optimization of drug candidates [59]. For the facilitation of rapid and accurate biological profiling and structural determination by HTS, significant emphasis has recently been directed toward the analysis, purification, and characterization of components prior to screening [60].

In parallel with the development of enantiospecific analytical methodology in the past few decades, the enantiomeric composition of biologically active compounds has attracted increasing attention [61]. The world market for single enantiomer drugs is still growing rapidly [62]. For the approval of new chiral drugs – whether racemic or enantiopure – enantiospecific methods are now required in all industrial countries [63].

In „chiral separations“ enantiomers are separated on the basis of stereoselectivity. „Chiral chromatography“ has developed with the need for enantiomerically pure drugs. Many chiral drugs have been used as their racemates because of difficulties in stereoselective synthesis and purification. As only one of the enantiomers may exhibit the pharmacological effect and the other may even show side effects, it is important to separate and determine the enantiomers of drugs [62].

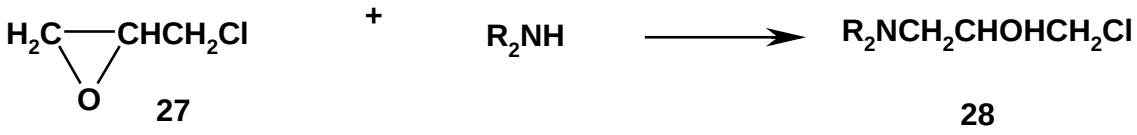
The alkylating capacity of epoxy functions is well-known [64], [65], [66] and the antineoplastic activity of bifunctional epoxides has been reported [61], [68], [69]. The investigation of active antitumor agents containing higher numbers of epoxy groups in their structure has been performed [70]. As a continuation of this work, we have synthesized a series of related epoxy compounds with varying chemical structure. Modification of one of

the epoxy groups in the molecule by reaction with nucleophiles permits wide variations of physicochemical properties without a concomitant loss of active centers for any biological activity, like antineoplastic activity. On the other hand, it is known that the chemical reactivity of epoxides in strongly dependent on the substituents of the oxirane ring and location of oxirane ring in the molecule [71]. A number of heterocycles containing a pyridine-type nitrogen atom and an oxirane ring have been designed as antitumor compounds. They are also potential synthons for other drug candidates in high throughput screening.

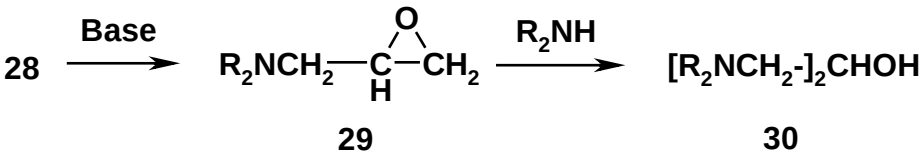
3.2. Fundamentals

3.2.1. General Procedure for Synthesis of the Epoxy Compounds

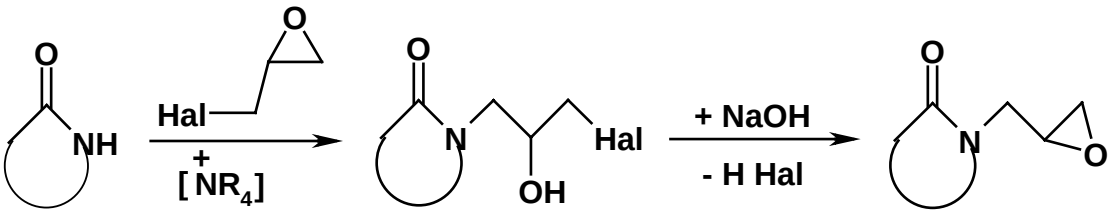
The reaction between amines and epichlorohydrin has been studied extensively in the past, most of them are intermediates in drug synthesis, but they also have a certain antitumor activity. Epoxides are alkylating agents, and they react with nucleophiles with opening of the epoxide ring [71], [62]. The reaction between secondary amines and epichlorohydrin is usually formulated as:



Treatment of the chlorohydrin (**27**) with base (either excess amine or alkali) affords the N-(2,3-epoxy-propyl) dialkylamine (**28**). When excess amine is used the 1,3-bis-(dialkylamino)-propanol-2 (**30**) can be isolated.



Nearly all glycidyl compounds were prepared according to the general reaction scheme shown in the following:



31 **32** **33**

The oxo-N-heterocycles (**31**) were alkylated by a large excess of halogen epoxy propane, mostly the chloroderivative epichlorohydrin, to give the halogenhydroxypropyl intermediates (**32**), which were subsequently converted into the epoxy derivatives **33**.

Often, epoxy compounds have antitumor activity [70], and other pharmacophores like a succinimide group give rise to activities such as CNS depressant [73], analgesic [74], antitumor [75], cytostatic [76], anorectic [77], nerve conduction blocking [78], etc.. A piperazine moiety has been reported to be present in some Ca-channel antagonists [75]. Hence, it is important to screen a set of oxiranes for different pharmacological effects. Moreover, the oxirane ring can be used as a linker of different pharmacophores in the HTS approach.

3.2.2. Enantiomer Separation of Oxirane Drug Precursors by HPLC on Different Chiral Stationary Phases

Enantiomeric compounds cannot be separated directly in normal chromatographic systems since the groups attached to the stereogenic center are equally accessible to binding. If the enantiomers are combined with a chiral selector (enantiomeric reagent), however, two diastereomers are formed that may show differences in binding properties and therefore can be separated by chromatography. The use of chiral stationary phase (CSP) is a technique that relies on the formation of transient, temporary diastereoisomers between the sample enantiomers and chiral stationary phase [79]. Differences in stability between the diastereoisomers are reflected in differences in retention times. The ability of the analyte and CSP to form transient-diastereomeric complexes utilizing hydrogen bonding, π-π interactions, dipole stacking, inclusion complexing, and steric bulk is the driving force behind enantioseparation [79]. The enantiomer that forms the least stable complex is eluted first. The most important considerations are the type of substituent groups present in the analyte

molecule and their ability to either π- or H-bonding (attractive interaction) or steric interference with bonding (repulsive interaction). The spatial arrangement of the substituents around the analyte stereogenic center plays an important role in enantiomer separation. In most cases, the closer a group is to the stereogenic center, the more likely is chiral recognition and enantioselectivity. If the analyte does not contain groups that can bind to the stationary phase, derivatization of the analyte may be necessary.

Within the framework of this thesis, the enantiomers of epoxy compounds were directly separated by HPLC on five different chiral stationary phases. The following chromatographic columns were chosen: Chiralcel OJ, OG, OD-H (all three based on cellulose), Chiralcel AD and AS (both based on amylose). Retention factors, enantioselectivity, efficiency and resolution were tested while modifying the composition of the mobile phase. The impact of the structure of the analyte on the mechanism of chiral recognition of drug precursors by the different chiral phases was thereby investigated.

3.3. Results and Discussion

3.3.1. Enantiomer Separation of 14 Drug Precursors on Five Chiral Stationary Phases by HPLC

Based on the impact of different substructures on the separation data, we choose to divide the total of 14 drug precursors (see Table 3-1) into two classes, according to their chemical structure, one class where the substructure π is present, and another class where π is absent. In Tables 3-2 to 3-6, the separation data are compiled for the 14 analytes where π is present and absent, respectively.

The quality of an HPLC separation is adequately described in terms of the resolution achieved in a certain time. In order to evaluate the chromatographic performance of the five selected columns in the enantiomer separation of the 14 oxiranes, several factors were investigated. The retention factors (*k'*), the separation factor of the enantiomers (α), and the resolution factor (R_s). Various mathematical functions have been proposed to evaluate separation quantitatively [80], [81]. Thus, the retention factor k' is given as in Equation (3-1)

$$k' = (t_R - t_0) / t_0 \qquad (3\text{-}1)$$

where t_R is the band retention time and t_0 is the column dead time. *k'* is the average retention factor for two bands. The separation factor α is given as in Equation (3-2)

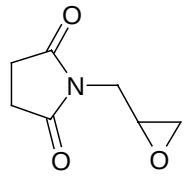
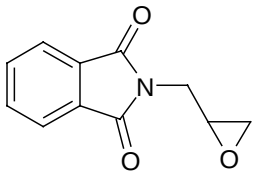
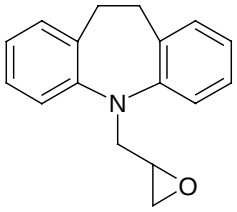
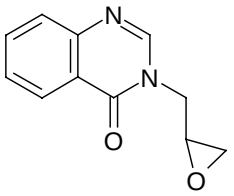
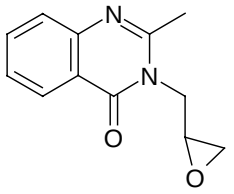
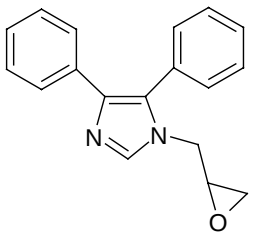
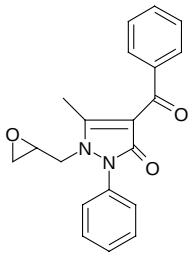
$$\alpha = k_2 / k_1 \qquad (3\text{-}2)$$

where k_2 and k_1 are values of *k* for adjacent bands 1 and 2. The resolution factor R_s is defined as in Equation (3-3)

$$R_s = 2(t_2 - t_1) / (w_1 + w_2) \qquad (3\text{-}3)$$

Here, t_1 and t_2 are the retention times of the first and second adjacent bands, respectively, and w_1 and w_2 are their baseline bandwidths. R_s is used to describe the degree of separation between neighboring solute bands or peaks.

Table 3-1: Names and structures of 14 drug precursors (# old numbering as in an unpublished study)

Number	Name	Structure
34 (Nr.01#)	1-(2,3-epoxypropyl)-2,5-pyrrolidinedione	
35 (Nr.02#)	N-oxiranylmethyl-phthalimide	
36 (Nr.04#)	5-oxiranylmethyl-10,11-dihydro-5H-dibenz[b,j]azepine	
37 (Nr.05#)	3-oxiranylmethyl-3H-quinazolin-4-one	
38 (Nr.06#)	2-methyl-3-oxiranylmethyl-3H-quinazolin-4-one	
39 (Nr.20#)	1-oxiranylmethyl-4,5-diphenyl-1H-imidazole	
40 (Nr.21#)	4-benzoyl-5-methyl-1-oxiranylmethyl-2-phenyl-1,2-dihydro-pyrazol-3-one	

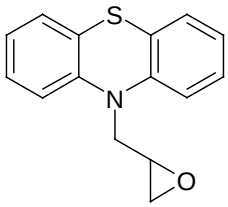
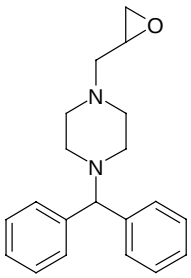
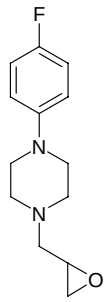
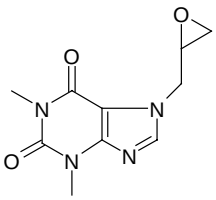
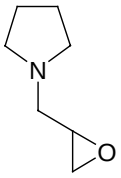
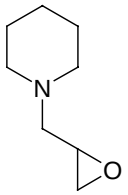
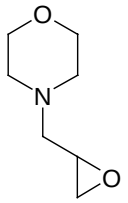
41 (Nr.23#)	10-oxiranylmethyl-10H-phenothiazine	
42 (Nr.25#)	1-benzhydryl-4-oxiranylmethyl-piperazine	
43 (Nr.27#)	1-(4-fluoro-phenyl)-4-oxiranylmethyl-piperazine	
44 (Nr.32#)	1,3-dimethyl-7-oxiranylmethyl-3,7-dihydro-purine-2,6-dione	
45 (Nr.24#)	1-oxiranylmethyl-pyrrolidine	
46 (Nr.30#)	1-oxiranylmethyl-piperidine	
47 (Nr.31#)	4-oxiranylmethyl-morpholine	

Table 3-2: Retention times (t); retention factors (k'), separation factors (α) and resolution factors (R_S) for HPLC of 14 oxiranes (# old numbering as in an unpublished study) on a Chiralcel AD stationary phase; mobile phase: heptane / iso-propanol (70/30), flow rate: 0.5ml/min, t_0 = 1.329.

oxirane with π-system	CSP: Chiralcel AD t_1	t_2	k'	α	R_S
34 (Nr.01#)	4.446	7.574	3.522	2.004	3.476
35 (Nr.02#)	3.125	3.811	1.609	1.382	1.247
36 (Nr.04#)	1.889	-	0.421	1.000	0
37 (Nr.05#)	3.395	4.873	2.111	1.715	2.111
38 (Nr.06#)	2.929	5.362	2.119	2.521	3.476
39 (Nr.20#)	2.753	-	1.710	1.000	0
40 (Nr.21#)	2.859	5.209	2.035	2.536	3.357
41 (Nr.23#)	2.118	2.390	0.696	1.345	1.360
42 (Nr.25#)	1.878	2.075	0.487	1.359	0.985
43 (Nr.27#)	1.820	1.999	0.437	1.365	0.895
44 (Nr.32#)	1.978	-	0.488	1.000	0
without π-system					
45 (Nr.24#)	4.441	-	2.342	1.000	0
46 (Nr.30#)	1.495	-	0.125	1.000	0
47 (Nr.31#)	1.645	-	0.238	1.000	0

Table 3-3: Retention times (t); retention factors (k'), separation factors (α) and resolution factors (R_S) for HPLC of 14 oxiranes (# old numbering as in an unpublished study) on a Chiralcel OG stationary phase; mobile phase: heptane / iso-propanol (70/30), flow rate: 0.5ml/min, t_0 = 1.151.

oxirane with π-system	CSP: Chiralcel OG t_1	t_2	k'	α	R_S
34 (Nr.01#)	12.852	-	10.166	1.000	0
35 (Nr.02#)	5.848	-	4.081	1.000	0
36 (Nr.04#)	2.202	-	0.913	1.000	0
37 (Nr.05#)	9.337	11.043	7.853	1.208	1.706
38 (Nr.06#)	7.230	8.815	5.970	1.261	1.761
39 (Nr.20#)	8.905	10.155	7.280	1.161	1.250
40 (Nr.21#)	3.547	-	2.082	1.000	0
41 (Nr.23#)	2.737	2.882	1.441	1.091	0.725
42 (Nr.25#)	1.826	-	0.586	1.000	0
43 (Nr.27#)	2.503	-	1.175	1.000	0
44 (Nr.32#)	2.417	-	1.100	1.000	0
without π-system					
45 (Nr.24#)	1.749	-	0.520	1.000	0
46 (Nr.30#)	1.536	-	0.334	1.000	0
47 (Nr.31#)	1.680	-	0.460	1.000	0

Table 3-4: Retention times (*t*); retention factors (*k'*), separation factors (α) and resolution factors (R_S) for HPLC of 14 oxiranes (# old numbering as in an unpublished study) on a Chiralcel OJ stationary phase; mobile phase: heptane / iso-propanol (70/30), flow rate: 0.5ml/min, t_0 = 1.212.

oxirane with π-system	CSP: Chiralcel OJ t_1	t_2	k'	α	R_S
34 (Nr.01#)	8.531	-	6.039	1.000	0
35 (Nr.02#)	8.917	-	6.357	1.000	0
36 (Nr.04#)	7.361	8.435	5.517	1.175	0.826
37 (Nr.05#)	9.918	11.557	7.631	1.189	1.261
38 (Nr.06#)	5.616	-	3.634	1.000	0
39 (Nr.20#)	6.213	-	4.126	1.000	0
40 (Nr.21#)	13.358	-	10.021	1.000	0
41 (Nr.23#)	8.430	9.812	6.526	1.191	1.256
42 (Nr.25#)	3.873	-	2.196	1.000	0
43 (Nr.27#)	3.300	3.870	1.958	1.273	1.425
44 (Nr.32#)	17.233	21.217	23.031	1.242	2.656
without π-system					
45 (Nr.24#)	1.498	-	0.236	1.000	0
46 (Nr.30#)	1.424	-	0.175	1.000	0
47 (Nr.31#)	1.920	-	0.584	1.000	0

[a)] mobile phase: 90/10 n-heptane/iso-propanol [b)] flow rate: 0.8 ml/min

Table 3-5: Retention times (t); retention factors (k'), separation factors (α) and resolution factors (R_S) for HPLC of 14 oxiranes ($^{\#}$ old numbering as in an unpublished study) on a Chiralcel OD stationary phase; mobile phase: heptane / iso-propanol (90/10), flow rate: 0.5ml/min, t_0 = 1.304.

oxirane with π-system	CSP: Chiralcel OD t_1	t_2	k'	α	R_S
34 (Nr.01$^{\#}$)	12.036	13.427	8.763	1.13.0	1.546
35 (Nr.02$^{\#}$)	4.408	4.611	2.458	1.065	0.677
36 (Nr.04$^{\#}$)	2.518	-	0.915	1.000	0
37 (Nr.05$^{\#}$)	6.519	6.792	4.104	1.052	0.546
38 (Nr.06$^{\#}$)	4.592	-	2.521	1.000	0
39 (Nr.20$^{\#}$)	7.019	-	4.383	1.000	0
40 (Nr.21$^{\#}$)	6.444	7.100	4.150	1.128	0.729
41 (Nr.23$^{\#}$)	2.633	2.901	1.104	1.203	1.072
42 (Nr.25$^{\#}$)	2.004	-	0.537	1.000	0
43 (Nr.27$^{\#}$)	2.290	-	0.756	1.000	0
44 (Nr.32$^{\#}$)	5.375	6.119	3.370	1.183	0.827
without π-system					
45 (Nr.24$^{\#}$)	1.587	-	0.207	1.000	0
46 (Nr.30$^{\#}$)	1.534	-	0.167	1.000	0
47 (Nr.31$^{\#}$)	1.728	-	0.314	1.000	0

[c)] mobile phase: 70/30 n-heptane/iso-propanol

Table 3-6: Retention times (*t*); retention factors (*k'*), separation factors (α) and resolution factors (R_S) for HPLC of 14 oxiranes (# old numbering as in an unpublished study) on a Chiralcel AS stationary phase; mobile phase: heptane / iso-propanol (90/10), flow rate: 0.5ml/min, t_0 = 0.479.

oxirane with π-system	CSP: Chiralcel AS t_1	t_2	k'	α	R_S
34 (Nr.01#)	5.217	-	9.891	1.000	0
35 (Nr.02#)	1.584	-	2.307	1.000	0
36 (Nr.04#)	0.789	-	0.647	1.000	0
37 (Nr.05#)	2.700	-	4.637	1.000	0
38 (Nr.06#)	1.491	-	2.113	1.000	0
39 (Nr.20#)	1.919	-	3.006	1.000	0
40 (Nr.21#)	6.782	-	13.159	1.000	0
41 (Nr.23#)	0.916	-	0.912	1.000	0
42 (Nr.25#)	0.673	-	0.405	1.000	0
43 (Nr.27#)	1.275	2.184	2.611	2.142	0.909
44 (Nr.32#)	3.235	-	5.754	1.000	0
without π-system					
45 (Nr.24#)	0.642	-	0.340	1.000	0
46 (Nr.30#)	0.607	-	0.267	1.000	0
47 (Nr.31#)	0.684	-	0.428	1.000	0

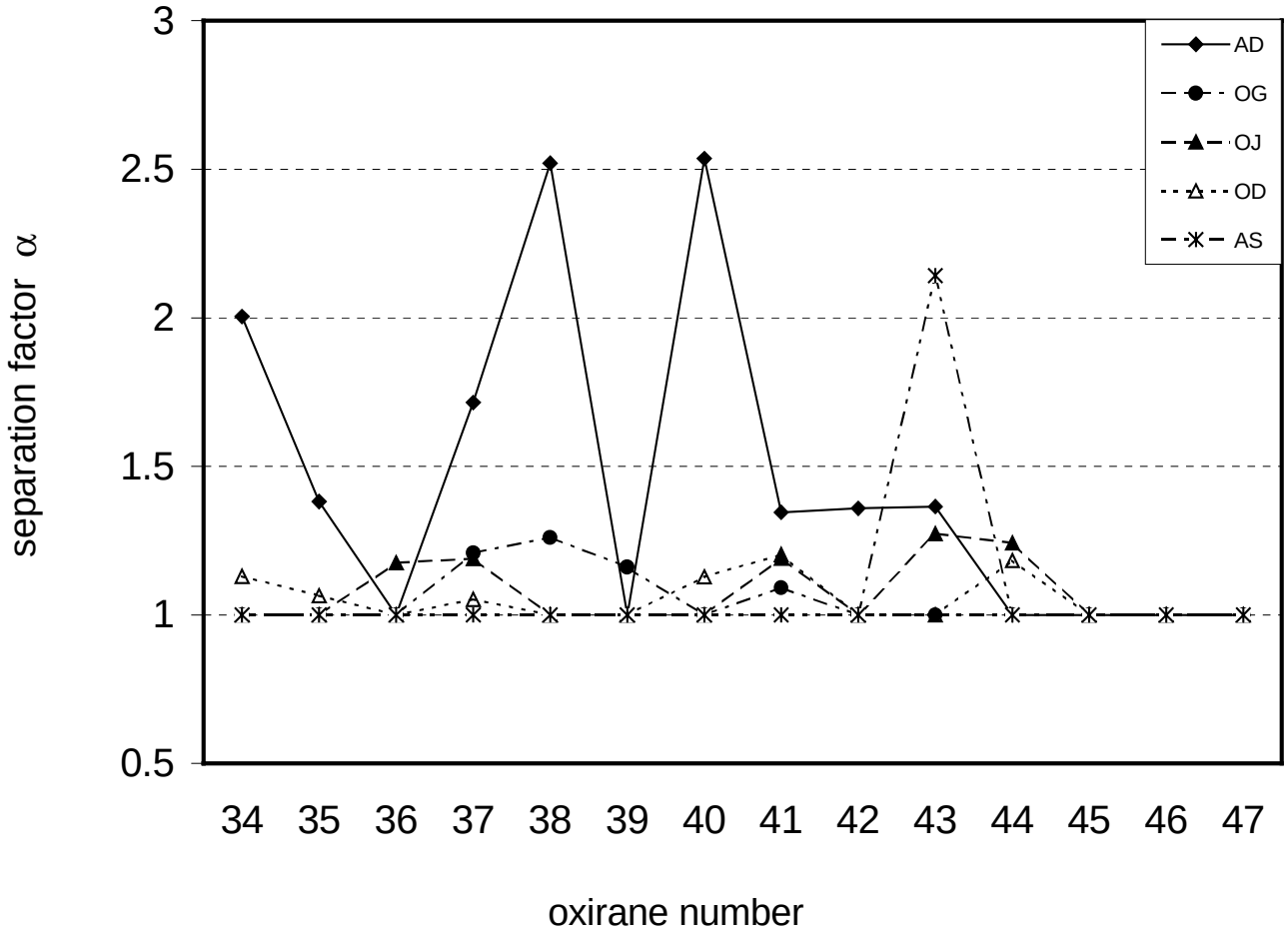


Figure 3-1: Enantiomer separation of oxiranes **34** to **47** on 5 CSPs by HPLC

In Figure 3-1, the situation of 14 different oxiranes is compared for 5 different CSPs. While linear cellulose derivatives form the basis of most polysaccharide stationary phases, helical amylose derivatives can provide widely different selectivities. The tris(3,5-dimethylphenylcarbamate) derivative of amylose (Chiralcel AD) often exhibits the highest enantioselectivity in this class of polysaccharides. Here it was successful for 8 out of 14 oxiranes tested. It is interesting to note that the corresponding cellulose derivative, cellulose tris(3,5-dimethylphenyl carbamate) (Chiralcel OD) proved to be the second best phase in this selection, with a success for 6 entries. The separation capability of these five stationary phases is decreasing in the order: AD > OD > OJ > OG > AS.

3.3.2. Comparison of Enantiomer Separations on Five Different CSPs

In order to compare the behaviour of the 14 oxiranes on 5 chiral stationary phases, the relationship between the net capacity factor (*k'*) and the separation factor (α) is shown in Figures 3-2 to 3-6.

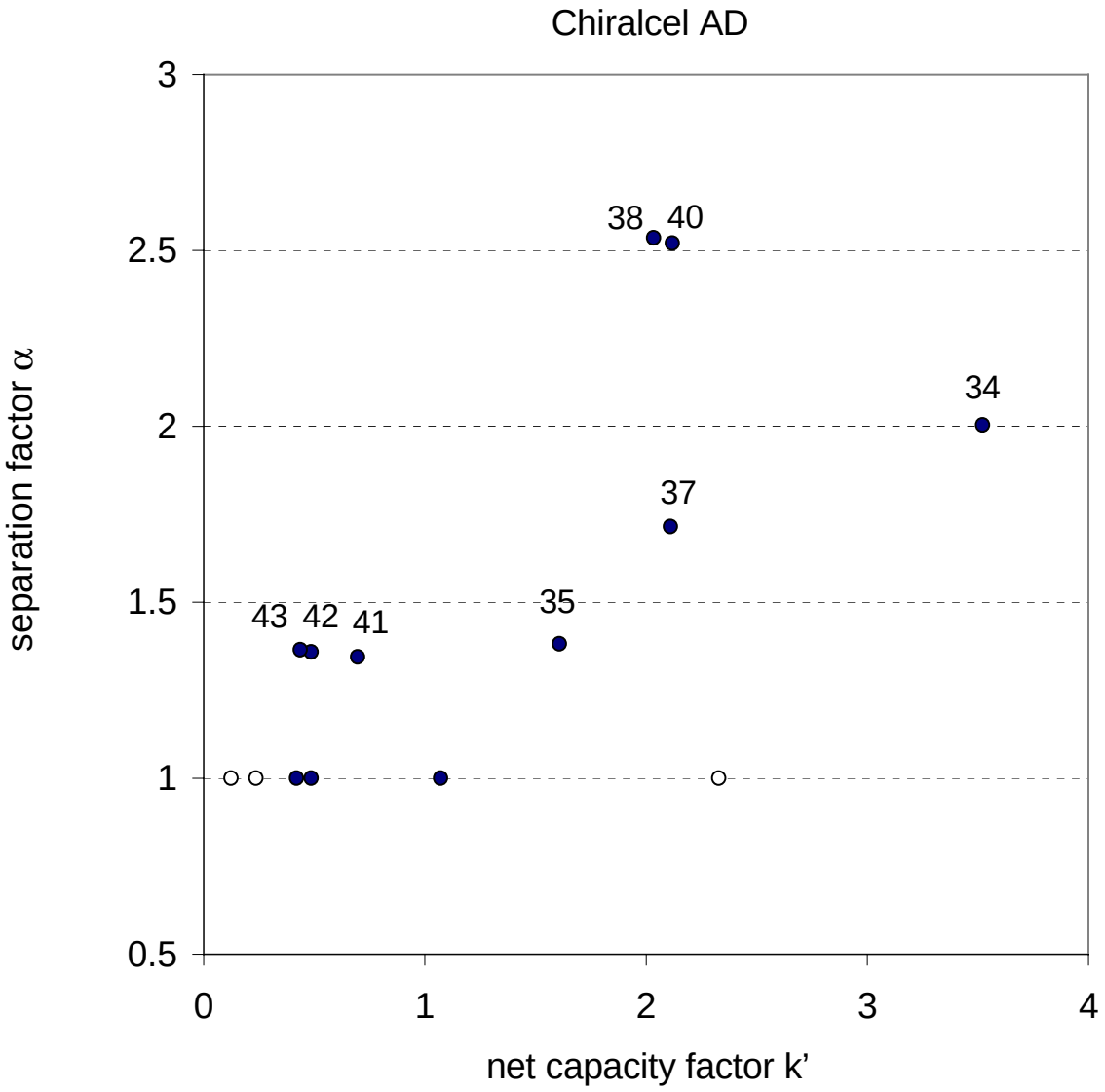


Figure 3-2: Separation factor α versus net capacity factor *k'* for the CSP Chiralcel AD

Chiracel AD appears to be quite versatile, being successful for 8 out of 11 oxiranes with π-system, yet zero success without π-system.

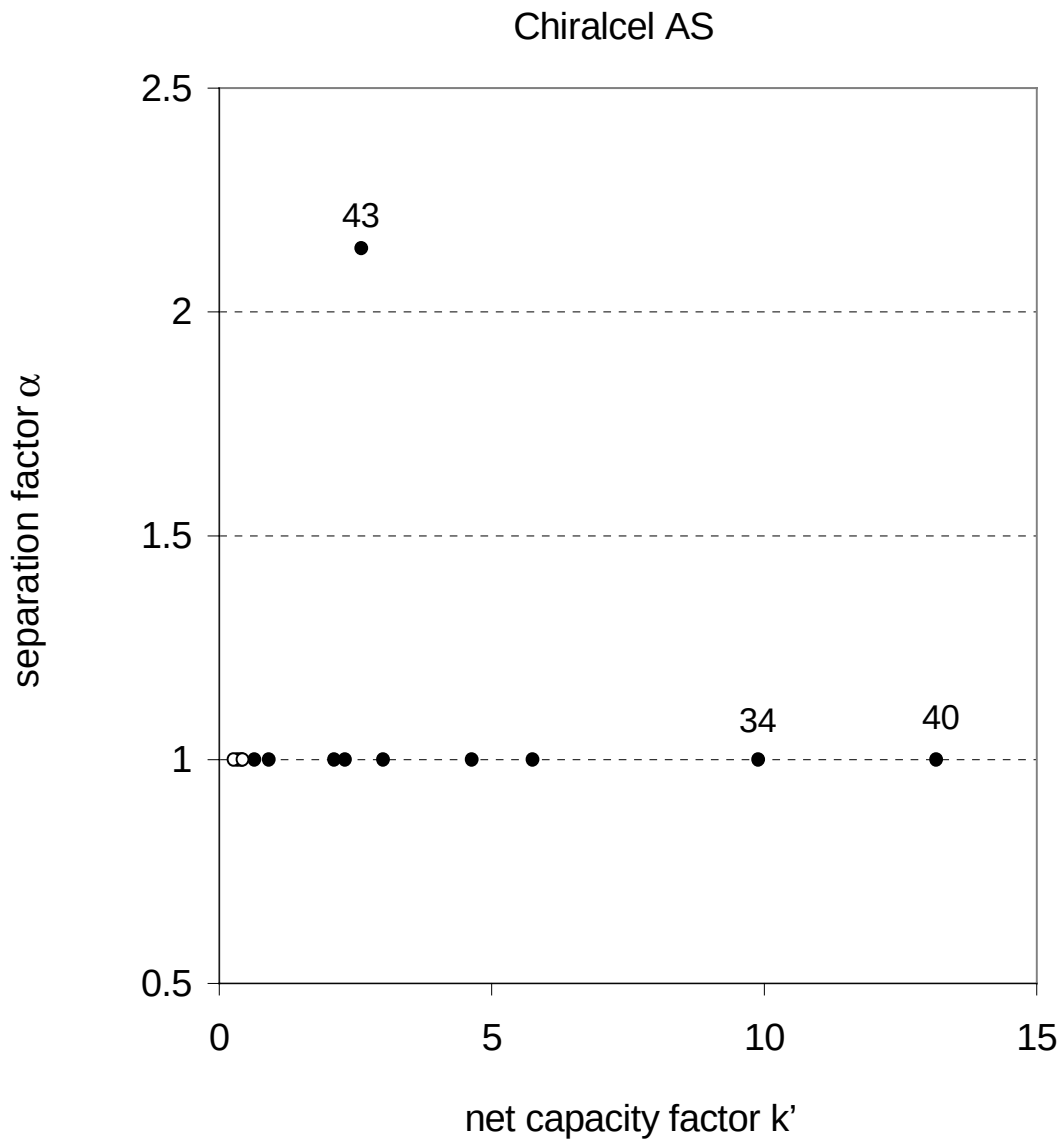


Figure 3-3: Separation factor α versus net capacity factor *k'* for the CSP Chiralcel AS

The other amylose phase Chiralcel AS, however, allows merely the separation of entry **43**, probably due to its unique rod-like molecular structure.

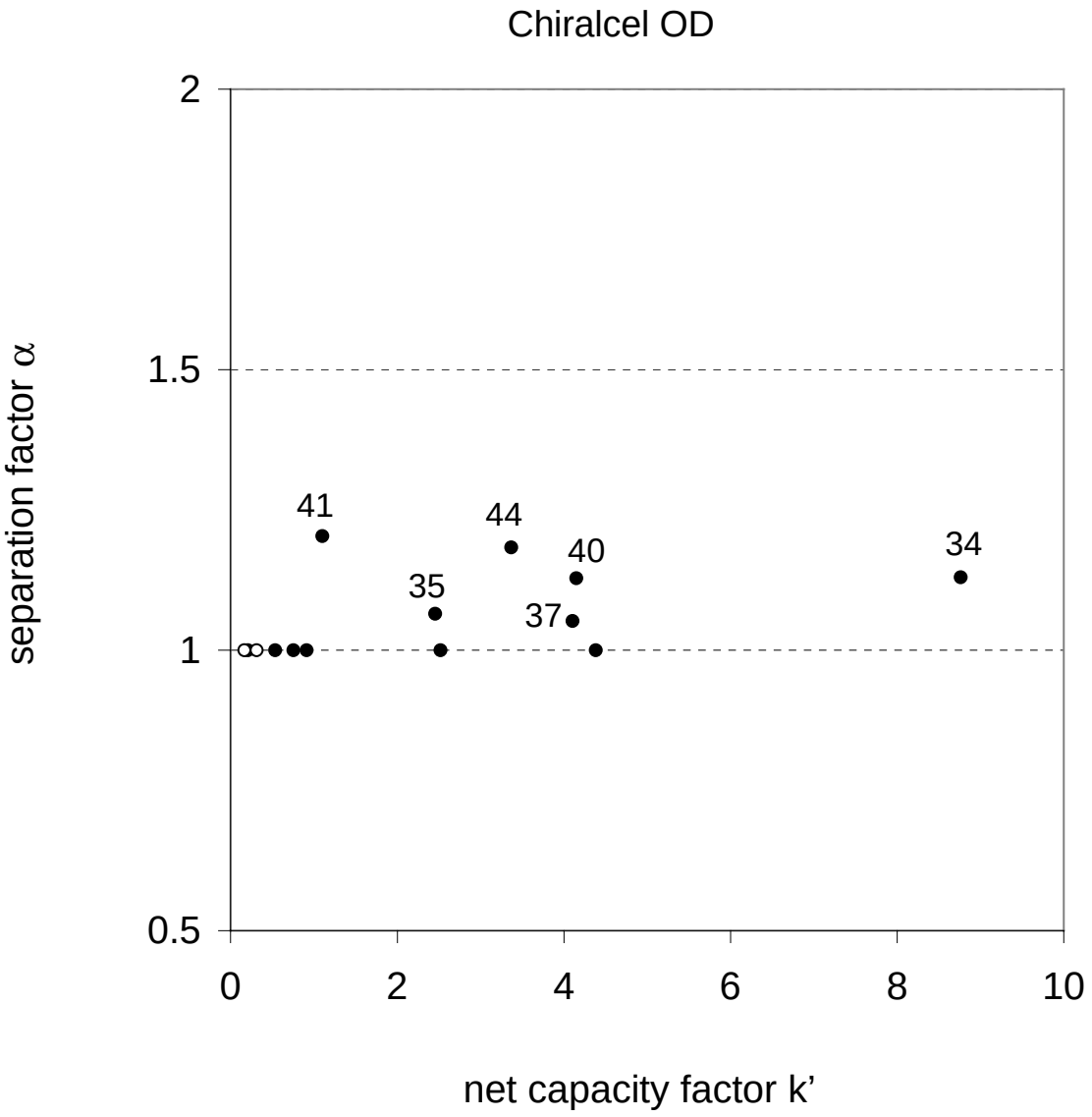


Figure 3-4: Separation factor α versus net capacity factor *k'* for the CSP Chiralcel OD

In analogy to Chiracel AD, the similar cellulose derivative Chiralcel OD is also versatile, but not as effective; overall, the separation factors (α) are much smaller, and entry **43**, *inter alia*, is not separated at all.

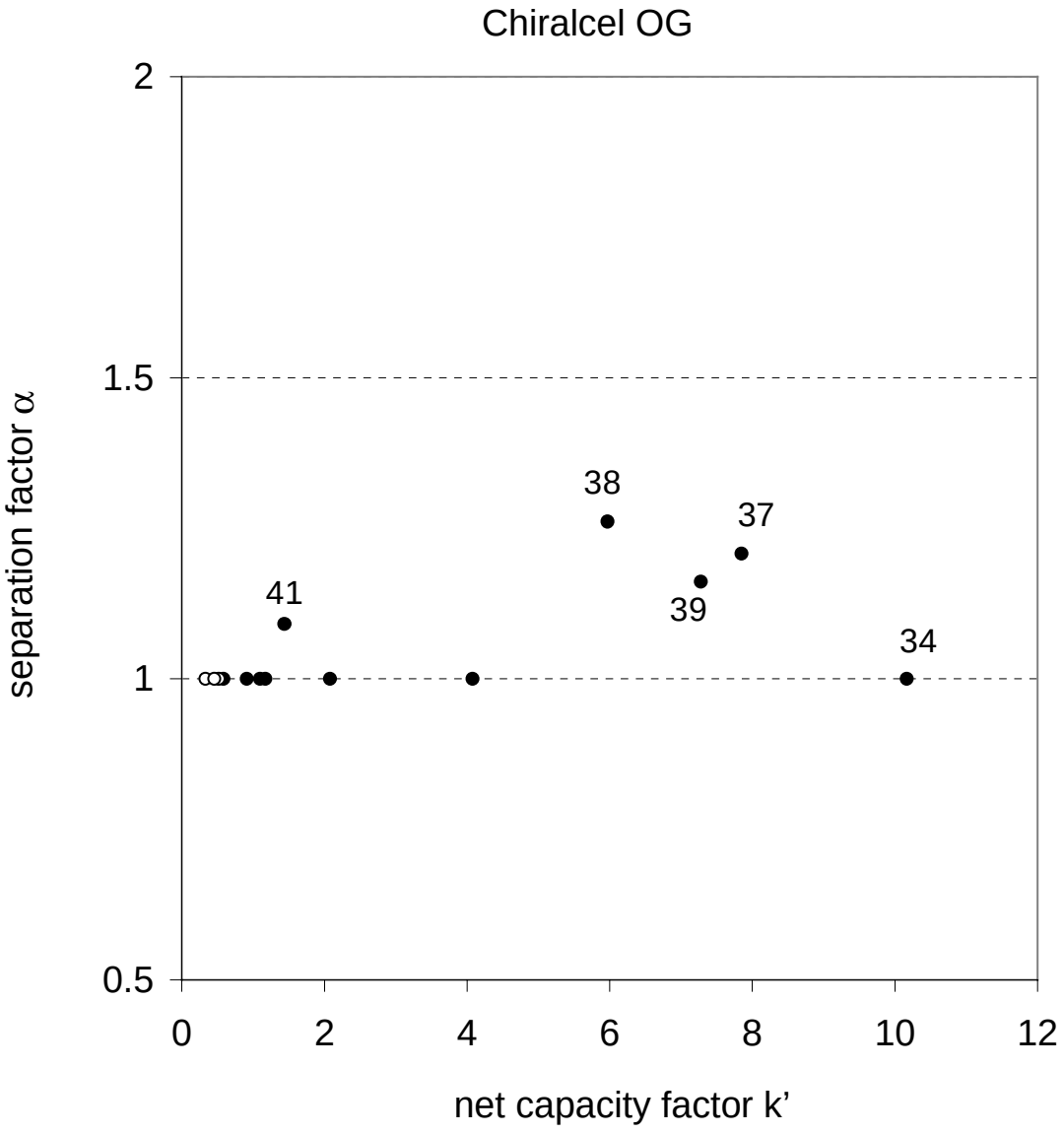


Figure 3-5: Separation factor α versus net capacity factor *k'* for the CSP Chiralcel OG

Chiralcel OG is also of limited applicability, but the selectivity is entirely different from Chiralcel OD. The methyl substituents play an important role in chiral recognition, with a mostly steric effect for the 3,5-dimethylphenylcarbamate (OD) and an electronic +M-effect for the 4-methyl derivative (OG).

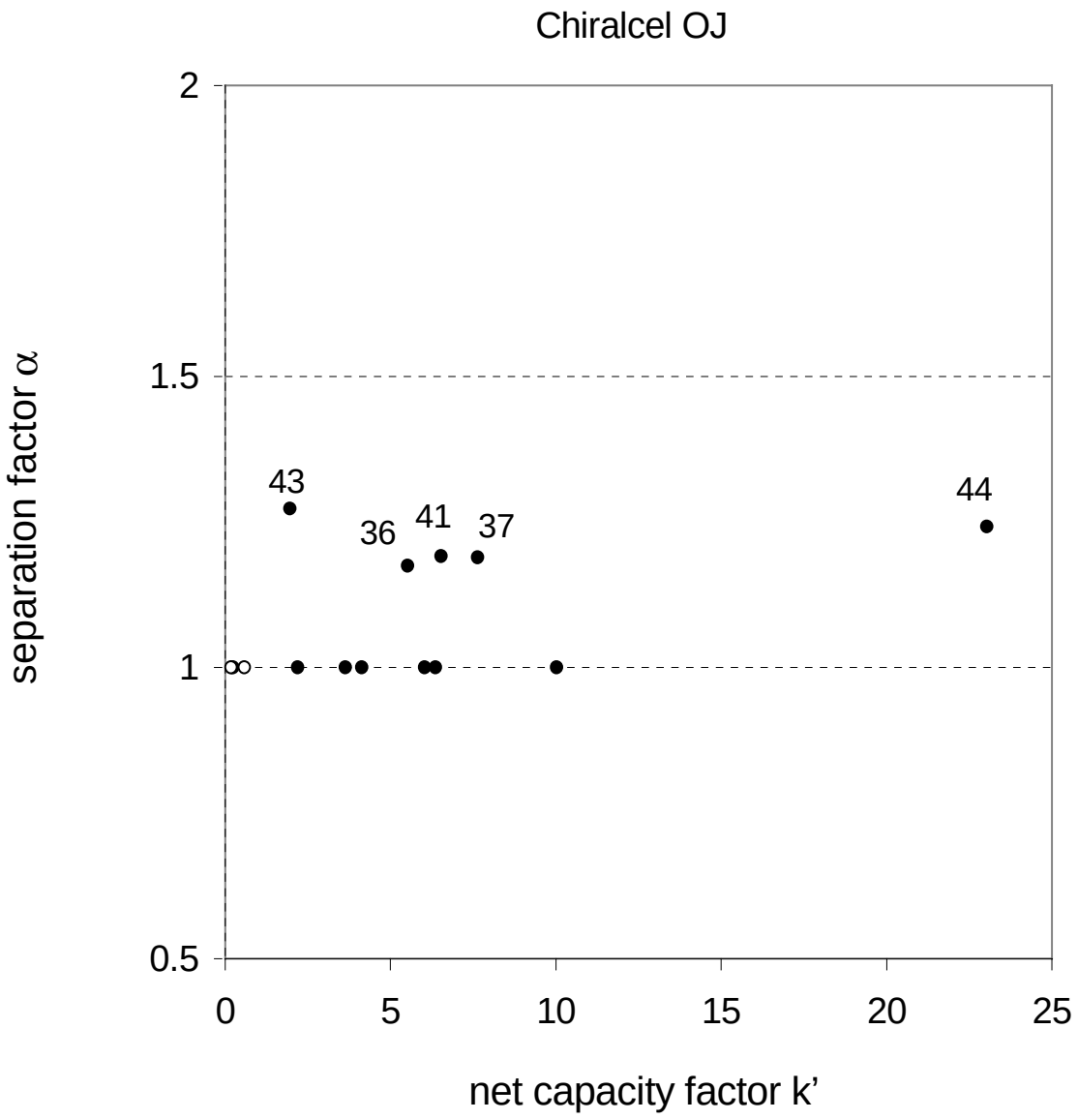


Figure 3-6: Separation factor α versus net capacity factor *k'* for the CSP Chiralcel OJ

Likewise, the 4-methyl-benzoate Chiralcel OJ is not very effective; however, the selectivity is again quite different from Chiralcel OG. Notably, the rod-like compound **43** is separated best, like on Chiralcel AS.

3.3.3. Influence of the Analyte Structure on the Enantiomer Separation

The molecular structure of the analytes will also influence the enantiomer separation and retention behaviour. The 14 analytes can be divided into two groups, one where π is present (entries **34** to **44** in Table 3-1), and the other where π is absent (entries **45** to **47**). From Figures 3-2 to 3-6, it is obvious that without an additional π system (represented by hollow points in the Figures), these oxiranes are not likely to be separated, and they also have a rather short retention time. Hence, they are not sufficiently interacting with this type of CSPs. None of the 14 oxiranes can be separated on all five columns, but entries **37** and **41** can be separated on four of them, while **43** can be separated on three different CSPs. Together with Chiralcel OJ, the separation task can be solved with these three phases almost as good as with all five phases, apart from the intriguingly wide separation of the rod-like compound **43** on Chiralcel AS.

Compound **34** has a strong retention due to the high polarity of this molecule, despite the lack of an aryl group. This behaviour is not due to the small size, as entries **45**, **46** and **47** are also small, but these are lacking the carbonyl groups as well, hence they have only a weak interaction with any of the five CSPs. However, the enantiomer separation of **34** not as good as for some of the oxiranes bearing an aryl group. The entries **36** and **44** do have aryl groups, but they do not bind very strongly to the stationary phases. In entry **39**, the aryl groups are from the stereogenic center, so there is only a small enantioselectivity.

We conclude that dipole interactions have a strong impact on the retention mechanism, and extended π systems are mandatory. The arrangement in space of the substituent groups around the analyte stereogenic center plays an important role in enantiomeric separations. The closer a group is to the chiral center, the more likely is chiral recognition and enantioselectivity. If there are no groups in the analyte molecule that bind to the stationary phase, the enantiomers are not likely to be separated.

3.4. Experimental Section

3.4.1. Instruments

3.4.1.1 HPLC

Spectra Physics SP8800 HPLC Pump, Spectra Physics SP8880 Autosampler, Spectra Physics Spectra 100 Detector, Spectra Physics Chromjet Integrator, Computer 486DX2, 16MB, Software PC1000 Version 3.0, Mobile phases: heptane / isopropanol and 0.1 % diethylamine, HPLC-grade (Merck). Chemical reagent: diethylamine (Fluka) >= 99.7 %. Sample volume: 10µl

3.4.1.2 IR-Spectrometer

Perkin-Elmer 281 B. All wave numbers in cm^{-1}.

3.5.1.3 NMR-Spectrometer

Bruker AC 250 (250 MHz) and Bruker WM 400 (400 MHz). Chemical shift δ in ppm (TMS and TSP, respectively, as standard)

3.4.1.4 Elemental Analysis

C, H, N: Carlo Erba Elemental Analyzer Mod. 1106, Mikroanalytisches Labor der Universitaet Tuebingen.

3.4.1.5 MS-Spectrometer

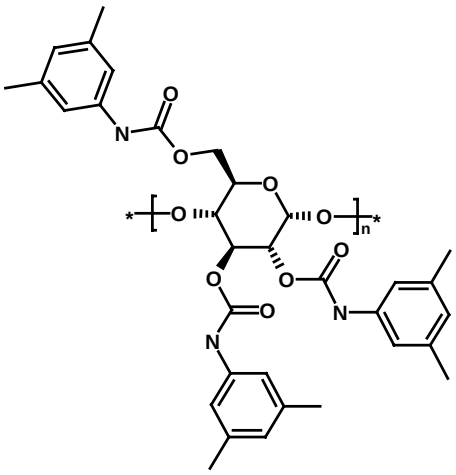
Double Physical Focus Sector Field-MS (AMD Intectra), and Tri-Stage-Quadrupol-MS TSQ 70 (Finnigan-MAT).

3.4.2. Daicel-HPLC-Phases

We have synthesized the drug precursors (see Table 3-1), the aim was to separate these compounds into enantiomers on five chiral stationary phases (DAICEL chiral AD, chiral OG, chiral OJ, chiral OD and chiral AS), in order to study the impact of the molecular structure on separation. The chiral stationary phases from the Fa. Daicel [11] (Illustration Table 3-7) was offered for HPLC-Phase. They are composed of the derivates from amylosecarbamate [82], cellulosecarbamate [82] or celluloseester [82], which were coated on a silica-gel substrate.

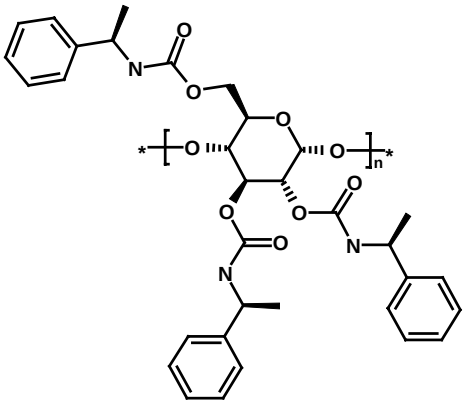
Table 3-7 Daicel HPLC-Phases

Amylosecarbamate-Derivatives



CHIRALCEL AD

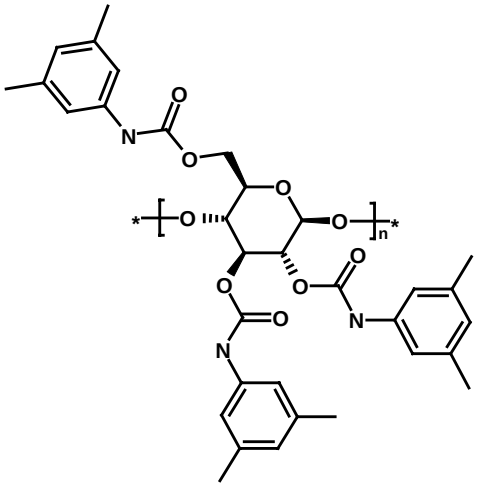
Column: 250 x 2 mm (L x I.D.) column material: Amylose tris[3,5-dimethylbenzyl-carbamate], coated on a 10 µm silica-gel substrate



CHIRALCEL AS

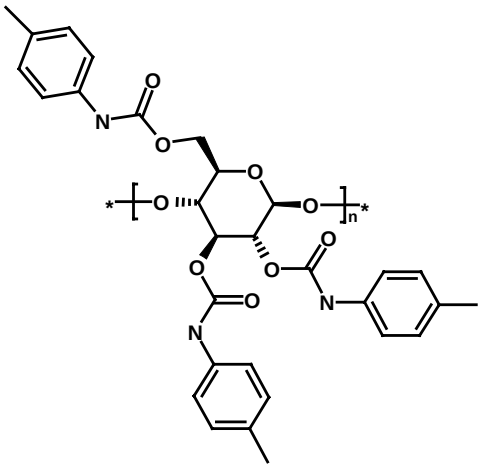
Column: 250 x 1 mm (L x I.D.), column material: Amylose tris[(S)-α-methylbenzyl-carbamate], coated on a 10 µm silica-gel substrate

Cellulosecarbamate-Derivatives



CHIRALCEL OD-H

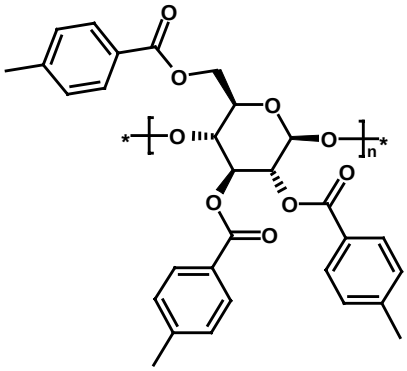
Column: 250 x 2 mm (L x I.D.) column material: Cellulose tris[3,5-dimethylphenyl-carbamate], coated on a 5 µm silica-gel substrate



CHIRALCEL OG

Column: 250 x 2 mm (L x I.D.) column material: Cellulose tris[4-methylphenylcarbamate], coated on a 10 µm silica-gel substrate

Celluloseester-Derivatives



CHIRALCEL OJ

Column: 250 x 2 mm (L x I.D.), column material: Cellulose tris[4-methylbenzoate], coated on a 8 μm silica-gel substrate

The chiral columns are really sensitive to polar mobile phases. The suitable mobile phases are included in the Table 3-8:

Table 3-8: The suitable mobile phases in five different chiral stationary phases

Column type	*n*-heptane / 2-propanol or *n*-hexane / 2-propanol	*n*-heptane / ethanol or *n*-hexane / ethanol
AD	100/0 to 0/100 v/v	100/0 to 85/15 v/v 40/60 to 0/100 v/v
AS	100/0 to 0/100 v/v	100/0 to 0/100 v/v
OD-H	100/0 to 0/100 v/v	100/0 to 0/100 v/v
OG	100/0 to 50/50 v/v	100/0 to 80/20 v/v
OJ	100/0 to 0/100 v/v	100/0 to 0/100 v/v
Suitable Mobile Phase Modifiers include N,N-Diethylamine for a basic sample, typical 0.1%, maximal 0.5% Trifluoroacetic for an acidic sample, typical 0.1%, maximal 0.5%		

3.4.3. Chemicals

Basic chemicals were purchased from ABCR, Aldrich, Fluka, Merck, and Schuetz & Co.

TLC Plates: Silica gel 60 F_{254} (E. Merck, Darmstadt). UV detection, staining with $Ce(SO_4)_2$ / H_2SO_4 / $(NH_4)_6Mo_7O_{24} \cdot 4H_2O$

LC column filling: Silica gel 60 (0.032-0.063 mm) (E. Merck, Darmstadt); this silica gel was impregnated with triethylamine and suspended in petrolether (30 - 50 ^oC) / diethyl ether / triethylamin (9 / 3 / 7), filtered, and finally dried in vacuo at 50°C.

General procedures. All non-aqueous reactions were performed under a positive pressure of N_2 gas. Flash column chromatography was performed as described by Still et al.[83] employing 32-63 μm (220-440 mesh ASTM) silica gel.

Reagent. [84]

Tetrahydrofuran was permeated through a basic Al_2O_3 column to remove peroxides, then it was refluxed with sodium in the presence of benzophenone under N_2 gas until the blueviolet colour persisted, distilled under N_2 gas, and finally stored over CaH_2.

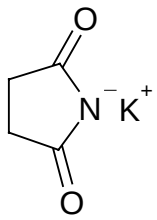
Dichloromethane, diisopropylamine, triethylamine were distilled under nitrogen from calcium hydride.

Dry methanol was prepared by distillation from magnesium methylate.

3.4.4. Synthesis

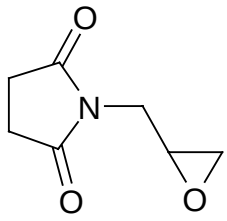
3.4.4.1. 1-(2,3-Epoxypropyl)-2,5-pyrrolidinedione (34)

3.4.4.1.a.Succinimide potassium salt



Following a literature procedure [85], potassium hydroxide (5.66 g / 0.1 mol) was dissolved in 25 ml of methanol, then succinimide (9.94 g / 0.1 mol) was added into the solution, and the mixture was stirred at room temperature for 1 h. The solvent was evaporated under reduced pressure, the residue was rinsed twice with diethyl ether to remove last traces of methanol. The slurry was filtered to get light brown crystals of succinimide potassium salt, yield 13.45 g (96 %).

3.4.4.1.b. 1-(2,3-Epoxypropyl)-2,5-pyrrolidinedione



In analogy to a general procedure [85], to a mixture of epichlorohydrin (6.0 ml, 0.075 mol) and acetonitrile (20 ml), the potassium salt of succinimide (6.85 g, 0.05 mol) was gradually added while stirring at 40 to 50°C. After the addition was complete, the temperature was raised to about 80 to 90°C, and stirring was continued at reflux temperature for another 6 h. The solution was filtered to remove the residual KCl and unreacted succinimide potassium salt, and acetonitrile was removed by distillation. Excess epichlorohydrin was removed by extraction with petrol ether (60 to 80°C) (3 × 10 ml), and fractional distillation in vacuo afforded the product as a clear colourless oil with a tendency to form white crystals.

Yield: 4.38 g (56.5 %), b.p. 210°C / 0.02 mbar, purity > 97 %

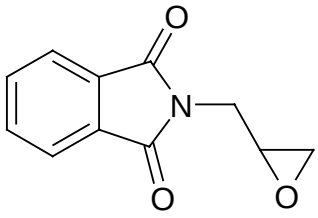
Anal. Calculated for $C_7H_9NO_3$: C, 54.2; H, 5.1; N, 9.0
Found: C, 52.5; H, 5.8; N, 8.9

^{1}H-NMR ($CDCl_3$): δ = 2.57 - 2.60 (CH_2O), 2.70 - 2.76 (CH_2-CH_2), 3,11 - 3.14 (CHO), 3.53 - 3.73 (NCH_2) ppm

^{13}C-NMR ($CDCl_3$): δ = 28.22, 29.66 (CH_2-CH_2), 40.60 (CH_2O), 46.12 (NCH_2), 48.51 (CHO), 176.99, 178.04 (C=O) ppm

MS: m/z = 155.7 $[M]^+$

3.4.4.2. N-Oxiranylmethyl-phthalimide (35)



In analogy to a general procedure [86], epichlorohydrin (35 ml / 0.4471 mol) was dropped into potassium phthalimide (15.05 g / 0.0813 mol) that was placed in a flask equipped with stirrer and reflux condenser. The mixture was heated in a bath warmed to 160° for 10 h, during which the original pasty yellow substance was gradually transformed into a suspension of finely divided powder in a dark brown liquid. The epichlorohydrin was distilled from the reaction mixture in vacuo with a water-pump, the residue was dissolved in 100 ml hot ethanol. The insoluble inorganic residue was filtered from the hot solution by filtration and washed with 15 ml of hot ethanol. After cooling, the combined ethanol solutions deposited the product as yellowish white crystals. Recrystallization from 10 ml of ethanol eventually afforded yellowish white crystals.

Yield: 12.51g (75.76%), m.p. 95-97°C, purity > 98%

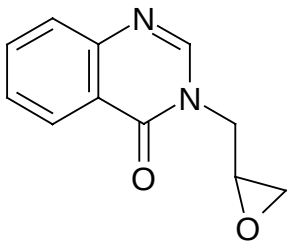
Anal. Calculated for $C_{11}H_9NO_3$: C, 65.03; H, 4.43; N, 6.90
Found: C, 64.43; H, 4.31; N, 6.88

^{1}H-NMR ($CDCl_3$): δ = 2.64 - 2.79 (CH_2O), 3.17 - 3.24 (CHO), 3.73 - 3.97 (NCH_2), 7.67 - 7.87 (CH_{arom}) ppm

^{13}C-NMR ($CDCl_3$): δ = 39.70 (CH_2O), 46.14 (CHO), 49.09 (NCH_2), 123.46 - 134.17 (CH_{arom}), 168.00 (CO) ppm

MS: m/z = 203.3 $[M]^+$

3.4.4.3. N-Oxiranylmethyl-3H-quinazolin-4-one (37)



In analogy to a general procedure [87], 3H-quinazolin-4-one (14.6 g / 0.1 mol) was dissolved in 100 ml of 1 *N* sodium methoxide, and epichlorohydrin (37 ml / 0.47 mol) was added dropwise. The reaction mixture was allowed to stand at room temperature for 2 h, while keeping the reaction temperature below 35° by cooling with a water bath. After 2.5 h, the solution was filtered from the salt, and the solvent was evaporated in vacuo. The residue was dissolved in 300 ml of chloroform, the brown solution was dried over magnesium sulfate, filtered and evaporated in vacuo. Recrystallization from EtOAc / petrol ether (30-50°C) afforded white crystals.

Yield, 10.61g (52.47%), m.p. 79-80°C (Lit. 78-80°C), purity > 98%.

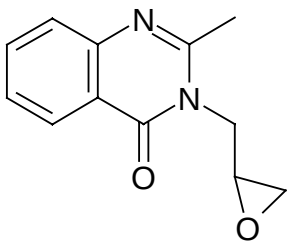
Anal. Calculated for $C_{11}H_{10}N_2O_2$: C, 65.25; H, 4.97; N, 13.90
Found: C, 64.87; H, 5.03; N, 13.84

^{1}H-NMR ($CDCl_3$): δ = 2.52 - 2.83 (CH_2O), 3.26 - 3.33 (CHO), 3.73 - 4.53 (CH_2N), 7.40 - 8.25 (CH_{arom}), 7.97 (CHN) ppm

^{13}C-NMR ($CDCl_3$): δ = 45.50 (CH_2O), 47.72 (NCH_2), 49.74 (CHO), 126.74 - 134.51 (CH_{arom}), 146.58 - 148.14 (NCH), 161.14 (CO) ppm

MS: m/z = 202.2 $[M]^+$

3.4.4.4. 2-Methyl-3-oxiranylmethyl-3H-quinazolin-4-one (38)



In analogy to a general procedure [87], 2-methyl-3H-quinazolin-4-one (8.01 g / 0.05 mol) was dissolved in 58.0 ml of 1 *N* sodium methoxide. To this solution, 20 ml of epichlorohydrin were added dropwise, followed by tetraethylammonium bromide (5.2 g / 0.025 mol). The reaction mixture was allowed to stand at room temperature for 3 h (not longer), keeping the reaction temperature below 35° by cooling with a water bath. Then, the solution was filtered from the salt and the solvent was evaporated in vacuo. The residue was dissolved in 250 ml of chloroform, dried over magnesium sulfate, and the solution was evaporated in vacuo. Recrystallization from EtOAc / petrol ether (60-90°C) afforded white crystals.

Yield, 7.25g (67.65%), m.p. 90-92°C (Lit. 90-92°C), purity > 96%.

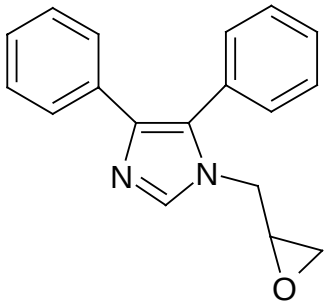
Anal. Calculated for $C_{12}H_{12}N_2O_2$: C, 66.60; H, 5.60; N, 12.95
Found: C, 64.59; H, 5.96; N, 12.83

^{1}H-NMR ($CDCl_3$): δ = 2.56 - 2.86 (CH_2O), 2.65 (CH_3), 3.31 - 3.37 (CHO), 3.98 - 4.69 (CH_2N), 7.39 - 8.24 (CH_{arom}) ppm

^{13}C-NMR ($CDCl_3$): δ = 23.65 (CH_3), 45.37 (CH_2O), 45.71 (NCH_2), 49.94 (CHO), 126.57 - 126.85 (CH_{arom}), 134.53 (NC), 154.63 (CO) ppm

MS: m/z = 216.2 $[M]^+$

3.4.4.5. 1-Oxiranylmethyl-4,5-diphenyl-1H-imidazole (39)



In analogy to a general procedure [88], 4,5-diphenyl-1H-imidazole (17.68 g / 0.08 mol) was mixed with 25.6 g of 50% aqueous sodium hydroxide, and 25.2 ml of epichlorohydrin were added dropwise to this mixture, then tetraethylammonium bromide (0.84 g / 0.04 mol) was added. The mixture was vigorously stirred for 3 h at 20°C, then it was heated for another 0.5 h at 30°C. The reaction mixture was dissolved in EtOAc, filtered, and evaporated in vacuo. The residue was recrystallized from EtOAc / petrol ether (30-50°) to afford white crystals.

Yield, 14.87 g (67.35%), m.p. 99-102°C (Lit. 98-100°C), purity > 98%.

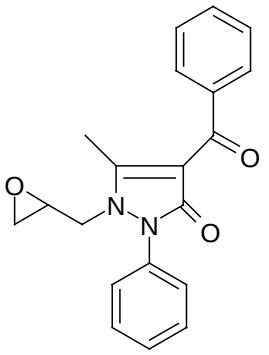
Anal. Calculated for $C_{18}H_{16}N_2O$: C, 78.17; H, 5.79; N, 10.13
Found: C, 75.43; H, 5.53; N, 9.55

^{1}H-NMR ($CDCl_3$): δ = 2.32 - 2.74 (CH_2O), 3.03 - 3.09 (CHO), 3.80 - 4.12 (CH_2N), 7.10 - 7.49 (CH_{arom}), 7.77 (CHN) ppm

^{13}C-NMR ($CDCl_3$): δ = 45.61 (CH_2O), 46.63 (NCH_2), 50.54 (CHO), 126.46 - 134.45 (CH_{arom}), 130.47 - 131.07 (NC-CN), 138.33 (CHN) ppm

MS: m/z = 276.3 $[M]^+$

3.4.4.6. 4-Benzoyl-5-methyl-1-oxiranylmethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (40)



4-Benzoyl-5-methyl-2-phenyl-1,2-dihydro-pyrazol-3-one (27.90 g / 0.1 mol) was dissolved in 110 ml of 1 *N* sodium methoxide, and epichlorohydrin (100 ml / 1.28 mol) was added dropwise and slowly. Then, the mixture was refluxed at 110°C for 4 h, filtered and evaporated under reduced pressure. The residue was dissolved in 250 ml of chloroform and dried over magnesium sulfate, the solution was filtered and evaporated to a yellowish-brown clear liquid. Recrystallization from EtOAc / diisopropyl ether afforded white crystals.

Yield: 17.42 g (51.56%), m.p. 129-131°C, purity > 96%.

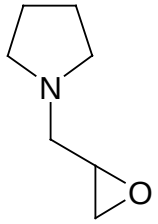
Anal. Calculated for $C_{20}H_{18}N_2O_3$: C, 71.77; H, 5.38; N, 8.37
Found: C, 70.46; H, 4.66; N, 8.18

^{1}H-NMR ($CDCl_3$): δ = 2.40 - 2.42; 2.71 - 2.74 (CH_2O), 2.63 (CH_3), 2.98 - 3.02 (CHO), 3.71 - 4.12 (NCH_2), 7.25 - 7.90 (CH_{arom}) ppm

^{13}C-NMR ($CDCl_3$): δ = 12.64 (CH_3), 45.28 (CH_2O), 48.31 (NCH_2), 49.05 (CHO), 126.28 - 134.34 (CH_{arom}), 138.46 (CN), 159.19 (C=C), 163.85 (C=O), 190.49 (C=O) ppm

MS: m/z = 334.2 $[M]^+$

3.4.4.7. 1-Oxiranylmethyl-pyrrolidine (45)



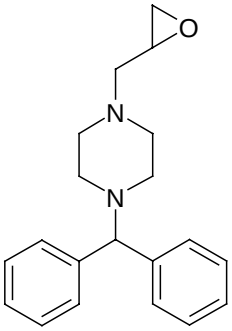
Pyrrolidine (33.2 ml / 0.4 mol) was dissolved in 200 ml of diethyl ether, and epichlorohydrin (32 ml / 0.4 mol) was added dropwise and slowly during appr. 2 h. Stirring was continued while heating with a bath warmed to 40° for 24 h, during which the clear organic phase changed into a translucent light yellow liquid. The diethyl ether was removed by evaporation under reduced pressure. After addition of 50% NaOH (40 ml / 0.5 mol), the mixture was stirred at room temperature for 2 h (warming up should be prevented by cooling with a water bath, otherwise, 2,5-bis-pyrrolidinemethyl-p-dioxane will be formed). Then it was washed with 80 ml of water, the aqueous layer was extracted with diethyl ether four times, and the combined organic solutions were dried over K_2CO_3 for 2 h. After removal of diethyl ether in vacuo, the residue was distilled under reduced pressure to afford the product as a colourless, transparent liquid.

Yield: 36.88 g (72.61%), b.p. 25 ~ 26°C / 0.1 mbar, purity > 98%

^{1}H-NMR ($CDCl_3$): δ = 1.74 - 1.79 (CH_2-CH_2), 2.34 - 2.56 (CH_2O), 2.34 - 2.78 (NCH_2), 2.46 - 2.59 (CH_2-CH_2N), 3.05 - 3.08 (CHO) ppm

^{13}C-NMR ($CDCl_3$): δ = 23.52 (CH_2-CH_2), 45.60 (CH_2O), 51.06 (CH_2N), 54.67 (NCH_2), 58.66 (CHO) ppm

3.4.4.8. 1-Benzhydryl-4-oxiranylmethyl-piperazine (42)



Diphenylmethylpiperazine (17.68 g / 0.07 mol) was dissolved in 350 ml of dry acetone, then epibromohydrin (12 ml / 0.14 mol) was added drop by drop while stirring slowly at the beginning and faster towards the end. During addition of half of the epibromohydrin, the solution turned white and muddy. After addition of all epibromohydrin, K_2CO_3 (9.7 g / 0.07 mol) was added into the mixture, and it was refluxed at 65°C for 6 h. After cooling, the inorganics were filtered off, the filtrate was evaporated to dryness, and an oily yellow residue was obtained. Repeated recrystallization (twice) from hot ethanol afforded light yellow crystals.

Yield: 16.44 g (76.15 %), m.p. 103-104°C, purity > 99%.

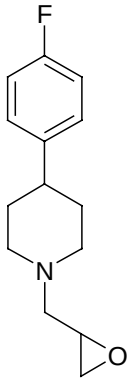
Anal. Calculated for $C_{20}H_{24}N_2O$: C, 77.8; H, 7.78; N, 9.08
Found: C, 77.4; H, 7.83; N, 8.98

^{1}H-NMR ($CDCl_3$): δ = 2.27 - 2.48 (CH_2O), 2.28 - 2.77 (NCH_2), 2.45 - 2.69 (CH_2-CH_2), 3.05 - 3.12 (CHO), 4.24 (CH), 7.20 - 7.44 (CH_{arom}) ppm

^{13}C-NMR ($CDCl_3$): δ = 45.13, 61.08 (CH_2-CH_2), 50.22 (CH_2O), 51.81 (NCH_2), 53.98 (CHO), 126.96 - 128.51(CH_{arom}), 142.75 (CH) ppm

MS: m/z = 308.4 $[M]^+$

3.4.4.9. 1-(4-Fluoro-phenyl)-4-oxiranylmethyl-piperazine (43)



1-(4-Methylphenyl)-2-methylpiperazine (19.07 g / 0.1 mol) was dissolved in 100 ml of ethanol under stirring at 40°C, and epichlorohydrin (7.8 ml / 0.1 mol) was added dropwise into the mixture. The reaction mixture was stirred for 6 h at 40°C. After addition of 50% NaOH (4 g / 0.2 mol) into this solution, the mixture was stirred for another 15 h at room temperature, then it was filtered. After evaporation of the ethanol, the residue was dissolved in 160 ml of diethyl ether and again filtered. The ether solution was concentrated in vacuo and the crude 1-[1-(4-methylphenyl)-4-(2-methylpiperazino)]-2,3-epoxypropane was obtained as an oil. Recrystallization from EtOAC / petrol ether (ratio 2/1), afforded white crystals.

Yield: 5.16 g (43.7%), m.p. 44-47°C, purity > 96%

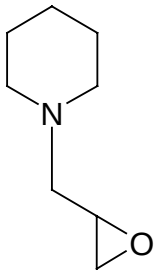
Anal. Calculated for $C_{13}H_{17}FN_2O$: C, 66.03; H, 7.20; N, 11.85
Found: C, 65.69; H, 7.21; N, 11.83

^{1}H-NMR ($CDCl_3$): δ = 2.29 - 2.31; 2.61 - 2.70 (CH_2O), 2.26 - 2.34; 2.49 - 2.52; 2.84 - 2.86 (NCH_2), 2.73 - 2.80; 3.09 - 3.12 (NCH_2-CH_2N), 3.14 - 3.16 (CHO), 6.84 - 6.98 (CH_{arom}) ppm

^{13}C-NMR ($CDCl_3$): δ = 44.85, 61.00 (CH_2-CH_2), 50.11 (CH_2O), 50.24 (NCH_2), 53.68 (CHO), 115.35 - 147.96(CH_{arom}), 155.31 - 159.11 (CH_2-CH_2) ppm

MS: m/z = 236.0 $[M]^+$

3.4.4.10. 1-Oxiranylmethyl-piperidine (46)



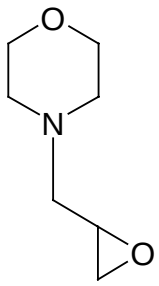
Piperidine (39 ml / 0.4 mol) was dissolved in 200 ml of diethyl ether, and epichlorohydrin (32 ml / 0.4 mol) was added dropwise and slowly during appr. 2 h. Stirring was continued while heating with a bath warmed to 40° for 8 h, during which the clear organic phase changed into a translucent light yellow liquid. The diethyl ether was removed by evaporation under reduced pressure. After addition of 50% NaOH (40 ml / 0.5 mol), the mixture was stirred at room temperature for 45 min at 30°C (warming up should be prevented by cooling with a water bath, otherwise, 2,5-bis-piperidinemethyl-p-dioxane will be formed), then it was washed with 80 ml of water, the aqueous layer was extracted with diethyl ether four times, and the combined organic solutions were dried over K_2CO_3 for 2 h. After removal of diethyl ether in vacuo, the residue was distilled under reduced pressure to afford the product as a colourless, transparent liquid.

Yield: 36.12g (64.05%), b.p. 30 ~ 31°C / 0.06 mbar, purity > 98%

^{1}H-NMR ($CDCl_3$): δ = 1.37 - 1.63 (CH_2-CH_2), 2.19 - 2.53 (CH_2N), 2.40 - 2.53; 2.72 - 2.76 (NCH_2), 2.36 - 2.46; 2.60 - 2.67 (CH_2O), 3.04 - 3.10 (CHO) ppm

^{13}C-NMR ($CDCl_3$): δ = 24.15 - 25.92 (CH_2-CH_2), 45.20 (CH_2O), 50.39 (NCH_2), 55.04 (CH_2N), 61.88 (CHO) ppm

3.4.4.11. 4-Oxiranylmethyl-morpholine (47)



Morpholine (35 ml / 0.4 mol) was dissolved in 200 ml of diethyl ether, and epichlorohydrin (32 ml / 0.4 mol) was added dropwise and slowly during appr. 2 h. Stirring was continued while heating with a bath warmed to 40° for 6 h, and then stirring at room temperature for another 24 h, during which the clear organic phase changed into a translucent light yellow liquid. The diethyl ether was removed by evaporation under reduced pressure. After addition of 50% NaOH (40 ml / 0.5 mol), the mixture was stirred at room temperature for 45 min at 30°C (warming up should be prevented by cooling with a water bath, otherwise, 2,5-bis-morpholinemethyl-p-dioxane will be formed), then it was washed with 80 ml of water, the aqueous layer was extracted with diethyl ether four times, and the combined organic solutions were dried over K_2CO_3 for 2 h. After removal of diethyl ether in vacuo, the residue was distilled under reduced pressure to afford the product as a colourless, transparent liquid.

Yield: 13.16g (23%), b.p. 36-39° / 0.01 mbar, purity: > 98%.

^{1}H-NMR ($CDCl_3$): δ = 2.21 - 2.48 (CH_2-CH_2N), 2.18 - 2.26; 2.67 - 2.75 (NCH_2), 2.23 - 2.26; 2.50 - 2.58 (CH_2O), 3.02 - 3.40 (CHO), 3.64 - 3.74 (OCH_2-CH_2) ppm

^{13}C-NMR ($CDCl_3$): δ = 44.78 (CH_2O), 50.14 (NCH_2), 54.09 (CH_2N), 61.41 (CHO), 66.88 (OCH_2) ppm

3.5. Summary

Epoxy compounds with vary chemical structure are of antitumor active. their enantiomers can be separated on chiral stationary phases by HPLC.

The molecular stucture of the analytes will influence the enantiomer separation and retention behaviour. The dipole interactions have a strong impact on the retention mechanism, and extended π system are mandatory. The arrangement in space of the substituent groups around the analyte stereogenic center plays an important role in enantiomeric separations. The closer a group is to the stereogenic center, the more likely is chiral recognition and enantioselectivity. If there are no groups in the analyte molecule that bind to the stationary phase, the enantiomers are not likely to be separated.

4. References

[1] E.L. Eliel; S.H. Wilen, *Stereochemistry of Organic Compounds*, John Wiley & Sons Inc., New York (1994)

[2] R.S. Atkinson, *Stereoselective Synthesis*, John Wiley & Sons Ltd, New York (1995)

[3] A.J. Kirby, "The Anomeric Effect and Related Stereoelectronic Effects at Oxygen. Reactivity and Structure", *Concepts in Organic Chemistry* **15**, Springer-Verlag, Berlin (1983)

[4] C.R. Noe; M. Knollmüller; P. Ettmayer; P. Gärtner; M. Letschnig, *Österr. Chem. Z.* **91**, 36-41 (1990)

[5] G. Helmchen; R. Wierzchowski, *Angew. Chem.* **96**, 59-60 (1984)

[6] W. Oppolzer, *Pure and Appl. Chem.* **60**, 39-48 (1988)

[7] C.R. Noe; M. Knollmüller; P. Ettmayer; Gärtner; M. Letschnig, *Österr. Chem. Z.* **91**, 36-41 (1991)

[8] B. Koppenhoefer; A. Jakob; X.F. Zhu; B.C. Lin, *J. High Resolut. Chromatogr.* **23(6)**, 413-329 (2000)

[9] L. Olsen; K. Bronnum; P. Helboe; G.H. Jorgensen and S. Kryger, *J. Chromatogr.*, **636,** 231 (1993)

[10] Th. Jira; Ch. Toll; Ch. Vogt and Th. Beyrich, *Pharmazie*, **46** 432 (1991)

[11] DAICEL CHEMICAL INDUSTRIES, LTD, Chiral Chemicals, Division, 2-5, Kasumigaseki 3-chome,Chiyoda-ku 100-607 7, Tokyo, JAPAN

[12] Y. Zhou; P. Luan; L. Liu; Z.P. Sun, *J. Chromatogr. B*, **659**, 109-126 (1994)

[13] C.R. Noe, *Chem. Ber.*, **115,** 1576-1590 (1982)

[14] C.R. Noe; M. Knollmüller; G. Göstl; B.G. Steinbauer; H. Völlenkle, *Chem. Ber.*, **119**, 792 (1986)

[15] C.R. Noe; M. Knollmüler; I. Ziebarth-Schroth; M. Letschnig, *Liebig Ann. Chem.*, 1009; (1996)

[16] E. Juaristi; G. Cuevas, *Tetrahedron*, **48**, 5019 (1992)

[17] L.H. Easson; E. Stedman, *Biochem., J.* **27**, 1257-1266 (1933)

[18] C.C. Pfeiffer, *Science*, **124**, 29-31 (1956);

[19] K. Williams; E. Lee, *Drugs*, **30**, 333-354 (1985)],

[20] C.R. Noe; M. Knollmüller; G. Steinbauer; E. Jangg; H. Völlenkle, *Chem. Ber.*, **121**, 1231-1239 (1988)

[21] E. Jangg, *Dissertation*, TU Wien (1990)

[22] G. Gmeiner, *Dissertation*, TU Wien(1992)

[23] G. Steinbauer, *Dissertation*, TU Wien (1985)

[24] E. Jangg, *Dissertation*, TU Wien (1990)

[25] B. Koppenhoefer; M. Schwierskott, H.G. Brendle, C.R. Noe and E. Jangg, *J. Org. Chem.*, **61**, 4476-4479 (1996)

[26] B. Koppenhoefer; H. Allmendinger: *Chromatographia* **21(9)**, 503-508 (1986)

[27] B. Koppenhoefer: *Habilitation Thesis*, (1992)

[28] N.P. Franks; W.R. Lieb, *Nature* **367**, 607-613 (1994)

[29] M. Hummel: *Dissertation*, University of Tuebingen, (1991)

[30] H. Frank; G.J. Nicholson; E. Bayer, *J. Chromatogr. Sci.* **15**, 174-176 (1977)

[31] B. Koppenhoefer; H. Allmendinger; G.J. Nicholson; E. Bayer; *J. Chromatogr.* **63**, 260 (1983)

[32] B. Koppenhoefer; S. Abdalla; M. Hummel; *Chromatographia* **31(1-2)**, 31-40 (1991)

[33] T.J. Leitereg; D.G. Guadagni; J. Harris; T.R. Mon; R. Teranishi, Evidence for the difference between the odors of the optical isomers (+)- and (-)-carvone. *Nature* **230**, 455-456 (1997)

[34] L. Friedman; J.G. Miller, Odor in congruity and chirality. *Science* **172**, 1044-1046 (1971)

[35] K. Bodenhöfer; A. Hierlemann; J. Seemann; G. Gauglitz; B. Koppenhoefer & W. Göpel, Chiral discrimination using piezoelectric and optical gas sensors, *Nature* **387**, 577-580 (1997)

[36] B. Koppenhoefer; U. Mühleck & K. Lohmiller, Backbone modification of Chirasil-Val: effect of nonpolar side chains on enantiomer separation in GC, *Chromatographia* **40**, 718-723 (1995)

[37] L. Lepori; B. Koppenhoefer, *J. Phys. Chem.* **98**, 6862-6864 (1994)

[38] B. Koppenhoefer; H. Allmendinger; G.J. Nicholson and E. Bayer, *J. of Chromatography*, **260**, 63-73 (1983)

[39] W.B. Smith, *"Introduction to theoretical organic chemistry and molecular modeling"*, Weinheim VCH, (1996)

[40] U. Burkert and N.L. Allinger, *Molecular Mechanics*, American Chem. Soc., Washington, DC, (1982)

[41] John Zeng Hui Zhang *"Theory and Application of Quantum Molecular Dynamics"* World Scientific Publishing o. Pte. Ltd. (1999)

[42] P. Comba; T.W. Hambley, *"Molecular Modeling"*, Weinheim; VCH, (1995)

[43] M. Saunders, *Journal of Computational Chemistry*, **10(2)**, 203-208 (1989)

[44] C. Karlsson; H. Wikstrom; D.W. Armstrong; D.K. Owens, *J. Chromatogr. A*, **897**, 349-363 (2000)

[45] W.B. Schweizer, *Structure Correlation*, H.-B. Bürgi; J.D. Dunitz, (eds) VCH, New York 1994, Vol. 1, p.370

[46] M. Saunders; K.N. Houk; Y.D. Wu; W.C. Still; M. Lipton; G. Chang and W.C. Guida, *J. Am. Chem. Soc.* **112**, 1419-1427 (1990)

[47] M. Lipton; W.C. Still, *J. Comput. Chem.* 343, 9 (1988)

[48] R.A. Dammkoehler; S.F.B. Karasek; G.R. Marshall, *J. Computer-Aided Molec. Design* **3**, 3 (1989)

[49] J.J. Gajewski and K.E. Gilbert, PCMODEL (Version 4.0), SERENA-SOFTWARE, Bloomington, IND, USA.

[50] J.J. Gajewski; K.E. Gilbert; J. Mckelvey, *Adv. Mol. Model.*, 2, 65-92 (1990)

[51] N.L. Allinger, *J. Am. Chem. Soc.,* **99**, 8127 (19**77**)

[52] W.H. Pirkle; D.J. Hoover. *"NMR Chiral Solvating Agent,"* Section 6-5.c, p. 231; *Top. Stereochem.,* **13**, 205 (1982)

[53] D.A.Lightner; J.E.Gurst, *"Organic conformational Analysis and Stereochemistry from Circular Dichroism Spectroscopy"*, A John Wiley & Sons, Inc. WILEY-VCH (2000)

[54] J. Otto; P. Argos; M.G. Rossmann, *Eur. J. Biochem.*, **109**, 325 (1980)

[55] B. Koppenhoefer; E. Bayer, *J. Chrom. Lib.*, **32**, 1 (1985)

[56] B. Christian; B. Koppenhoefer, (*unpublished paper)*

[57] G.N. Ramachandran; V. Sasisekharan, *Adv. Protein Chem.*, **23**, 263-438 (1968)

[58] R.W. Spencer, *Biotechnol. Bioeng. (Comb. Chem.)* **61**, 61-67 (1998)

[59] K.R. Oldenburg; J. Zhang; T. Chen; A. Maffa; K.F. Blom; A.P. Combs; T.D.Y. Chung, *J. Biomol. Screening*, **3 (1)**, 55-62 (1998)

[60] M. Greig, *Am. Lab. 31 (24),* 28-32 (1999)

[61] C. Brown(ed), *Chirality in Drug Design and Synthesis*, Academic Press, London, 1990

[62] S.C. Stinson, *Chem. Eng. News* **oct 9**, 44-74 (1995)

[63] B. Campbell, in: P. A. Barnacal (ed), *Pharmaceutical Biotechnology International 1996*, Sterling Publications, London, 1996, pp.27-30.

[64] C.C. Price; G.M. Gaucher; P. Koneru; R. Shibakawa; J.R. Sowa; M. Yamaguchi, *J. Ann. N.Y. Acad. Sci.*, **163**, 593 (1969)

[65] W.C.J. Ross, *J.Chem. Soc. (London)*, 2257 (1950)

[66] W.C.J. Ross, *J. Ann. N.Y. Acad. Sci.*, **68**, 669 (1958)

[67] M. Fuzy; P. Lelieveld; L.M.van Putten, *Eur.j.Cancer* **11**, 169 (1975)

[68] K. Gerzon; J.E. Cochran; L.A. White; R. Monahan; E.V. Krumkalns; R.E. Scroggs; J. Mills, *J.Med.Pharm.Chem.* **1**, 223 (1959)

[69] L. Nemeth; L. Institoris; S. Somfai; F. Gal; I. Palyi; J. Sugar; O. Csuca; Z. Szentirmay; B. Kellner, *Cancer Chemother, Rep.* **56**, 593 (1972)

[70] G. Atassi; F. Spreafico; P. Dumont; P. Nayer; J. Klastersky, *Eur.J.Cancer* **16**, 1561 (1980)

[71] A. Rosowsky, in: A. Weissberger, Ed., *"Heterocyclic compounds with three- and four membered rings"*, Interscience, New York (1964)

[72] G. Dittus, in: Houben-Weyl, 4th ed., *"Methoden der organischen Chemie"*, **Vol. 6/3,** pp. 371-487, Thieme, Stuttgart (1965)

[73] L. Sabstel; B. Zeik; O. Jolanta, *Arch Immunol Ther Exp,* **25,** 285 (1977)

[74] S. Laila and K.J. Mattila, *Psycopharmacologia,* **35**, 221 (1974)

[75] J.R. Dahlbon and B.L. Karlen, *Chem Abstr,* **82**, 139969 (1975)

[76] G. Weitzel and F. Schneider, *J. Phys. Chem.*, **336**, 107 (1964)

[77] P.E. Crass; R.P. Dickinson; G. Halliwell and J.E.G. Kemp, *Eur. J. Med. Chem. Chim. Ther.*, **12**, 173 (1977)

[78] R. Sandberg and K.E. Domeji, *Acta. Pharm. Sues.*, **16**, 386 (1979)

[79] L.R. Snyder and J.J. Kirkland, *"Introduction to Modern Liquid Chromatography,"* 2nd Ed. Wiley, New York, 1979

[80] J.C. Berridge, *Techniques for the Automated Optimization of HPLC Separation*, Wiley, New York (1985) pp. 10-27

[81] P.J. Schoenmarkers, *Optimization of Chromatographic Selectivity*, Elsevier, Amsterdam, (1986) Chapter 4

[82] http://www.daicel.co.jp/chiral/

[83] W.C. Still; M. Kahn; A. Mitra, *J. Org. Chem.* **43(14)**, 2923-2925 (1978)

[84] D.D. Perrin; W.L.F. Armarego, *Purification of Laboratory Chemicals.* 3rd Ed, Pergamon Press. Oxford, (1988)

[85] B.M. Khadilkar; S.R. Bhayade, *Indian J. Chem. Sect. B*, **32 (3)**, 338-342 (1993)

[86] M. Zakerinia; H. Davary; G.H. Hakimelahi, *Helv. Chim. Acta*, **74 (4)**, 912-915 (1990)

[87] B.R. Baker; M.V. Querry; A.F. Kadish; J.H. Williams, *J. Org. Chem.*, **17**, 35-42 (1952)

[88] N.I. Korotkikh; O.P. Shvaika, *Russ. J. Org. Chem.*, **32 (7)**, 1037-1046 (1996)

Appendix I. Energies and Parameters of all stable conformations in N-TFA-Phe-O-3'-pentyl ester

N-TFA-Phe-O-3'-pentyl ester, conformations

Force field energies and geometries with PCMODEL Version 4 (without Pi): files *.inp

files t*.inp	Rel. E	DHf	MMXE	Φ	Ψ	χ	C*COC_3	COC_3C_2	COC_3C_4	$OC_3C_2C_1$	$OC_3C_4C_5$	$C_1C_2C_3C_4$	$C_2C_3C_4C_5$	$C_FC_ONC^*$
	(Kcal/mol)											ω2,3	ω3,4	
0001.inp	0	-236.03	38.05	-72.5	115.7	-177.7	179.6	-138.4	99.7	58.7	-65.6	178.7	175	179.2
0002.inp	0.96	-235.08	39.01	-70.2	123.9	-176.3	-179.2	-147.7	87.9	61.8	62.2	-176.3	-59.3	179.6
0003.inp	0.89	-235.15	38.94	-68.1	123.8	-176.4	-178.9	-149	87.9	56.5	-174.2	176	66.1	179.8
0004.inp	3.59	-232.45	41.64	-67.3	133.1	-176.7	178.6	-142.5	90.3	-32	61.4	91.5	-62.4	179.7
0004a.inp	3.64	-232.4	41.69	-76.2	143.4	-178.1	177.8	-145.2	87.7	-61.1	32.3	63.2	-91.3	179
0005.inp	1.09	-234.95	39.14	-71.7	131.9	-178.4	178.2	-130.8	105	-56.5	-68.1	64.7	171.1	179.4
0006.inp	1.9	-234.13	39.95	-68.1	135.8	-178.6	-179.8	-131.8	102.7	-61	-179.2	59.7	60	179.8
0007.inp	3.63	-232.41	41.68	-67.1	131.6	-177	179.3	-149.7	86.4	176.6	-143.9	-63.6	97.1	179.6
0007a.inp	3.43	-232.6	41.48	-66.8	133.7	-177.4	176.5	-145.1	90.9	143.6	-178.1	-97.2	62.7	179.8
0008.inp	1.49	-234.55	39.54	-71.9	126.4	-178.4	176.1	-136.4	100.7	170.5	-63.3	-69.5	177.8	179.2
0009.inp	1.94	-234.1	39.99	-67.2	134.8	-177.6	180	-146.9	87.6	178	61.5	-61	-59.1	179.6
0010.inp	1.67	-234.37	39.72	-78.6	110.6	-179.5	178.1	61.2	-67.6	51.3	-58.5	178.1	174	178.7
0011.inp	4.48	-231.56	42.53	-76.6	126.6	-176.7	-179.9	52.3	-81.4	53.3	78.4	-175.4	-53.8	178.9
0012.inp	2.83	-233.21	40.88	-78.3	118.1	-178.9	176.7	62.3	-67.2	48.9	-168.4	175.2	64.2	179
0013.inp	9.18	-226.86	47.23	-66.7	119.3	177.9	177	76.8	-63.7	-53.8	97.9	83.9	-40	179.6
0013a.inp	9.42	-226.62	47.47	-66.4	132	-180	-173.7	57.9	-82.3	-105	57.7	32.1	-79.4	179.4
0014.inp	4.34	-231.7	42.39	-66.7	114.3	176	-175.4	78.5	-54.8	-66.7	-55.1	65.2	173.8	179.2
0015.inp	5.09	-230.94	43.14	-65	120.8	179.7	-176.4	79.7	-54.4	-70.8	-165.5	60.4	63.7	179
0016.inp	4.82	-231.22	42.87	-68.1	121.6	-179.6	-178.6	67.3	-62.2	171	-140	-63.3	94.6	179.9
0016a.inp	4.64	-231.4	42.69	-66.6	126.5	-178.5	-179.2	59.7	-69.9	140.5	-172.3	-94.2	61.9	179.6
0017.inp	2.73	-233.31	40.78	-68.4	117.7	-179.7	-177	61.4	-68	163.1	-58.2	-70.2	175.3	179.6
0018.inp	5.04	-231	43.09	-67.2	123.4	-179.8	-178.6	51.9	-82.5	166.3	80	-62.6	-51.6	179.9
0019.inp	1.4	-234.63	39.45	68	-28.2	-177.1	-178.7	-103.3	135.3	66.7	-59.8	-174.1	-179.6	177.5
0020.inp	2.74	-233.3	40.79	-66.2	-25.4	-176.3	179.3	-99	137.4	69.9	61	-169.7	-60	176.8
0021.inp	2.97	-233.07	41.02	-68.4	-24.4	-176.5	-179.4	-100.4	137	65.5	-170.9	-175.9	69.5	177.2
0022.inp	5.18	-230.86	43.23	-66.3	-30.7	-174.5	-179.2	-89.2	143.9	-64.4	31.1	59.3	-92.4	-178.9
0022a.inp	4.99	-231.05	43.04	-77.6	-34.3	-175.8	-177.3	-83.3	149.9	-30.4	64.2	92.8	-60	177.9
0023.inp	2.15	-233.89	40.2	-67.3	-33.4	-175	-178.5	-89	146.5	-60.4	-63.5	60.9	174.9	-178.9
0024.inp	3.21	-232.83	41.26	-66.9	-34.6	-175.1	-179.5	-86	148.5	-60.4	-178	57.2	60.7	-178.9
0025.inp	4.98	-231.06	43.03	-62.6	-31	-175.9	177.4	-89.4	146.9	178.7	-146.8	-62.3	94.6	178.7
0025a.inp	4.94	-231.1	42.99	-63.1	-32.1	-176.2	176.9	-86.7	149.7	144.6	-177.4	-96.7	63.2	178.5
0026.inp	2.27	-233.77	40.32	-61.5	-31.5	-176.1	177.8	-91.6	145.4	175	-57.8	-65.7	-176.9	178.5
0027.inp	3.23	-232.81	41.28	-60.2	-32.4	-176.9	176.5	-86	148.8	179.6	64	-59.8	-56.6	177.6
0028.inp	3.07	-232.97	41.12	-72	-22.8	-176.8	-177.3	66	-62.9	57.6	-54.2	-174.4	178.9	177.3
0029.inp	5.7	-230.34	43.75	-63.6	-25.6	-176.6	173.5	53.9	-79.5	54.4	68.3	-174.6	-63.7	178.8
0030.inp	4.05	-231.99	42.1	-65.7	-22.8	-176.1	-179.3	68.1	-61.4	56	-162.5	-177.3	71	179.1
0031.inp	10.34	-225.7	48.39	-70.3	-40.3	-178.6	178.5	53.8	-85.2	-107.6	54.4	27.9	-81.8	178.6
0031a.inp	10.73	-225.3	48.78	-62.7	-50	178.9	173.5	78.3	-62.5	-57.9	101.8	79.7	-36.2	179.3
0032.inp	5.64	-230.4	43.69	-70.9	-29.4	-178.3	-179.1	81.4	-52.2	-74.3	-53.5	58	175.3	178
0033.inp	6.31	-229.73	44.36	-63.3	-32.1	-177.8	179	81.8	-52.7	-77.9	-166.3	53.7	62.6	179.3
0034.inp	5.89	-230.15	43.94	-62.6	-30.6	-178.2	179.6	70	-59.5	172	-140.1	-62.3	94.8	179.2
0034a.inp	5.97	-230.07	44.02	-63.4	-28.6	-178.3	177.7	61.8	-67.8	140.4	-171	-94.2	63.1	179.2
0035.inp	3.88	-232.16	41.93	-73.5	-29.8	-178.2	-177.2	65.7	-63.9	167.5	-51.2	-65.1	-177.8	177.8
0036.inp	6.2	-229.84	44.25	-60.8	-31.4	179.9	176.6	53.7	-80.5	165.7	71.8	-63.5	-59.6	178.8
0037.inp	0.66	-235.37	38.71	-69.5	143.9	-179.4	-174.8	-98.8	139.8	73.4	-58.6	-168.1	-179.9	179.1
0038.inp	1.57	-234.47	39.62	-72.9	150.4	-177.5	-176.6	-95.2	141.6	72.6	61.5	-179.5	-59.8	179.4
0039.inp	2.04	-234	40.09	-71.4	141.3	-178.6	-175.6	-98.6	139	71.4	-169.4	-170	71	179.6
0040.inp	3.49	-232.55	41.54	-68.6	127	-178	-177.8	-89.6	143.4	-64.8	31.5	59.1	-92	179.7
0041.inp	0.65	-235.39	38.7	-70.1	124.5	-178.2	-179.5	-87.2	148.6	-62.3	-65	59.1	173.7	179.7
0042.inp	1.45	-234.59	39.5	-68.9	124.4	-178.2	-179.1	-87.3	147.2	-64.2	-177.9	56.8	60.8	179.8
0043.inp	3.5	-232.51	41.55	-68.8	134.5	179.6	179.5	-87.3	149.1	179.4	-147.1	-61.5	94.2	179.7
0043a.inp	3.64	-232.4	41.69	-69.1	133.2	178.8	-179.1	-85.1	151.3	145.6	-177.2	-95.6	63.1	179.7
0044.inp	0.98	-235.06	39.03	-69.4	135.4	179	-179.6	-88.9	148.1	176.1	-57.4	-64.4	-176.8	179.7
0045.inp	1.78	-234.26	39.83	-68.9	135.1	178.6	179.8	-85.2	149.7	179.5	64.5	-59.7	-56.5	179.6
0046.inp	2.95	-233.09	41	-71.9	142.2	-179.6	-173.1	67.8	-60.8	59.8	-51.6	-172.2	-178.4	179.7
0047.inp	4.53	-231.51	42.58	-76	139.6	-175.3	-179.2	53.2	-80.4	53.7	73	-174.9	-59	179.1
0048.inp	2.84	-233.19	40.89	78.4	130.5	-178.7	177.7	63.8	-65.8	51.1	-168.3	177.7	64.4	179.3
0049.inp	9.06	-226.97	47.11	-68.6	125.1	178.9	178.9	80.9	-58.6	-54.5	104.7	82.2	-31.8	179.3
0049a.inp	9.49	-226.55	47.54	-66.7	137.4	-178.4	-173.2	-59.6	-80.9	-103.7	58	33.8	-79.3	179.2
0050.inp	4.64	-231.4	42.69	-69.5	126.2	-178	-171.4	80.7	-52.2	-68.5	-53	63.6	176.4	179.2
0051.inp	5.11	-230.93	43.16	-66.9	128.4	-176.6	-176.3	81.4	-52.6	-70.6	-164.9	60.7	64.5	179.2
0052.inp	4.94	-231.1	42.99	-67.6	140.2	-177.6	-177.3	70.3	-58.8	171.8	-137.9	-62.2	97.1	179.1
0052a.inp	4.7	-231.33	42.75	-67.8	133.5	-178.6	-179.7	60.4	-69.2	140.6	-172.8	-94	61.3	179.6
0053.inp	2.71	-233.33	40.76	-66.8	117.4	179.5	-176.3	61.8	-67.7	164	-57.4	-69.3	176.1	179.2
0054.inp	5.08	-230.95	43.13	-69	137.6	-176.9	-179.2	53.4	-81	166.8	76.1	-62	-55.4	179.7
0055.inp	1.83	-234.11	39.88	-65.7	-56.3	171.3	176	-142.9	95.7	58.7	-72.4	178.9	168.5	178.9
0056.inp	2.5	-233.54	40.55	-63.5	-43.6	172	-179.9	-152.7	83.1	63.6	62.5	-175	-58.7	-179.9
0057.inp	2.17	-233.87	40.22	-64.4	-43.7	174	179.5	-152.4	84.6	56.4	-175.2	176.2	65	-179.8
0058.inp	4.74	-231.3	42.79	-61.7	-37.8	173.9	179.7	-145.6	87.4	-32.3	64	91.2	-59.9	178.6
0059.inp	2.67	-233.36	40.72	-59.5	-38.9	174.7	174.1	-136.7	99.5	-59.6	-72.7	61.8	167	176.9
0060.inp	2.98	-233.06	41.03	-58.9	-29.8	178.6	176	-144.9	89.5	-63.1	-179.9	57.9	59.3	176.8
0061.inp	4.89	-231.15	42.94	-63.3	-40.5	175	178.3	-153.7	82.5	176.7	-144.3	-63.2	96.6	178.2

0061a.inp	4.75	-231.29	42.8	-60.9	-39.7	175.6	178.1	-150.1	86.1	146.2	-179.2	-94.8	61.6	178.6
0062.inp	3.28	-232.76	41.33	-61.5	-48.2	174.7	174.5	-140.8	96.6	168.1	-71.9	-71.9	169.6	178.8
0063.inp	2.94	-233.1	40.99	-60.8	-36	175.7	179.7	-149.4	85.3	177.9	63.6	-60.9	-57.2	178.5
0064.inp	4.42	-231.62	42.47	-71.9	-67.2	172.2	171.7	58.2	-70.3	48	-56.2	174.4	175.5	178.5
0065.inp	6.23	-229.81	44.28	-66.8	-50.3	172.1	174.3	48.7	-84.1	50.8	67.1	-178.8	-65.2	177.9
0066.inp	4.58	-231.46	42.63	-59.8	-41	175.7	173.8	63.6	-66	50.5	-168	176.9	64.6	178.8
0067.inp	10.8	-225.23	48.85	-62.2	-49.7	173.7	-179.5	68.8	-73.3	-69.5	56.7	70.5	-83.5	179
0068.inp	5.37	-230.67	43.42	-69.1	-54	175.2	179.5	78.8	-54.9	-70.9	-53.5	61.1	174.9	178.8
0069.inp	6.19	-229.85	44.24	-60.2	-45.1	178	178.2	79.8	-54.7	-77.3	-167	54.2	61.6	179.7
0070.inp	6.08	-229.96	44.13	-61.4	-46.4	176.2	176.7	58.4	-70.8	139.3	-171.8	-95.8	62.2	179.3
0070a.inp	5.93	-230.1	43.98	-61.1	-42.6	176.8	179	68.4	-61.3	172.8	-140.2	-61.3	94.2	179.2
0071.inp	3.97	-232.07	42.02	-70.4	-49.2	176.1	179.8	62.6	-67	165.5	-53.1	-67.5	180	179.3
0072.inp	6.3	-229.74	44.35	-60.9	-43.4	174.7	177.7	50.7	-83.3	164.7	71.3	-65	-60.1	178.4
0073.inp	3.72	-232.32	41.77	-98.5	-124.3	-178	-175.9	-134.7	103.8	59.9	-59.4	179.5	-178.7	178.5
0074.inp	4.25	-231.79	42.3	-103.4	-126.5	-174.1	178.2	-153.9	82	61	52.8	-177.2	-68.5	178.5
0075.inp	4.8	-231.24	42.85	-102.5	-116.2	-177.3	-178.7	-153.5	83.8	55.1	-175.3	174.7	65.1	179.2
0076.inp	7.87	-228.16	45.92	-99.2	-126.3	-174.5	178.6	-152.7	79.6	-70.6	32.2	54.6	-92.5	178.6
0076a.inp	7.83	-228.21	45.88	-101.6	-110.8	-178.9	-176.7	-150.1	82.1	-33.8	64	91.2	-61.2	179.3
0077.inp	4.73	-231.31	42.78	-101.1	-112	176.5	-175.2	-134.5	101.4	-57.4	-67.6	64	171.2	179.4
0078.inp	5.05	-230.99	43.1	-92.9	-86.8	169.9	-175.6	-154.6	80.2	-63.3	-179.1	58	59.8	179.8
0079.inp	6.43	-229.6	44.48	-93.7	-92.8	176.7	-176.9	-157.7	79	176.7	-142.6	-63.3	98.4	179.9
0079a.inp	7.01	-229.03	45.06	-91.9	-100.7	174.9	-178.4	-156.1	80.5	145.8	-178.2	-95.1	62.8	179.2
0080.inp	4.38	-231.66	42.43	-94.4	-102.8	178.3	179.9	-138.8	98.5	173	-57.7	-66.7	-176.6	179.2
0081.inp	6.17	-229.87	44.22	-91.5	-92.6	176.7	174.7	-154.3	79.8	177.3	65.3	-60.1	-56.2	179.6
0082.inp	5.14	-230.89	43.19	-99.7	-115.3	-177.3	-179.6	62.5	-66.4	52.9	-52.9	179.9	179.7	178.4
0083.inp	7.65	-228.99	45.7	-95.2	-106.5	179.6	-177.6	48.8	-84.4	52.6	65	-176.5	-67	179.2
0084.inp	6.1	-229.94	44.15	-97.3	-112.4	-178.5	-179.7	62	-67.5	50.2	-167.2	176.7	65.5	178.8
0085.inp	13.24	-222.8	51.29	-97.3	-108.1	176.6	-174.2	52.3	-86.8	-107	53.1	28.7	-83.2	178.7
0085a.inp	11.02	-225.02	49.07	-73.6	-67	171.5	178.9	79.1	-60.9	-57.1	105.8	79.8	-31.2	179.3
0086.inp	8.95	-227.09	47	-102.9	-135.2	-175.9	-178	80.7	-52.9	-66.5	-51.8	65.5	177	178.2
0087.inp	8.67	-227.37	46.72	-92.7	-102.1	174.9	-173.9	80	-53.7	-65.9	-162.7	65.4	66.6	179.5
0088.inp	8.27	-227.77	46.32	-93.4	-100.2	177.9	-174.3	65.8	-63.8	170	-140.2	-64.1	94.4	179.6
0089.inp	5.88	-230.15	43.93	-91.4	-91.8	173.4	-175.7	61.8	-67.6	163.5	-50.4	-69.7	-176.9	179.1
0090.inp	9.25	-226.79	47.3	-97.2	-107.5	177	-172.8	48.3	-85.9	163.2	68.6	-65.8	-62.7	179
0091.inp	3.24	-232.8	41.29	-100.6	117.6	179.5	-179.8	-137.8	100.6	58.9	-63.1	178.8	177.4	-0.6
0092.inp	5.44	-230.6	43.49	-73.2	128.4	-175.1	175.5	-147.2	88.5	62.3	67	-175.4	-54.9	2.8
0093.inp	4.06	-231.98	42.11	-92.4	127.8	179.6	179.3	-153	84.2	57.1	-173	176.9	67.2	0.3
0094.inp	6.74	-229.3	44.79	-87.5	140	179.7	176.7	-141.2	90.9	-35.8	67	88.6	-57.6	0.7
0095.inp	4.25	-231.79	42.3	-96.1	134.9	179	177.1	-132.7	103.3	-57.1	-69.8	64.1	169.5	-0.4
0096.inp	4.84	-231.19	42.89	-90.4	140.9	179.8	179.9	-137.8	96.6	-61.6	-179.5	59.3	59.7	0.5
0097.inp	6.66	-229.38	44.71	-91.9	135.9	-179.2	176.5	-151.4	84.6	176.2	-144.2	-63.8	96.8	0.1
0097a.inp	6.36	-229.68	44.41	-89.7	138.1	-179.2	175.1	-147.3	88.8	143.1	-178.1	-97.6	62.6	0.4
0098.inp	4.67	-231.37	42.72	-96.3	129.5	179.3	175.2	-137.3	99.9	169.7	-64	-70.3	177.2	-0.5
0099.inp	5.11	-230.93	43.16	-91.1	142.3	-179.7	177.5	-144.7	89.7	177.5	66.5	-61	-54.6	1.2
0100.inp	4.84	-231.2	42.89	-106.4	110.6	176.7	178.8	61.5	-67.3	51.5	-57.9	178.2	174.9	-0.9
0101.inp	7.62	-228.42	45.67	-100.5	123.7	177.4	178.2	51.8	-81.8	52.5	79.9	-176.5	-52.2	-0.6
0102.inp	5.97	-230.07	44.02	-103.1	120.4	176.4	175.3	62.1	-67.4	47.9	-169.1	174.1	63.6	-0.9
0103.inp	12.52	-223.52	50.57	-92.5	125.4	175.7	176.1	74.6	-66.5	-53	90.9	85.6	-48	0.4
0103a.inp	12.6	-223.44	50.65	-91.5	137.3	178.1	-176.1	57.6	-82.5	-105.9	58.3	31	-78.7	0
0104.inp	7.94	-228.1	45.99	-103.7	111.2	174.5	-178.6	78.8	-54.7	-68	-56.2	63.9	172.5	-0.2
0105.inp	8.35	-227.68	46.4	-92.8	129	177.2	179.9	80.5	-53.7	-70.8	-166.9	60.6	62.1	0.2
0106.inp	7.83	-228.21	45.88	-94.9	126.9	177.2	177	58.9	-70.5	140.6	-172.7	-94.5	61.5	0.4
0106a.inp	8.08	-227.96	46.13	-96.2	125.3	175.8	179.2	67.5	-62.1	171.4	-139.9	-63.2	94.6	0.4
0107.inp	6.04	-230	44.09	-100.3	116.1	176.6	179	59.8	-69.6	160.9	-60.1	-72.8	173.3	0
0108.inp	8.05	-227.99	46.1	-91.1	135.7	179.3	179.3	52.3	-82	166.4	77.5	-62.6	-54	0.7
0109.inp	7.91	-228.13	45.96	-118.2	99.4	-177.8	-4.6	-125.1	113.8	64.1	-62.3	-176.6	178.9	179.6
0110.inp	8.6	-227.44	46.65	-110.9	111.3	-177.1	-6.4	-147.6	89.1	63	48.8	-175.4	-71.6	179.7
0111.inp	8.85	-227.19	46.9	-108.9	111.4	-176.8	-5.3	-145.9	91.6	60.4	-168.2	-179.9	72.4	179.4
0112.inp	11.11	-224.93	49.16	-111.4	109.7	-177.6	-4	-145.3	88.3	-65.3	31.8	58.7	-91.3	179.9
0112a.inp	11.88	-224.15	49.93	-105.1	115.6	-176.3	-7.4	-145.8	87.9	-33.3	56.1	90.7	-67.5	179.9
0113.inp	9.87	-226.17	47.92	-111.4	103.2	-178.1	-6.1	-120.2	115.9	-59.1	-64.5	61.2	174.8	180
0114.inp	10.24	-225.8	48.29	-122	101.6	-177.7	-4.2	-143.5	91.3	-65.4	-176.5	55.8	62.5	-179.4
0115.inp	10.34	-225.69	48.39	-108.9	112.1	-176.3	-4	-150.5	86.6	176.2	-141	-64	100	179.8
0115a.inp	11.29	-224.75	49.34	-107.8	112.7	-176.8	-6.1	-145	91.7	145.1	-175.9	-95.8	64.9	179.7
0116.inp	9.25	-226.79	47.3	-103.4	104.6	-177.3	-5.5	-115.4	121.6	171.4	-60.9	-69.2	-179.7	179.2
0117.inp	9.44	-226.59	47.49	-106.6	114.3	-176.1	-6.2	-147.9	87.6	176.1	56	-62.5	-64.3	179.9
0118.inp	10.62	-225.42	48.67	-150.9	104.5	179.3	-1	73.6	-61.1	47.1	-46	-175.4	-179.1	179.6
0119.inp	15.96	-220.08	54.01	-159.1	115.4	179.1	-1.3	63.3	-78.3	55.8	80.8	-164.3	-59.4	-178.2
0120.inp	11.65	-224.39	49.7	-151.2	107.8	179.4	-0.5	73.3	-61.9	47.6	-158.7	-179.6	68.5	-179.1
0121.inp	19.38	-216.66	57.43	-155.1	117.9	-176.4	-1.5	60.4	-84.6	-127.7	59.8	14.2	-82.5	-179.4
0122.inp	15.66	-220.38	53.71	-151.7	96.6	-176.7	-0.7	90.8	-48.8	-68.5	-52.7	70.5	169.5	179.6
0123.inp	16.02	-220.02	54.07	-152.7	94.2	-175.6	0.2	93.9	-44.6	-65.3	-152.9	72	71.3	-179.7
0124.inp	13.49	-222.55	51.54	-145.9	110.9	-179.3	-2.5	67.8	-66.6	131.8	-168.2	-97.3	60.5	-179.1
0124a.inp	13.54	-222.5	51.59	-146.2	111.6	-179.5	-1	75.3	-58.9	165.2	-130.6	-63.5	98.6	-179
0125.inp	12	-224.04	50.05	-146.8	108.7	178.8	-1.3	72.6	-62.4	157.1	-43.9	-69.8	-176.5	179.7
0126.inp	15.79	-220.24	53.84	-154.2	122.1	-178.4	-3.1	58	-82.5	154.8	73.8	-67.2	-65	-178.9
0127.inp	1.59	-234.45	39.64	-74.5	114.5	-60.6	-179.6	-137.3	101	60.6	-65.2	-179.5	175.4	179.6
0128.inp	2.53	-233.51	40.58	-72.2	123.1	-59.3	-177.9	-146	89.7	64.4	62.4	-174.3	-58.9	-179.7
0129.inp	2.55	-233.49	40.6	-70.1	123.5	-58.7	-177.7	-145.9	91	58.3	-174	177.7	66.4	-179.7

0130.inp	5.37	-230.67	43.42	-71.9	123.3	-58.7	-179.1	-145.9	87	-31.9	64.3	91.7	-59.7	-179.5
0130a.inp	5.2	-230.83	43.25	-86.6	126.8	-58.4	179.1	-152.5	80.7	-64.5	29.5	59.6	-93.9	-179.6
0131.inp	2.74	-233.3	40.79	-73.1	119	-58.8	-178.7	-136.8	99.2	-61.5	-68.6	59.8	170.5	179.9
0132.inp	3.46	-232.58	41.51	-69.2	125.2	-58.3	-176.4	-146.8	87.7	-64.8	-178.9	56.3	59.9	-179.7
0133.inp	4.86	-231.17	42.91	-68.2	122.9	-58.4	-176.3	-149.4	86.9	146.9	-178.4	-94.4	62.3	-179.8
0133a.inp	4.77	-231.27	42.82	-69.5	123.6	-58.5	-176.3	-151.4	85	177.3	-143.7	-63.2	97.2	-179.8
0134.inp	2.66	-233.37	40.71	-74	117	-58.3	179.6	-137.9	99.3	170.9	-63.6	-69.2	177.4	179.8
0135.inp	3.19	-232.65	41.24	-71	125.5	-57.7	-177	-147.3	87.3	178.2	64.5	-60.6	-56.5	-179.5
0136.inp	3.15	-232.89	41.2	-81.1	116	-59.3	179	63.5	-65.1	53.1	-52.9	-179.9	179.9	-179.4
0137.inp	5.64	-230.4	43.69	-79	124.9	-56.9	-179.1	51	-82.2	51.7	66	-177.3	-65.9	-179.6
0138.inp	4.05	-231.98	42.1	-80.8	120	-57.4	177.9	62.6	-66.8	49.1	-167.8	175.5	64.9	-179.9
0139.inp	10.4	-225.64	48.45	-68.2	126.6	-57.2	-175.7	55.3	-83.9	-106.7	53.5	29.2	-82.7	-179.8
0139a.inp	10.19	-225.85	48.24	-71.4	117.2	-58.4	-178.1	81.5	-57.7	-54.6	107.5	81.6	-28.3	180
0140.inp	5.45	-230.59	43.5	-68	118.8	-58.6	-177.1	79.6	-53.7	-65.9	-51.7	65.8	177.3	179.9
0141.inp	6.14	-229.9	44.19	-67.5	120.8	-58	-174.1	80.2	-53.8	-70.8	-169.2	60.5	64.2	179.5
0142.inp	6.04	-229.99	44.09	-74.2	121.8	-56.7	-178.1	67.6	-61.9	171.1	-140.2	-63.1	94.4	-178.8
0142a.inp	5.99	-230.04	44.04	-70.3	126.2	-57.7	-176.7	60	-69.5	140.2	-171.3	-94.4	62.9	-179.7
0143.inp	3.98	-232.06	42.03	-71.6	123.1	-56.1	-177.9	64.2	-65.3	166.5	-50.4	-66.6	-176.9	-179.3
0144.inp	6.53	-229.51	44.58	-69.6	129.7	-55.1	-177.4	51.9	-82.2	165.5	71.3	-63.5	-60	-179.8
0145.inp	1.84	-234.2	39.89	-72.7	-5.3	-59.6	177.8	-102	136.5	64.4	-60.5	-176.5	179.9	178.2
0146.inp	2.68	-233.36	40.73	-71.8	-4.4	-60.9	176	-98.6	137.8	67	59.3	-172.5	-61.6	177.8
0147.inp	3	-233.04	41.05	-73.4	-3.5	-60.4	177.1	-100.2	137.2	62.2	-172.2	-179.1	68.3	178.3
0148.inp	4.99	-231.05	43.04	-76	-7.9	-60.5	179.9	-90.6	142.5	-64.7	31.5	58.9	-92	178
0148a.inp	4.78	-231.26	42.83	-82.1	-11.1	-60.1	-179.3	-82.1	151.5	-28.9	63.4	94	-60.6	177
0149.inp	2.55	-233.49	40.6	-77.3	-10.2	-60.1	-179.7	-89.1	146.6	-60.9	-63.8	60.3	174.7	178.7
0150.inp	3.3	-232.74	41.35	-76.9	-11.6	-59.4	179.1	-85.6	149	-64.2	-178.3	56.8	60.3	179.1
0151.inp	5.14	-230.9	43.19	-69.6	-11.7	-59.6	174.8	-88.4	148.1	178.6	-147.3	-62.3	94.3	179.1
0151a.inp	5.02	-231.02	43.07	-68.8	-14	-59.6	175.3	-84.2	152.4	143.9	-177.5	-97.3	63.1	179
0152.inp	2.7	-233.34	40.75	-68.8	-12.5	-59.7	175.9	-88.9	148.4	174.5	-58	-66.3	-177	178.7
0153.inp	3.17	-232.87	41.22	-67.5	-14.7	-59.8	174.9	-83.7	151.2	179.7	63.2	-59.6	-57.5	178.4
0154.inp	3.42	-232.62	41.47	-78.8	-6.5	-58.8	-179.2	65.1	-63.8	53.1	-53.4	-179.5	179.5	179
0155.inp	6.11	-229.93	44.16	-69.7	-10.5	-61.7	174	53.4	-79.8	51.4	65.7	-177.7	-66.2	179.6
0156.inp	4.42	-231.61	42.47	-70.2	-12.5	-61.7	176.2	65.6	-63.9	50.2	-166.2	176.7	66.8	179.8
0157.inp	10.77	-225.27	48.82	-72.6	-7.8	-58.3	175.7	56.6	-82.4	-108.2	53.8	27.2	-82.3	179.8
0157a.inp	10.94	-225.1	48.99	-70.7	-12.5	-60.9	177.2	85.3	-53.7	-53.3	107.6	82.9	-28	180
0158.inp	6.04	-229.99	44.09	-73.7	-9.7	-58.7	-179.7	83.1	-50.1	-65.2	-51.7	66.8	177.3	179.8
0159.inp	7.06	-228.98	45.11	-74.8	-8	-59	-179.4	84.3	-49.6	-68.5	-163.2	62.8	66.3	-179.9
0160.inp	6.56	-229.48	44.61	-73.3	-6.8	-59.6	178.4	70.9	-58.6	171.8	-140.2	-62.3	94.6	180
0160a.inp	6.51	-229.52	44.56	-74.4	-5.5	-58	177.2	62.3	-67.3	139.9	-170.9	-94.6	63.1	-179.9
0161.inp	4.44	-231.6	42.49	-77.3	-3.3	-59.1	-179.4	67.2	-62.4	167.8	-49.2	-64.8	-175.8	179.1
0162.inp	7.12	-228.91	45.17	-77	-0.6	-59.1	176.4	55	-79.3	166.1	72.4	-62.8	-59.2	-179.8
0163.inp	1.68	-234.36	39.73	-71.8	142.6	-57.7	-179.5	-104.5	133.6	62.6	-60.6	-177.9	179.5	179.7
0164.inp	3.3	-232.74	41.35	-77.3	153.7	-57.6	178	-106.3	129.4	65.3	60	-173.5	-61.2	-179.9
0165.inp	3.07	-232.97	41.12	-77	152.6	-57.6	179.1	-104.1	132.9	59.8	-173.1	179	67.2	-179.9
0166.inp	5.83	-230.21	43.88	-76.5	146.8	-58.3	177.6	-94.3	139	-61.8	30.2	61.8	-92.7	-179.6
0166a.inp	5.25	-230.79	43.3	-73.7	138.3	-58.4	-179.4	-82.8	150.3	-30.9	64.8	92.5	-59.4	-179.6
0167.inp	2.72	-233.32	40.77	-75.1	142.9	-58.8	178.1	-90.6	145.2	-56.6	-63.5	64.4	175.4	-179.4
0168.inp	3.54	-232.5	41.59	-74.8	141.4	-59.2	177.4	-86	148.8	-61	-178.5	59.8	60.6	-179.4
0169.inp	5.27	-230.77	43.32	-76	145.6	-58.1	177.8	-90.3	145.9	178.4	-147.3	-62.4	94.1	-179.6
0169a.inp	5.05	-230.99	43.1	-73.8	141.7	-58.5	179	-84.9	151.5	143.2	-177	-97.7	63.3	-179.6
0170.inp	2.76	-233.28	40.81	-74.5	144.4	-58.1	179	-91.4	145.5	174.3	-58.1	-66.2	-177.4	-179.6
0171.inp	3.77	-232.27	41.82	-74	142.4	-58.3	178.6	-86.5	148	179.1	64.7	-59.8	-56.4	-179.7
0172inp	3.16	-232.87	41.21	-74	146.3	-57	-179.6	65.3	-63.4	54.9	-52.9	-177.9	-179.9	179.5
0173.inp	5.95	-230.09	44	-74.7	153.8	-57.5	179.9	52.8	-80.5	52.2	66.5	-176.7	-65.2	179.5
0174.inp	4.22	-231.81	42.27	-74.9	152.5	-57.6	-178.9	65.6	-63.8	51.8	-164.8	178.4	68.4	179.8
0175.inp	10.44	-225.59	48.49	-73.8	142.5	-58.5	178.4	83.4	-55.8	-53.7	107	82.5	-28.8	-179.9
0175a.inp	10.56	-225.48	48.61	-71.3	146.8	-58.6	-179	56.4	-82.7	-107	53.6	28.7	-82.5	179.7
0176.inp	5.66	-230.38	43.71	-72.3	145.4	-57.4	-177.8	82.1	-51	-65.5	-51.8	66.3	177.4	179.6
0177.inp	6.46	-229.57	44.51	-71.2	145.2	-57.7	-177.6	83.2	-50.5	-68.8	-163.4	62.4	66.2	179.4
0178.inp	6.25	-229.78	44.3	-73.2	148.6	-56.7	-178.8	69.8	-59.5	171.9	-140.1	-62.4	94.8	179.9
0178a.inp	6.17	-229.87	44.22	-71.7	144.9	-57.7	-179.4	61.3	-68.2	140.1	-171	-94.4	63.2	-179.9
0179.inp	4.15	-231.89	42.2	-72.2	147.2	-56.9	-178.3	66.5	-63	167.7	-49.6	-65.1	-176	179.7
0180.inp	6.78	-229.26	44.83	-74.1	150.1	-55.6	179.2	53.6	-80.6	166.3	72.1	-62.7	-59.3	179.9
0181.inp	1.66	-234.38	39.71	-70.3	-36.1	-58.1	-178.2	-135.8	102.6	63	-62.7	-177.4	177.9	180
0182.inp	2.49	-233.55	40.54	-68.3	-35	-57.7	-177.8	-149.9	86.1	64.7	57.8	-174.2	-63.2	-179.3
0183.inp	2.64	-233.4	40.69	-69.5	-34.1	-57.3	-177.6	-149	88.1	59.5	-173.6	178.8	66.8	-178.8
0184.inp	4.9	-231.15	42.95	-67.5	-27.5	-56.5	178	-147.9	85.4	-63	29.9	60.9	-92.9	178
0184a.inp	5.18	-230.86	43.23	-68	-28.6	-56.1	178.5	-148.4	84.5	-33.8	60.8	89.9	-63.2	-179.9
0185.inp	2.54	-233.5	40.59	-62.7	-32.7	-57.6	176.8	-133.9	102.1	-59.7	-65.7	61.9	173.8	178.2
0186.inp	3.22	-232.82	41.27	-63.2	-27.1	-56.7	178.1	-139.2	95.4	-63.1	-179.5	57.5	60.1	177.6
0187.inp	5.05	-230.99	43.1	-67.5	-30.8	-56.5	-179.8	-150	86.3	177.1	-144.2	-63.3	97	179.4
0187a.inp	5.03	-231.01	43.08	-65	-28.1	56.5	178.1	-146.9	89.3	146.5	-178.6	-94.7	62.4	-179.9
0188.inp	2.85	-233.19	40.9	-63.7	-34.9	-58	178.1	-135.4	101.7	172.5	-59.6	-67.7	-178.5	179.2
0189.inp	3.38	-232.66	41.43	-64	-26.8	-57	-177.7	-144.8	90	178.5	60.9	-60.8	-59.4	178.4
0190.inp	3.24	-232.8	41.29	-72.5	-38.3	-58.3	-179.9	62.6	-66.3	52.9	-55.8	-179.9	176.8	179.2
0191.inp	5.87	-230.17	43.92	-65.2	-38.1	-59	178	50.8	-82.5	51.8	66.5	-177.3	-65.4	179.5
0192.inp	4.28	-231.76	42.33	-63.3	-37.2	-59.2	177.9	63	-66.6	49.6	-167.5	176	65.2	179.9
0193.inp	10.72	-225.32	48.77	-69.1	-33.5	-60.7	-179.8	54.7	-84.4	-108	54.5	27.7	-81.8	179.4
0193a.inp	10.87	-225.17	48.92	-63.8	-37.8	-59.1	178.7	82.3	-56.9	-53.7	106.9	82.5	-29	180

0194.inp	6.14	-229.9	44.19	-72.2	-44.8	-59.9	-179.7	79.4	-54.1	-67.5	-53.1	64.4	175.5	179.4
0195.inp	6.93	-229.11	44.98	-63.8	-35.5	-60.5	178.4	80.9	-53.5	-72.5	-166.2	58.9	62.7	-179.9
0196.inp	6.41	-229.63	44.46	-64.1	-37.3	-57.7	178.6	67.9	-61.8	170.9	-140.2	-63.3	94.2	179.9
0196a.inp	6.3	-229.74	44.35	-64.1	-31	-56.9	179.1	60.6	-68.9	139	-171.2	-94.8	62.9	179.9
0197.inp	4.26	-231.78	42.31	-73.9	-38.3	-58.4	-179.8	62.4	-67.2	163.6	-54.3	-69.5	179	179.4
0198.inp	6.56	-229.48	44.61	-63.5	-26.4	-58.7	176.8	52.8	-81.3	164.8	70.6	-64.5	-60.8	179.7
0199.inp	4.48	-231.56	42.53	-98.2	-115.6	-58.3	179	-107.9	130.2	61.6	-60.8	-179	179.5	-179.5
0200.inp	5.6	-230.44	43.65	-97.3	-120.4	-59	179.2	-104.3	131.5	65.1	60.4	-173.9	-60.9	-179.9
0201.inp	5.41	-230.63	43.46	-102.8	-127.1	-58.6	178.5	-102.6	134.5	58.1	-173.5	177.3	66.8	-179.7
0202.inp	8.11	-227.93	46.16	-97.7	-122.1	-57	178.7	-83.4	150	-61	31.2	62.8	-92.2	-179
0201a.inp	7.54	-228.5	45.59	-99.2	-126.8	-56.5	177.2	-78.9	154.7	-30.2	64.2	92.8	-59.5	-179.3
0203.inp	5.23	-230.81	43.28	-100.5	-123.9	-56.8	179.3	-82.7	153.4	-54.7	-63.1	66.3	175.7	-178.9
0204.inp	5.99	-230.05	44.04	-103.5	-124.2	-57.1	178.7	-81.6	153.2	-60.1	-178.1	60.5	60.8	-178.8
0205.inp	7.6	-228.44	45.65	-106	-130.2	-54.8	178.6	-85.7	150.7	178.7	-146.7	-62.2	94.5	-178.9
0205a.inp	7.06	-228.98	45.11	-136.7	-122.5	-56.6	179.4	-82.2	154.3	142.9	-176.7	-98.1	63.4	-176.6
0206.inp	5.18	-230.85	43.23	-107.2	-132	55	179.6	-86.4	150.7	174.3	-57.7	-66.2	-177.2	-178.8
0207.inp	5.92	-230.12	43.97	-106.6	-136.9	-55.1	178.6	-82.6	152.2	179.5	64.7	-59.5	-56.5	-179.1
0208.inp	5.96	-230.08	44.01	-102.3	-121	-58.9	179.3	65.1	-63.8	51.5	-52.5	-179.3	-179.7	-179.4
0209.inp	8.69	-227.35	46.74	-102.3	-106	-62.1	179.3	51.4	-82	52.1	66.1	-176.7	-65.9	-179.4
0210.inp	6.88	-229.15	44.93	-106.5	-117.6	-60	-178.3	64.8	-64.8	51.1	-165.4	178	67.7	-178.9
0211.inp	13.3	-222.74	51.35	-104.1	-105.9	-62.1	178.2	54.1	-84.7	-108.5	53	26.8	-83	-179.4
0211a.inp	12.73	-223.31	50.78	-136.7	-135.5	-56.4	179.9	85.5	-53.4	-53.4	108.3	82.7	-27	-177.3
0212.inp	8.73	-227.31	46.78	-103.4	-111.3	-61	-178.2	81.5	-51.8	-66.5	-51.5	65.6	177.4	-178.4
0213.inp	9.49	-226.55	47.54	-105.7	-111.1	-60.8	-177.9	82.1	-52	-71	-164.3	60.5	64.8	-178.4
0214.inp	8.89	-227.15	46.94	-108.1	-114.9	-59.7	-179.3	69.3	-60.2	171.7	-140	-62.4	94.7	-178.3
0214a.inp	8.46	-227.58	46.51	-137.7	-113.7	-62.9	-179.6	60.7	-68.9	139.9	-171	-94.6	63	-177.3
0215.inp	6.94	-229.1	44.99	-94.2	-111	-60.7	178.2	65.3	-64.3	155	-49.9	-67	-176.7	-179.5
0216.inp	9.4	-226.64	47.45	-112.4	-105.7	-64.5	-179.2	52.1	-82.2	165.1	70.8	-63.8	-60.7	-178.7
0217.inp	2.36	-233.68	40.41	-95.1	57	-59.9	-178.7	-129.8	108.5	60.9	-60.5	-179.7	-179.8	178.5
0218.inp	2.96	-233.08	41.01	-97.8	68.8	-58.4	-178.7	-146.3	89.6	63.5	56.1	-175.4	-64.8	180
0219.inp	3.4	-232.64	41.45	-98.7	68.7	-58	-179.9	-144.7	92.3	58	-174.1	177.3	66.5	-179.4
0220.inp	5.03	-230.97	43.08	-97	71.4	-57.9	-177.9	-148.5	85	-64.2	29.9	59.4	-93	179.2
0220a.inp	5.55	-230.49	43.6	-97.1	69.3	-58.1	-179.5	-145.4	88	-30.5	61.6	92.5	-62.4	-179.9
0221.inp	3.34	-232.7	41.39	-98.6	60.3	-59.3	-179.7	-133	103	-60.3	-64.9	60.8	174.2	179.5
0222.inp	4.07	-231.97	42.12	-98.6	66.2	-58.7	-178.1	-142.5	92.1	-64.1	-179.3	56.7	59.8	179.8
0223.inp	5.63	-230.41	43.68	-99	70.2	-58.1	-179	-148.3	88.1	177.3	-144.2	-63.3	97	-179.4
0223a.inp	5.74	-230.3	43.79	-99.2	69.4	-58.1	179.5	-146.1	90.2	146.5	-178.6	-94.7	62.3	-179.1
0224.inp	3.33	-232.7	41.38	-100	60.6	-59.5	-179.4	-132.4	104.8	173.4	-57.8	-67.1	-176.8	179.8
0225.inp	3.73	-232.31	41.78	-99.9	70.5	-57.6	-177.3	-145.2	89.6	178.7	61.4	-60.5	-59.2	-178.9
0226.inp	3.74	-232.3	41.79	-96.6	65.1	-58	-176.3	64.5	-64.4	53.2	-53.5	-179.5	179.6	178.7
0227.inp	6.6	-229.44	44.65	-101.7	63.7	-59.4	179.3	51.8	-81.6	52	66.4	-176.9	-65.5	-179.8
0228.inp	4.63	-231.41	42.68	-102.2	60.6	-60.1	-179.3	64.3	-65.2	50.3	-166.8	176.9	66.3	179.8
0229.inp	11.53	-224.51	49.58	-101.3	64.3	-58.7	176.6	53.9	-84.6	-108.2	53.1	26.9	-82.7	-178.8
0229a.inp	11.39	-224.65	49.44	-102.6	49.7	-59.8	-179.8	83.9	-55.1	-53.3	107.5	82.8	-28	-179.4
0230.inp	6.81	-229.06	44.86	-100.3	62.7	-62.3	178.7	81.3	-52.1	-66.6	-52.5	65.2	176.3	-179.5
0231.inp	7.41	-228.63	45.46	-99.2	67.1	-61.8	-179.2	81.6	-52.5	-71.3	-165.5	63.7	60	-179.7
0232.inp	7.02	-229.01	45.07	-101.3	56.4	-60.3	179.4	68.8	-60.7	171	-140.3	-63.1	94.3	-179.2
0232a.inp	6.97	-229.07	45.02	-103.6	62.2	-59	-179.5	60.6	-68.9	139.8	-171.3	-94.8	62.9	-179
0233.inp	4.11	-230.93	42.16	-100.2	53.1	-60.9	176.3	65	-64.5	165.6	-51.3	-67.6	-178.1	-179.5
0234.inp	7.52	-228.52	45.57	-103.4	62.5	-58.6	178.2	52.1	-82	164.6	71	-64.6	-60.4	-178.9
0235.inp	4.54	-231.5	42.59	-104.1	116.8	-59.4	-178.6	-133.7	104.5	60.9	-62.8	-179.4	177.7	0
0236.inp	5.8	-230.24	43.85	-95.2	137.8	-56.5	178.9	-143.1	92.2	64.1	66.4	-174.1	-55.1	1.4
0237.inp	5.58	-230.45	43.63	-96.5	126.7	-58.7	-179.7	-150	87	58	-173.5	177.6	66.9	0.4
0238.inp	8.54	-227.5	46.59	-94.3	138.1	-57.6	178.8	-138.8	93.8	-32.3	66.9	91.6	-57.2	1.2
0238a.inp	8.26	-227.78	46.31	-120.6	140.1	-60.8	-179.5	-149.2	84	-64.6	29.7	59.4	-93.6	2
0239.inp	5.86	-230.18	43.91	-100.7	133.5	-58.9	179.1	-133.2	102.6	-61	-68.6	60.4	170.4	0.5
0240.inp	6.54	-229.5	44.59	-96.4	138.2	-58.2	-178.1	-142	92.3	-64.6	-179	56.5	59.9	1.2
0241.inp	7.81	-228.22	45.86	-98.8	127.7	-59.4	-178.9	-151.3	85.1	177.1	-144.3	-63.2	96.7	0.7
0241a.inp	7.93	-228.11	45.98	-99.2	127.1	-59.4	-179.7	-148.3	87.9	146.2	-178.1	-94.9	62.6	1
0242.inp	5.58	-230.45	43.63	-104.4	118.8	-60.4	-179.8	-135.8	101.4	172.5	-60.1	-67.8	-179.1	0.1
0243.inp	6.53	-229.51	44.58	-113.5	124.7	-60.8	-179.4	-139.6	94.7	178.2	65.7	-60.4	-55.4	1.1
0244.inp	6.01	-230.03	44.06	-107.6	112.7	-61.7	-179.9	63.4	-65.3	51.6	-53.1	178.6	179.8	-0.4
0245.inp	8.76	-227.28	46.81	-102.9	133.1	-56.6	176.6	51.1	-81.8	51.1	65	-178.3	-66.8	0.8
0246.inp	6.9	-229.14	44.95	-109.4	116.4	-60	179.3	63.2	-66.2	48.9	-167.4	175.4	65.5	0.4
0247.inp	13.3	-222.74	51.35	-102	122.8	-58.9	-178.7	82.6	-56.4	-53.3	107.3	82.7	-28.2	0.9
0247a.inp	13.46	-222.58	51.51	-95.6	136.7	-58.1	-177.4	55.7	83.4	-106.9	53.5	28.9	-82.7	1
0248.inp	8.73	-227.31	46.78	-106.4	121.1	-58.9	179.8	80.8	-52.5	-65.9	-51.9	65.9	177	1.2
0249.inp	9.54	-226.49	47.59	-104.2	120.1	-55	-177.1	80.9	-53.1	-70.2	-165.2	61.1	64.1	0.8
0250.inp	9.12	-226.92	47.17	-109.3	113.9	-61.5	-179.2	68.2	-61.3	171	-140	-63.2	94.7	0.8
0250a.inp	9.11	-226.9	47.16	-107.7	118.8	-60.7	-177.5	60.4	-69.2	139.9	-171.2	-94.6	63	0.9
0251.inp	7.13	-228.91	45.18	-110.8	111.7	-61.3	178.3	64.3	-65.2	165.3	-51	-67.9	-177.6	0.7
0252.inp	9.62	-226.42	47.67	-113.6	122.5	-59.2	178	51.7	-82.2	164.6	70.6	-64.7	-60.8	1.6
0253.inp	9.02	-227.02	47.07	-90.8	118.9	-64.6	-4.9	-133.9	106	63.5	-62.5	-177.3	179.2	-179.2
0254.inp	9.28	-226.76	47.33	-80	122.3	-57.3	-2.9	-150.6	85.7	64.8	55.3	-173.8	-65.4	-179.2
0255.inp	9.04	-227	47.09	-77.9	122.9	-57.6	-3.6	-150.3	87	60.4	-170.5	-180	70.2	-179.3
0256.inp	12.66	-223.38	50.71	-79.1	123.3	-58.8	-3.7	-148.8	84.7	-32.1	61.4	91.6	-62.3	-179.2
0256a.inp	11.79	-224.25	49.84	-78.1	124.5	-58.1	-2.7	-151.9	81.7	-65.4	30.9	58.8	-92.2	-179.3
0257.inp	10.3	-225.73	48.35	-77.8	119.8	-61.1	-4.5	-126.9	109.5	-60.4	-65.5	60.7	173.9	-179.4
0258.inp	10.26	-225.78	48.31	-75.6	122.9	-59.1	-2.8	-150.2	84.6	-65.7	-177.9	55.7	61.1	-179.2

0259.inp	10.83	-225.21	48.88	-77.4	124.7	-59.5	-4.5	-154.8	82	176.7	-144.1	-63.3	97.1	-179.2
0259a.inp	11.45	-224.59	49.5	-76	124.7	-60	4.3	-150.9	85.8	145.4	-177	-95.4	63.8	-179.4
0260.inp	9.82	-226.22	47.87	-80.9	117.8	-62.1	-4.7	-128.2	109.3	171.6	-60.2	-68.8	-178.8	-179.2
0261.inp	10.2	-225.84	48.25	-77.9	123	-56.8	-2.8	-150.6	84.6	178	60.8	-60.7	-59.7	-179.2
0262inp	11.88	-224.15	49.93	-114.3	130.3	-58.9	1.4	65.3	-69.1	49.7	-39.3	-176.8	-172.5	-177.9
0263.inp	15.5	-220.54	53.55	-145.2	130.4	-62.7	-1.8	57.4	-83.2	52.7	72.7	-168.8	-66.7	-176.8
0264.inp	12.59	-223.45	50.64	-136.7	123.6	-63.6	-1.4	67.4	-68.2	45.9	-162.6	178.7	64	-176.9
0265.inp	18.74	-217.3	56.79	-146.3	127.7	-62.2	-5.1	59.5	-84.6	-133.6	60.1	6.8	-80.9	-176.8
0265a.inp	19.04	-217	57.09	-143.6	107.7	-64.1	0.3	88.2	-56.1	-60.9	138.1	80.1	-2.4	-176.7
0266.inp	15.08	-220.96	53.13	-143.2	105.9	-67.4	0.5	87	-52.9	-71.3	-47.2	47.2	167.9	-178.7
0267.inp	15.78	-220.26	53.83	-143.3	104.4	-68	-0.1	90.2	-48.7	-69.4	-149	68.1	74.7	-177.6
0268.inp	13.8	-222.24	51.85	-136.8	124.3	-62.4	-3	63.1	-71.2	130.9	-169.8	-98.4	58.8	-176.8
0268a.inp	13.67	-222.37	51.72	-137	123.7	-61.3	0.8	70.8	-63.3	167.6	-128.4	-61.2	100.7	-176.2
0269.inp	12.61	-223.43	50.66	-97	135.3	-59.2	-0.3	63.2	-71.6	159.8	-41.5	-61.3	-174.2	-179.2
0270.inp	15.68	-220.36	53.73	-142.6	133	-61.2	-3.2	53	-86.3	151.1	70	-72.3	-67.8	-176.6
0271.inp	1.7	-234.34	39.75	-72.8	133.3	61.4	179.5	-137.8	100.4	60.5	-66.1	-179.3	174.5	178.5
0272.inp	2.53	-233.51	40.58	-66.6	135.5	61.6	-177.2	-151.4	84.4	64.1	59	-174.6	-62.2	178.9
0273.inp	2.62	-233.42	40.67	-66.4	136.3	61.5	-177.7	-148.9	88	58.3	-174.1	177.8	66.3	179.1
0274.inp	5.58	-230.45	43.63	-66.7	137.2	61.4	-178.2	-151.3	81.8	-31.9	61.5	91.7	-62.5	179.1
0274a.inp	5.38	-230.66	43.43	-79.1	143.8	59.8	178.9	-152.9	80.1	-65.2	31.3	59.4	-92.3	178.8
0275.inp	3.14	-232.9	41.19	-70.6	133.1	61.9	-179.2	-139.8	96.3	-62	-69.8	59.5	169.4	179
0276.inp	3.7	-232.34	41.75	-67.2	139.2	62	-177	-148.5	85.9	-64.9	-179.1	56.3	59.7	179
0277.inp	4.95	-231.09	43	-67	139.3	61.5	-177.6	-151.5	84.8	177.1	-143.8	-63.2	97.2	179.2
0277a.inp	5.08	230.96	43.13	-67	139.1	61.6	-178.7	-149.4	86.8	146	-178.3	-95	62.4	179.2
0278.inp	3.01	-233.03	41.06	-72.8	133.7	61.6	-178.9	-139.3	97.9	170.9	-64.2	-69.1	176.9	178.9
0279.inp	3.35	-232.69	41.4	-67.5	141.1	62.3	-176.5	-150.4	84.3	178.4	60.6	-60.7	-60.1	178.9
0280.inp	2.92	-233.11	40.97	-74.9	137.2	61.3	177.9	62.2	-66.5	53.9	-57.1	-179.3	175.4	178.7
0281.inp	5.66	-230.37	43.71	-73.9	146.7	64.2	-178.7	53.9	-79.9	54.6	81.5	-172.9	-50.7	178.5
0282.inp	3.74	-232.3	41.79	-73	145.9	63.6	179.1	64.1	-65.5	52.3	-167	178.8	65.9	178.4
0283.inp	10.1	-225.94	48.15	-70.3	138.3	64.5	-179.8	81	-58.5	-55	105.8	81.6	-30.6	178.5
0283a.inp	10.98	-225.06	49.03	-68.5	146	67.5	-169.6	60.7	-80.7	-101.8	59	36.4	-78.8	178.5
0284.inp	5.49	-230.55	43.54	-66.4	131.9	62	-174.6	78.2	-55.3	-69.2	-56.2	62.7	172.6	178.6
0285.inp	6.14	-229.89	44.19	-66.1	136.6	64.1	-175.5	80.1	-54	-72.4	-165.4	59	63.8	178.4
0286.inp	5.88	-230.16	43.93	-68	139.9	64.1	-177.2	67.5	-61.9	171.1	-140.7	-63.1	94.1	178.9
0286a.inp	5.76	-230.28	43.81	-67.8	145.5	64.1	-178.6	60.2	-69.2	140.1	-171.5	-96.7	62.7	178.6
0287.inp	3.82	-232.22	41.87	-67.2	137.8	63.2	-179.6	61.2	-68.2	162.4	-57.3	-71.1	176.2	179
0288.inp	6.3	-229.74	44.35	-67.7	144.9	65.6	-176.5	54.4	-80.2	166.9	80.7	-61.7	-50.9	178.6
0289.inp	0.41	-235.62	38.46	-71.8	-4.2	62.3	178.8	-99	139.8	63.8	-57.3	-177.1	-177	177.5
0290.inp	0.87	-235.16	38.92	-67	-18.9	60.1	-179.4	-109.3	127.1	69.1	53.8	-170.6	-66.8	175.8
0291.inp	1.74	-234.29	39.79	-68.4	-15.2	58.5	178.1	-101.6	135.7	64.3	-171.2	-177	69.2	177
0292.inp	3.17	-232.87	41.22	-67	-21.4	58.8	-176.6	-92.4	140.3	-64.4	32.7	59.4	-91.1	179.1
0292a.inp	3.56	-232.48	41.61	-78	-22.7	58.8	-176.2	-85.9	147.5	-29.7	62.2	93.3	-62	176.7
0293.inp	0.9	-235.13	38.95	-75.9	-11.4	64	-178.1	-85.7	150.2	-60.2	-61	61.1	177.3	177.7
0294.inp	1.93	-234.11	39.98	-68.9	-23	61.7	-177.3	-86.4	148	-64	-177.8	57	60.7	179.2
0295.inp	3.71	-232.33	41.76	-62.7	-22.6	58.7	178.6	-92.2	144.1	178.5	-145.4	-62.3	95.9	178
0295a.inp	3.77	-232.27	41.82	-63	-23.7	58.8	177.8	-88.6	147.8	144.6	-177.4	-96.6	63.2	177.7
0296.inp	1.07	-234.97	39.12	-69	-10.4	62.5	178.5	-86.4	150.8	175.1	-55.6	-65.6	-174.9	177.9
0297.inp	1.71	-234.33	39.76	-60.7	-22.3	61.1	178.1	-84.1	150.9	-180	62.2	-59.6	-58.5	176.4
0298.inp	2.48	-233.56	40.53	-78.5	5.3	60.3	-179.9	68.4	-60.7	58.5	-51.8	-174	-178.6	178.4
0299.inp	5.69	-230.35	43.74	-79.7	7.4	64.7	179.4	57	-77	57.8	70.6	-170.4	-61.3	178.9
0300.inp	3.46	-232.58	41.51	-75.1	0.1	64.2	179.3	69.6	-60	59.4	-161.7	-173.8	71.9	178.7
0301.inp	9.87	-226.17	47.92	-69.8	-8.1	61.9	177.1	59.2	-80.3	-105.8	54.1	30.3	-82.5	178.7
0301a.inp	10.49	-225.55	48.54	-64.3	-25.1	60	170.3	81.1	-59.9	-60.5	102.8	77.5	-35.5	178.8
0302.inp	5.02	-231.01	43.07	-72.6	-14.2	67.7	179.3	81.7	-52.3	-82.5	-53.5	49.9	175	177.8
0303.inp	5.76	-230.28	43.81	-66.9	-17.9	61.7	176	81.9	-52.8	-80.4	-166.6	51.4	61.9	178.8
0304.inp	5.2	-230.84	43.25	-68.2	-13.3	62.2	178.9	71	-58.6	172.5	-140.3	-61.6	94.4	178.9
0304a.inp	5.38	-230.66	43.43	-69.3	-11.3	64.7	176.4	62.9	-66.8	140.3	-170.9	-94.2	63	179.1
0305.inp	3.19	-232.85	41.24	-75.4	-7.5	63.4	-177.9	67.8	-61.9	168.8	-49	-63.7	-175.6	178.3
0306.inp	5.68	-230.36	43.73	-68.3	-14.5	63.6	177.2	55	-79.4	167.2	72.2	-61.7	-59.4	179.3
0307.inp	2.8	-233.24	40.85	-79.8	167.3	64.9	-172.1	-96.4	142.1	76.6	-59.9	-164.4	179.7	178.5
0308.inp	3.85	-232.19	41.9	-81.3	171.1	62.3	-173.9	-93.6	143	77.2	62.6	-162.4	-59.2	178.6
0309.inp	4.05	-231.99	42.1	-81.7	171.4	63	-172.7	-95.2	142.4	75.2	-167.5	-166.2	72.3	178.5
0310.inp	5.26	-230.78	43.31	-70.9	149.6	62.3	-178.6	-83.9	149.2	-60.2	31.7	63.7	-91.9	178.9
0311.inp	2.39	-233.65	40.44	-74.9	154.1	62.1	-178.6	-84.6	151.4	-59.4	-64.1	61.8	174.4	179.1
0312.inp	3.11	-232.92	41.16	-73.9	152.8	62.3	-179	-83.3	151.4	-61.6	-177.9	59.3	60.7	178.9
0313.inp	5.03	-231.01	43.08	-75.6	154.9	63	-176.7	-84	152.3	180	-146.4	-60.8	94.3	178.9
0313a.inp	4.98	-231.06	43.03	-72	147.8	64	-174.2	-82.4	153.8	142.9	-176.4	-97.8	63.1	179
0314.inp	2.53	-233.51	40.58	-71.7	147.4	62.4	-176.2	-87.3	149.5	175.7	-57.4	-64.6	-177.2	178.7
0315.inp	3.55	-232.48	41.6	-70.6	145.4	60.4	-177	-83.2	151.4	179.7	65.3	-59.2	-56.1	179.2
0316.inp	5.6	-230.44	43.65	-83	175.6	65.8	-165.5	70.1	-57.9	54.7	-47.6	-176.6	-173.8	178.2
0317.inp	5.59	-230.45	43.64	-72.8	156.4	65.8	-177.3	54.3	-79.5	53.9	78.6	-174.4	-53.5	178.2
0318.inp	3.76	-232.28	41.81	-72.5	150.8	64.2	-178.8	64.5	-65.2	52.2	-167.6	178.9	65.4	178.3
0319.inp	10.46	-225.58	48.51	-74.6	157.7	68.3	-176.4	86.2	-52.2	-52.9	107.7	83.1	-27.2	178.1
0319a.inp	11.07	-224.96	49.12	-72.7	161.3	67.2	-171.2	63.2	-77.8	-100.2	59.3	38.4	-78.7	178.3
0320.inp	6.99	-229.05	45.04	-77.1	148.6	65	-166.8	84.9	-47	-66.1	-51.8	66.3	178.5	178.1
0321.inp	6.17	-229.86	44.22	-68.8	156.4	64.6	-176.5	82.1	-51.9	-70.7	-165.1	60.7	64.3	178.3
0322.inp	5.9	-230.13	43.95	-67.6	141.2	65.6	-176.7	68	-61.5	171.4	-140.8	-62.8	94	178.8
0322a.inp	5.82	-230.22	43.87	-70.5	152	64.4	-179	60.7	-68.9	140	-172.3	-94.5	61.9	178.8
0323.inp	3.82	-232.22	41.87	-65.9	136.6	63.8	-177.1	61.9	-67.6	163.7	-56.8	-69.7	176.8	178.9

0324.inp	6.3	-229.73	44.35	-70.6	154.4	64.7	-177.1	55.1	-79.4	167.1	80.4	-61.4	-51.2	178.5
0325.inp	1.75	-234.29	39.8	-73.8	-45.3	56.7	173.5	-144.8	94	58.7	-70.4	179.4	170.3	-179.7
0326.inp	0.78	-235.26	38.83	-68.6	-19.6	63.2	-178.6	-118.2	118.2	69.2	55.3	-170	-65	175.4
0327.inp	1.51	-234.53	39.56	-70.9	-35.8	65.6	175.6	-156.5	80.8	56	-172.6	-172.6	67.5	-179.7
0328.inp	3.66	-232.38	41.71	-75.1	-14.4	65.9	177.8	-145.7	86.8	-35.1	65.7	89.3	-58.8	-178.8
0328a.inp	3.78	-232.26	41.83	-71.7	-10.7	67.4	177	-141.2	89.4	-53.9	54.5	71.1	-70.3	179.5
0329.inp	1.81	-234.23	39.86	-67.4	-19.6	65.1	170.4	-133.5	103.1	-62.9	-79.9	58.3	160.3	178.4
0330.inp	1.57	-234.47	39.62	-64.9	-18.4	64.5	176.3	-141.7	92.9	-64	179.7	56.9	59.2	177.5
0331.inp	3.82	-232.2	41.87	-68.4	18.7	64.6	175.6	-145.2	91.1	177	-144.7	-63.2	96.6	177.9
0331a.inp	3.62	-232.42	41.67	-65.9	-16.6	64	176.5	-141.9	94.3	146.6	-179.8	-94.5	61.1	178
0332.inp	2.59	-233.45	40.64	-67.3	-18.7	65.2	169.9	-135.1	102.5	167.8	-77	-72.4	164.7	178
0333.inp	1.43	-234.61	39.48	-66.2	-13.4	65.3	176.6	-140.9	93.9	178.3	63.3	-60.9	-57	177.2
0334.inp	4.87	-231.17	42.92	-75.1	-55.6	53.8	169.8	54.4	-73.9	49	-59.7	175.2	171.7	-179.8
0335.inp	6.49	-229.55	44.54	-73.6	-49.5	60.3	170.9	43.5	-88.4	52.6	66	-178	-66.2	177.8
0336.inp	5.73	-230.31	43.78	-69.2	-42.6	52.6	166.1	58	-71.1	45	-169.7	171	61.6	179
0337.inp	10.12	-225.92	48.17	-73.7	-38.6	61.2	177.9	49.3	-89.2	-107.3	53.3	27.5	-82.9	178
0337a.inp	10.36	-225.68	48.41	-61.4	-39.1	61.2	172.8	77.1	-63.9	-58.5	99.9	79.5	-38.7	178.8
0338.inp	5.24	-230.8	43.29	-75.7	-37.3	59.6	176.8	79	-54.7	-70.3	-54	61.8	173.9	177.9
0339.inp	5.8	-230.24	43.85	-67.4	-28.4	62.6	176.3	80.5	-54.1	-77.4	-167.1	54.4	61.1	179.6
0340.inp	5.32	-230.71	43.37	-64.2	-29.3	64.9	174.8	59	-70.3	138.4	-171.9	-96.5	61.8	179.1
0340a.inp	5.14	-230.9	43.19	-64	-24.4	64.9	176.3	69.6	-60.2	173	-139.9	-61	94.3	178.7
0341.inp	3.33	-232.71	41.38	-77.7	-27.3	64.7	178.3	63.3	-66.4	166.4	-54.3	-66.5	178.5	177.8
0342.inp	5.49	-230.55	43.54	-65.5	-22.1	66.6	176.3	53.4	-80.8	166.4	70.9	-62.8	-60.6	179.2
0343.inp	2.32	-233.72	40.37	-154.5	-158.3	69.2	-177.6	-97.3	140.9	62.9	-60.4	-177.6	-179	-178.1
0344.inp	3.12	-232.92	41.17	-155.8	-160.2	70.1	-178.3	-95.7	140.1	64.8	60.1	174	-62.3	-178
0345.inp	3.31	-232.73	41.36	-155.4	-158.3	69.4	-177.7	-96.4	140.8	61.1	-172.3	-179.8	67.2	-178
0346.inp	7.02	-229.02	45.07	-156.8	-149.4	69.6	-174.3	-75.2	156.7	-32.7	70.3	92.5	-55.9	-178.1
0346a.inp	7.56	-228.48	45.61	-157.4	-149.9	69.4	-174	-78	153.9	-60.2	34.7	65.2	-91.1	-177.7
0347.inp	3.92	-232.12	41.97	-154.1	-129.1	64.5	-178.9	-76.7	159.3	-51.7	-60.9	69.7	176.9	-178.2
0348.inp	4.95	-231.09	43	-154.1	-126.9	63.7	-180	-76.4	158.3	-56.6	-175.3	64.4	62.7	-178.2
0349.inp	6.35	-229.69	44.4	-156.3	-143.8	68.2	176.5	-78.8	157.9	178.4	-146.1	-62.5	94.9	-178
0349a.inp	5.26	-230.78	43.31	-156.9	-163.3	69.4	179	-76.3	160.2	142.8	-176.6	-98	63.1	-177.9
0350.inp	3.85	-232.19	41.9	-156.4	-147.5	68.5	177.6	-79.7	157.8	172.6	-57	-67.7	-176.9	-178.2
0351.inp	4.69	-231.34	42.74	-161	-162.9	81.1	176.1	-79.1	155.8	178.6	63.7	-60.3	-57.6	-177.9
0352inp	4.51	-231.52	42.56	-152.1	-146.4	65.7	-176.9	68.2	-60.4	54.4	-51.2	-177.9	-177.9	-178.3
0353.inp	6.08	-229.96	44.13	-156.6	-168.6	68.8	-179.5	53.2	-79.9	51.5	62.4	-176.9	-69.5	-177.8
0354.inp	4.9	-231.14	42.95	-156.3	-164.4	68.4	179.4	68.6	-60.7	52.4	-162.4	179.2	70.9	-178
0355.inp	10.82	-225.22	48.87	-156.8	-174.1	65.9	-180	88.1	-50.4	-52.8	108.2	83.1	-26.7	-177.6
0355a.inp	10.7	-225.34	48.75	-155.3	-164.1	65.5	-179	59.3	-80.2	-106.5	54.1	30.1	-82.5	-177.6
0356.inp	6.93	-229.11	44.98	-155.6	-143.8	66.2	176.8	85.3	-47.8	-65.7	-52.6	66.4	176.5	-178.2
0357.inp	7.1	-228.93	45.15	-157.2	-168.8	69	177.2	86.9	-46.8	-67.9	-161.2	63.4	68.4	-177.8
0358.inp	6.31	-229.67	44.36	-156.5	-173.3	68.6	179.5	72.3	-56.8	171.3	-135.7	-62.5	98.9	-178
0358a.inp	6.78	-229.26	44.83	-155.9	-167.5	67.7	-179.3	63.3	-66.3	139.6	-171.6	-94.5	62.5	-177.8
0359.inp	5.44	-230.6	43.49	-154.8	-163.5	68.1	-171.7	68.7	-60.4	168.1	-46.5	-63.9	-172.6	-177.9
0360.inp	6.72	-229.31	44.77	-156.9	-171.1	68.6	-179.1	52.7	-81	162.3	65.1	-66.5	-66.2	-177.7
0361.inp	3.31	-232.73	41.36	-100	69.3	51.1	-178.2	-103.5	134.8	63.2	-60.8	-177.6	179.4	178.8
0362.inp	4.79	-231.25	42.84	-100.5	78.5	51.6	-179.6	-104.3	131.5	66.2	59.3	-172.9	-62	179.1
0363.inp	4.85	-231.19	42.9	-98.6	80.1	51.3	-178.7	-105.4	131.6	59.3	-173	178.4	67.3	179.4
0364.inp	7.09	-228.95	45.14	-95.4	82	50.9	179.3	-83.7	149.5	-30.3	63.8	92.8	-60	179.8
0365.inp	4.28	-231.75	42.33	-95.2	83.8	50.7	-178.1	-87.9	147.8	-56.1	-63.6	64.9	175.1	178.9
0366.inp	5.48	-230.57	43.53	-93.2	80.1	51.5	-178.7	-87.6	147	-61.6	-178.2	59.1	60.6	179.3
0367.inp	7.01	-229.03	45.06	-93.9	81.2	51.4	-177.9	-92.4	143.7	178.3	-146.4	-62.5	94.7	179.4
0368.inp	4.26	-231.78	42.31	97.2	80	51.1	-178.8	-91.8	145.2	173.7	-58.8	-66.8	-178.3	179.6
0369.inp	5.42	-230.62	43.47	-96.6	77.7	51.1	-179.7	-87.3	147.2	179.4	64.2	-59.7	-57	179.5
0370.inp	4.84	-231.2	42.89	-100.1	69.1	54	-177.3	65.2	-63.8	53	-53	-179.7	-179.9	177.7
0371.inp	7.53	-228.51	45.58	-96.9	85.8	55.5	-177	50.9	-82.6	51.5	65.8	-177.2	-66.1	178.5
0372.inp	5.48	-230.56	43.53	-107.1	58.5	53.8	-176.6	66.4	-63.2	51.3	-164.3	178.2	69.1	177.9
0373.inp	12.12	-223.91	50.17	-103.3	58.5	55.8	-175.4	86.9	-51.2	-51.6	107.7	83.9	-26.7	178.4
0373a.inp	12.62	-223.42	50.67	-105.6	84.6	56.8	-179.3	54	-84.8	-108.1	53.4	27.3	-82.6	-179.9
0374.inp	7.62	-228.42	45.67	-105	58.4	55.4	-175.7	83.3	-49.5	-63.7	-51.8	68.1	177.8	178.9
0375.inp	8.19	-227.85	46.24	-107.1	55.7	55.1	-176.2	84.7	-48.7	-66.7	-162.2	64.5	67.8	178.9
0376.inp	7.94	-228.1	45.99	-102	56.8	53.6	-179.1	70.4	-59	171.9	-140.4	-62.2	94.5	179.5
0376a.inp	7.73	-228.3	45.78	-104.7	48.1	52	178.5	62.4	-67.2	140.1	-171	-94.4	63.2	179.8
0377.inp	5.86	-230.18	43.91	-106.2	52.2	53.9	179.4	66.9	-62.7	167.4	-50.1	-65.5	-176.6	179.7
0378.inp	8.5	-227.55	46.55	-112.8	58	55.6	179.3	54.8	-79.6	166.6	73.7	-62.1	-57.9	-179.9
0379.inp	4.89	-231.15	42.94	-98.2	147	60.8	177.2	-136.4	101.9	60.2	-68.3	-179.6	172.3	0.6
0380.inp	5.39	-230.64	43.44	-85.2	153.1	60.2	-179.3	-146.1	89.5	63.4	59.4	-175.3	-61.8	0.8
0381.inp	5.49	-230.55	43.54	-86.3	151.7	60	-179.6	-145.2	91.6	58.1	-174.8	177.7	65.5	0.4
0382.inp	8.52	-227.52	46.57	-85.7	154.4	61.3	-179.3	-141.7	91.5	-30.4	61.6	92.8	-62.1	0.6
0382a.inp	8.56	-227.47	46.61	-86.3	165.2	60.8	-178.6	-134.9	97.6	-63.6	34.4	60.3	-89.2	0.8
0383.inp	6.38	-229.66	44.43	-94.2	147.3	60.3	177.5	-136.4	99.6	-61.7	-72.5	59.9	166.8	0.3
0384.inp	6.72	-229.32	44.77	-86.6	153.4	60.8	-179.3	-145.5	88.9	-64.8	-179.3	56.4	59.6	0.5
0385.inp	8.1	-227.94	46.15	-88.4	154.9	59.8	179.7	-149.8	86.3	176.9	-143.9	-63.2	97	0.6
0385a.inp	8.12	-227.91	46.17	-87	154.2	60.4	179.6	-145.7	90.4	146	-178.5	-95	62.2	0.6
0386.inp	6.35	-229.69	44.4	-97	147.1	59.8	175.8	-136.8	100.4	170	-66.9	-70	174.2	0.4
0387.inp	6.43	-229.61	44.48	-86.3	15.5	60.9	-178.9	-147.2	87.4	178.1	62	-60.8	-58.8	0.7
0388.inp	6.47	-229.57	44.52	-108.3	134.6	60	177.3	62.3	-66.3	51.5	-55.4	178.2	177.2	0.3
0389.inp	9.32	-226.72	47.37	-107.1	135.1	61.8	-177.7	52.2	-81.4	52.2	75.3	-176.3	-56.9	0.2
0390.inp	7.33	-228.7	45.38	-111.8	147.2	60.8	178.8	63.9	-65.6	50.4	-167.2	176.9	65.6	0.9

0391.inp	14.24	-221.8	52.29	-94.5	136.7	61.6	-171.2	57.7	-82.6	-104	56.9	33.6	-80.6	0.6
0391a.inp	13.48	-222.55	51.53	-93.1	138.2	61.2	18.9	80.3	-59.4	-56	105.2	80.7	-31.5	0.2
0392.inp	8.87	-227.17	46.92	-91.3	134	59.5	-176.6	78.4	-55.1	-68	-56.6	63.9	172.1	0.5
0393.inp	9.35	-226.68	47.4	-88.3	145.4	61.3	-177.6	80.5	-53.3	-74.5	-166.5	56.9	62.5	0.2
0394.inp	9.14	-226.9	47.19	-90.4	140.6	61.1	-178.6	67.5	-62.1	171.7	-140.6	-62.4	93.9	0.9
0394a.inp	8.96	-227.08	47.01	-88.3	150.5	60.8	180	60.2	-69.2	139.9	-171.6	-94.9	62.5	0.5
0395.inp	7.06	-228.97	45.11	-89.7	140.6	58.1	180	62.7	-66.8	164.9	-55.7	-68.5	177.6	0.9
0396.inp	9.46	-226.57	47.51	-87	150.3	61.3	-178	54	-80.5	166.5	82.2	-62.2	-49.5	0.7
0397.inp	10.39	-225.65	48.44	-86.9	126.4	61.4	-4.6	-130.4	109.7	64.5	-61.6	-176.5	-179.8	179
0398.inp	10.09	-225.94	48.14	-71.6	127.1	62.4	-4.8	-150.1	86.4	64.3	52.3	-174.3	-68.2	179.2
0399.inp	10.15	-225.89	48.2	-71.3	127.5	62.8	-6	-148.3	89.2	60	-172.4	179.6	68.4	179
0400.inp	12.52	-223.52	50.57	-72.3	128.7	62.2	-4.2	-150.9	82.6	-65.3	31.4	58.8	-91.6	179
0400a.inp	13.58	-222.46	51.63	-72.1	128.8	62.3	-6.8	-148.4	85.3	-32.3	58.3	91.6	-65.3	179.2
0401.inp	9.11	-226.92	47.16	-72.6	145.6	61.4	2.1	-94.9	141.4	-54.4	-63.9	66.3	174.8	178.6
0402.inp	11.4	-224.64	49.45	-72.1	126.6	61.9	-5.1	-148.1	86.8	-65.5	-179.2	55.9	60	179.4
0403.inp	12.09	-223.95	50.14	-72.5	128	63.1	-5.3	-152.9	84.1	176.1	-140.6	-63.9	100.5	179.2
0403a.inp	12.67	-223.37	50.72	-73	128.5	63.1	-7.9	-148.2	88.7	144.9	-178.5	-95.8	62.4	179.4
0404.inp	11.1	-224.94	49.15	-76.3	126.7	61.8	-4.9	-121.5	116.1	171.9	-60.5	-68.9	-178.9	179.4
0405.inp	11.12	-224.92	49.17	-71.2	128.4	62.4	-4.8	-149.4	86	177.9	58.5	-60.9	-61.7	179
0406.inp	12.74	-223.3	50.79	-115.8	130.3	54.6	-0.4	66.2	-68.5	49.5	-39.2	-176.9	-172.5	-179.9
0407.inp	16.2	-219.83	54.25	-150.6	132.7	57.8	-1.8	57.6	-83.2	53.4	73.7	-167.8	-65.9	-177.2
0408.inp	13.37	-222.66	51.42	-152.4	132	57.3	-2.4	65.8	-69.8	49.1	-161.8	-178.1	64.8	-176.9
0409.inp	20.08	-215.96	58.13	-153.4	129.5	59.1	-5.5	60.5	-83.8	-130.1	60.4	10.6	-81	-177.7
0410.inp	16.84	-219.2	54.89	-147.5	110	57.4	-3.2	88.1	-52.6	-76.3	-45.5	63.5	175.6	-179.1
0411.inp	17.57	-218.47	55.62	-149.4	108	56.5	-4.1	91	-49	-73.5	-150.6	64.8	71.9	-177.9
0412.inp	14.72	-221.32	52.77	-153.6	132.3	56.1	-1.6	68.4	-65.5	163.1	-127.7	-65.7	101.2	-177
0412a.inp	14.99	-221.05	53.04	-153.5	131	56.6	-3.3	62.6	-72.2	135.5	-170.3	-93.5	58.1	-176.9
0413.inp	13.35	-222.69	51.4	-153.4	133.4	55.1	-2.4	64.8	-70.3	158.6	-43.1	-68.4	-176	-177.5
0414.inp	16.46	-219.58	54.51	-153.3	134.8	53.8	-3.5	55.1	-85.1	156.6	73.7	-66	-64.7	-177.3
0415.inp	0.9	-235.14	38.95	-157.9	116.8	-178.9	179	-136.9	101.4	58.8	-62	178.9	177.7	-179
0416.inp	1.68	-234.36	39.73	-157.2	125.5	-178.1	-179.4	-150.5	85.4	61.2	55.3	-177.4	-66	-179.2
0417.inp	1.61	-234.43	39.66	-157.8	125.2	-178.1	179.4	-149.4	87.6	56.8	-174.1	176.5	66.1	-178.8
0418.inp	4.17	-231.87	42.22	-158.6	141.9	-179.4	178.6	-150.9	82.3	-62.2	30.7	61.2	-92.6	-179.2
0418a.inp	4.28	-231.75	42.33	-159.4	140	-179.1	176.2	-145.8	86.6	-34.2	61.7	89.9	-62.5	-178.6
0419.inp	1.66	-234.37	39.71	-159.1	137.2	178.3	177.8	-132.4	103.5	-57.8	-65.5	63.5	173.5	-179.1
0420.inp	2.34	-233.7	40.39	-158.8	141.7	178.5	179.5	-135.5	99	-62.1	-179.1	58.9	59.9	-179
0421.inp	4.08	-231.96	42.13	-158.7	138.1	-178.5	176.5	-151.3	84.9	176.1	-143.4	-63.9	97.5	-179.2
0421a.inp	3.81	-232.23	41.86	-159.3	140.5	-179.2	174.2	-146.7	89.5	142.3	-177.8	-98.2	62.7	-179
0422.inp	2.06	-233.98	40.11	-159.5	133	179.5	176.1	-135.4	101.8	171.3	-60.1	-68.8	-179.1	-179.1
0423.inp	2.59	-233.45	40.64	-158.7	142.5	179.6	179.3	-146.3	88.4	178.4	61.8	-60.5	-59	-179
0424.inp	2.44	-233.6	40.49	-157.2	110.4	179.5	-179.5	63	-65.8	52.1	-56.6	179	176.3	-179
0425.inp	5.04	-231	43.09	-157.5	127.8	178.2	-178.8	52.5	-81.3	53.1	77	-175.5	-55.1	-179.3
0426.inp	3.39	-232.64	41.44	-157.8	123.7	178	179.7	62.9	-66.7	49.6	-168.5	176.1	64.4	-179.2
0427.inp	10.1	-225.94	48.15	-159.5	117.9	175.8	172	76.3	-64.7	-53.9	93.5	84.4	-45.4	-179
0427a.inp	10.1	-225.94	48.15	-157.8	132.8	176.9	-176	57	-83.1	-106.2	58.4	30.6	-78.6	-178.2
0428.inp	10.33	-230.71	48.38	-158.8	107.9	176.2	179.4	79.7	-53.9	-68.3	-56.4	63.7	172.2	-178.5
0429.inp	6.05	-229.99	44.1	-158.2	121	177.6	178.7	80.4	-54	-73	-167	58.5	61.8	-179.1
0430.inp	5.5	-230.55	43.55	-158.7	123.3	177.8	179.5	68	-61.5	171	-140.2	-63.1	94.4	-179
0430a.inp	5.24	-230.8	43.29	-158.5	129.2	178.4	178.7	60	-69.6	140.4	-172.6	-94.3	61.5	-178.9
0431.inp	3.37	-232.67	41.42	-159.7	115.2	178.1	180	62	-67.4	162.8	-59	-70.5	174.4	-178.3
0432.inp	5.55	-230.49	43.6	-158.3	129.5	178.4	179.3	52.4	-82	166	80.8	-63	-50.8	-179
0433.inp	3.69	-232.35	41.74	-148	0.3	-172.5	-178.3	-103.9	134.4	63.1	-60.2	-177.6	179.9	-179.3
0434.inp	4.73	-231.3	42.78	-146.6	-6.5	-175.3	179.7	-100.8	135.3	66.8	59.8	-172.5	-61.4	-179.9
0435.inp	4.88	-231.16	42.93	-148	1	-171.7	-179.8	-102.5	134.7	59.8	-172.6	178.8	67.7	-179.5
0436.inp	7.18	-228.86	45.23	-146.4	3.3	-171.4	180	-84.8	148.7	-61.1	29.9	62.4	-93.3	179.9
0436a.inp	6.87	-229.17	44.92	-144.5	0.7	-172.1	178	-79.7	153.8	-30.4	63.6	92.5	-60.1	179.5
0437.inp	4.5	-231.54	42.55	-147.6	4	-171.3	-179.2	-84.5	151.6	-55.7	-63	65.2	175.7	-179.9
0438.inp	5.39	-230.64	43.44	-147.4	4.4	-171.3	-179.9	-82.9	151.9	-60.7	-178	59.9	60.8	-179.8
0439.inp	7.02	-229.01	45.07	-148.5	5.5	-171.7	-179	-87.9	148.4	178.5	-146.2	-62.4	94.8	-179.5
0439a.inp	6.91	-229.13	44.96	-149.5	7.8	-171.9	-178.2	-82.2	154.1	142.4	-176.4	-98.4	63.5	-179.6
0440.inp	4.51	-231.53	42.56	-148.1	6.5	-172.5	-177.6	-87.4	149.6	173.7	-57.3	-66.8	-177	-179.7
0441.inp	5.34	-230.7	43.39	-148	5.8	-172.5	-179.4	-84.5	150.1	179.5	64	-59.7	-57.2	180
0442inp	5.21	-231.83	43.26	-149	9.1	-171.7	-178.2	64.4	-64.5	52.5	-53.1	179.9	179.7	-179.5
0443.inp	7.86	-228.18	45.91	-149.4	11.6	-171.5	-178.9	52.2	-81.4	51.3	67.3	-177.3	-64.8	-179.5
0444.inp	5.01	-230.03	43.06	-149.6	10.2	-171.8	-177.3	64.5	-65.2	50.1	-165.7	177	67.4	-179.3
0445.inp	12.64	-223.4	50.69	-150.5	13	-171.6	-179	55.5	-83.7	108.1	54	27.7	-82.3	-179.4
0445a.inp	12.38	-223.65	50.43	-150.4	11.6	-176.6	-176.6	84.8	-53.8	-52.9	108.8	83	-26.1	-179.4
0446.inp	7.83	-228.21	45.88	-149.5	12.4	-171.8	-177.3	81.7	-51.5	-65.2	-51.7	66.9	177.4	-179.6
0447.inp	8.52	-227.52	46.57	-149.6	11.9	-171.8	-176.7	82.9	-51	-68.3	-162.4	63.1	67.1	-179.5
0448.inp	8.17	-227.87	46.22	-149.3	11.3	-170.8	-178.8	69.1	-60.4	171.4	-139.7	-62.6	94.9	-179.5
0448a.inp	8.19	-227.85	46.24	-151.5	11.5	-172.9	-179.3	60.9	-68.7	139.7	-171	-94.7	63	-179
0449.inp	6.23	-229.81	44.28	-149.6	11.9	-171.6	179.5	65.2	-64.5	165.9	-50.9	-67	-177.7	-179.6
0450.inp	8.74	-227.3	46.79	-149	11.5	-171.2	179.1	52.5	-81.8	164.9	72.1	-64	-59.6	-179.5
0451.inp	1.33	-234.7	39.38	-159.3	153	-177.8	-176.6	-98.2	140.5	70.8	-60.2	-170.3	179.9	-178.6
0452.inp	1.79	-234.25	39.84	-158.7	152.8	-178.3	-177.5	-96.3	140.5	72.5	60.7	-167.2	-60.6	-178.8
0453.inp	2.42	-233.62	40.47	-158.4	153.5	-178.2	-176.6	-97	140.7	69.4	-169.7	-172.1	70.5	-178.8
0454.inp	5.17	-230.87	43.22	-157.7	147	-175.5	-171.9	-81.2	151.3	-68.7	34.2	55.7	-90.7	-178.8
0454a.inp	5.01	-231.03	43.06	-157.3	144.3	-176.9	-170.2	-75.5	157.7	-28.9	64.6	94.7	-60.8	-178.9
0455.inp	1.48	-234.56	39.53	-159.9	128.1	-178.7	-178.9	-87.6	149.8	-63.8	-64.5	57.5	174	-178.3

0456.inp	2.12	-233.92	40.17	-159.1	127.4	-178.1	-179	-86.3	148.2	-65.5	-177.7	55.5	60.9	-178.7
0457.inp	4.08	-231.96	42.13	-159.8	144.2	-179.5	-179.5	-86	150.5	177.8	-146.5	-63.1	94.6	-178.7
0457a.inp	4.08	-231.96	42.13	-159.3	143.7	179.3	-178.7	-82	154.5	146.1	-177.3	-95.1	62.9	-178.8
0458.inp	1.72	-234.32	39.77	-159.6	143.4	180	-179.6	-87.2	150.1	174.1	-58.2	-66.4	-177.7	-178.7
0459.inp	2.1	-233.94	40.15	-159.5	143.1	179.2	-179.8	-83.2	151.7	178.3	64.4	-60.9	-56.8	-178.9
0460.inp	3.95	-232.08	42	-156	160.3	-175.9	-171.6	68.7	-59.7	54.7	-49.5	-177.1	-176.1	-178.8
0461.inp	5.2	-230.84	43.25	-158.4	150.1	-175.6	-178.7	53.3	-80.2	52.6	68.1	-175.9	-63.8	-178.9
0462.inp	3.81	-232.23	41.86	-158.1	152.2	-177.3	-178	66.9	-62.5	51.9	-164.5	-177.7	68.9	-178.8
0463.inp	10.37	-225.67	48.42	-156.7	160.4	-171.4	-177.8	60.7	-79.2	-104.4	55.4	32.6	-81.5	-179.1
0463a.inp	10.07	-225.97	48.12	-159.7	144	-177.1	-179.6	85.3	-53.5	-53.1	107.5	82.9	-27.8	-178.8
0464.inp	6.01	-230.02	44.06	-158.2	157.4	-176.9	-174.8	85	-47.4	-64.7	-51.4	67.3	178.5	-178.7
0465.inp	6.24	-229.79	44.29	-158.8	154.2	-176.4	179.7	86.2	-47.4	-68.2	-162.1	63	67.7	-179
0466.inp	5.56	-230.48	43.61	-158.1	151.6	-177.7	-178.7	71.6	-57.5	171.8	-136.5	-62	98.3	-178.9
0466a.inp	5.5	-230.54	43.55	-159.2	142.8	-177.8	-179.8	61	-68.7	140.4	-173	-94.1	61.1	-178.6
0467.inp	4.71	-231.33	42.76	-156.3	155.5	-176.3	-171.7	69	-60.2	169	-46.6	-62.9	-172.8	-178.8
0468.inp	5.68	-230.36	43.73	-159.4	145.7	-177.4	179.8	53.2	-81	166.2	73.1	-62.6	-58.4	-178.8
0469.inp	2.37	-233.67	40.42	-156.4	-59.6	178.4	176	-141.4	97.1	61.3	-72.9	-178.6	168	-179
0470.inp	2.92	-233.12	40.97	-158.8	-45.2	178	178.8	-147.8	87.9	63.7	64.8	-174.9	-56.4	-178.6
0471.inp	2.91	-233.13	40.96	-158.5	-45.2	177.5	178.8	-147.5	89.3	58.2	-175.2	177.8	65.2	-178.8
0472.inp	5.63	-230.41	43.68	-159.5	-44.4	177.8	178.7	-144.4	88.5	-32.3	65.8	91.4	-58.2	-178.2
0473.inp	3.52	-232.52	41.57	-158.3	-49.9	177	175.8	-136.4	99.9	-60.3	-75.8	60.9	163.9	-178.2
0474.inp	3.87	-232.16	41.92	-158.9	-43.9	177.5	179.6	-147.3	87.2	-63.8	-179.9	57.3	59.2	-178.5
0475.inp	5.53	-230.51	43.58	-159.3	-44.9	177.2	177.6	-150.8	85.4	177.1	-145.6	-63.1	95.5	-178.4
0475a.inp	5.42	-230.62	43.47	-158.8	-46.5	177.5	178.3	-148.4	87.8	146.3	-178.8	-94.6	61.9	-178.6
0476.inp	3.72	-232.32	41.77	-157.7	-54.8	177.3	174.9	-139.1	98.4	168.6	-72.2	-71.6	169.3	-178.5
0477.inp	3.75	-232.29	41.8	-159.2	-43.7	177	179.2	-145.6	89	177.7	65.5	-61.1	-55.3	-178.6
0478.inp	4.67	-231.37	42.72	-155.5	-65.1	172.9	174.4	61	-67.5	50.7	-55.3	177.6	176.6	-179.1
0479.inp	6.77	-229.26	44.82	-156.6	-63.8	175	172	47.8	-84.5	50.1	63.7	-179.9	-68.4	-179.1
0480.inp	5.69	-230.34	43.74	-156.5	-62.2	176.6	170.7	60.5	-68.8	45.5	-168.6	171.6	63.3	-178.8
0481.inp	10.96	-225.08	49.01	-158	-66	174.4	176.4	79.9	-60.2	-56.9	105.3	80.1	-31.9	-178.6
0481a.inp	11.14	-224.94	49.19	-160.2	-50.2	173.7	-179.9	54.8	-84.2	-107.6	53.5	28	-82.7	-178.5
0482.inp	5.91	-230.13	43.96	-157.3	-61.3	174.6	177.7	80	-53.5	-67.7	-52.2	64.2	176.2	-179
0483.inp	6.75	-229.29	44.8	-157.9	-60	174.5	179.9	80.6	-53.6	-71.4	-165.3	60.1	63.4	-178.6
0484.inp	6.78	-229.25	44.83	-158.2	-57.5	176.7	178.3	67.9	-61.7	173.1	-139.9	-61	94.3	-178.6
0484a.inp	6.74	-229.3	44.79	-159.3	-51.4	176.1	179.1	59.6	-69.8	138.7	-171.3	-96	62.7	-178.5
0485.inp	4.61	-231.43	42.66	-157	-58.4	175.9	176.9	63.3	-66.2	166	-51.1	-67.2	-178.1	-178.9
0486.inp	7.17	-228.86	45.22	-158.5	-51.8	176.1	178.2	50.6	-83.3	164.3	70.6	-65.1	-60.9	-178.8
0487.inp	2.76	-233.28	40.81	-154.3	-114.4	-178.3	-178.3	-135.1	103.3	60.5	-59	-179.6	-178.4	-179
0488.inp	3.65	-232.39	41.7	-153.6	-117.1	-177.8	174.8	-155.7	80	60.4	52	-177.3	-69.4	-179.2
0489.inp	4.02	-232.01	42.07	-152.7	-116.2	-177.7	-179.8	-152.7	84.6	55	-175.6	174.6	64.8	-179.3
0490.inp	6.93	-229.1	44.98	-153.1	-115.8	-176	177.2	-152.7	79.1	-72	33.1	53.7	-92.2	-179.4
0490a.inp	7.12	-228.92	45.17	-153.4	-112.4	-177.9	176.8	-148.6	83.5	-33.9	63.9	91.2	-61.3	-179.3
0491.inp	3.96	-232.08	42.01	-153.7	-113.9	177.8	-175.2	-132.8	103	-57	-66.7	64.3	172	-179.2
0492.inp	4.48	-231.56	42.53	-156.6	-91.2	170.8	-175.4	-152.4	82.2	-63.1	-178.7	58.2	60	-178.9
0493.inp	5.67	-230.37	43.72	-157.1	-88	174	-177.8	-158.5	78.5	176.6	-142.3	-63.3	98.7	-178.6
0493a.inp	6.28	-229.76	44.33	-154.9	-101.9	176.8	-178.8	-153.9	82.6	146	-177.5	-94.9	63.2	-179.1
0494.inp	3.78	-232.25	41.83	-154.2	-110.9	178.6	-178.7	-137.8	99.6	173	-57.5	-66.9	-176.5	-179.1
0495.inp	4.65	-231.38	42.7	-154	-120.2	-176.8	176.5	-155.6	78.9	176.1	57.5	-61.9	-63.6	-179.4
0496.inp	4.42	-231.62	42.47	-153.6	-118.3	-177.4	-179.2	62.6	-66.3	53.1	-53	-179.9	179.7	-179.3
0497.inp	7.13	-228.91	45.18	-153.8	-114.2	-177.6	-175.5	49.3	-84.2	52.7	65.5	-176	-66.5	-179.4
0498.inp	5.46	-230.58	43.51	-153.3	-122.9	-174.7	-176.4	62.6	-67.1	50.9	-166.6	177.6	66.3	-179.5
0499.inp	12.94	-223.1	50.99	-152.7	-125.8	-172.6	176.4	52.3	-86.2	-107.9	52.6	26.8	-83.2	-179.6
0499a.inp	12.92	-223.11	50.97	-154.4	-151	-167.5	179.5	86.2	-52.7	-53	107.7	83	-27.6	-179.4
0500.inp	8.12	-227.92	46.17	-152.7	-132.2	-176.1	-177.8	79.9	-53.7	-66.9	-51.9	65	176.9	-179.6
0501.inp	8.21	-227.82	46.26	-153.9	-111.9	178	-172.5	79.6	-54.3	-68.1	-164	63.3	65.3	-179.2
0502.inp	7.79	-228.25	45.84	-154.3	-109.2	179.8	-172.7	66	-63.6	170.2	-140.4	-63.8	94.4	-179.2
0502a.inp	6.86	-229.76	44.91	-157	-83.1	172.6	-174.9	57.1	-72.3	135.9	-171.2	-98.5	62.7	-178.9
0503.inp	5.47	-230.57	43.52	-155.4	-100.2	175.6	-174.5	61.9	-67.7	164	-50.6	-69.1	-177.1	-179.1
0504.inp	9	-227.04	47.05	-153.4	-129.5	-173.9	178.9	49.5	-84.3	163.1	68.6	-66.5	-62.7	-179.4
0505.inp	3.53	-232.5	41.58	-135.1	114.9	179.9	178.5	-133.6	104.6	58.9	-62.1	178.9	178.3	0.9
0506.inp	4.34	-231.7	42.39	-132.9	122.9	-179.3	-179.2	-146.8	89.1	61.1	55	-177.8	-66.2	0.7
0507.inp	4.36	-231.68	42.41	-133.5	122	-179.8	179.6	-145.5	91.4	56.8	-174.2	176.3	66.1	0.6
0508.inp	7.35	-228.69	45.4	-133.3	126.7	-178.9	-179.9	-151.9	81.3	-64.5	30.4	59.3	-92.7	0.6
0508a.inp	7.13	-228.91	45.18	-133.2	135.3	-179.9	177	-142.3	90.4	-32.3	61.2	91.3	-62.6	0.8
0509.inp	4.53	-231.51	42.58	-133	131.8	177.5	178.2	-126.1	109.7	-56.2	-64.1	64.9	175	0.5
0510.inp	5.31	-230.72	43.36	-134.1	132.8	177.4	178.1	-122.2	112.4	-61.2	-179.2	59.4	60.1	0.7
0511.inp	6.99	-229.05	45.04	-135.8	135.4	177.7	176.9	-148.7	87.4	176.4	-144.2	-63.7	96.8	0.9
0511a.inp	6.72	-229.32	44.77	-136.1	137.4	177.9	174	-144.9	91.2	143.1	-178.1	-97.5	62.6	0.8
0512.inp	4.89	-231.14	42.94	-134.3	130.4	174.5	178.1	-130.4	106.6	172.9	-58.4	-67.4	-177.5	0.7
0513.inp	5.88	-230.16	43.93	-131.5	124.8	-179.5	-179.2	-148.4	86.2	178.1	60.6	-60.9	-60.1	0.4
0514.inp	4.99	-231.05	43.04	-130.9	109.2	176.5	178.3	62.7	-66.2	52.2	-57.4	179	175.4	0.2
0515.inp	8.02	-228.02	46.07	-135	117.4	178.7	178.3	52.7	-81.1	53.3	79.1	-175.5	-53.1	0.7
0516.inp	6.16	-229.88	44.21	-135.1	119.4	177.5	176.6	63.1	-66.5	49.3	-168.4	175.6	64.5	0.5
0517.inp	12.83	-223.2	50.88	-135.6	105.1	176	179.6	54.4	-84.6	-107.3	53.4	28.5	-82.8	1
0517a.inp	12.92	-223.12	50.97	-129.8	112	174.4	173.8	80.1	-59.9	-54.2	102.1	82.8	-35.1	0
0518.inp	7.94	-228.09	45.99	-134.7	107.7	175	179.3	80.2	-53.3	-68	-55.8	63.9	172.9	0.6
0519.inp	8.79	-227.25	46.84	-137.3	125.2	175.6	177.6	81	-53.4	-73.1	-167.4	58.3	61.4	0.9
0520.inp	8.06	-227.98	46.11	-137.1	122.7	174.8	174.3	60.1	-69.3	140.6	-171.9	-94.6	62.2	1
0520a.inp	8.33	-227.71	46.38	-137.3	120	173.6	176.3	68.3	-61.4	170.8	-140.1	-63.4	94.3	1.1

0521.inp	5.97	-230.07	44.02	-135.5	111.2	177.3	177.2	62	-67.4	162	-58.1	-71.5	175.2	0.9
0522.inp	8.58	-227.45	46.63	-134.1	118.7	178.4	177.7	53.2	-81.2	166	81.7	-63	-49.9	0.4
0523.inp	8.07	-227.97	46.12	-152.7	119.5	-178.8	2.6	-99.1	131	64.5	-63.3	-176.6	177.4	180
0524.inp	9.19	-226.85	47.24	-151.7	130.9	179	3.6	140.8	64.3	63.2	-177.4	177.5	-179.7	-179.8
0525.inp	8.38	-227.66	46.43	-151.9	132.3	179.4	4.6	-104.1	133.8	62.7	-169.3	-178.7	71.1	-179.7
0526.inp	11.25	-224.79	49.3	-156.8	133.3	178.2	2	-86.8	147.2	-27.5	64.7	95.1	-59	-178.9
0526a.inp	11.68	-224.36	49.73	-156.6	135.3	179.3	3.2	-91.7	142	-62.5	28.9	61.1	-94.3	-179.1
0527.inp	8.48	-227.56	46.53	-155.8	126	178	1.4	-84.4	152.7	-56.8	-66.1	63.5	173	-178.6
0528.inp	9.14	-226.9	47.19	-156.9	135.2	177.4	2.1	-91.3	143.3	-62.9	-175.7	58.1	62.9	-179
0529.inp	9.8	-226.23	47.85	-156.5	136.2	-179.8	4.2	-89	147	143.2	-173.8	-97.5	65.8	-178.8
0529a.inp	10.35	-225.69	48.4	-156.7	134.4	-178.6	2.9	-90	146.4	175.1	-151	-66.1	90.4	-178.8
0530.inp	8.15	-227.89	46.2	-156.5	128.5	-178.4	4.8	-85.1	153.2	165	-62.4	-75.9	178	-178.4
0531.inp	9.47	-226.57	47.52	-155.9	133.5	-177.8	2.7	-88.8	145.9	177.4	65.4	-61.6	-55.9	-179.2
0532inp	10.58	-225.46	48.63	-148.6	106.9	-178	0	73.2	-61.5	49.3	-45.3	-177.1	-178.4	179.1
0533.inp	15.97	-220.07	54.02	-159.5	114.8	-176.2	-1.5	64.6	-77	55.8	85.1	-164.2	-55.2	-173.7
0534.inp	11.67	-224.37	49.72	-152.5	109.1	-177.9	-1.1	74	-61.1	49.3	-155.8	-178	71.5	-178.7
0535.inp	19.4	-216.64	57.45	-155.6	117.4	-172.3	-0.9	60.5	-84.7	-127.4	60	14.6	-82.4	-179.6
0536.inp	15.62	-220.42	53.67	-151.7	96.6	-174.2	-0.3	90.6	-49.1	-68.3	-52.6	70.7	169.3	179.7
0537.inp	16.02	-220.02	54.07	-152.2	94.8	-174.2	-0.4	94.2	-37.8	-65.6	-152.5	72.3	71.7	-179.8
0538.inp	13.55	-222.48	51.6	-152.1	116.9	-175.4	-1	73.6	-60.3	164	-129.5	-64.8	99.7	-178.6
0538a.inp	13.43	-222.61	51.48	-151.5	112.5	-174.6	-1.2	67.1	-67.4	132.6	-168.9	-96.4	59.8	-178.8
0539.inp	11.96	-224.07	50.01	-147.8	115.3	-174.8	-0.1	70.7	-64.2	158.8	-41.9	-68.1	-174.5	-179.7
0540.inp	15.77	-220.26	53.82	-154.9	121.7	-175.2	-2.9	58.5	-82.2	155.7	74.9	-66.1	-64	-179.3
0541.inp	2.27	-233.77	40.32	-144.2	117.2	-60.4	179.5	-135.7	102.5	60.8	-62.2	-179.3	178.3	-176.9
0542.inp	3.1	-232.93	41.15	-142.8	127.5	-59.6	-177.9	-148.7	87.3	63.7	55.7	-175.1	-65.4	-176.7
0543.inp	3.06	-232.98	41.11	-143.4	127.5	-59.3	-179.2	-147	89.9	58.4	-173.9	177.8	66.5	-176.6
0544.inp	5.57	-230.47	43.62	-142.6	130.7	-59.6	-176.7	-150.6	82.6	-64.7	30.8	59.1	-92.6	-176.7
0544a.inp	6.03	-230	44.08	-143.3	129.6	-59.3	-179.6	-146.2	86.9	-31.1	61.7	92.4	-62.3	-176.6
0545.inp	3.52	-232.52	41.57	-143.7	122.5	-59.3	179.5	-136.9	99	-61.4	-66.5	60.1	172.4	-176.5
0546.inp	4.01	-232.03	42.06	-143.2	129.7	-58.8	-178.6	-146.7	87.7	-64.9	-179.1	56.4	59.7	-176.5
0547.inp	4.08	-231.96	42.13	-143.5	129.8	-59.2	-178.9	-151.2	85.1	177	-143.3	-63.2	97.5	-176.5
0547a.inp	5.4	-230.64	43.45	-143.6	129.4	-59.1	179.4	-148	88.1	146	-178.3	-94.9	62.3	-176.5
0548.inp	1.72	-234.32	39.77	-143.7	122.2	-58.7	179.7	-136	101.1	172.2	-59.5	-67.8	-178.7	-176.4
0549.inp	2.1	-233.94	40.15	-142.8	131.2	-58.6	-177.5	-148	86.7	178.3	61.5	-60.6	-59.4	-176.7
0550.inp	3.62	-232.42	41.67	-143.9	120.8	-59.1	-179.8	63.4	-65.3	52.6	-53.3	179.6	179.5	-176.8
0551.inp	6.2	-229.84	44.25	-143	130.7	-57.7	-177.5	51.7	-81.7	52.1	66.4	-176.6	-65.5	-176.8
0552.inp	4.5	-231.54	42.55	-144.4	126.4	-57.7	179.4	63.1	-66.4	49.6	-167.7	176.1	65.2	-176.4
0553.inp	10.86	-225.18	48.91	-143.6	127	-57.6	-179	54.8	-84.1	-107.4	53.4	28.2	-82.7	-176.7
0553a.inp	11	-225.04	49.05	-143.6	116.3	-58.2	179.5	82.6	-56.6	-53.8	107.4	82.5	-28.4	-176.4
0554.inp	6.3	-229.74	44.35	-144	119.2	-57.7	178.8	80.5	-52.9	-76.2	-52.2	64.6	176.4	-176.2
0555.inp	7.04	-229	45.09	-144.4	122.2	-57	179.8	80.5	-53.8	-72.6	-166.4	58.9	62.5	-176.2
0556.inp	6.51	-229.52	44.56	-144.5	125.1	-57.1	-179.7	68	-61.5	171	-140.2	-63.1	94.3	-176.1
0556a.inp	6.48	-229.56	44.53	-143	129.9	-57	178.7	60.2	-69.2	140	-171.3	-94.6	62.8	-176.3
0557.inp	4.44	-231.6	42.49	-143.8	127.5	-56.5	-179.7	64.7	-64.8	166.3	-50.7	-66.3	-177.3	-176.3
0558.inp	6.91	-229.13	44.96	-143.4	136.4	-55.5	-179.5	52.2	-81.9	165.3	71	-63.9	-60.4	-176.3
0559.inp	2.66	-233.38	40.71	-138.2	-0.2	-56.6	179.5	-133.2	105.2	60.6	-62	-179.7	178.7	-177.4
0560.inp	3.4	-232.64	41.45	-138.7	0.9	-58.8	-178.3	-149.5	86.6	62.9	54.8	-176.2	-66	-177.8
0561.inp	3.51	-232.53	41.56	-138.4	0.8	-57.9	-180	-147.4	89.6	57.4	-174.1	176.8	66.5	-177.7
0562.inp	5.58	-230.46	43.63	-138.5	5.1	-57.6	-176.6	-150.9	82.6	-63.6	30.5	59.9	-92.4	-177.9
0562a.inp	5.87	-230.17	43.92	-135.8	4.8	-56.9	-179.6	-147.3	86.3	-30	60.8	92.9	-62.5	-178.8
0563.inp	3.62	-232.42	41.67	-136.7	-6	-58	178.9	-134.4	101.6	-59.3	-65.8	61.9	173.5	-177.6
0564.inp	4.22	-231.82	42.27	-138.4	3.1	-56.9	-178.7	-146.5	88.1	-63.6	-179.4	57.3	59.8	-177.8
0565.inp	5.78	-230.25	43.83	-137.9	3.5	-56.8	-179.6	-150.5	85.9	177.2	-144.1	-63.2	97.1	-177.3
0565a.inp	5.91	-230.13	43.96	-137.8	2.8	-56.7	179.3	-148.1	88.2	146.2	-178.4	-94.8	62.4	-177.1
0566.inp	3.72	-232.32	41.77	-137.3	-6.3	-57.7	178.9	-135.1	102.1	172.7	-59.4	-67.5	-178.4	-176.6
0567.inp	4.17	-231.86	42.22	-138.5	4.8	-57	-176.7	-148.7	86.2	178.6	60.5	-60.6	-60	-177.3
0568.inp	4.24	-231.8	42.29	-136	0	-58.7	178.6	63.8	-65.1	52.4	-53.5	179.5	179.2	-177.2
0569.inp	6.98	-229.06	45.03	-136.9	0.1	-60	178.2	51.5	-81.8	51.7	66.5	-177.2	-65.5	-177.1
00570.inp	5.11	-230.93	43.16	-137.4	0.3	-60.6	179.7	64	-65.6	50.1	-166.6	176.7	66.3	-177
0571.inp	11.8	-224.24	49.85	-137.6	0.1	-62.4	177.6	54.3	-84.5	-108.6	53.4	26.6	-82.6	-177.1
0571a.inp	11.65	-224.39	49.7	-137.4	-15	-61.6	179.9	83.8	-55.3	-53.5	108	82.7	-27.5	-176.7
0572.inp	7.03	-229	45.08	-135.1	0.7	-61.1	178.9	81.4	-52.1	-66.6	-52.3	65.4	176.3	-177.3
0573.inp	7.73	-228.31	45.78	-136.6	0.3	-62	170.7	81.6	-52.6	-71.4	-165.4	60.1	63.6	-177.2
0574.inp	7.19	-228.85	45.24	-136.4	0.1	-59.1	179.3	68.7	-60.9	171.2	-139.9	-62.8	94.6	-176.8
0574a.inp	7.15	-228.89	45.2	-139.1	6.8	-58.4	-179.1	60.6	-69	139.8	-171.1	-94.6	62.9	-176.9
0575.inp	5.19	-230.85	43.24	-137.6	1.5	-59.1	-180	65.2	-64.5	167.1	-50.9	-65.8	-177.6	-176.9
0576.inp	7.76	-228.28	45.81	-137.8	0.9	-59.4	177.9	51.5	-82.6	164.5	70.9	-64.6	-60.6	-176.8
0577.inp	2.15	-233.88	40.2	-146.2	151.3	-61.1	179.7	-128.2	109.8	62.1	-62.2	-178.1	178.2	-176.6
0578.inp	3.23	-232.81	41.28	-145.2	154.4	-60.7	-179.6	-130.9	104.7	64.5	57.9	-174.4	-63.2	-176.6
0579.inp	3.13	-232.91	41.18	-145.3	153.7	-60.6	-179.8	-129.2	107.6	59.6	-173.4	179	66.9	-176.3
0580.inp	5.84	-230.2	43.89	-143.7	160.2	-60.3	-177.1	-138.4	94.7	-64.1	30.7	59.5	-92.5	-176.3
0580a.inp	6.03	-230	44.08	-144.5	157.9	-60.4	179.8	-133.4	99.7	-30.9	62.5	92.4	-61.3	-176.2
0581.inp	3.41	-232.63	41.46	-145	154	-60.1	179.3	-129.1	106.5	-59.8	-65.7	61.5	173.2	-176.4
0582.inp	4.14	-231.9	42.19	-145.1	154.9	-59.8	179.6	-128.7	105.6	-63.7	-179.1	57.2	59.9	-176.2
0583.inp	5.29	-230.75	43.34	-144.8	154.5	-60.6	179	-150.6	85.7	176.8	-143.2	-63.3	97.6	-176.4
0583a.inp	5.41	-230.63	43.46	-144.9	153.9	-60.1	179	-145.1	91	146.2	-178.3	-94.8	62.4	-176.4
0584.inp	3.26	-232.78	41.31	-145	152.9	-60.1	178.8	-131.3	105.8	173.2	-59.3	-67	-178.4	-176.2
0585.inp	4.01	-232.03	42.06	-144.2	158	-60.1	-178.7	-138.7	95.8	178.7	62.3	-60.4	-58.4	-176
0586.inp	3.68	-232.36	41.73	-144	165.8	-57.8	179.7	65.5	-63.2	53.9	-53.1	-178.9	179.8	-176.4

0587.inp	6.22	-229.82	44.27	-144.7	156.6	-59.5	179.2	52.5	-80.7	52.3	66.2	-176.7	-65.6	-176.4
0588.inp	4.49	-231.54	42.54	-146.7	148.6	-59.9	178.4	64.4	-65.1	50.5	-166.7	-166.7	66.3	-176.3
0589.inp	10.81	-225.23	48.86	-143.9	152.2	-56.3	179.5	55.7	-83.2	-107.6	53.4	27.9	-82.7	-176.1
0589a.inp	10.93	-225.11	48.98	-145.6	136.8	-57.3	177.9	82.7	-56.5	-53.9	106.8	82.5	-29.2	-175.7
0590.inp	6.16	-229.88	44.21	-146.8	140.6	-57.6	177.9	81.1	-52.4	-67.2	-52.4	64.7	176.2	-176.2
0591.inp	6.92	-229.12	44.97	-145.6	138.1	-58.3	-178.2	81.8	-52.3	-71.3	-165.4	60.2	63.7	-176.2
0592.inp	6.44	-229.59	44.49	-146.6	145.2	-59.9	178.2	68.7	-60.9	171.2	-140.1	-63	94.4	-176
0592a.inp	6.43	-229.61	44.48	-144.8	149.3	-59.4	-179.9	61.6	-68.4	140	-171	-94.6	63.1	-176.2
0593.inp	4.4	-231.64	42.45	-146.7	146.3	-59.3	178.2	64	-65.5	164.6	-52.7	-68.5	-179.4	-176
0594.inp	6.86	-229.18	44.91	-145.5	153.7	-58.9	177.4	52.6	-81.4	165	70.6	-64.3	-60.8	-176.1
0595.inp	2.47	-233.57	40.52	-143.1	-50.3	-60.3	179.8	-135.9	102.5	60.1	-62.6	179.8	178.2	-177.4
0596.inp	3.31	-232.72	41.36	-144.6	-45.6	-60.1	-179.6	-146.9	88.9	62.9	58.5	-175.8	-62.5	-177.1
0597.inp	3.33	-232.7	41.38	-143.5	-43.5	-59.6	179.7	-147.2	89.8	57.8	-173.9	177.2	66.7	-177.1
0598.inp	5.88	-230.16	43.93	-143.7	-41.1	-59.2	179	-148.5	84.9	-63.7	29.5	60.3	-93.5	-176.4
0598a.inp	6.07	-229.97	44.12	-142	-40.6	-58.8	179.5	-148	85.3	-30.9	61.6	92.6	-62.2	-176.7
0599.inp	3.67	-232.37	41.72	-142.7	-47.3	-59.6	179.6	-135.6	100.5	-59.3	-65.9	61.9	173.4	-176.5
0600.inp	4.36	-231.68	42.41	-143.4	-40.9	-58.8	-178.9	-142.3	92.2	-63.5	-179.3	57.4	59.9	-176.6
0601.inp	5.8	-230.23	43.85	-143.6	-40.5	-58.4	-179.9	-150	86.4	177.1	-144.2	-63.3	97	-176.9
0601a.inp	6.07	-230.13	44.12	-142.7	-41	-58.2	179.2	-147.8	88.5	146.2	-178.4	-94.9	62.4	-176.7
0602.inp	3.69	-232.35	41.74	-142.6	-47.5	-58.9	179.4	-136.2	101	172.3	-59.7	-67.9	-178.7	-176.4
0603.inp	4.26	-231.78	42.31	-143.5	-39.1	-58.2	-178.1	-145.2	89.6	178.6	62.2	-60.5	-58.4	-176.4
0604.inp	4.02	-232.02	42.07	-141.9	-52.6	-60.3	178.4	62.9	-65.9	52.7	-53.2	179.8	179.4	-177.7
0605.inp	6.89	-229.15	44.94	-141.8	-50.9	-60.7	177.9	50.1	-83.1	52	65.4	-177.2	-66.6	-176.9
0606.inp	5.06	-230.98	43.11	-141.6	-49.6	-60.1	178.9	62.9	-66.7	49.9	-167.2	176.4	65.5	-176.7
0607.inp	11.73	-224.3	49.78	-141.2	-53.7	-63.2	176.5	51.2	-87.1	-107.8	52.1	26.9	-83.6	-177.3
0607a.inp	11.63	-224.41	49.68	-142.4	-52.7	-59.5	-178.4	81.9	-57.2	-53.7	107.4	82.5	-28.3	-176.4
0608.inp	6.94	-229.1	44.99	-141.3	-56.2	-60.4	179.6	79.6	-54	-67.4	-52.2	64.5	176.3	-177.3
0609.inp	7.75	-228.29	45.8	-142	-54.3	-61.3	-177.5	79.7	-54.6	-72.7	-166.2	58.8	62.8	-176.6
0610.inp	7.2	-228.83	45.25	-142.1	-51.2	-58.4	-179.4	67.4	-62.2	170.9	-140.2	-63.2	94.3	-176.5
0610a.inp	7.18	-228.86	45.23	-143.6	-45.6	-58	-178	60	-69.6	140.2	-171.3	-94.4	62.8	-176.4
0611.inp	5.01	-231.02	43.06	-141	-52.4	-59.3	177.3	63	-66.6	164.4	-51.6	-68.9	-178.4	-177.5
0612.inp	7.67	-228.36	45.72	-141.4	-46.4	-59.9	178.3	50.6	-83.4	163.8	70	-65.6	-61.4	-176.6
0613.inp	3.88	-232.16	41.93	-138	-122.7	-58.1	178.9	-103.8	134.5	62.1	-61	-178.6	179.4	-177
0614.inp	4.97	-231.07	43.02	-138.3	-124	-58.1	178.2	-101.7	134.2	65.7	60	-173.4	-61.2	-176.8
0615.inp	4.85	-231.19	42.9	-137.9	-127.1	-57.5	177.9	-102	135.1	58.9	-172.9	178	67.4	-176.9
0616.inp	7.46	-228.57	45.51	-138	-125.2	-58.9	179.5	-82.1	151.2	-60.6	31.2	63.3	-92.3	-177
0616a.inp	6.88	-229.16	44.93	-138.1	-130.3	-57	177.1	-78.3	155.2	-30	64.1	93	-59.6	-176.9
0617.inp	4.61	-231.42	42.66	-137.5	-128	-58.5	-179.9	-81.8	154.3	-54.5	-63	66.5	175.7	-177.5
0618.inp	5.45	-230.58	43.5	-137.7	-123.6	-58.1	178.7	-81.4	153.4	-60	-178.1	60.7	60.8	-176.9
0619.inp	7.01	-229.02	45.06	-137.6	-124.2	-58.5	-179.5	-81.6	154.8	142.4	-176.5	-98.4	63.4	-176.9
0367a.inp	6.91	-229.13	44.96	-95.7	79.4	51.1	-178.8	-85.8	150.5	143.3	-176.6	-97.7	63.5	179.6
0620.inp	4.74	-231.3	42.79	-138	-125	-58	-179.4	-86.9	150.1	173.8	-58.1	-66.7	-177.7	-176.9
0621.inp	5.56	-230.48	43.61	-138	-124.3	-58.7	179.7	-83.1	151.5	179.4	64.5	-59.6	-56.8	-176.9
0622inp	5.42	-230.62	43.47	-137.8	-120.7	-59.1	178.3	65.4	-63.5	53.6	-52.4	-179.2	-179.7	-177
0623.inp	8.2	-227.9	46.25	-137.8	-110.8	-61.9	179.2	52	-81.5	52.2	66.3	-176.6	-65.8	-177.2
0624.inp	6.37	-229.67	44.42	-137.2	-124.5	-58.9	179.5	65.3	-64.3	51.2	-165.4	177.9	67.6	-177.2
0625.inp	12.81	-223.23	50.86	-137.7	-111.2	-62.1	178.2	54.8	-84.1	-108.3	53.2	27	-82.8	-177.2
0625a.inp	12.89	-223.15	50.94	-137.5	-121.4	-58.8	179.9	85	-53.9	-53.5	108.3	82.7	-27.2	-177
0626.inp	8.17	-227.87	46.22	-137.9	-117.7	-61.6	-179	81.9	-51.5	-66.7	-51.7	65.4	177.2	-177.1
0627.inp	8.99	-227.05	47.04	-136.6	-116.8	-61.4	-177.6	82.7	-51.3	-70.5	-163.8	61	65.4	-177.2
0628.inp	8.44	-227.6	46.49	-137.4	-109.2	-60.6	179.6	69.1	-60.4	171.2	-139.8	-62.8	94.8	-176.9
0628a.inp	8.48	-227.56	46.53	-137.8	-110.4	-62.8	-178.8	60.6	-69	139.9	-171	-94.4	63	-177
0629.inp	6.3	-229.74	44.35	-137.7	-109.8	-61.9	178.3	65.5	-64.2	166.2	-50.2	-66.8	-176.1	-177.2
0630.inp	8.9	-227.13	46.95	-138.4	-112.4	-62.8	178	52.3	-81.8	164.8	70.8	-64.3	-60.8	-177.3
0631.inp	2.26	-233.78	40.31	-138.7	56.2	-58.7	-179.4	-128.8	109.4	61.2	-61.1	-179.2	179.4	-177.6
0632.inp	3.01	-233.02	41.06	-137.6	62.8	-59.1	-177.1	-141.7	94.2	63.8	55.2	-175.5	-65.6	-178.6
0633.inp	3.33	-232.7	41.38	-137.5	62.1	-58.9	-178.4	-140	96.9	58.7	-174	177.8	66.6	-178.2
0634.inp	5.37	-230.67	43.42	-134.1	65.8	-58	-177.8	-143.5	89.8	-64.2	30.2	59.3	-92.8	-178.9
0634a.inp	5.75	-230.29	43.8	-133.8	61.7	-59.2	-178.4	-141.7	91.7	-30.5	60.4	92.3	-63	-179.2
0635.inp	3.35	-232.69	41.4	-136.1	53.6	-58.5	-178.4	-129	106.9	-59.3	-64.5	61.8	174.5	-178.1
0636.inp	4.14	-231.9	42.19	-136.4	61.2	-58.6	-178.7	-139.5	95	-64.2	-179.1	56.6	59.9	-178
0637.inp	5.5	-230.54	43.55	-137.5	64.1	-58.6	-178.7	-145.6	90.8	177.5	-144.6	-63.1	96.6	-177.7
0637a.inp	5.59	-230.45	43.64	-137.6	63	-58.6	179.6	-143.8	92.3	146.8	-178.4	-94.4	62.4	-177.4
0638.inp	3.24	-232.79	41.29	-137.5	55.8	-59.4	179.8	-133.4	103.8	173.1	-58.5	-67.2	-177.5	-177.7
0639.inp	3.68	-232.36	41.73	-136.1	62.6	-59.3	-176.3	-145.3	89.6	178.8	60.2	-60.7	-60.3	-178.9
0640.inp	3.73	-232.31	41.78	-138.7	51.1	-58.8	-179.5	64.2	-64.7	52.9	-53.7	-179.9	179.2	-177.4
0641.inp	6.4	-229.64	44.45	-139.7	58.6	-59	179.7	52.2	-81.2	52	67	-176.7	-65	-177.2
0642.inp	4.48	-231.5	42.53	-138.9	54.9	-59	-178.6	64.7	-64.9	50.9	-165.8	177.7	67.2	-177.7
0643.inp	11.27	-224.76	49.32	-139.3	54.5	-58.9	179.6	54.6	-84.3	-108	53.6	27.4	-82.5	-177.1
0643a.inp	11.07	-224.97	49.12	-139.4	61	-60.8	-179.2	84.3	-54.5	-53	108	83	-27.3	-177.3
0644.inp	6.51	-229.53	44.56	-139.2	58.6	-59.7	-179.3	81.5	-51.7	-66.3	-52.4	65.6	176.6	-177.1
0645.inp	7.16	-228.88	45.21	-139.5	59.3	-59.5	-178	82.4	-51.6	-70.1	-164.5	61.3	64.9	-177
0646.inp	6.72	-229.32	44.77	-138.9	62.4	-58.3	-178.7	69.2	-60.2	171.4	-140.2	-62.8	94.7	-177
0646a.inp	6.73	-229.3	44.78	-139.1	53.8	-59	-179.1	60.5	-69	139.9	-171.4	-94.6	62.8	-177.4
0647.inp	4.86	-231.18	42.91	-138	48.2	-58.9	178	64.5	-65.1	165.2	-51.7	-68	-178.4	-177.2
0648.inp	7.3	-228.74	45.35	-138.4	54.9	-59.2	178.4	51.9	-82.2	164.5	71	-64.7	-60.5	-177.3
0649.inp	4.53	-231.51	42.58	-110.3	118.9	-60.8	-179.4	-129	109	60.6	-61.6	-179.7	178.9	1.1
0650.inp	5.89	-230.15	43.94	-113.7	120.4	-60.9	179.5	-127.9	107.5	64.5	63.3	-174.1	-57.9	1.3
0651.inp	5.74	-230.3	43.79	-110.7	121.6	-60.2	179.7	-127.8	108.9	57.9	-174.2	177.2	66.4	1.4

0652.inp	7.78	-228.26	45.83	-115.5	115.9	-61.1	-178.9	-151.3	81.9	-64.5	30.1	59.5	-93.2	0.6
0652a.inp	8.41	-227.63	46.46	-115.3	113	-61.2	178.1	-146	87	-31.5	62.9	92.3	-61.3	0.9
0653.inp	5.74	-230.3	43.79	-109	106	-60.9	-178.5	-135	100.9	-60.6	-64.9	60.6	174.3	0.4
0654.inp	6.43	-229.61	44.48	-105.9	114.5	-59.8	-176.9	-147.1	87.6	-64.4	-179.2	56.5	59.9	0.6
0655.inp	7.89	-228.15	45.94	-113.3	119.7	-60.5	-179.7	-151.7	84.6	176.9	-143.1	-63.2	97.7	1.5
0655a.inp	7.97	-228.07	46.02	-108.8	119.6	-60.1	179.6	-147.9	88.3	146.1	-178.4	-94.9	62.3	1.3
0656.inp	5.56	-230.48	43.61	-107.7	111.3	-60.4	-178.5	-134.8	102.4	172.9	-58.3	-67.4	-177.4	0.5
0657.inp	6.46	-229.58	44.51	-116.9	118.1	-61.2	-179.2	-142.5	91.9	178.4	64.6	-60.2	-56.5	1.1
0658.inp	6	-230.04	44.05	-109.7	114.9	-60.9	179.1	63.4	-65.3	51.7	-53.2	178.7	179.6	0.6
0659.inp	8.62	-227.41	46.67	-106.9	126	-58.8	-179.6	51.5	-81.7	51.4	65.8	-177.5	-66	0.8
0660.inp	6.89	-229.15	44.94	-110.3	118.8	-60.2	179.5	63.4	-66.1	49	-167.1	175.6	65.8	0.8
0661.inp	13.65	-222.38	51.7	-115.3	109.5	-60.1	176.1	52.8	-85.6	-108.1	52.7	26.7	-83	1.7
0661a.inp	13.57	-222.47	51.62	-117.3	92	-64.6	179	83.4	-55.6	-53.4	107.3	82.8	-28.4	0.7
0662.inp	8.95	-227.09	47	-117	88.3	-63.3	178.8	81.4	-52	-66.3	-52.1	65.6	176.7	0.7
0663.inp	9.64	-226.4	47.69	-117.2	87	-62.2	-179.4	82.3	-52.2	-71.1	-165.4	60.3	63.7	0.7
0664.inp	9.17	-226.87	47.22	-114.8	114.8	-62.1	179.6	68.5	-61	171.2	-140.2	-62.9	94.4	1.3
0664a.inp	9.14	-226.9	47.19	-111.2	110.6	-61.6	-178	60.4	-69.2	140	-171.2	-94.5	63	0.8
0665.inp	7.17	-228.87	45.22	-112.3	105	-61	178.7	64.3	-65.2	165.3	-51	-67.9	-177.5	0.8
0666.inp	9.65	-226.39	47.7	-114	115.4	-59.5	178	51.2	-82.7	164	69.6	-65.4	-61.7	1.7
0667.inp	7.76	-228.28	45.81	-136.5	84.4	-65.1	-4.6	-126.7	112	63.7	-64.7	-176.8	176.2	-177.2
0668.inp	9	-227.04	47.05	-134.6	86	-65.4	-1.5	-136.7	99.1	66.1	58.6	-172.6	-62.4	-177.9
0669.inp	8.58	-227.46	46.63	-135.1	84.7	-64.7	-2.2	-138.6	98.2	61.3	-169.9	-179	70.5	-178.1
0670.inp	11.77	-224.27	49.82	-136.7	85.4	-63	-2.6	-142.7	91.3	-64.7	26.9	59.1	-95.7	-176.5
0670a.inp	12.43	-223.61	50.48	-136.9	85	-63.1	-5	-136.9	96.3	-31.6	63	92.1	-60.8	-176.3
0671.inp	9.81	-226.23	47.86	-135.3	88.6	-64.7	-5.7	-127.2	109.3	-61.3	-68.4	59.8	171.2	-176.4
0672.inp	10.03	-226	48.08	-136.2	84.2	-63.5	-2.6	-138.7	95.8	-63.5	-177	56.1	61.8	-176.7
0673.inp	10.43	-225.61	48.48	-136.3	85.4	-62.7	-3.2	-146.1	90.5	176.3	-142.8	-63.8	98.1	-177
0673a.inp	11	-225.04	49.05	-135.6	84	-62.5	4	-138.7	97.5	143.8	-175.6	-96.7	64.8	-177.2
0674.inp	9.25	-226.79	47.3	-133.9	84.6	-67	-4.5	-125.2	112.1	170.4	-62.6	-70	178.5	-178
0675.inp	9.96	-226.08	48.01	-136.6	82.5	-63.8	-1.8	-137.2	97.4	177.8	63.1	-60.9	-57.8	-177.4
0676.inp	11.79	-224.25	49.84	-144.3	107.8	-60.6	-2.4	72.3	-62.3	43.8	-45.2	177.2	-178.6	-177.6
0677.inp	15.57	-220.47	53.62	-146.2	127.8	-57.9	-3.7	58.3	-82.2	50.9	72.7	-170.6	-66.9	-176.6
0678.inp	12.85	-223.19	50.9	-145.1	106	-60.1	-5.6	72.4	-62.5	36.9	-162.6	169.4	64	-176.8
0679.inp	18.74	-217.3	56.79	-146.9	127.1	-60.2	-4.9	59.4	-84.6	-133.2	60	7	-81.4	-177.1
0679a.inp	15.72	-220.31	53.77	-143.8	105.2	-64.9	-0.7	90.1	-48.9	-70.2	149	67.4	-74.5	-177.1
0680.inp	15.01	-221.03	53.06	-144.1	103.8	-65.2	-0.03	87.1	-52.9	-71.5	-47.6	67.7	174.3	-178.7
0681.inp	15.72	-220.32	53.77	-145.2	101.3	-66.9	-0.4	90.5	-48.4	-69.2	-149.7	68.3	74.1	-177.8
0682.inp	13.99	-222.05	52.04	-142.7	107.5	-58.8	-0.1	75.9	-58.4	169.9	-131.6	-58.7	97.6	-177.1
0682a.inp	13.95	-222.08	52	-143.8	110.1	-58.7	-3.8	67.2	-66.7	128.6	-167.2	-100.7	61.7	-176.7
0683.inp	12.68	-223.36	50.73	-144.9	102.7	-59.9	-1.1	74	-61.2	161.4	-44.1	-65.3	-176.7	-178.5
0684.inp	15.73	-220.31	53.78	-144.2	130.1	-57.5	-3.3	53.2	-86.1	149.2	69.5	-74.2	-68.3	-176.7
0685.inp	1.56	-234.47	39.61	-158.4	147	60.6	179.5	-137	101.2	60	-62.9	-179.9	177.5	-178
0686.inp	2.31	-233.73	40.36	-158.2	156.2	59.2	-179.6	-148.3	87.5	63	56.6	-175.6	-64.7	-177.7
0687.inp	2.22	-233.82	40.27	-158.4	157	58.8	179.8	-147.4	89.5	58.2	-174.1	177.8	66.1	-177.4
0688.inp	5.16	-230.88	43.21	-158.5	160	58.7	-179.2	-149.5	83.5	-64.7	30.9	59.3	-92.4	-177.5
0688a.inp	5.47	-230.57	43.52	-159.2	159.1	58.6	178	-144.7	88.2	-31.2	62	92.5	-61.9	-177.6
0689.inp	3.03	-233.01	41.08	-159.3	153.2	58.9	177.9	-136.3	99.5	-61.4	-66.9	60.2	172.1	-177.6
0690.inp	3.47	-232.57	41.52	-159	160.4	58.6	179.7	-145	89.3	-64.8	-179	56.5	59.8	-177.6
0691.inp	4.76	-231.27	42.81	-159	160	58.1	178.8	-148.9	87.3	176.9	-144.1	-63.3	96.9	-177.4
0691a.inp	4.83	-231.21	42.88	-159.2	160.1	58.1	177.4	-145.8	90.2	145.6	-178.2	-95.2	62.4	-177.4
0692.inp	2.78	-233.26	40.83	-159.8	154.3	58.6	177.2	-135.1	101.9	171.9	-60.2	-68.1	-179.2	-177.6
0693.inp	3.37	-232.68	41.42	-158.8	162.3	58.3	179.9	-144.3	90.2	178.1	61.9	-60.7	-58.9	-177.5
0694.inp	3.04	-233	41.09	-159	144.4	58.4	-179	61.3	-67.5	52.5	-60.2	179.3	172.4	-177.4
0695.inp	5.61	-230.43	43.66	-157.7	154.1	60.3	-177.1	53.7	-80.1	53.6	77.2	-174.8	-54.9	-177.9
0696.inp	3.81	-232.23	41.86	-158.6	150.6	60	179.8	63.2	-66.4	50.1	-168.4	176.6	64.5	-177.5
0697.inp	10.5	-225.54	48.55	-159.9	145.1	60.8	175	76.5	-64.3	-54	95.4	84.2	-43.1	-177.7
0697a.inp	10.86	-225.18	48.91	-157.8	156.1	62.1	-172.6	59.3	-81.1	-104.5	59.4	33.3	-78.1	-177.7
0698.inp	6.02	-230.01	44.07	-158.5	138.6	58.9	179.6	77.6	-56.2	-70.5	-60.4	61.5	167.8	-177.6
0699.inp	6.38	-229.66	44.43	-159.2	144.7	58.2	-179.4	80.1	-54.2	-73.2	-166.8	58.2	62	-177.8
0700.inp	5.94	-230.1	43.99	-159.1	148.2	60.2	-178.6	67.9	-61.6	171.1	-141.1	-63	93.5	-177.5
0700a.inp	5.68	-230.35	43.73	-158.4	153.6	59.3	-179.8	60.2	-69.3	140.1	-172.1	-94.6	62.1	-177.7
0701.inp	3.92	-232.12	41.97	-158.3	145.5	59	179.6	60.8	-68.6	161.7	-60.4	-71.8	172.9	-177.6
0702.inp	6.13	-229.9	44.18	-157.9	153.6	59.8	-178.2	54.1	-80.3	166.6	80.6	-62.1	-51	-177.7
0703.inp	1.07	-234.97	39.12	-152.2	7.1	59.6	-175.5	-106.8	131.4	62.4	-57.9	-177.8	-177.8	-177.8
0704.inp	1.48	-234.56	39.53	-152.2	3.6	59.9	-175.1	-148.9	87.3	63.5	55.3	-175.9	-65.4	-177.8
0705.inp	2.37	-233.67	40.42	-152.5	0.1	59.6	179.6	-146.8	90.1	57	-175.1	176.3	65.5	-177.8
0706.inp	4.17	-231.87	42.22	-152.1	8.2	61.2	-175.7	-145.3	86.9	-62.9	38.4	61.1	-85.3	-178.4
0706a.inp	3.94	-232.1	41.99	-149.7	-0.9	61.4	-176.9	-144.8	89	-29.8	60.1	92.5	-62.8	-178.8
0707.inp	2.93	-233.11	40.98	-151.8	3.4	62.6	175.3	-135.5	101.1	-60.7	-72.8	60.6	166.9	-178.4
0708.inp	2.88	-233.16	40.93	-152.1	-1.6	61.3	-177.1	-148.2	86.6	-63.6	179.5	57.1	58.9	-177.9
0709.inp	4.68	-231.36	42.73	-152.9	1	59.7	-178.9	-148.5	88	177.2	-143.8	-63.3	97.4	-177.8
0709a.inp	4.66	-231.38	42.71	-153.1	-2.3	59.7	-178.8	-146.8	89.5	147	-179.5	-94.4	61.4	-177.4
0710.inp	3.55	-232.49	41.6	-152.5	-8.8	61.8	172.7	-136.3	101.4	168.2	-73.7	-72	167.9	-177.7
0711.inp	2.19	-233.85	40.24	-152.3	0.1	61.6	-176.7	-150.2	84.8	178.4	60.8	-60.9	-59.6	-177.7
0712inp	2.74	-233.3	40.79	-152.7	14.5	57.2	-176.2	65.1	-63.9	55.7	-52.8	-176.9	-179.7	-177.6
0713.inp	5.77	-230.27	43.82	-151.6	12.8	61.1	179.5	52.8	-80.8	55.6	68	-173	-64.2	-178
0714.inp	3.47	-232.56	41.52	-154	12.9	60.3	-174.7	66.1	-63.5	55.4	-163.1	-178	70.4	-177.4
0715.inp	10.65	-225.39	48.7	-154.3	5.9	60.8	-179.3	55.8	-83.5	-106.6	53.9	29.5	-82.7	-177.1
0715a.inp	10.68	-225.37	48.73	-154.1	4.6	62.5	-174.2	59.1	-81	-103.1	54.5	34.2	-82.7	-177.4

0716.inp	6.14	-229.9	44.19	-151.7	2.1	58	-178	80.4	-53.7	-76.7	-53.5	55.6	174.7	-177.4
0717.inp	6.6	-229.44	44.65	-152.5	2.6	58.5	-179.4	80.3	-54.4	-81.7	-166.4	50.3	62.1	-177.2
0718.inp	5.9	-230.14	43.95	-153.6	-1.4	57.7	-177.7	69	-60.6	171.5	-140.2	-62.5	94.5	-177.1
0718a.inp	6.08	-229.96	44.13	-154.3	4.3	59.3	-177.7	61.1	-68.7	140.3	-171	-94.1	63.1	-177.3
0719.inp	3.99	-232.05	42.04	-152.3	-3.3	59.3	-179.6	65.5	-64.3	167	-50.6	-65.9	-177.3	-177.4
0720.inp	6.64	-229.4	44.69	-152.5	-1.5	60.1	-179.1	52.9	-81.6	165.9	72.5	-62.8	-59.1	-177.5
0721.inp	2.52	-233.52	40.57	-157.6	152.7	62.4	-171.2	-100.9	137.9	74.7	-60.1	-166.1	179.6	-177.5
0722.inp	3.48	-232.55	41.53	-157.4	152.6	62.3	-173	-98.6	137.7	77.3	62.4	-162.1	-59.2	-177.5
0723.inp	3.58	-232.46	41.63	-157.4	157	62	-172.4	-98.6	138.9	75.7	-167.4	-165.6	72.5	-177.5
0724.inp	5.19	-230.85	43.24	-159.4	146.6	59.3	180	-92.4	139.3	-38	64.6	94.6	-60.2	-177.2
0724a.inp	5.08	-230.96	43.13	-159.5	154.3	57.7	-179.8	-87.9	145.2	-60.2	31.5	63.7	-91.9	-177.2
0725.inp	2.16	-233.88	40.21	-159.2	153.7	57.4	-179.5	-87.1	148.7	-56.9	-63.9	64.3	174.8	-177.1
0726.inp	2.83	-233.21	40.88	-159.7	154.2	57.5	-179.8	-84.4	150.3	-60.8	-178.2	60	60.5	-177.1
0727.inp	4.71	-231.33	42.76	-159.7	156.4	57.7	-178.8	-86.7	149.5	180	-146.7	-60.7	94.3	-177.2
0727a.inp	4.75	-231.29	42.8	-159.4	152.7	58.2	-177	-84.1	152.1	142.7	-176.6	-98	63.1	-177.2
0728.inp	2.45	-233.59	40.5	-158.9	155.3	58.1	-177.4	-87.5	149.3	175	-58.2	-65.3	-178	-177.2
0729.inp	3.23	-232.81	41.28	-158.9	155.7	58	-178.7	-84.3	150.1	180	65	-58.7	-56.5	-177.3
0730.inp	3.07	-232.97	41.12	-159	143.5	59.3	178.8	61.2	-67.7	52.2	-60.1	179.1	172.5	-177.4
0731.inp	5.65	-230.38	43.7	-158.9	153.3	61.9	-179.6	53.3	-80.5	53.6	80.9	-175	-51.2	-177.6
0732.inp	3.85	-232.19	41.9	-159.8	150.2	60.5	177.5	63.1	-66.5	49.6	-168.8	176.1	64	-177.5
0733.inp	10.85	-225.19	48.9	-158.1	158	61.6	-173.1	59.3	-81.3	-104.8	59.7	32.8	-77.8	-177.6
0733a.inp	10.38	-225.66	48.43	-159.5	146.5	61.5	178.2	80	-59.8	-54.2	102.6	83	-34.4	-177.5
0734.inp	6.03	-230.01	44.08	-158.5	140.1	58.6	-179.5	77.6	-56.2	-70.5	-61.2	61.5	167.1	-177.6
0735.inp	6.35	-229.68	44.4	-159.4	148.7	61.1	-179.9	80.2	-54.2	-73.5	-167.4	58.1	61.4	-177.8
0736.inp	5.69	-230.35	43.74	-159.3	151.4	59.3	178.1	60.1	-69.3	140.3	-171.9	-94.6	62.2	-177.5
0736a.inp	5.93	-230.11	43.98	-159.5	147.2	59.6	-179.1	68	-61.6	171.2	-141.1	-62.9	93.4	-177.4
0737.inp	3.97	-232.07	42.02	-159.7	145.5	59.6	177.4	60.1	-69.2	161	-60.5	-72.6	172.7	-177.4
0738.inp	6.1	-229.94	44.15	-159.4	157.3	61.2	179.8	53.8	-80.6	166.2	81.7	-62.6	-50	-177.4
0739.inp	1.83	-234.21	39.88	-155.1	-51.3	58.1	175.3	-143.8	95	61	-67.4	-178.4	173.4	-178.1
0740.inp	4.25	-231.78	42.3	-154.9	-49.5	59.7	166.3	-157.1	77.8	63.9	66.1	-172	-56.4	-178
0741.inp	2.13	-233.91	40.18	-157.1	-44.2	60	176.1	-157.1	80.3	58.5	-170.4	178.8	70	-177.7
0742.inp	6.09	-229.94	44.14	-154.3	-46.1	57	165.5	-152.6	79	-35.4	72.1	91.1	-53.1	-177.9
0742a.inp	6.02	-230.02	44.07	-154.2	-43.5	57.5	165.5	-158.8	73.8	-64.3	29.7	62	-94.2	-178
0743.inp	2.22	-233.82	40.27	-154.8	-49.5	55.3	174.1	-141.8	94.5	-58.8	-68.9	63.3	170.6	-177.7
0744.inp	2.37	-233.67	40.42	-157.9	-38.8	57.5	176.1	-153.6	81.2	-62.9	-177.2	58.9	61.9	-177.3
0745.inp	4.57	-231.47	42.62	-157.9	-42.6	60.2	176.4	-158.1	78.4	177	-145.7	-62.7	95.6	-177.5
0745a.inp	4.61	-231.43	42.66	-157.7	-33.7	59.8	175.3	-150.2	86.1	145.4	-177.1	-95	63.6	-177.7
0746.inp	3.2	-232.84	41.25	-155.7	-52.1	57.7	174.2	-142.7	94.8	170.4	-65.6	-69	175.8	-177.8
0747.inp	5.42	-230.62	43.47	-153.9	-55.3	57.7	165.7	-155.7	77.7	175.7	69.5	-60	-52.7	-178
0748.inp	4.64	-231.4	42.69	-151.3	-62.4	56.3	173.2	56.8	-71.5	49.4	-56.5	176	175.2	-178.9
0749.inp	6.6	-229.44	44.65	-155.1	-51.1	57.5	171.1	45.4	-86.6	40	63.6	-178.5	-68.4	-178.3
0750.inp	5.69	-230.35	43.74	-153.6	-58.5	55.6	170.8	58	-71.1	46.7	-169	172.7	62.7	-178.3
0751.inp	10.79	-225.24	48.84	-157.9	-45.2	53.4	179.2	49.8	-88.5	-107.9	52.1	26.7	-83.7	-177.6
0751a.inp	10.83	-225.21	48.88	-156.9	-46.7	52.2	176.7	79.3	-60.7	-55.9	104.5	81.2	-32.7	-177.9
0752.inp	5.82	-230.22	43.87	-157.3	-41.9	52.8	176.1	80.3	-53.3	-66.2	-52.3	65.7	175.8	-177.9
0753.inp	6.57	-229.47	44.62	-157.6	-38	54.5	177.2	80.9	-53.4	-70.9	-165.6	60.6	62.8	-177.5
0754.inp	6.15	-229.89	44.2	-158.3	-40.2	57.1	177.9	57.9	-71.3	138.8	-171.7	-97.9	62	-177.5
0754a.inp	6.18	-229.86	44.23	-158	-35.9	57.6	177	68.8	-61	173.7	-139.9	-60.3	94	-177.6
0755.inp	4.1	-231.94	42.15	-157.3	-43.1	56.9	175.4	62.4	-67.1	164.8	-51.6	-68.6	-178.7	-178.2
0756.inp	6.76	-229.28	44.81	-158.7	-45.6	57.1	-180	46.2	-87.2	161.3	67.1	-68.6	-64.2	-177.5
0757.inp	2.8	-233.24	40.85	-153.5	65.8	-175.2	-178.6	-131.8	106.4	61.2	-62	-179.1	178.6	-179.7
0758.inp	3.56	-232.48	41.61	-152.8	66.6	-174.8	-177	-151.3	84.9	64	55	-175.1	-65.9	179.7
0759.inp	3.85	-232.19	41.9	-154.2	66	-175.3	-179.4	-150.7	86.5	58.3	-173.8	177.8	66.7	-179.5
0760.inp	6.01	-230.03	44.06	-149.1	68.7	-174.5	-179.6	-152.1	81.2	-64.7	30.6	59.4	-92.6	179.1
0760a.inp	6.47	-229.57	44.52	-151.9	66.6	-174.6	-178.8	-150	83.4	-31.1	59.9	92.1	-63.7	179.6
0761.inp	4.21	-231.83	42.26	-152.8	58.7	-175.2	-179.5	-137.2	98.9	-61.1	-66	60.2	173.2	-179.8
0762.inp	4.71	-231.33	42.76	-153.5	68.1	-175	-178	-149.1	85.6	-64.6	-179.3	56.4	59.7	-179.6
0763.inp	6.06	-229.98	44.11	-154.5	66.4	-175.3	180	-154.9	81.5	176.7	-142.5	-63.3	98.3	-179.4
0763a.inp	6.14	-229.9	44.19	-154.6	69.5	-175.2	179.6	-149.9	86.4	146.3	-178.6	-94.8	62.2	-179.3
0764.inp	3.99	-232.05	42.04	-154.3	60.9	-176.5	-179.7	-136.5	100.8	172.5	-59.4	-67.7	-178.5	-179.5
0765.inp	4.3	-231.74	42.35	-153.3	70.4	-176.2	-175.6	-149.3	85.7	178.5	59.8	-62.8	-60.7	179.7
0766.inp	2.74	-233.3	40.79	-153	14.1	57.3	-176.4	65	-64	55.8	-53.1	-176.8	-179.9	-177.6
0767.inp	5.72	-230.32	43.77	-153.2	21.6	55.9	-177.4	53	-80.8	53.5	68.3	-174.9	-63.6	-177.9
0768.inp	3.5	-232.54	41.55	-153.9	15.8	57.5	-173.8	65.9	-63.7	54.2	-163.3	-178.9	70.3	-177.7
0769.inp	10.67	-225.37	48.72	-153.8	7.2	58.2	-176.3	57.2	-82.4	-106	54.4	30.5	-82.3	-177.4
0769a.inp	10.37	-225.67	48.42	-152.8	24.2	59.6	-176.7	86.5	-51.9	-50.6	108.3	85.1	-26.5	-178.1
0770.inp	5.99	-230.05	44.04	-152.7	24.8	59.9	-176.6	82.6	-50.6	-65.3	-52	66.8	177.1	-178.2
0771.inp	6.63	-229.4	44.68	-152.7	24.7	59.5	-176.1	83.5	-50.4	-70.1	-163.8	61.5	65.7	-178.1
0772.inp	6.11	-229.93	44.16	-154.1	7.9	58.6	-177.3	61.1	-68.6	140	-170.8	-94.3	63.3	-177.4
0773.inp	3.97	-232.07	42.02	-153	-3	59.3	-178.3	65.5	-64.3	167.2	-50.5	-65.6	-177.2	-177.5
0774.inp	6.71	-229.33	44.76	-153.7	1.2	56.5	-179	52.9	-81.6	166	72.9	-62.7	-58.8	-177.3
0775.inp	6.41	-229.63	44.46	-164.8	147.1	59	179.4	-136.6	101.7	60.1	-62.7	-179.8	177.6	1.3
0776.inp	7.2	-228.84	45.25	-165.6	154.3	58.8	-179.6	-147.7	88.1	63	56.6	-175.6	-64.7	1.6
0777.inp	7.12	-228.91	45.17	-165.6	154.9	58.3	179.5	-146.8	90	58.4	-173.8	178	66.4	1.8
0778.inp	10.06	-225.98	48.11	-165.1	158	58.1	-179.1	-148.6	84.4	-64.7	30.9	59.3	-92.4	1.9
0778a.inp	9.29	-226.75	47.34	-140.4	151.2	49.2	-179.5	-126.7	106.3	-30.7	62.8	92.4	-60.8	2.7
0779.inp	7.91	-228.13	45.96	-165.5	151.3	58.1	178	-135.8	99.9	-61.3	-66.9	60.3	172.1	1.5
0780.inp	8.39	-227.65	46.44	-164.9	157.8	57.6	179.6	-142.9	91.4	-64.7	-178.9	56.7	59.9	1.8
0781.inp	9.68	-226.35	47.73	-165.1	157.5	57.6	179	-148.5	87.7	176.8	-144	-63.3	96.9	1.9

0781a.inp	9.79	-226.24	47.84	-163.8	157	55.5	177.9	-143.1	92.9	146.3	-178.4	-94.6	62.3	2.3
0782.inp	7.69	-228.35	45.74	-165.7	151.8	57.9	177.6	-135	102	171.7	-60.1	-68.3	-179.3	1.6
0783.inp	8.29	-227.75	46.34	-165	159.3	57.6	-179.7	-143.5	91	178.2	61.9	-60.6	-58.9	2
0784.inp	7.91	-228.13	45.96	-163.8	140.5	58.5	178.9	61.6	-67.2	52.7	-59.1	179	173.5	1.3
0785.inp	10.58	-225.46	48.63	-166.1	150.3	61.4	-179.8	53.7	-80	53.6	81.6	-174.9	-50.6	1.1
0786.inp	8.74	-227.3	46.79	-166.6	147.7	59.8	177.4	63	-66.5	49.6	-168.6	176	64.1	1.4
0787.inp	15.92	-220.12	53.97	-166	127.9	62.3	-177	53	-86	-107.4	53.8	28.6	-82.7	0.5
0787a.inp	13.76	-222.27	51.81	-140.2	140.3	55.7	177.9	81.7	-57.8	-54.1	105.5	82.4	-30.8	2.2
0788.inp	9.24	-226.8	47.29	-140.7	138.5	54.7	179.8	78.7	-55.1	-69.5	-58.2	62.4	170.2	2.5
0789.inp	11.28	-224.76	49.33	-166.6	145	60.4	179.1	79.9	-54.5	-73.6	-167.7	57.9	60.9	1
0790.inp	10.59	-225.45	48.64	-165.5	148.4	58.7	177.9	60.2	-69.1	140.2	-171.5	-94.7	62.6	1.5
0791a.inp	10.82	-225.22	48.87	-165.4	144.1	58.8	-179.4	68.2	-61.4	171.2	-141	-62.9	93.5	1.3
0791.inp	8.82	-227.22	46.87	-165.9	143.3	58.7	177.5	60.5	-68.9	161.1	-60	-72.4	173.1	1.4
0792.inp	11.08	-224.96	49.13	-164.6	154.8	57.6	-179.9	55	-79.5	166.8	82	-61.8	-49.8	1.8
0793.inp	8.36	-227.68	46.41	-156.5	147.2	58.2	4.5	-107.9	131.8	64.3	-60.8	-177.1	-180	-178
0794.inp	9.83	-226.2	47.88	-156.8	149.6	55.1	4.6	-110.8	125.5	67.5	60.9	-172.1	-60	-177.9
0795.inp	9.47	-226.57	47.52	-157	150.7	55	4.1	-111.2	126.4	61.7	-172.2	-179.8	68.5	-177.8
0796.inp	12.16	-223.88	50.21	-159.8	153.6	57.3	0.3	-96.9	136.4	-29.8	64.7	93.2	-59	-177
0796a.inp	12.47	-223.57	50.52	-158.8	152.8	56.8	3.4	-101	132.2	-63	30.7	60.6	-92.6	-177.4
0797.inp	9.07	-226.97	47.12	-158.9	151.8	57.6	2.5	-96.4	139.8	-56.3	-63.6	64.5	175.1	-177.2
0798.inp	10.15	-225.89	48.2	-158.6	151	57.6	2.2	-95.3	139.6	-62.6	-178.2	57.9	60.7	-177.3
0799.inp	11.45	-224.59	49.5	-158.9	152.2	55.8	2	-99.2	137.2	177.6	-146.2	-63.3	95.1	-177.3
0799a.inp	11.03	-225.01	49.08	-158.9	149.8	57.3	2.5	-90.7	145.9	143.6	-176.7	-97.6	63.5	-177
0800.inp	8.77	-227.27	46.82	-159.3	151.9	56.3	2.3	-98	139.3	172.2	-59	-68.5	-178.2	-177.1
0801.inp	10.25	-225.79	48.3	-159.1	151.3	56.5	2	-96.1	138.6	178.2	65.1	-60.9	-56	-177.1
0802inp	12.54	-223.5	50.59	-154.7	133	59.2	-1.7	65.7	-69.1	50.2	-44	-176.4	-177.6	-177.3
0803.inp	16.19	-219.85	54.24	-153.5	130.7	54.5	-1.8	58	-82.9	53.2	73.7	-168	-66	-178
0804.inp	13.44	-222.6	51.49	-157	135.4	58.4	-1.9	65.5	-69.6	50.1	-156.7	-177.3	70.1	-176.9
0805.inp	20.68	-215.35	58.73	-150.1	111.2	57	-2	90.3	-53.8	-56.3	132.8	84.8	-7.8	-177.6
0805a.inp	19.92	-216.12	57.97	-154.5	126.8	52.4	-5.3	60.9	-83.2	-135.8	59.7	4.4	-81.2	-178.2
0806.inp	16.93	-219.11	54.98	-145.9	109.5	59.4	-2.6	88.1	-52.4	-75.3	-45.7	64.4	175.5	-179.3
0807.inp	20.58	-215.46	58.63	-155.8	131.7	58.3	15.7	96.7	-40.4	-66.4	-159.3	71.2	66.4	-176.9
0808.inp	14.84	-221.2	52.89	-157.3	136.9	58.6	-3	67.7	-66.1	161	-127.2	-67.9	101.5	-177.1
0808a.inp	15.03	-221.01	53.08	-154.9	131.7	59.1	-3.6	62.8	-72.2	136.2	-170.4	-92.9	57.9	-177.2
0809.inp	13.44	-222.6	51.49	-156.3	137.4	58.7	-2	63.7	-71	157.9	-42.1	-69.3	-175	-177.3
0810.inp	16.47	-219.57	54.52	-154.2	137	53.6	-3.6	55	-85.4	158.5	74.6	-64	-64	-177.5
0811.inp	2.5	-233.54	40.55	50	63.8	-172.7	178.7	-99.8	138	62.1	-60	-178.4	-179.9	-179.2
0812.inp	4.26	-231.75	42.31	49.7	68	-171.5	176.3	-97.8	137.9	64.9	60.2	-174.1	-61.1	-179.1
0813.inp	4.04	-232	42.09	50.5	68.4	-171.9	177	-98.7	138.4	58.5	-173	177.7	67.1	-179.4
0814.inp	6.21	-229.83	44.26	49.4	47.2	-170.8	-178	-87.4	145.7	-61.7	31.1	62	-92.4	-178.6
0814a.inp	5.94	-230.09	43.99	49.6	42	-170.6	-178	-83.8	149.4	-30.1	63.6	72.9	-60.2	-177.8
0815.inp	3.41	-232.63	41.46	52.5	45.8	-170.8	179.2	-84.6	151.5	-56.3	-65.2	65	173.5	-178.5
0816.inp	4.39	-231.65	42.44	50.2	45.3	-171	-178	-85	149.5	-61.2	-177.9	59.5	60.8	-178.9
0817.inp	6.32	-229.71	44.37	51.3	59.1	-172	178.6	-86.6	149.5	178.6	-147	-62.1	94.2	-179.6
0817a.inp	5.86	-230.18	43.91	49.6	48.4	-171.3	-176.9	-82.8	153.3	142.6	-176.3	-98.1	63.5	-178.8
0818.inp	3.37	-232.67	41.42	50.8	56.8	-171.8	-179.5	-86.8	150.2	174.6	-56.1	-65.6	-175.9	-179.9
0819.inp	4.69	-231.35	42.74	50.7	53.8	-171.5	-179.8	-83.9	150.6	179.5	64.7	-59.5	-56.6	-179.1
0820.inp	4.06	-231.97	42.11	51	67.7	-172.2	176.7	67.5	-61.3	55	-50.4	-177.8	-177.5	-178.9
0821.inp	6.73	-229.31	44.78	54.1	72.4	-172.1	177.7	54.6	-78.9	52.5	65.6	-177.2	-66.3	-178.4
0822.inp	5.16	-230.88	43.21	53.3	65.7	-173	176.5	66.4	-63.2	52.8	-165.4	179.5	67.5	-179.1
0823.inp	11.54	-224.5	49.59	50.9	69.2	-173.8	179.1	58.5	-80.7	-107.5	53.7	28.4	-82.4	-179.4
0823a.inp	11.61	-224.43	49.66	54.8	54.3	-172.8	175.9	83.3	-56.5	-56.3	106.7	80.6	-30	-178.7
0824.inp	6.68	-229.36	44.73	51	57	-173.5	177.4	81.9	-51.8	-68.8	-51.1	63.2	177.5	-179.1
0825.inp	7.4	-228.64	45.45	51.1	56	-173	-179.3	82.2	-52.1	-74.4	-165.5	57.2	63.5	-178.9
0826.inp	7.24	-228.8	45.29	50.2	61	-173.3	179.2	70	-59.5	171.7	-140.2	-62.5	94.6	-179.7
0826a.inp	7.11	-228.93	45.16	50.6	56.5	-172.5	-179.8	61.7	-67.9	140	-171	-94.5	63.2	-179.3
0827.inp	5.07	-230.96	43.12	49.5	59.7	-173.4	179.6	66.9	-62.6	167.3	-48.7	-65.6	-175.2	-179.4
0828.inp	7.64	-228.4	45.69	50.1	64	-173.2	178.6	54.2	-80	165.1	70.7	-63.9	-60.7	-179.4
0829.inp	5.28	-230.76	43.33	68.1	-10.7	-173.7	-177.5	60.5	-68.3	50.4	-53.8	177.5	178.7	-179.1
0830.inp	7.68	-228.37	45.73	65	-3.8	-171.3	-175.4	48	-85.3	50	65.5	-178.1	-66.6	-179.5
0831.inp	6.09	-229.95	44.14	68	-10.2	-173.6	-177	60.7	-68.8	48	-167.3	174.7	65.4	-179.3
0832.inp	13.56	-222.48	51.61	77.2	-37.6	-175.8	-178.3	52.5	-86.3	-107.3	53.1	28	-83	-178.7
0832a.inp	13.97	-222.07	52.02	80.4	-46.4	-170.9	175.3	81	-59.2	-57.1	105	80	-32.2	-178.6
0833.inp	8.71	-227.33	46.76	80	-43.9	-171.8	178.8	79.4	-54.5	-75.8	-53.4	56.2	175	-177.9
0834.inp	9.42	-226.62	47.47	79.9	-42.2	-171.3	-178	78.7	-55.8	-80.8	-166.5	50.8	62.2	-179
0835.inp	8.91	-227.13	46.96	76.2	-32.7	-172.2	-175	66.4	-63.1	170.9	-139.9	-63.3	94.9	-179.1
0835a.inp	9.32	-226.72	47.37	79.3	-51.1	-175.3	178.7	59.7	-69.7	139.5	-171.3	-95.3	62.7	-178.7
0836.inp	6.87	-229.17	44.92	74.9	-29.6	-173.5	-176.1	62.6	-67	165.8	-51	-67.2	-177.6	-178.9
0837.inp	9.72	-226.32	47.77	79.5	-48.8	-175.6	178.6	51.1	-82.9	165.3	71.3	-64.1	-60.1	-178.3
0838.inp	5.4	-230.63	43.45	120.8	-60.7	-179.7	173.6	-139	99.4	60.2	-73.4	-179.8	167.6	-176.1
0839.inp	5.71	-230.23	43.76	123	-48.7	-179.7	178.4	-145.5	90.3	62.7	60.3	-176.2	-60.6	-176.5
0840.inp	5.8	-230.24	43.85	122.3	-53.7	-179.5	176.9	-147.9	88.9	56.8	-175.7	176.5	64.8	-176.6
0841.inp	8.36	-227.67	46.41	122.5	-49.3	-179.4	179.4	-142.7	90.7	-29.6	62.4	93.4	-61.2	-176.8
0842.inp	6.63	-229.41	44.68	121.6	-52.8	-180	173.5	-134.9	101.4	-60	-75.7	61.1	164.1	-175.1
0843.inp	6.87	-229.17	44.92	121.8	-52.9	179.2	178.7	-148.2	86.3	-63.2	179.9	58	59.2	-175.5
0844.inp	8.6	-227.44	46.65	124	-52.8	178.9	177.8	-148.3	87.9	146.4	-179.4	-94.6	61.5	-176.4
0844a.inp	8.71	-227.32	46.76	120.7	-54.1	-179.7	177	-153.1	83.1	176.9	-145	-63.1	96	-176.7
0845.inp	7.01	-229.03	45.06	120.8	-63.9	-179.7	173.7	-139.1	98.4	168.1	-72.8	-72.2	168.8	-176.4
0846.inp	6.81	-229.22	44.86	123.7	-48.9	179.4	179.9	-146.6	88.1	178.2	63.6	-60.8	-57	-176.6

0847.inp	3	-233.04	41.05	55.3	29	-168.1	178.6	-140.2	98.4	60.3	-71.8	-179.8	169.3	-179.7
0848.inp	3.42	-232.61	41.47	53.7	42.1	-167.8	179.2	-150	85.6	64.5	64.6	-173.8	-56.9	-179.8
0849.inp	3.45	-232.59	41.5	51.2	41.8	-168.4	178.7	-148.9	88.2	58	-174.6	-177.4	65.9	-179.8
0850.inp	6.1	-229.94	44.15	53.6	40.6	-168.1	178.4	-148.4	84.3	-32.8	66.3	91.4	-57.9	178.9
0850a.inp	6.45	-229.59	44.5	60.5	48.6	-168.3	172.7	-150.6	82.1	-65.2	33	60.2	-90.4	-178.3
0851.inp	3.67	-232.37	41.72	55.7	22.1	-167.6	-178	-142.3	94.5	-61.1	-72.6	60	167.3	-176.5
0852.inp	4.03	-232.01	42.08	50.8	40.3	-168.9	-176.6	-150.2	84.6	-64.6	-179.6	56.3	59.6	-177.8
0853.inp	5.74	-230.3	43.79	52.7	42.6	-168.7	-178.5	-149.7	84.7	177.2	-145	-63.2	96.2	-178.5
0853a.inp	5.72	-230.31	43.77	50.8	41.9	-168.9	-178	-148.2	88.1	146.4	-178.9	-94.8	62	-178.9
0854.inp	4.09	-231.95	42.14	55.4	34.5	-168.6	177.6	-139.2	98.4	169.1	-71.3	-71.1	-170.1	-177.9
0855.inp	3.97	-232.07	42.02	52.6	45.6	-168.8	-179.2	-147.8	86.7	177.8	65.8	-60.8	-55.3	177.9
0856.inp	5.3	-230.74	43.35	61.3	14.5	-170.8	174.2	61.6	-67	51.1	-54	178.1	177.9	-178.5
0857.inp	7.57	-228.47	45.62	60	11.8	-173.8	179.6	48	-85	50.4	65	-178.9	-67.2	-179.4
0858.inp	6.13	-229.91	44.18	63.4	4.9	-172.4	177.9	60.4	-69.1	46.4	-168.2	173	63.9	-179.3
0859.inp	11.71	-224.33	49.76	57.7	16.3	-170.6	-176.7	79.8	-59.8	-55.9	107.6	80.7	-28.6	-179.2
0859a.inp	11.44	-224.59	49.49	51.7	38.9	-169.9	-177	53.9	-85.1	-107.6	53.5	28.1	-82.7	-179.2
0860.inp	7.37	-228.67	45.42	60.5	7.1	-172.1	-173.4	78.2	-55.1	-64.6	-51.1	67.4	177.8	-179.7
0861.inp	7.37	-228.67	45.42	53.8	28.5	-171	-175	79	-55.3	-72.1	-165.5	59.6	63.4	-178.8
0862.inp	6.98	-229.06	45.03	52.5	35.1	-169.6	-176.2	67.6	-62	172	-140.1	-62	94.4	-179.1
0862a.inp	7.01	-229.02	45.06	52.3	41.6	-169.8	-177.5	59.9	-69.7	139.5	-171.4	-94.9	62.6	-178.9
0863.inp	5.12	-230.92	43.17	52.9	33.8	-169.6	-178	63.4	-66.3	165.9	-50.8	-67.1	-177.6	-179.2
0864.inp	7.51	-228.53	45.56	50.7	41.4	-170.4	-179.1	50.3	-83.7	163.4	69.2	-65.9	-62.2	-179.2
0865.inp	1.87	-234.17	39.92	55.4	-128.9	-174.6	-175	-141.1	97.8	58.6	-60.2	178.2	-179.6	-179.7
0866.inp	2.14	-233.9	40.19	54.8	-123.3	-172.7	174.8	-156.2	79.7	59.5	51.8	-178.4	-69.6	-179.8
0867.inp	2.64	-233.4	40.69	54.2	-120.7	-173.5	178.5	-154.3	83.1	53.8	-175.6	173.4	64.7	-179.8
0868.inp	5.52	-230.52	43.57	54.6	-115	-174.3	173.5	-151.2	80.8	-70	32.3	55.6	-92.6	-179.7
0868a.inp	5.66	-230.38	43.71	54.6	-113.9	-176	172.6	-145.5	86.6	-33.1	63.3	91.8	-61.6	-179.6
0869.inp	2.38	-233.66	40.43	54.7	-114.5	-180	179.7	-128	107.7	-55.5	-65.3	65.8	173.6	-179.7
0870.inp	3.63	-232.41	41.68	54.9	-111.7	179.5	179.1	-126.5	107.8	-60.6	-178	60.2	61	-179.6
0871.inp	5.03	-231.01	43.08	54.8	-113	-175.8	-179.3	-151.6	84.9	176.4	-143.4	-64	97.8	-179.7
0871a.inp	5.17	-230.87	43.22	54.6	-113.8	-176.1	178.7	-148.6	87.8	146.2	-178.1	-95	62.9	-179.6
0872.inp	2.55	-233.49	40.6	54.9	-117.5	-176.4	179.5	-135.2	102.1	173.5	-56.9	-66.7	-175.8	-179.7
0873.inp	3.56	-232.48	41.61	54.6	-118.7	-174.8	172.5	-154.2	80.2	176.2	57.1	-61.6	-63.9	-179.5
0874.inp	3.74	-232.3	41.79	56.3	-129	-171.7	-174.5	59.5	-69.5	52.5	-62.9	179.9	169.7	-178.9
0875.inp	5.52	-230.52	43.57	55.1	-116.3	-175.6	-178.9	51.1	-82.4	52.6	67.3	-176.2	-64.6	-179.1
0876.inp	4.04	-232	42.09	54.9	-119.6	-173.9	179.1	62.8	-66.8	50.1	-168	176.7	64.8	-179.4
0877.inp	11.16	-224.88	49.21	57.8	-114.2	-174.5	-176.8	55.6	-84	-106.8	55.8	29.5	-80.8	-179.1
0877a.inp	10.58	-225.45	48.63	54.3	-112.1	-178.5	-178.2	84.3	-54.4	-51.6	107.7	84.2	-27.4	-179.4
0878.inp	6.24	-229.8	44.29	59.1	-115.7	-177.8	-172.3	81.2	-51.4	-61.7	-50.4	70.2	179.1	-179.4
0879.inp	6.97	-229.07	45.02	54.4	-114.3	-178.5	-177.7	81.2	-52.8	-69	-164.7	62.3	64.6	-179.6
0880.inp	6.67	-229.37	44.72	54.7	-116.9	-175.4	-176.2	68	-61.6	170.6	-140.5	-63.5	94.3	-179.6
0880a.inp	6.48	-229.56	44.53	54.8	-109.8	-176.6	-176.1	60.3	-69.5	138	-171.5	-96.3	62.8	-179.7
0881.inp	5.56	-230.48	43.61	56	-127	-173	-176.1	57.8	-71.8	159.2	-65.2	-74	168.2	-179.1
0882.inp	7.06	-228.98	45.11	55.2	-116.2	-175.6	179.6	50.5	-83.6	164.3	71	-65	-60.4	-179
0883.inp	4.57	-231.46	42.62	76.4	-36.5	-175.6	174.3	-140.9	97.9	59.5	-68.5	179.5	172.7	-177.2
0884.inp	4.41	-231.63	42.46	73.2	-26.3	-174.6	-178.7	-158.6	77.7	61.6	52.1	-177.2	-68.5	-177.1
0885.inp	4.89	-231.15	42.94	72.5	-25	-174.5	-178	-155	82.4	58.9	-174.5	176.1	66.4	-177.4
0886.inp	6.6	-229.44	44.65	70.2	-13.4	-172.3	-179.3	-157.5	75.4	-66.6	31.6	58.1	-92.2	179.5
0886a.inp	7.29	-228.75	45.34	72.6	-15.5	-172	179.9	-152.6	80.3	-30.4	63	93.8	-61.4	179.4
0887.inp	5.95	-230.09	44	82.8	-47.9	-172.4	175.5	-139.2	96.8	-65.9	-74.9	56	164.2	-177
0888.inp	6.06	-229.98	44.11	81.4	-46.4	-173.4	-179.6	-151.7	82.6	-67.1	-179.5	54.5	59.1	-177.3
0889.inp	7.24	-228.8	45.29	70.1	-18.2	-174.7	-176.3	-158.1	78.6	176.8	-142.2	-63.4	98.9	-179.1
0889a.inp	7.74	-228.3	45.79	79.1	-48.5	-174.3	179.1	-149.4	86.8	146.5	-179.5	-94.6	61.5	-177.7
0890.inp	4.42	-231.61	42.47	65.5	-6.1	-173.3	-174.8	-140.3	97.1	173	-59.9	-67.4	-178.7	-179
0891.inp	5.52	-230.52	43.57	74	-27.6	-174.4	-177.5	-158.1	77	177.7	57.9	-61.2	-62.4	-178.2
0892.inp	7.15	-228.57	45.2	46.3	72	-172.1	177	-96.2	142.5	61.6	-60	-179	-179.8	1.1
0893.inp	8.74	-227.29	46.79	43.3	69.2	-171.8	177.1	-96.7	139.2	65.3	60.5	-173.7	-60.9	0.3
0894.inp	8.49	-227.55	46.54	44	66.9	-170.5	177	-99.6	137.5	57.9	-173.4	177.1	66.8	0.1
0895.inp	11.51	-224.52	49.56	42.7	62.8	-170.7	177.6	-87.7	145.6	-61.2	29.6	62.5	-93.5	0.7
0895a.inp	11.02	-225.02	49.07	43.5	60.7	-170.2	176.3	-82.4	150.9	-29.5	64.1	93.6	-59.4	0.6
0896.inp	8.46	-227.58	46.51	45.5	62.5	-170.8	178.1	-80.5	155.9	-53.4	-62.6	67.5	176.3	1.4
0897.inp	9.44	-226.6	47.49	43.6	63.2	-170.2	178.7	-80.8	153.9	-59.3	-177.6	61.4	61.2	0.2
0898.inp	10.94	-225.1	48.99	44	58.6	-169.4	179.3	-89.9	146.2	178.3	-145.9	-62.3	95.2	0.6
0898a.inp	10.93	-225.11	48.98	45.3	55.2	-168.2	-179.5	-84.3	152	142.9	-176.7	-97.9	63.4	0.7
0899.inp	8.66	-227.38	46.71	46.7	60.2	-169	-178.3	-81.9	155.6	173.8	-58.2	-66.7	-177.8	1.6
0900.inp	9.63	-226.41	47.68	44.3	59.7	-168.1	-179.3	-82.8	151.8	179.4	65	-59.5	-56.4	0.5
0901.inp	9.32	-226.72	47.37	48.1	80.4	-169	175.3	70.7	-58.2	59.4	-51	-173.2	-178	1.2
0902.inp	12.75	-223.29	50.8	49.3	81.7	-169.1	176	59.5	-74.6	62.3	71.5	-165.7	-60.6	1.9
0903.inp	11	-225.04	49.05	48.6	75.7	-169.3	177.4	72.1	-57.5	60	-160.5	-173.1	72.7	2.1
0904.inp	16.43	-219.61	54.48	47.5	75.2	-168.4	171.1	56.7	-82	-106.1	52.5	29.4	-83.9	-0.1
0904a.inp	18.33	-217.71	56.38	46	67.3	-165.9	163.7	78.2	-63.8	-63	95.6	75.9	-44.3	-1.9
0905.inp	12.95	-223.09	51	76.3	65.5	-165.8	177.2	85.7	-47.4	-64.4	-51.1	67.5	178.2	0.6
0906.inp	13.49	-222.55	51.54	47.1	68.9	-164.6	172.2	81.9	-52.9	-86.2	-164.9	45.7	63.1	-0.9
0907.inp	12.55	-223.49	50.6	47.9	69.2	-168.2	174.4	71.1	-58.5	172.2	-139.8	-61.8	94.4	-0.2
0907a.inp	12.96	-223.08	51.01	48.8	76	-167.5	172.4	64.8	-65	142.9	-170.6	-91.7	63.2	0.2
0908.inp	10.04	-226	48.09	46.5	75.1	-164.9	174.1	69.3	-60.3	168.7	-48	-64.2	-174.8	0.6
0909.inp	12.56	-223.48	50.61	46.2	74	-167.4	172.1	56	-78.3	168.3	71.6	-60.8	-60.1	0.2
0910.inp	9.9	-226.14	47.95	52.8	69.6	-174.1	0.2	-128.9	110.3	64.3	-63.1	-176.7	178.1	-178.6
0911.inp	11.24	-224.8	49.29	50.7	68.2	-173.7	2.1	-135.6	100.5	66.9	58.3	-172.3	-62.4	180

0912.inp	11.02	-225.01	49.07	50.1	68.4	-173.5	1.3	-136.5	100.5	62.2	-171.6	-178.7	69.1	-179.9
0913.inp	14.39	-221.64	52.44	47.9	67.8	-173.1	1.9	-140.1	93.5	-64.5	28	59.1	-94.9	-178.8
0913a.inp	14.91	-221.13	52.96	47.4	68	-173.1	-1.7	-133.4	99.6	-31.1	62.7	92.2	-61	-178.8
0914.inp	11.71	-224.33	49.76	49.2	68.8	-172.9	-1.5	-122.4	113.4	-60.2	-66	60.8	173.2	-178.5
0915.inp	12.74	-223.29	50.79	47.9	65.9	-172.3	0.4	-125.3	108.9	-63.9	-178.8	56.9	60.2	-178.6
0916.inp	13.52	-222.51	51.57	48.2	68.1	-173	0.8	-143.8	92.6	176.7	-143	-63.6	97.9	-178.7
0916a.inp	13.7	-222.33	51.75	46.9	67.9	-173.4	-1.3	-135.6	100.5	144.1	-177.3	-96.9	63.3	-177.9
0917.inp	11.21	-224.83	49.26	48.8	67.2	-172.2	-0.9	-122	114.9	171.3	-61	-69.3	-180	-178
0918.inp	12.57	-223.46	50.62	47.4	64.5	-171.8	0.5	-123	111.2	177.6	63.5	-61.2	-57.3	-178.1
0919.inp	14.63	-221.41	52.68	52	84.8	-176.2	4	70.7	-63.7	42.8	-47.8	176.4	179	-177.1
0920.inp	21.27	-214.77	59.32	58.3	84.9	-171.2	-13.2	47.5	-90.7	54.1	66.6	-169.4	-72.4	178.9
0921.inp	15.86	-220.18	53.91	46.2	79.9	-175.8	3.1	71.7	-62.5	39.7	-154.4	172.5	72.9	-178
0922.inp	25.12	-210.91	63.17	55.6	86.2	-173.1	-8.8	52.5	-92.9	-110.2	57.6	32.6	-86.9	179.9
0923.inp	19	-217.04	57.05	53.6	80.6	-172.1	6.6	87.7	-51.4	-68	-56.2	70.7	166.8	-179.4
0924.inp	19.12	-216.91	57.17	48	75.2	-171.5	9.3	89.7	-48.3	-67.5	-158.5	69.6	66.5	-178.4
0925.inp	18.6	-217.44	56.65	49.2	71.4	-172.6	-5	65.4	-69.1	145.4	-138.2	-83.1	89.8	-179.1
0925a.inp	17.8	-218.23	55.85	45.8	80.5	-175.8	4.9	67.4	-66.3	128.5	-157.4	-100.1	71.6	-178
0926.inp	16.61	-219.43	54.66	49.5	75.1	-172.9	-3.1	63.8	-70.8	148.5	-46	-78.3	-179.5	-179.2
0927.inp	21.49	-214.54	59.54	59.2	84	-171.7	-16.7	43.3	-93.7	162.4	67.7	-63.5	-69.4	179.1
0928.inp	1.83	-234.21	39.88	54.1	51.3	-57.3	178.2	-100	138.5	63.1	-61.7	-177.3	178.4	178.3
0929.inp	2.73	-233.31	40.78	49.6	44.7	-60.4	-177.6	-105.3	130.4	65.6	58	-173.7	-63.3	-178.6
0930.inp	2.85	-233.19	40.9	50.1	43.7	-59.8	-177.4	-104.1	133	59.7	-173	178.6	67.2	-179.6
0931.inp	5.25	-230.79	43.3	52.2	40.8	-58.9	-179.2	-91.9	140.8	-62.3	33.7	61.7	-90	178.8
0931a.inp	4.84	-231.2	42.89	51.2	34.1	58.4	-177.8	-88.6	144.6	-30.2	62.6	92.6	-61	-178.2
0932.inp	2.46	-233.57	40.51	55.1	39.1	-56.9	177.5	-86	150.1	-57.2	-66.4	64	172.6	178.2
0933.inp	3.38	-232.66	41.43	52.3	40.3	-56.7	-179.6	-87.1	147.5	-61.9	-178.3	58.9	60.5	179.5
0934.inp	4.89	-231.15	42.94	51.1	38	-59.2	-178	-92.9	143.3	178.6	-147	-62.4	94.3	-179.8
0934a.inp	4.76	-231.28	42.81	51.3	36.6	-58.7	-176.9	-88.7	147.5	144.1	-176.9	-97	63.4	-179.6
0935.inp	2.45	-233.59	40.5	55.3	40.8	-54.9	177.6	-88.1	149	172.8	-59.9	-67.2	-179.4	177.1
0936.inp	3.17	-232.87	41.22	52.1	37.8	-55.6	-178	-89	145.1	179.6	63.3	-59.6	-57.7	-179.3
0937.inp	3.47	-232.57	41.52	54.9	53.8	-58	176.9	67.5	-61.4	59.1	-52.6	-173.5	-179.9	179.6
0938.inp	6.35	-229.68	44.4	55.9	60.7	-57.5	177.5	55.6	-78	55.8	69.4	-172.6	-62.8	179.9
0939.inp	4.35	-231.69	42.4	56.1	54.3	-57.4	175.7	67.4	-62.1	56.1	-164.1	-177.3	68.7	179.4
0940.inp	11.38	-224.66	49.43	50.6	50.2	-58.6	-178.5	70.4	-71.3	-70.3	56.5	70	-83.4	179
0940a.inp	10.66	-225.38	48.71	54.7	39.6	-58	176.8	82.2	-57.8	-57	106.5	80	-30.4	179.9
0941.inp	5.8	-230.23	43.85	52	42.5	-59.3	179.8	80	-52.9	-69.7	-52.6	62.3	176.1	179.6
0942.inp	6.31	-229.74	44.36	51.5	43	-58.8	-177.6	81.3	-53	-74.8	-166.1	56.8	62.9	179.8
0943.inp	5.96	-230.08	44.01	51.3	41.2	-58	-177.3	69	-60.5	171.9	-139.9	-62.2	94.8	179.4
0943a.inp	6.03	-230.01	44.08	52.2	44	-55.8	-178.8	61.1	-68.5	139.7	-171	-94.7	63	179.5
0944.inp	4.47	-231.57	42.52	49.5	48.1	-62.2	179.4	65.6	-64	167	-50.4	-65.9	-177	179.8
0945.inp	7.06	-228.98	45.11	49.6	51.7	-61.6	179.2	53.6	-80.7	166.1	72.5	-62.8	-59	179.4
0946.inp	5.43	-230.61	43.48	72.4	122.7	-53.1	179.1	-107.4	130.7	62	-61.2	-178.5	179	-179.9
0947.inp	6.65	-229.38	44.7	72.5	122.1	-53.1	178.4	-104.8	131	65.6	60.4	-173.2	-60.9	180
0948.inp	6.42	-229.62	44.47	72.5	122.9	-52.9	179.3	-104.4	132	59.6	-173	178.8	67.2	-179.9
0949.inp	9.3	-226.74	47.35	71.8	121.5	-55.8	178.7	-85.2	148	-60.9	31.2	62.9	-92.2	-179.9
0949a.inp	8.78	-227.25	46.83	71.9	121.7	-54.7	179.9	-79.8	153.3	-30.9	65	92.6	-59.3	-179.9
0950.inp	6.3	-229.74	44.35	72.2	122.7	-53.3	179.6	-82.9	153.1	-54.7	-63.7	66.4	175	-179.9
0951.inp	7.04	-229	45.09	71.4	119.5	-55.4	177.9	-81.8	153	-60.1	-178.2	60.6	60.8	-179.8
0952.inp	8.68	-227.36	46.73	72.3	123.7	-54.1	179.3	-88.4	147.9	178.2	-146.3	-62.4	94.8	-179.9
0952a.inp	8.53	-227.57	46.58	72.2	122.2	-53.9	178.7	-83.1	153.3	142.5	-176.7	-98.3	63.4	179.8
0953.inp	6.37	-229.67	44.42	72.5	122.3	-53.6	-179.6	-89.5	147.7	173.4	-58.4	-67	-178	-179.8
0954.inp	7.27	-228.77	45.32	72.1	122.6	-54.4	178.3	-85	149.5	179.1	64.9	-59.7	-56.3	-179.9
0955.inp	6.84	-229.2	44.89	72.5	121.8	-53	179.6	64.9	-64	52.8	-52.8	-179.7	179.9	-179.6
0956.inp	9.48	-226.56	47.53	72.5	123.5	-53.3	178.6	52.2	-81.2	51.6	66.1	-177.2	-66	-179.5
0957.inp	7.76	-228.28	45.81	72.7	123.6	-53.2	-179.4	64.7	-64.9	50.6	-165.5	177.4	67.5	-179.5
0958.inp	14.17	-221.82	52.22	72.5	123.7	-54.2	-179.2	84.3	-54.6	-53.5	108.6	82.6	-26.8	-179.4
0958a.inp	14.09	-221.95	52.14	72.8	123	-53.2	178.6	55.1	-83.9	-108.8	53.5	26.7	-82.6	-179.8
0959.inp	9.44	-226.6	47.49	72.5	122.1	-53.5	-179.3	82	-51.4	-66.3	-51.7	65.8	177.2	-179.4
0960.inp	10.25	-225.79	48.3	73	123.2	-53.5	-178.4	82.3	-51.8	-70.8	-164.1	60.8	65	-179.6
0961.inp	9.72	-226.32	47.77	72.4	122.5	-52.4	179.1	69.4	-60.2	171.3	-139.8	-62.7	94.7	-179.8
0961a.inp	9.71	-226.33	47.76	72.4	120.5	-52.7	179.3	61.4	-68.3	139.8	-171.1	-94.6	62.9	-179.9
0962.inp	7.67	-228.37	45.72	72.6	122.9	-52.3	179.3	65.6	-64	166.2	-50.5	-66.6	-177.3	-179.8
0963.inp	10.2	-225.84	48.25	73	122.6	-50.5	178.3	52.8	-81.4	164.8	71.3	-64.2	-60.3	180
0964.inp	2.46	-233.58	40.51	56.5	-132.4	-52.9	178.4	-137.9	100.6	58.8	-62.9	178.8	177.4	179.2
0965.inp	3.12	-232.91	41.17	57	-125.4	-53.9	-179.2	-148.3	87.7	62.7	56	-176.2	-65.1	178.5
0966.inp	3.07	-232.96	41.12	56.4	-125.9	-54.3	178.3	-148.1	88.9	56.1	-174.2	175.6	66	178.6
0967.inp	5.7	-230.34	43.75	57	-123.3	-54.4	-179.3	-147.3	86	-63.8	30.2	59.7	-92.7	178.5
0967a.inp	5.94	-230.1	43.99	56.7	-122.7	54.7	178	-143	90.4	-29.7	61.6	93.5	-62	178.8
0968.inp	3.64	-232.39	41.69	56.6	-129.9	-54.2	176.9	-134.6	101.3	-60.3	-66.7	61.2	172.5	179.3
0969.inp	4.15	-231.89	42.2	57	-123.4	-54.3	178.1	-141.5	93	-64	-179.3	57	59.8	178.6
0970.inp	5.65	-230.39	43.7	56.1	-121.9	-57.3	176.3	-151.7	84.4	176.6	-142.8	-63.2	97.8	179.3
0970a.inp	5.69	-230.35	43.74	55.9	-122.2	-56.5	175.3	-146	90.1	145.7	-178.2	-95.2	62.5	179.2
0971.inp	3.59	-232.45	41.64	55.9	-124.1	-58	178.5	-131.9	105.1	173.3	-58.5	-66.9	-177.7	179.4
0972.inp	4.33	-231.7	42.38	55	-115.8	-61.2	-179.9	-139.3	95.3	178.9	62.6	-60.2	-58.2	179.6
0973.inp	4.18	-231.86	42.23	57.3	-140.2	-50.7	178.2	61.6	-67.3	52.2	-61.1	179.3	171.4	179.6
0974.inp	6.39	-229.65	44.44	58	-129.4	-52.6	176.6	52.7	-80.8	52.7	71.1	-176.2	-61	179.7
0975.inp	4.81	-231.23	42.86	56.5	-130.8	-51.7	175.8	63.9	-65.6	49.7	-168	176.2	64.8	179.3
0976.inp	11.38	-224.66	49.43	58	-108.8	-60.4	178.7	60.8	-79.1	-105.7	56	31	-80.8	180
0976a.inp	11.29	-224.75	49.34	56.2	-122.7	-55.4	176.3	84.2	-55	-53.8	107	82.5	-28.9	179.5

0977.inp	7.05	-228.99	45.1	59.9	-150.6	-47.1	179.1	79.5	-54.2	-69.6	-56.4	62.5	172	179.7
0978.inp	7.41	-228.63	45.46	57	-133.3	-50.9	177.1	81.3	-53.1	-73.3	-166.6	58.2	62.1	179.2
0979.inp	6.84	-229.19	44.89	57	-133.8	-51.9	178.3	68.6	-61.1	170.7	-140.2	-63.3	94.2	179.3
0979a.inp	6.71	-229.33	44.76	56.9	-126.3	-53.5	177.9	60.8	-68.7	139.9	-171.7	-94.8	62.4	178.5
0980.inp	5.13	-230.91	43.18	57.3	-135.8	-53.5	-179.6	60.8	-68.6	161.1	-61.9	-72.1	171.4	179.5
0981.inp	7.05	-228.99	45.1	56	-119.5	-59.7	176.5	53.7	-80.5	165.6	72.9	-63.4	-58.6	-180
0982.inp	1.79	-234.25	39.84	56.7	29.1	-52	178	-137.4	101	60.3	-71.2	-179.8	-169.7	-179.6
0983.inp	2.23	-233.8	40.28	55.4	38.3	-51.2	-179.7	-145.6	90	64.8	64.8	-173.7	-56.6	177.1
0984.inp	2.35	-233.69	40.4	53.1	37.9	-51.4	-178.3	-145	91.9	58.2	-174.7	177.4	65.9	179.4
0985.inp	4.87	-231.17	42.92	55.2	36.8	-50.8	179.3	-144.6	88.1	-32.6	66.3	91.3	-57.9	177.8
0985a.inp	5.42	-230.62	43.47	62.5	42.6	-48.1	173.2	-144.9	87.5	-65.1	33.8	60.3	-90.3	-179.7
0986.inp	2.57	-233.47	40.62	56.2	30.7	-51.4	179.2	-137.4	99	-61.7	-73.6	59.4	166	-179.1
0987.inp	2.91	-233.13	40.96	52.7	36.9	-51.5	-177.2	-148	86.7	-64.6	-179.5	56.3	59.7	-179.7
0988.inp	4.63	-231.41	42.68	54.3	38.2	-51.6	-178.4	-147.5	88.9	177.4	-145.5	-63.1	95.8	179.9
0988a.inp	4.59	-231.45	42.64	52.8	37.4	-52.3	-177.5	-146.1	90.2	146.7	-178.8	-94.6	62	179.6
0989.inp	2.85	-233.19	40.9	57.1	30.1	-51.6	177.7	-138	99.5	169.3	-70.4	-71	171	-179.7
0990.inp	2.83	-232.21	40.88	55	39.6	-51.7	-179.2	-145.4	89.1	177.8	66.3	-60.9	-54.7	177.1
0991.inp	3.94	-232.1	41.99	61.6	19.3	-52.3	173.4	62.1	-66.5	52.5	-54.3	179.4	177.6	-179.9
0992.inp	6.1	-229.93	44.15	58.9	32	-51	174.9	50.7	-82.2	52.2	66.4	-177	-66	179.7
0993.inp	4.72	-231.32	42.77	61.9	24.2	-51.3	173.2	62.9	-66.5	48.7	-167.5	176.2	64.4	-179.8
0994.inp	10.5	-225.54	48.55	56.8	21.1	-54.1	-177.6	79.7	-60	-56.4	107	80.3	-29.5	179.6
0994a.inp	10.49	-225.54	48.54	53.3	37.9	-50.4	-176	56.3	-83.2	-106.2	54.1	30.1	-82.4	179
0995.inp	5.6	-230.44	43.65	55.3	25.9	-52.4	-175.5	79	-54.4	-67.9	-52.1	64.1	176.7	179.4
0996.inp	6.19	-229.85	44.24	54.9	27.3	-52.2	-174.9	79.7	-54.5	-71.7	-165.4	59.8	63.6	179.4
0997.inp	5.89	-230.15	43.94	54.3	30.9	-52.9	-176.7	67.6	-62	171.8	-140.1	-62.3	94.4	179.1
0997a.inp	5.93	-230.11	43.98	54.1	36.7	-51.3	-177.6	60.3	-69.3	139.4	-171.1	-95	62.9	179.1
0998.inp	4.06	-231.98	42.11	54.7	29.1	-52.9	-177.9	63	-66.6	165.5	-51.3	-67.6	-178.1	179.2
0999.inp	6.54	-229.5	44.59	53.6	33.5	-53.3	-178.3	50.6	-83.5	164.6	70.8	-64.5	-60.6	178.8
1000.inp	7.64	-228.4	45.69	67.5	39.3	-57.9	178.7	-99.4	139.2	64	-60.4	-176.6	179.8	-0.8
1001.inp	9.3	-226.74	47.35	66.8	40.9	-59.5	179.4	-98.7	137.2	66.7	59.7	-172.5	-61.7	-0.2
1002.inp	9.01	-227.03	47.06	66.4	38.1	-59	-179.6	-100.9	136.2	59.7	-172.7	178.7	67.4	-0.7
1003.inp	10.97	-225.06	49.02	66.7	35.7	-59.5	178.9	-90	141	-55.5	36.7	68.9	-87.5	-0.5
1003a.inp	11.23	-224.81	49.28	66.7	30.4	-59.6	176.3	-85.6	147.7	-29.5	61.7	93.6	-61.8	-0.5
1004.inp	8.38	-227.66	46.43	68.4	32.2	-59.3	177.6	-86	150.1	-55.9	-62.2	65.3	176.7	-1.5
1005.inp	9.46	-226.58	47.51	66.1	31.1	-58.8	178.2	-85	149.7	-60.9	-177.6	59.9	61.3	-1
1006.inp	11.08	-224.96	49.13	66.5	33.8	-58.6	178.7	-95.9	140.2	175.4	-149.4	-65.9	92.1	-0.5
1006a.inp	10.71	-225.32	48.76	66	25.6	-58.8	179.6	-86.4	150	142.5	-176.6	-98.6	63.8	-0.4
1007.inp	8.23	-227.8	46.28	68.3	31.4	-57.8	178.8	-86.9	150.2	174.3	-56.1	-65.7	-175.7	-2.2
1008.inp	9.4	-226.64	47.45	66.4	30.6	-57.8	179.1	-85.6	149	178.2	63.1	-60.9	-58	-1.3
1009.inp	9.37	-226.67	47.42	68.1	43.9	-57.2	-179	69.1	-59.9	60.9	-52.8	-171.6	-179.8	-0.8
1010.inp	13.24	-222.79	51.29	68.4	45.4	-57.1	-178.9	72	-61	58.3	112.5	-171.8	-16.8	-1.4
1011.inp	10.26	-225.77	48.31	68.3	44.5	-57.2	-179.6	70.3	-59.1	60.1	-160.7	-173	72.8	-1
1012.inp	16.85	-219.19	54.9	67.4	42	-57.3	-178.7	61.1	-78.9	-102.5	54.4	34.7	-82.8	-1.2
1012a.inp	17.28	-218.76	55.33	68.2	27.4	-55.7	170.7	81.9	-58.9	-59.4	104	78.5	-34.1	-0.8
1013.inp	12.18	-223.86	50.23	67.3	37.8	-56.1	178.9	82.3	-51.5	-79.6	-53.9	52.6	174.7	-0.9
1014.inp	12.67	-223.36	50.72	66.8	37.7	-56.5	179.6	82.6	-51.9	-81.8	-165.8	50	63	-0.7
1015.inp	11.98	-224.06	50.03	66.5	35.5	-57.4	-179.4	70.4	-59.1	172	-140.4	-62.1	94	-0.7
1015a.inp	12.21	-223.83	50.26	66.9	36.6	-55.4	178.5	62.9	-66.9	140.4	-170.5	-93.9	63.4	-1
1016.inp	10.07	-225.97	48.12	65.7	35.2	-55.6	-179.1	67.2	-62.5	168.6	-49.9	-64.2	-176.4	-0.4
1017.inp	12.72	-223.32	50.77	67	38.8	-54.7	179	55.1	-79.3	167.5	73.8	-61.1	-57.7	-2.1
1018.inp	9.44	-226.59	47.49	53.9	66.8	-55.3	1.5	-129.5	109.9	64.5	-64	-176.5	177.2	176.7
1019.inp	10.43	-225.61	48.48	51.6	65.2	-54.3	3.8	-136	100.2	67	58.6	-172.2	-62.1	177.9
1020.inp	10.19	-225.85	48.24	51.3	65.3	-53.9	3.3	-136.8	100.5	62.5	-171.8	-178.6	69	178
1021.inp	13.82	-222.22	51.87	48.9	63.2	-54.1	4.1	-133.5	99.6	-64.2	30.4	59.4	-92.7	179.6
1021a.inp	13.16	-222.88	51.21	51.2	59.1	-57.2	0.9	-106	128.1	-25.6	63.8	96.8	-59.6	178.6
1022.inp	10.86	-225.18	48.91	49.9	62.7	-56.4	-0.1	-118.7	117	-59.8	-66.4	61.2	172.6	179.4
1023.inp	11.66	-224.38	49.71	49.8	61.2	-56.6	0.9	-116.4	118.1	-63.5	-179	57.2	60	179.1
1024.inp	12.77	-223.27	50.82	48.7	64.1	-53.6	2.8	-140.5	95.7	176.9	-143.4	-63.6	97.5	179.7
1024a.inp	12.15	-223.89	50.2	50.7	59.5	-56.3	1.5	-109.2	127.2	147.6	-177.7	-94	63.2	-170
1025.inp	10.24	-225.8	48.29	49.7	60.9	-57.6	-0.1	-115.4	121.5	168.4	-61.2	-72	179.5	-179.5
1026.inp	11.51	-224.53	49.56	49.8	59.6	-57.6	0.7	-114.2	120.1	175.3	63.8	-63.5	-57.3	179.8
1027.inp	15.02	-221.02	53.07	50.9	79.4	-53.7	3.6	69.2	-65.2	41.5	-48	175.3	178.4	-179.7
1028.inp	20.77	-215.27	58.82	60	82.1	-52.9	-13.5	45.5	-92.2	56	66.7	-168.1	-71.9	176.9
1029.inp	16.18	-219.86	54.23	49.7	68.3	-55.1	-4.1	63.8	-71	42	-151.7	175.3	74.1	178.8
1030.inp	24.55	-211.49	62.6	56	84.7	-56.4	-7.2	51.8	-93.7	-110	57.8	33.1	-86.9	178.2
1030a.inp	22.7	-213.34	60.75	50	80.4	-57.7	6.1	88.2	-57	-61.1	116.8	82.2	-25.4	-179.9
1031.inp	18.3	-217.74	56.35	54	81.8	-57.3	8	85.1	-54.1	-71.1	-54	67.5	168.9	-180
1032.inp	18.71	-217.32	56.76	47.1	75.6	-58.3	8.7	88.4	-49.8	-70.6	-157.7	66.6	66.7	-180
1033.inp	17.62	-218.42	55.67	54.1	64.5	-55.9	-6.5	61	-73.5	154.3	-130.5	-73.9	96.7	177.7
1033a.inp	17.79	-218.25	55.84	48.7	68.2	-54.7	-0.9	62.5	-72	140.1	-145.2	-88.4	82.9	179
1034.inp	15.92	-220.12	53.97	51.4	70.8	-56.1	-2.1	61	-73.6	150	-45	-76.6	-178.7	178.9
1035.inp	20.58	-215.46	58.63	50.5	79.4	-56.3	-16	40.1	-96.6	165.3	68.6	-61	-68.3	176.7
1036.inp	2.71	-233.33	40.76	46.6	48.6	57.4	176.7	-95.6	143.3	63.4	-62.3	-176.7	177.7	178.4
1037.inp	2.94	-233.1	40.99	44.1	39.3	56.4	176.2	-102.9	133.1	66.1	59.2	-173.2	-62.2	-180
1038.inp	3.17	-232.87	41.22	44.4	38.8	56.3	-176.1	-102.4	134.8	60	-172.9	178.9	67.3	179.9
1039.inp	5.42	-230.62	43.47	44.2	38.3	55.1	-177.3	-82.8	150.4	-30.7	63.7	92.4	-60.3	-179.9
1039a.inp	5.64	-230.4	43.69	44.3	38.8	54.7	-175.3	-84.9	147.6	-61.4	35.1	62.8	-89.1	178.6
1040.inp	3.11	-232.93	41.16	47.2	38.6	56.2	178.3	-79.4	157.1	-55.7	-66.6	65.7	172	177.1
1041.inp	3.76	-232.29	41.81	44.2	37.6	55.9	-176.5	-84.9	149.7	-61.5	-178	59.3	60.6	179.5

1042.inp	5.28	-230.76	43.33	43.8	39.5	55.3	-176.3	-87.5	148.7	178.7	-146.1	-62.2	94.9	179.3
1042a.inp	5.16	-230.88	43.21	44.3	37.1	55.1	-175.8	-86.1	150.1	143.8	-176.7	-97.3	63.4	179.5
1043.inp	3.18	-232.23	41.23	47.6	39.5	55.8	178.3	-82.3	155	172.7	-58.7	-67	-178.5	176
1044.inp	3.59	-232.45	41.64	44.3	36.6	55.5	-176.7	-88.9	145.6	179.7	63	-59.5	-58.1	-179.5
1045.inp	4.48	-231.56	42.53	46.7	49.8	59.4	176.4	69.9	-59.1	65.8	-51.9	-166.6	-179.3	179.8
1046.inp	7.56	-228.48	45.61	47	56.7	56.7	175.5	58.4	-75.4	61.7	71.9	-166.5	-60.5	-179.6
1047.inp	5.36	-230.68	43.41	47.6	49.2	49.2	174.9	70.4	-59.1	63.9	-160.7	-169.4	72.4	179.5
1048.inp	11.28	-224.75	49.33	45.4	34.9	58.7	-176.8	70.5	-71.9	-61	65.3	79.3	-74.9	179.1
1048a.inp	11.27	-224.77	49.32	45.5	34.7	58.6	-176.1	69.8	-72.6	-63.2	61.9	77.1	-78.2	178.9
1049.inp	5.77	-230.26	43.82	46.8	30.9	57.3	-177.5	79.5	-53.9	-68	-52.1	64	176.6	179
1050.inp	6.39	-229.65	44.44	47.1	31.2	57.7	-176.1	80.7	-53.5	-71.4	-164.8	60.1	64.2	179.1
1051.inp	6.45	-229.59	44.5	44.7	40.7	57.7	-178.8	70.1	-59.5	172.9	-140.1	-61.1	94.6	179
1051a.inp	6.56	-229.48	44.61	45.5	39.1	57.6	179.6	61	-68.6	139.6	-170.9	-94.9	63	179.2
1052.inp	4.55	-231.48	42.6	45.1	39	57.8	-178.3	66.2	-63.5	169	-49.7	-63.7	-176.4	179.2
1053.inp	7.16	-228.88	45.21	43.9	41.3	59.6	-178.4	54	-80.5	167.6	73.9	-61	-57.8	172.2
1054.inp	2.94	-233.1	40.99	48.3	-132.2	54.6	-177.7	-135	103.3	61.9	-62.1	-178.2	177.9	179.7
1055.inp	3.45	-232.59	41.5	48.2	-124.7	54.2	-177.8	-145.9	90.1	63.9	56.9	-175	-64.6	179.4
1056.inp	3.7	-232.34	41.75	47.9	-123.9	54.1	-178.3	-145.5	91.5	60.7	-173.1	-179.9	66.9	179.4
1057.inp	7.04	-229	45.09	48.1	-127.2	52.3	174.9	-153.9	78.2	-73.7	33.5	51.6	-91.3	-179.9
1058.inp	5.39	-230.65	43.44	49.2	-138.3	51.9	177.3	-139.4	96.3	-73.5	-67.2	48.9	171	180
1059.inp	5.36	-230.68	43.41	49.2	-133.4	50.6	177.6	-152.4	82	-69.9	-177.3	52.1	60.8	179.7
1060.inp	6.35	-229.69	44.4	48	-121	53.7	177.5	-146.8	89.3	175.1	-143.8	-65	96.9	179.5
1060a.inp	6.23	-229.8	44.28	47.6	-118.2	53.2	175.7	-139.7	96.4	147.3	-178.5	-93.9	62.4	179.7
1061.inp	4.23	-231.81	42.28	48	-126.6	53.4	176	-133.4	103.6	169.5	-60.3	-70.5	-179.7	-179.9
1062.inp	4.59	-231.45	42.64	47.9	-117.7	52.5	177.9	-141	93.5	176.3	61.4	-95	-59.6	179.5
1063.inp	4.54	-231.5	42.59	49	-138.8	55.4	-178	62.5	-66.4	52.8	-59.3	-179.7	173.4	-180
1064.inp	7.28	-228.76	45.33	49.7	-130.1	53.3	175.5	54.5	-79.3	53.1	75.8	-175.5	-56.4	-179.8
1065.inp	5.63	-230.4	43.68	48.1	-133.6	53.7	173.8	64.7	-65.1	49.8	-168	176.2	64.7	-180
1066.inp	12.44	-223.6	50.49	51.8	-144.1	54.9	-175.6	57.2	-82.8	-106.1	56.3	31	-80.8	179.7
1066a.inp	12.41	-223.63	50.46	49.6	-145.4	55.5	175.2	82.2	-57.6	-54.4	105.3	82.3	-31.4	179.6
1067.inp	7.35	-228.69	45.4	50	-147.7	57.8	-178.5	79.3	-54.3	-69.5	-56.8	62.8	171.6	-180
1068.inp	8.44	-227.6	46.49	49.1	-142.9	54.3	175.6	81.2	-53.4	-73.8	-166.6	57.7	61.9	179.7
1069.inp	7.67	-228.37	45.72	48.8	-138.6	55.9	175.5	69.3	-60.5	171	-139.9	-63.1	94.3	180
1069a.inp	7.53	-228.51	45.58	48.7	-134	54.7	175.1	61.7	-67.9	140.1	-171.2	-94.6	62.8	179.5
1070.inp	5.46	-230.58	43.51	47.9	-135.5	56.1	180	61.1	-68.4	160.9	-61.4	-72.1	171.9	179.9
1071.inp	7.87	-228.17	45.92	49.3	-122.9	51.3	174.3	55.1	-79.3	166.4	77.6	-62.5	-54.1	-179.8
1072.inp	2.06	-233.98	40.11	49.8	21.6	62.6	179.8	-141.1	97.4	60.5	-70.2	-179.5	170.7	180
1073.inp	3.24	-232.8	41.29	49.5	28.7	62.8	179.4	-142.3	92.9	64.5	69.8	-173.5	-51.9	178.1
1074.inp	2.92	-233.12	40.97	46.5	31.3	61.6	-178.5	-147.4	89.6	58	-174.5	177.5	66	179.8
1075.inp	5.69	-230.35	43.74	49.1	29	62.2	178.1	-142.6	89.7	-33.9	70.8	90.6	-53.8	179.4
1075a.inp	6.03	-230.01	44.08	53.2	21.7	61.3	169.8	-159.2	73.7	-64.8	28.8	61.3	-95.1	179.7
1076.inp	2.74	-233.3	40.79	48.5	25	61.2	-179.8	-140.3	96.2	-61.6	-72.8	59.7	166.8	-179.1
1077.inp	3.35	-232.69	41.4	46.6	30.4	60.5	-177.1	-150.1	84.7	-64.3	-178.8	56.8	60.3	-179.2
1078.inp	5.21	-230.83	43.26	47.2	31.5	60.5	-179.6	-152.1	84.2	177.4	-146.2	-62.8	95	179.8
1078a.inp	5.17	-230.87	43.22	46.6	31.4	59.6	-178.7	-150.2	86.2	146	-178.2	-94.9	62.6	179.6
1079.inp	3.13	-232.91	41.18	49	24	60	179.2	-144.2	96.4	169.5	-69.6	-70.6	171.7	179.7
1080.inp	3.7	-232.34	41.75	48.7	32.1	60.1	179	-144.5	89.6	176.6	70.1	-61.4	-51.4	178
1081.inp	4.42	-231.61	42.47	53.5	12.9	63.4	175.6	58.3	-70.1	49.1	-54.6	175.7	177.2	179
1082.inp	6.5	-229.54	44.55	50.4	22.1	63.2	176.9	48.6	-84.1	49.5	65.2	-179.9	-67.1	179.2
1083.inp	5.24	-230.8	43.29	52.8	16.6	62.1	174.5	58.9	-70.4	45.7	-168.8	171.9	62.9	179
1084.inp	10.58	-225.46	48.63	48.8	23.5	59.7	-178.1	78.9	-61	-56.6	106.4	80.3	-30.4	178.7
1084a.inp	11.01	-225.03	49.06	45.7	34.3	60.5	-176.8	55.8	83.6	-106.5	54.1	29.7	-82.4	179.3
1085.inp	5.79	-230.25	43.84	48.1	25.6	60.7	-176.2	78.8	-54.6	-66.5	-51.8	65.5	176.9	179.1
1086.inp	6.47	-229.57	44.52	48.6	24.6	62.1	-175.4	79.9	-54.1	-69.1	-164.1	62.4	64.9	179.1
1087.inp	6.47	-229.57	44.52	47.8	28.3	58.8	-177	67	-62.6	172.5	-140	-61.5	94.5	178.9
1087a.inp	6.5	-229.54	44.55	46.9	31.6	59.3	-178.7	59.2	-70.2	138.9	-171.3	-95.6	62.6	179.2
1088.inp	4.62	-231.42	42.67	47.8	27.6	58.9	-178.3	62.6	-67.1	165.7	-51.3	-67.3	-178.1	178.8
1089.inp	7.06	-228.98	45.11	46.8	29.4	59.6	-177.6	49.7	-84.4	164.4	70.5	-64.8	-61	178.7
1090.inp	10.3	-225.74	48.35	54.7	48.1	59.2	176.7	-92.8	146.4	64.8	-57.1	-175.7	-177.2	-0.03
1091.inp	10.46	-225.58	48.51	47.3	45.1	60.3	176.7	-93.5	143.1	67.3	58.4	-171.8	-63.1	0.2
1092.inp	10.41	-225.63	48.46	46.7	45.4	61.2	176.1	-94.3	143.8	61.3	-171.8	-179.8	68.6	1.1
1093.inp	12.14	-223.89	50.19	46.1	38.4	60.7	176.5	-82.6	150.7	-60.6	32.5	63.4	-91	1.3
1093a.inp	12.14	-223.9	50.19	47.3	35.4	61.6	174.3	-77.6	155.9	-30.4	60.7	93.2	-63.2	0.4
1094.inp	10.57	-225.47	48.62	54.7	37.1	61.1	176.3	-75.8	161.1	-53.4	-59.9	67.9	178.9	1.1
1095.inp	10.54	-225.5	48.59	48.6	38.3	61.1	177.2	-78.4	156.6	-60.2	-177.9	60.6	60.8	-0.1
1096.inp	12.06	-223.97	50.11	47.7	38.4	61	176	-82.8	153.9	178.5	-144.8	-62.1	96.3	-0.1
1096a.inp	11.88	-224.16	49.93	47.4	36.3	61.9	176	-78.9	158	141.2	-176.9	-99.5	63.4	0.6
1097.inp	10.5	-225.54	48.55	53	39.7	61.3	176.1	-78	160	174	-55	-66.1	-174.5	1.1
1098.inp	10.6	-225.44	48.65	47.9	39.2	60.9	177	-78.8	156.2	179.8	63.9	-59.2	-57.3	0.1
1099.inp	12.38	-223.66	50.43	54.4	54.3	61.1	176.4	73.8	-55.5	65.5	-52	-166.5	-177.1	0.6
1100.inp	15.69	-220.35	53.74	54.5	59.5	65.2	173.6	61.2	-73	61.2	75.5	-166.6	-56.8	1
1101.inp	13.37	-222.66	51.42	54.2	52	63	178	76.4	-52.9	68.5	-157.2	-164.3	76.6	0.5
1102.inp	18.43	-217.61	56.48	44.4	46.3	65.4	170.8	74.3	-67.9	-60.9	64.4	79.3	-76.3	0
1103.inp	13.53	-222.51	51.58	46.2	48.1	64.4	174.1	85.8	-47.7	-73.2	-53.5	59.2	174.9	2.7
1104.inp	13.95	-222.08	52	49.2	44.6	65.2	174.2	87.6	-46.6	-75.8	-164.4	56	64.3	0.8
1105.inp	13.53	-222.51	51.58	48.6	44.4	64.6	176.6	73.2	-56.1	174.8	-140.3	-59.3	94.5	0.1
1105a.inp	12.89	-223.15	50.94	45.1	37.2	66	173.1	62	-67.1	136.8	-170.3	-97.9	63.4	-0.4
1106.inp	11.74	-224.3	49.79	48.1	46.2	64.3	177.4	70.4	-59.1	171.9	-48.7	-60.6	-175.3	0.3
1107.inp	13.11	-222.93	51.16	45.3	33.2	65.3	175	52.4	-81.4	164.8	71.4	-64.6	-60.1	-0.6

1108.inp	11.09	-224.95	49.14	45.3	65.8	52.5	2.1	-132	108	64.6	-63.9	-176.6	177.5	177.1
1109.inp	11.7	-224.33	49.75	42.5	64.2	52.8	4.2	-139.9	96.6	67.3	58.3	-172	-62.4	178.1
1110.inp	11.46	-224.58	49.51	41.7	64.4	52.6	3.1	-140.7	96.9	62	-171.2	-179.1	69.7	178.1
1111.inp	14.78	-221.26	52.83	38.2	62	53.3	3.7	-136.2	97	-64.4	30	59.2	-93.1	179.5
1111a.inp	14.47	-221.57	52.52	40.5	57.3	52.8	1.5	-116.1	117.8	-26.8	63.4	95.7	-59.9	177.3
1112.inp	11.95	-224.09	50	39.8	60.2	53.9	1	-120.3	115.7	-59.6	-66.3	61.3	172.8	178.1
1113.inp	12.7	-223.34	50.75	40.1	58.8	54.1	2	-120.4	114.2	-63.8	-178.8	56.9	60.2	178.1
1114.inp	13.8	-222.23	51.85	37.9	62.5	53.1	2.2	-141.2	95	176.5	-143.5	-63.8	97.4	179.9
1114a.inp	13.33	-222.71	51.38	41.7	57.8	53.6	3.1	-116.8	119.4	148.5	-177.9	-93.2	63	177.3
1115.inp	11.3	-224.74	49.35	40.3	58.7	53.7	1.2	-119.3	118	167.4	-61.5	-73.1	179.3	179.4
1116.inp	12.51	-223.53	50.56	40.2	57	53.8	2.6	-120.9	113.7	175.3	63.6	-63.7	-57.4	178.9
1117.inp	16.82	-219.22	54.87	42.9	73.1	49.9	-2.4	64.4	-70.8	40.9	-49.3	175.3	175.8	178.7
1118.inp	23.31	-212.73	61.36	49.4	83.9	46.8	-11.6	46.4	-92.1	53.9	65.9	-169.3	-73.6	176.6
1119.inp	17.62	-218.42	55.67	41.9	67.3	49.6	-2.2	64.2	-70.8	41.8	-152.3	175.4	73.3	178.2
1120.inp	26.74	-209.3	64.79	46.8	83	46.5	-7.5	49.9	-95.6	-107.9	57	35.2	-88	177.1
1121.inp	20.33	-215.71	58.38	43.4	80.3	48.9	8.7	84.7	-54.8	-72	-55.9	67	166.7	178.4
1122.inp	20.42	-215.62	58.47	38.8	73.4	46	10.4	88.2	-50.2	-70.9	-159.1	66.5	65.4	178.3
1123.inp	19.26	-216.78	57.31	46.4	63.9	51.5	-5.3	60.2	-74.6	153.1	-133.4	-74.8	93.7	177.2
1123a.inp	18.86	-217.18	56.91	36.1	74.5	48.6	5.2	66.6	-67.5	129.9	-157.1	-98.2	71.5	178.8
1124.inp	17.55	-218.49	55.6	45.2	69.4	47.4	-4.5	59.4	-75.4	150.7	-46.7	-75.9	179.3	177.8
1125.inp	22.72	-213.32	60.77	49.1	75.5	51	-14.2	32.9	-103.5	169.3	70	-57.3	-67	176.9
1126.inp	5.12	-230.92	43.17	111.3	103.2	-174.4	179	-134	104.2	59	-61.9	178.9	178.5	-177.6
1127.inp	5.91	-230.13	43.96	107.5	113.8	-173.6	177.6	-154.1	81.9	61.8	53.9	-176.6	-67.3	-177.8
1128.inp	5.86	-230.18	43.91	122	112.9	-178.5	178.8	-150.2	86.8	57.5	-173.2	177.2	67	-178.6
1129.inp	8.56	-227.47	46.61	118.6	130.5	-176.7	177.9	-144.4	87.9	-34.9	61.7	89.2	-62.7	-178
1714.inp	5.16	-230.88	43.21	70.2	120.7	-176.1	-176.2	-101.2	137.3	72.1	-60.4	-168.9	179.8	-178.5
1715.inp	6.07	-229.97	44.12	69.8	119.7	-177.3	-178.4	-98.3	138.3	75.8	62	-163.9	-59.1	-178.5
1716.inp	6.26	-229.78	44.31	70.3	121.6	-177.4	-176.9	-99.9	137.8	71.5	-169.1	-170	71.4	-178.6
1717.inp	8.76	-227.28	46.81	70.6	121.3	-173.7	-170.9	-76.5	156.6	-29.9	65	93.6	-60.4	-178.5
1718.inp	5.28	-230.76	43.33	71.7	120.7	-173.7	177.2	-121.4	114.3	-56	-64.4	65	174.7	-178.6
1719.inp	7.79	-228.25	45.84	70	123	-179.2	178.6	-82.5	154	144.2	-177.2	-96.8	63.1	-178.8
1719a.inp	7.63	-228.41	45.68	70.5	123.7	-178.4	178.7	-86.9	149.5	179.6	-146.8	-61.2	94.5	-178.7
1720.inp	5.37	-230.67	43.42	70.4	123.4	-178.1	178.6	-88.3	148.8	175.8	-58.2	-64.8	-177.5	-178.6
1721.inp	5.94	-230.1	43.99	70.1	124.3	-178.2	177.9	-83.5	151.3	179.8	64.6	-59.4	-56.4	-178.6
1130.inp	5.54	-230.5	43.59	-73.1	116.7	-119.2	179.7	-138.8	99.6	59.6	-65.6	179.5	175.2	178.9
1131.inp	6.34	-229.7	44.39	-70.1	126.8	-120.5	-179.7	-150.2	85.4	63.2	61.4	-175.1	-60	179.3
1132.inp	6.37	-229.67	44.42	-67.1	124.3	-119.9	-179	-149.9	87.1	56.6	-174.2	176.2	66.2	179.7
1133.inp	9	-227.04	47.05	-67.3	131.6	-120.2	-177.9	-145	88	-32.2	62.3	91.2	-61.6	179.6
1133a.inp	8.84	-227.2	46.89	-77.4	145.3	-119.3	178.1	-149.3	83.7	-63.4	31.4	60.9	-91.9	178.7
1134.inp	6.6	-229.44	44.65	-71.6	124.6	-118.4	-179.4	-135.5	100.5	-59.7	-69.5	61.5	169.8	178.9
1135.inp	7.29	-228.74	45.34	-65.8	129.5	-120.5	-176.2	-148.2	86.4	-63.8	-179.4	57.1	59.7	179.4
1136.inp	8.71	-227.33	46.76	-67.7	131.7	-121.8	-178.8	-152.6	83.7	176.7	-142.9	-63.4	97.9	179.5
1136a.inp	8.82	-227.21	46.87	-65.7	131.4	-117.2	-178.2	-146.8	89.4	146.5	-178.4	-94.8	62.4	179.4
1137.inp	6.73	-229.31	44.78	-74.2	126	-118.7	178.6	-135.9	101.3	171.1	-63.7	-69	177.3	179
1138.inp	7.08	-228.96	45.13	-66.8	134.8	-119.4	-178.4	-149.7	84.9	178.1	61.9	-60.7	-58.8	179.4
1139.inp	7.23	-228.8	45.28	-80.3	112.4	-120.3	178.4	62.1	-66.5	51.9	-54.1	178.8	178.5	178.9
1140.inp	9.59	-226.45	47.64	-73.4	127.2	-117.2	177.3	50.1	-82.8	51.6	64.7	-177.8	-67.1	178.9
1141.inp	8.21	-227.8	46.26	-80.1	118.9	-120.8	177.9	62.6	-66.9	49.4	-167.7	175.7	65.3	178.9
1142.inp	14.36	-221.68	52.41	-69.9	119.5	-118.8	-178.7	81.1	-58.2	-54.9	107.3	81.4	-28.6	178.8
1143.inp	9.28	-226.76	47.33	-67.4	122.8	-120.9	-175.4	79.8	-53.4	-66.9	-51.1	64.9	178	178.8
1144.inp	10.28	-225.76	48.33	-66.8	122.8	-120.7	-173.9	80.2	-53.7	-71.2	-164.9	60.1	64.5	178.7
1145.inp	10.01	-226.03	48.06	-67.1	123.4	-121.4	-177	67.3	-62.2	171.1	-140	-63.2	94.8	179.6
1145a.inp	9.95	-226.09	48	-66.6	128.9	-120.2	-178.1	59.6	-69.8	140.1	-171.3	-94.6	62.9	179.3
1146.inp	7.91	-228.13	45.96	-66.9	123.6	-120.1	-177.6	63.4	-66.1	165.7	-50.8	-67.5	-177.3	179.6
1147.inp	10.48	-225.56	48.53	-66.9	125.4	-120.2	-179.6	50.2	-83.7	164.2	69.2	-65.4	-62	179.4
1148.inp	8.46	-227.58	46.51	-103.3	118.7	-119.1	-179.4	-136.2	102.1	60.2	-62.9	179.9	177.8	-0.5
1149.inp	9.6	-226.43	47.65	-114.2	129.7	-122	177.7	-149.1	86.5	62.6	58.9	-175.5	-62.6	1.1
1150.inp	9.33	-226.71	47.38	-97	128.6	-119.6	179.6	-150.5	86.5	56.5	-173.9	176.1	66.5	0.5
1151.inp	12.25	-223.78	50.3	-108.9	135.9	-119.4	177.7	-144.1	88.6	-32.8	63.9	91.1	-60.2	0.9
1152.inp	9.49	-226.55	47.54	-101.7	134.7	-120.5	179.3	-131.6	104.2	-59.6	-68.6	61.6	170.7	0.1
1153.inp	9.93	-226.11	47.98	-90.1	148.8	-120.4	-178.7	-145.6	88.9	-63.6	-179.5	57.4	59.6	0.6
1154.inp	11.76	-224.28	49.81	-95.2	137.8	-119.7	178.8	-153.5	82.8	176.4	-143.2	-63.5	97.6	0.7
1154a.inp	11.75	-224.29	49.8	-92.7	140	-120.2	179.7	-148	88.2	145.8	-178.3	-95.2	62.5	0.8
1155.inp	9.7	-226.34	47.75	-106.6	125.6	-120.2	-180	-133.8	103.4	172.1	-61.1	-68.2	179.9	-0.02
1156.inp	9.98	-226.06	48.03	-90.4	153.4	-119.5	179.9	-148.5	86.1	178.4	63	-60.4	-57.8	1
1157.inp	10.03	-226.01	48.08	-109.2	113.3	-119.9	179.7	62.8	-65.9	51.9	-53.9	178.8	178.9	-0.3
1158.inp	12.61	-223.43	50.66	-104	124.2	-121.6	179.1	50.7	-82.4	51.2	64.6	-178	-67.2	0.2
1159.inp	11.05	-224.99	49.1	-112.3	119.4	-119.7	-179.5	63.4	-66.1	49.4	-166.8	175.8	66.2	-0.2
1160.inp	17.38	-218.66	55.43	-99.5	126.4	-120.5	-178.2	83	-55.9	-53.7	108.1	82.2	-27.3	0.1
1160a.inp	17.26	-218.78	55.31	-92.1	143.9	-119.7	-179.2	54.7	-84.3	-107.4	53.5	28	-82.6	0.8
1161.inp	12.3	-223.74	50.35	-93.2	142.2	-119.4	-178.3	80.9	-52.5	-67.9	-52.6	64	176.3	0.5
1162.inp	13.4	-222.64	51.45	-96.2	131.4	-121.1	-176.4	81.5	-52.4	-69	-164.1	62.2	65.3	0.4
1163.inp	13.02	-223.02	51.07	-94.7	136.5	-118.9	-179.7	59.6	-69.8	139.8	-171.5	-95	62.8	0.5
1163a.inp	13.04	-223	51.09	-96.4	132.9	-120.3	179.8	68.2	61.4	171.3	-139.9	-63	94.7	1
1164.inp	11.07	-224.97	49.12	-105.1	117.9	-121.1	179.9	63.3	-66.2	164.6	-51.8	-68.7	-178.4	0.5
1165.inp	13.35	-222.69	51.4	-94.2	135.9	-120.6	177.7	50.3	-83.4	163.6	69	-66.1	-62.2	1
1166.inp	6.26	-229.78	44.31	-158.8	-49.7	-119.6	178.4	-136.5	101.8	61	-64.9	-179.1	175.8	-178.9
1167.inp	7.07	-228.97	45.12	-161.4	-42.6	-119.3	-179.8	-146.4	89.5	63	56.6	-175.9	-64.3	-178.8
1168.inp	7.17	-228.87	45.22	-161.2	-42.6	-119.3	179.9	-145.4	91.6	58.4	-173.9	177.7	66.6	-178.8

1169.inp	9.9	-226.14	47.95	-160.5	-34.3	-119.8	176.6	-146.5	86.2	-64	32.6	60.5	-91	-178.5
1169a.inp	9.97	-226.07	48.02	-159.4	-37.2	-119.7	-179.6	-145.5	87.7	-30.8	61.1	92.4	-62.8	-178.4
1170.inp	7.39	-228.65	45.44	-159.8	-44.4	-122.1	178.4	-132.2	103.8	-59.1	-67.7	62.1	171.6	-178.4
1171.inp	8.19	-227.85	46.24	-159.6	-36.9	-120.1	-179.7	-144.5	90	-63.6	-179.4	57.3	59.8	-178.4
1172.inp	9.61	-226.43	47.66	-160.7	-38	-120.6	178.8	-150.1	86.3	177	-143.8	-63.3	97.3	-178.6
1172a.inp	9.71	-226.33	47.76	-160.3	-39.6	-120.9	178.4	-146.3	89.9	146.2	-178.4	-94.9	62.4	-178.6
1173.inp	7.5	-228.54	45.55	-159.8	-46.1	-120.6	176.9	-134.1	103.1	171.6	-62.7	-68.6	178.4	-178.4
1174.inp	8.04	-228	46.09	-161	-38.4	-119.7	-178.7	-147.8	87	178.4	60.8	-60.7	-59.8	-178.6
1175.inp	6.82	-229.22	44.87	-144.2	-2.5	-121.2	-177.4	-110.5	127.7	62.5	-60.7	-178.3	179.7	-179
1176.inp	7.87	-228.17	45.92	-144.5	-1.8	-120.8	-179.1	-108.7	127.2	65.5	58.9	-173.7	-62.2	-179.4
1177.inp	7.91	-228.13	45.96	-146.2	-2	-121.4	-179.2	-107.5	129.6	59.3	-173.2	178.3	67.2	-179.1
1178.inp	10.27	-225.77	48.32	-144.4	-2.6	-121.5	-179.6	-102.4	131.2	-61.7	29.2	61.4	-93.3	-180
1178a.inp	9.89	-226.15	47.94	-143.4	-12.3	-122.8	176.4	-83.4	150.3	-30.1	64.5	92.6	-59.7	179.9
1179.inp	7.46	-228.58	45.51	-145.4	-10.5	-125.4	179.4	-87.2	148.9	-55	-63.4	65.7	175.6	-179.5
1180.inp	8.2	-227.84	46.25	-146	-10.3	-127.2	178.6	-85.8	149.1	-60.7	-178.5	59.8	60.7	-179.4
1181.inp	10.07	-225.96	48.12	-146.4	-9.5	-121.8	179.7	-91.4	144.9	178.5	-146.9	-62.4	94.4	-178.9
1181a.inp	9.93	-226.11	47.98	-147.3	-11.4	-122.4	179.4	-85.9	150.6	143.2	-177	-97.7	63.3	-178.9
1182.inp	7.64	-228.4	45.69	-146.1	-8.3	-119.4	-177.1	-91.3	145.7	174	-57.4	-66.5	-177	-178.8
1183.inp	8.41	-227.62	46.46	-147.3	-9.3	-119.4	-179.3	-86.7	147.9	179.3	64.1	-59.8	-57.1	-179.2
1184.inp	8.29	-227.75	46.34	-144.9	-3.8	-119.9	-178.5	63.9	-65	52.7	-53.5	180	179.3	-178.9
1185.inp	10.97	-225.01	49.02	-147.3	-0.8	-120.1	-178.9	51.9	-81.6	52	67.4	-176.7	-64.6	-178.6
1186.inp	9.12	-226.92	47.17	-147	-9.3	-119.9	-178.8	64.2	-65.4	50.5	-166.1	177.2	66.9	-178.7
1187.inp	15.71	-220.32	53.76	-146.9	-3.2	-119.9	-179.2	55.3	-83.9	-108	53.9	27.8	-82.4	-178.7
1187a.inp	15.58	-220.46	53.63	-145.8	-1.9	-120	-178.7	84.2	-54.7	-53.4	108.2	82.7	-27.3	-178.9
1188.inp	10.97	-225.07	49.02	-145.8	-0.9	-120.8	-178.1	81.5	-51.9	-66.4	-52.2	65.7	176.8	-178.8
1189.inp	11.64	-224.4	49.69	-146.3	-0.2	-122	-176.7	82.2	-51.8	-70.5	-164.3	61	65	-178.8
1190.inp	11.21	-224.83	49.26	-147.3	-3.4	-120.3	-178.9	68.8	-60.7	171.2	-139.8	-62.8	94.7	-178.7
1190a.inp	11.21	-224.83	49.26	-147.7	1.1	-120.4	-179	60.5	-69.1	139.7	-171.3	-94.7	62.7	-178.6
1191.inp	11.77	-224.27	49.82	-147.1	-0.9	-119.2	178.8	52	-82.2	164.8	71.9	-64.2	-59.7	-178.8
1192.inp	9.24	-226.8	47.29	-145.1	-1.4	-119	178.1	64.8	-64.8	165.3	-51.4	-67.7	-178.2	-178.9
1193.inp	8.5	-227.54	46.55	-130.7	140.7	-120.5	-179.4	-115.2	122.9	63.6	-60.8	-177.1	179.6	1.4
1194.inp	9.63	-226.4	47.68	-131.1	140.5	-120.8	179.3	-112.9	122.9	65.8	58.9	-173.3	-62.1	1.5
1195.inp	9.62	-226.42	47.67	-133.9	137.4	-119.7	179.8	-106.9	130.2	60.2	-172.5	179.3	67.8	1.6
1196.inp	11.83	-224.21	49.88	-138.3	139.3	-120.5	-177.8	-80.2	152.7	-32	64.6	91.7	-60.1	1.6
1197.inp	12.09	-223.95	50.14	-133.5	130.5	-119.5	178.2	-93.4	142.8	178.2	-146.8	-62.6	94.6	1.5
1197a.inp	11.93	-224.11	49.98	-133	132.7	-119.7	178.8	-85.2	151.2	142.8	-176.9	-98	63.4	1.4
1198.inp	9.59	-226.45	47.64	-130.4	136.6	-119.8	-179.5	-91.6	145.4	173.6	-57.9	-66.9	-177.3	1.3
1199.inp	10.4	-225.64	48.45	-132.9	136.9	-119.6	178.6	-86.2	148.5	179.3	64.3	-59.8	-56.6	1.3
1200.inp	10.03	-226.01	48.08	-130.9	142.7	-119.8	-178.7	64.5	-64.2	53.1	-53	-179.6	180	1.3
1201.inp	12.83	-223.21	50.88	-124.8	149.6	-121.1	178.7	52.2	-81	52.1	66.4	-177	-65.4	1.9
1202.inp	11.12	-224.92	49.17	-127.8	141.2	-118.2	-179.7	64.2	-65.3	50.4	-166.2	176.9	66.9	1.3
1203.inp	17.7	-218.34	55.75	-133.2	136.1	-118.8	179.3	83.6	-55.4	-53.4	107.6	82.6	-28	1.4
1203a.inp	17.65	-218.39	55.7	-122.6	154.4	-119.7	179.9	55.8	-83.3	-107.3	54.2	28.4	-82	1.9
1204.inp	12.72	-223.32	50.77	-132.6	136.3	-119.1	179.7	81.3	-52	-66.4	-52.6	65.5	176.2	1.4
1205.inp	13.74	-222.3	51.79	-131.5	138.1	-120.1	-179	82.3	-51.7	-71.3	-165	60	64.2	1.4
1206.inp	13.22	-222.82	51.27	-129.7	140.4	-117.5	179.7	69	-60.5	171.4	-140.1	-62.8	94.6	1.4
1206a.inp	13.23	-222.81	51.28	-128	145.9	-121.3	178.7	61.1	-68.4	140.1	-171	-94.7	63.2	1.6
1207.inp	13.65	-222.39	51.7	-123.5	153.4	-120.5	177.2	52.3	-81.6	164.8	70.7	-64.6	-60.6	1.6
1208.inp	10.99	-225.05	49.04	-132.7	144.3	-118.2	-180	64.9	-64.6	165.9	-51.9	-67	-178.6	1.7
1209.inp	13.84	-222.2	51.89	56.0	-126.6	125.2	174.2	-153.6	77.5	-79.4	34.8	46.7	-91.1	-179.5
1210.inp	12.61	-223.43	50.66	55.0	-127.2	123.4	172.7	-151.6	81.7	-77.9	-173.8	45.4	63	-179.5
1211.inp	5.43	-230.6	43.48	-157.6	149	-119.7	-178.7	-108.4	129.9	63.1	-61.1	-177.6	179.2	-178.2
1212.inp	6.42	-229.62	44.47	-158	149.6	-119.9	-179.5	-107.4	128.6	66.1	59.7	-173.1	-61.4	-178.2
1213.inp	6.41	-229.63	44.46	-158.8	147.4	-121	-178.8	-106.3	130.9	60.8	-172.2	179.8	68	-178.1
1214.inp	9.51	-226.52	47.56	-153.4	143.7	-119.8	-176.6	-112.6	120	-67.5	31.9	56.4	-91.6	-178
1215.inp	6.81	-229.23	44.86	-154.2	137.2	-120.5	-179.6	-108.8	126.7	-64.5	-64.8	56.7	174	-177.9
1216.inp	7.49	-228.55	45.54	-154.7	134.4	-120.8	178.7	-103.9	130.5	-66.3	-178.3	54.7	60.7	-177.8
1217.inp	8.61	-227.43	46.66	-160.4	145.8	-122.1	177.3	-87.5	149	143.7	-177.4	-97.4	63.3	-178.3
1217a.inp	8.76	-227.28	46.81	-158.8	146.4	-120	179.5	-90.2	146.2	178.2	-146.5	-62.7	94.8	-178.4
1218.inp	6.45	-229.59	44.5	-158.8	147.2	-120	179.4	-91.5	145.6	174	-58.4	-66.6	-177.6	-178.2
1219.inp	7.02	-229.02	45.07	-160.1	146.7	-120.3	178.2	-86.8	147.9	179.3	64.1	-59.8	-56.8	-178.3
1220.inp	6.96	-229.08	45.01	-157.5	151.3	-118.3	-178.2	64.1	-64.6	53.6	-54.7	-179.2	178.3	-178.2
1221.inp	9.73	-226.31	47.78	-156	158.4	-120.1	177.3	52.7	-80.5	52.5	66.8	-176.6	-65	-178.2
1222.inp	8.02	-228.01	46.07	-159	148.8	-121	178.5	64.9	-64.6	51.2	-165.4	177.6	67.7	-178.1
1223.inp	14.34	-221.7	52.39	-156.6	154.6	-120	-180	56.3	-83	-107.2	54.3	28.7	-82	-178.1
1223a.inp	14.53	-221.51	52.58	-159	149.1	-119.5	177.9	83.9	-55.2	-53.6	107.1	82.6	-28.7	-178.4
1224.inp	9.54	-226.5	47.59	-158.7	147	-121.2	-179.3	81.4	-52	-67	-53.3	65	175.5	-178.1
1225.inp	10.54	-225.5	48.59	-158.6	147.8	-120.6	-178.7	82.3	-51.7	-71.7	-165	59.7	64.2	-178.3
1226.inp	10	-226.04	48.05	-158.3	149.1	-119	179.5	69.2	-60.2	171.5	-140	-62.8	94.7	-178.1
1226a.inp	10	-226.04	48.05	-157.4	153.6	-119	178.9	61.2	-68.3	140.3	-171.1	-94.4	63.1	-178.2
1227.inp	7.79	-228.25	45.84	-159.2	150.2	-119.6	-179.3	64.3	-65.1	165.1	-52.8	-67.8	-179.4	-178.1
1228.inp	10.36	-225.68	48.41	-157.4	156	-119.9	176.6	53	-81	165.6	71.5	-63.8	-59.9	-178
1229.inp	5.98	-230.06	44.03	52.9	47.4	4.7	177.8	-98.2	140.5	63	-62.8	-177.2	177.3	176.6
1230.inp	6.62	-229.42	44.67	49.9	35.5	9.2	-176.2	-105.4	131.7	59.8	-173.2	178.7	67.1	179
1231.inp	6.35	-229.67	44.4	49.4	36.3	9.4	-175.7	-106.2	129.6	66.1	60.2	-173.2	-61	178.5
1232.inp	9.11	-226.93	47.16	49.4	37.8	9.3	-175.6	-86.1	146.4	-61.6	35.1	62.6	-89.1	177.9
1722.inp	6.52	-229.52	44.57	51.5	40.4	8.7	178.1	-82	154.3	-56.1	-66.4	65.1	172.4	176.2
1723.inp	7.23	-228.81	45.28	49.3	34.4	8.7	-175.6	-87.3	147.3	-61.5	-178.1	59.1	60.7	179
1724.inp	8.63	-227.4	46.68	50	32.7	7.8	-175.1	-86.7	149.4	143.7	-176.7	-97.3	63.4	178.9

1724a.inp	8.72	-227.32	46.77	50.1	33.4	7.9	-174.2	-90.6	145.6	178.4	-145.3	-62.4	95.6	178.4
1725.inp	6.49	-229.55	44.54	50.6	46.1	7.9	-180	-83.4	152.8	173.6	-57	-66.3	-176.9	175.6
1726.inp	6.95	-229.09	45	50	31.1	9.6	-175.5	-93.3	141.2	179.4	62.9	-59.8	-58.1	179.7
1233.inp	5.85	-230.19	43.9	-70.8	-22.1	-118.6	-178.3	-110.8	127.5	65.9	-60.6	-175	179.8	177.4
1234.inp	6.71	-229.33	44.76	-69.5	-8.5	-119.2	176.4	-98.6	138	68.3	59.4	-171.4	-61.3	176.5
1235.inp	7.04	-229	45.09	-71.6	-22.5	-117.9	-178.7	-107.4	129.8	63.8	-171.6	-177.4	68.9	177.5
1236.inp	9.11	-226.92	47.16	-71.3	-16.7	-119	-177.7	-86.3	146.9	-64.2	31.5	59.4	-92.1	177.4
1236a.inp	8.9	-227.14	46.95	-79.9	-10.3	-120.5	-178.4	-79.9	153.7	-28.8	63.4	94.1	-60.6	176.3
1237.inp	6.63	-229.41	44.68	-73.5	-18.6	-119.5	-177.6	-87.3	148.3	-59.7	-63.6	61.5	174.7	178.7
1238.inp	7.38	-228.66	45.43	-72.4	-19.1	-119.9	-178.7	-85.2	149.3	-64	-178	56.9	60.5	179.1
1239.inp	9.13	-226.91	47.18	-63.8	-22.4	-120	176.1	-90.6	145.9	178.7	-147	-62.4	94.6	178.4
1239a.inp	9.07	-226.97	47.12	-65	-21.9	-119.5	177.1	-84.7	151.9	143.9	-177.2	-97.3	63.3	178.2
1240.inp	6.73	-229.3	44.78	-63.5	-22.6	-119.8	177.1	-92	145.1	174.1	-58.3	-66.7	-177.3	178.2
1241.inp	7.26	-228.78	45.31	-62.6	-22.4	-118.8	175.4	-83.8	151.3	179.7	63.5	-59.8	-57	176.8
1242.inp	7.41	-228.63	45.46	-75	-22.6	-120	-178.3	63.8	-65.1	53.7	-55.3	-178.9	177.5	177.7
1243.inp	9.86	-226.18	47.91	-62.8	-28.2	-118.9	175.2	51.9	-81.3	52.1	67.7	-177.2	-64.2	178.5
1244.inp	8.36	-227.68	46.41	-66.7	-19.5	-118.9	178.8	65.4	-64.2	51.2	-165.7	177.8	67.3	179.2
1245.inp	14.69	-221.35	52.74	-67.6	-19.4	-119	177.8	56.2	-83	-107.9	54.8	27.8	-81.4	178.7
1245a.inp	14.91	-221.13	52.96	-67.7	-15.9	-118.1	177.8	85.3	-53.7	-53.4	107.5	82.7	-28	179.2
1246.inp	10.05	-225.99	48.1	-71.2	-15.1	-118.2	-179.4	82.6	-50.6	-65.9	-51.9	66.1	177.2	178.5
1247.inp	10.97	-224.07	49.02	-67.8	-16.5	-118.1	-180	83.9	-50.1	-69.5	-164	61.8	65.4	179
1248.inp	10.43	-225.61	48.48	-64.6	-24.5	-117.8	177.3	69.4	-60.2	171.3	-139.9	-62.9	94.6	179.2
1248a.inp	10.39	-225.65	48.44	-65.5	-20.3	-117.9	177.6	61.6	-68	139.9	-171.2	-94.8	62.9	179.1
1249.inp	8.4	-227.64	46.45	-76.1	-23.7	-119	-179.1	63.5	-66	164.5	-53.5	-68.4	179.8	177.9
1250.inp	10.67	-225.37	48.72	-63.8	-23.1	-117.4	173.8	52.4	-81.5	164.3	70.7	-65.2	-60.8	178.6
1251.inp	5.31	-230.73	43.36	-70.3	141.3	-119	-179.3	-106.2	132.1	63	-60.6	-177.5	179.6	179.3
1252.inp	6.56	-229.48	44.61	-69.5	140.8	-118.5	-179.9	-106.4	129.5	65.8	59.6	-173.4	-61.5	179.4
1253.inp	6.48	-229.56	44.53	-68.5	137.4	-118.8	-178.8	-105.6	131.5	61.1	-172.1	-179.9	68.2	179.5
1254.inp	8.95	-227.09	47	-69.5	131.9	-121.8	-175.8	-80.2	153.2	-28.9	64.7	94.4	-59.6	179.5
1255.inp	6.35	-229.68	44.4	-69	130.4	-119.3	-178.4	-86.5	149.3	-57.8	-63.5	63.4	175.1	179.6
1256.inp	7.26	-228.78	45.31	-68.5	130.5	-119.1	-178.9	-85.9	148.7	-62.4	-178.1	58.5	60.7	179.6
1257.inp	8.82	-227.22	46.87	-69.7	140.5	-119.4	-179.3	-83.1	153.3	142.7	-176.7	-98.2	63.4	179.3
1257a.inp	8.93	-227.11	46.98	-69.1	140.5	-118.6	-179.1	-88.5	147.8	178.5	-146.3	-62.4	94.9	179.3
1258.inp	6.37	-229.66	44.42	-67.6	133.6	-116.8	-179.1	-92.1	144.9	173.8	-57.5	-66.6	-176.9	179.4
1259.inp	7.25	-228.79	45.3	-69.6	142.7	-118.2	179.8	-84.4	150.4	179.5	64.3	-59.7	-56.7	179.3
1260.inp	6.9	-229.14	44.95	-71.4	145.1	-118.8	-179	65.2	-63.4	56	-52.8	-176.7	-179.9	178.6
1261.inp	9.6	-226.44	47.65	-72	146.4	-117.8	177.6	51.8	-81.4	52.5	66.3	-176.7	-65.5	178.8
1262.inp	8.01	-228.03	46.06	-74	140.1	-119	177.5	64.9	-64.5	52.9	-165.3	179.3	67.6	178.9
1263.inp	14.21	-221.83	52.26	-67.1	135.6	-119.8	-179.1	54.7	-84.3	-107.5	53.3	27.9	-82.7	179.3
1263a.inp	14.36	-221.68	52.41	-72.4	142.2	-119.2	-179.9	83.9	-55.1	-54.2	107.8	81.9	-27.9	178.8
1264.inp	9.28	-226.76	47.33	-67.9	138.3	-118.1	-178	81.1	-52.2	-66.7	-52.4	65.2	176.6	178.8
1265.inp	10.27	-225.77	48.32	-66.8	136.4	-118	-175.9	81.8	-52.1	-71.4	-164.6	59.9	64.9	178.6
1266.inp	9.95	-226.09	48	-65.7	132.7	-117.3	-178.5	68	-61.4	171.4	-140	-63	94.8	179.3
1266a.inp	9.92	-226.12	47.97	-67.1	135.9	-121.2	-179	60.5	-69	140.2	-171.1	-94.5	63.2	179.3
1267.inp	7.75	-228.29	45.8	-66.5	137.1	-120.4	-176	65.4	-64	167	-48.5	-65.8	-174.9	179
1268.inp	10.35	-225.69	48.4	-67.6	137.7	-118.8	178	50.8	-83	163.9	69.5	-65.7	-61.7	179.4
1269.inp	12.43	-223.61	50.48	-121.5	99	-120	-5.7	-128.3	110.1	63.9	-63.7	-176.5	177.3	179.2
1270.inp	12.99	-223.05	51.04	-73	123.9	-118.3	-4.9	-152.4	84.4	63.4	48.3	-174.9	-72.2	179.4
1271.inp	12.71	-223.33	50.76	-74.2	123.8	-122.2	-1.5	-153	84.8	62.7	-160.4	-177.8	80.1	179.5
1272.inp	15.41	-220.64	53.46	-73.8	124.7	-121.1	-2.8	-151.7	82	-65.2	30.2	58.8	-92.7	179.6
1273.inp	14.3	-221.74	52.35	-122.7	101	-119.6	-6.6	-128.9	107.6	-60.6	-66.8	60.6	172.7	-179.6
1274.inp	14.17	-221.87	52.22	-74.6	123.8	-121.6	-2.3	-150.8	84.3	-65.3	-175.9	56	63.2	179.6
1275.inp	14.2	-221.84	52.25	-75.2	124.5	-122.3	-3.4	-154.5	82.5	176.5	-142.4	-63.6	98.8	179.6
1275a.inp	15.37	-220.68	53.42	-75.7	123.1	-120.5	-3.4	-149.6	87	145.9	-173.7	-95.1	67	179.6
1276.inp	13.83	-222.21	51.88	-123	99.5	-119.2	-7.1	-129	108.7	170.9	-61.4	-69.5	-180	-179.9
1277.inp	14.02	-222.02	52.07	-76.2	124.4	-121.9	-5.2	-151.9	83.7	176	55	-62.4	-65.3	179.8
1278.inp	6.06	-230.44	44.11	-151.8	121.1	-119.9	-178.5	-137.5	100.9	61.4	-62.5	-178.7	177.9	-178.3
1279.inp	6.85	-229.19	44.9	-152.1	134	-119.2	-176.2	-153.3	82.9	66.6	55.9	-172.3	-65.4	-178.3
1280.inp	6.81	-229.23	44.86	-150.5	129.7	-119.9	-179	-150.5	86.5	57.3	-173.3	177	66.8	-178
1281.inp	8.67	-227.37	46.72	-158.5	151	-121.5	-179.8	-150	83.2	-63.6	30.7	60.3	-92.5	-178.6
1282.inp	6.52	-229.52	44.57	-159.1	141.1	-122.2	179.1	-133.3	102.5	-61.9	-66.3	59.5	172.7	-178.3
1283.inp	7.03	-229	45.08	-156.9	153.3	-121.3	179.5	-145.9	88.5	-64.9	-179	56.4	59.9	-178.1
1284.inp	8.66	-227.37	46.71	-157.7	153.3	-121.9	179.2	-149.7	86.5	177.5	-143.5	-62.6	97.4	-178.3
1284a.inp	8.9	-227.14	46.95	-157.2	151.6	-121.7	-179.7	-146	90.1	146.8	-178.2	-94.1	62.2	-178
1285.inp	6.58	-229.46	44.63	-160.5	143.4	-123	179.4	-132	105	173.4	-59.4	-66.8	-178.5	-178.4
1286.inp	7.18	-228.86	45.23	-158	153.7	-122.1	-180	-146.8	87.9	178.8	61.6	-60.1	-59.2	-178.2
1287.inp	6.84	-229.2	44.89	-152.9	61.4	-120.4	-178.8	-104	134.3	62.5	-60.1	-178.1	-180	-179.7
1288.inp	8.17	-227.87	46.22	-152.9	59.7	-120.2	179.3	-103.4	132.4	65.6	58.4	-173.5	-62.8	-179.8
1289.inp	8.1	-227.94	46.15	-154.1	59.2	-120.4	179.7	-102.9	134.2	59.3	-172.7	178.3	67.5	-179.3
1290.inp	10.23	-225.83	48.28	-146.6	24.3	-120.7	-179	-84.4	149	-61.3	30.8	62.4	-92.6	-179.4
1291.inp	7.45	-228.59	45.5	-147.8	21	-122.3	-178.2	-84	152	-55.1	-62.6	65.8	176	-179.4
1292.inp	8.43	-227.61	46.48	-148.2	19.4	-120.1	-179.4	-83	151.7	-60.8	-178	59.9	60.8	-179.3
1293.inp	9.88	-226.15	47.93	-148.8	15.3	-120.5	-178.6	-83.2	153.1	142.9	-176.6	-98	63.4	-179
1293a.inp	10	-226.04	48.05	-148.7	15.6	-121	-178.1	-88.6	147.7	178.5	-146.1	-62.3	94.9	-179
1294.inp	7.48	-228.56	45.53	-148.3	15.5	-121.1	-177.6	-89.7	147.3	174	-57.6	-66.5	-177.2	-179
1295.inp	8.3	-227.72	46.35	-148	14.5	-122.3	-178.5	-87.7	147	179.4	63.6	-59.8	-57.5	-179.6
1296.inp	8.37	-227.67	46.42	-154.3	62.5	-120.6	-179.9	65.4	-63.5	53.6	-52.4	-179.1	-179.6	-179.4
1297.inp	11.05	-224.99	49.1	-155.1	65.8	-119.8	179.5	52.3	-81.2	51.9	66.1	-176.9	-65.9	-179.1
1298.inp	9.27	-226.77	47.32	-154.3	65.2	-119.8	-179.2	65	-64.7	51.4	-165.7	178.2	67.3	-179.3

1299.inp	15.7	-220.34	53.75	-150.3	16.8	-121.2	-179.3	55.5	-83.7	-108	53.9	27.8	-82.4	-178.6
1300.inp	11.1	-224.94	49.15	-150.9	26.3	-117.9	-178.2	82.3	-51	-66.1	-52	66	177	-178.8
1301.inp	11.76	-224.27	49.81	-151.8	24.2	-118	-177.6	83.2	-50.8	-70.3	-163.9	61.3	65.4	-178.6
1302.inp	11.22	-224.82	49.27	-149.2	14.8	-119.1	-179.7	69.4	-60.2	171.3	-139.8	-62.7	94.8	-178.7
1302a.inp	11.24	-224.8	49.29	-150.3	19.3	-119.2	-179	61.1	-68.6	139.6	-171.1	-94.7	62.9	-178.7
1303.inp	9.27	-226.77	47.32	-149.2	15.5	-118.5	179.9	65.3	-64.3	165.6	-51	-67.3	-177.7	-178.8
1304.inp	11.78	-224.25	49.83	-151.5	20.7	-119.5	178.8	52.9	-81.4	165.2	72.6	-63.7	-90.5	-178.6
1305.inp	12.75	-223.28	50.8	-145.2	126	-119	2.3	-99.9	140.2	65	-65	-176.8	175.9	-178.8
1306.inp	13.43	-222.61	51.48	-135.6	146	-120.3	5	-108.2	128.2	68.4	62.2	-171.1	-59	-178.5
1307.inp	12.64	-223.4	50.69	-135.1	147.2	-119.4	4.8	-109.3	128.3	62.5	-171.8	-178.9	68.7	-178.5
1308.inp	15.64	-220.4	53.69	-146.5	136.9	-120.6	3.2	-86.6	147.8	-25.6	64.5	96.9	-59.2	-178.2
1308a.inp	16.25	-219.78	54.3	-142.1	144.4	-120	3.9	-94.8	138.6	-62.9	31	60.9	-92.5	-177.9
1309.inp	13.08	-222.96	51.13	-133.7	142.4	-121.3	4	-90.8	146.3	-56.2	-66.1	64.1	172.9	-178.2
1310.inp	13.46	-222.58	51.51	-140.5	146.8	-121	3.3	-95.6	138.8	-62.8	-176	58.3	62.3	-178
1311.inp	13.88	-222.16	51.93	-135.2	146.1	-120.5	6.1	-89.9	145.9	141.7	-174.3	-98.4	64.7	-178.2
1311a.inp	14.68	-221.36	52.73	-135.2	145.1	-120.2	4.2	-93	143.6	174.6	-147.6	-66.3	93.5	-178.2
1312.inp	12.52	-223.52	50.57	-132.6	144.5	-120.5	5.8	-90.9	147	163.8	-60.6	-76.7	179.6	-178.3
1313.inp	13.77	-222.27	51.82	-138.3	146.3	-119.3	3.3	-93.9	140.4	176.4	65.6	-62.2	-56	-178.2
1314.inp	15.2	-220.84	53.25	-143.7	111.1	-120.6	-1	71.8	-63	49.3	-43.9	-177.1	-177.3	-179.7
1315.inp	19.7	-216.34	57.75	-140	128	-121.4	-1.9	57.1	-83.7	51.8	72	-169.3	-67.7	-177.7
1316.inp	16.22	-219.81	54.27	-134.7	121.6	-120.6	-1	68	-67.5	46.8	-159.6	179.7	67.2	-178.5
1317.inp	22.73	-213.31	60.78	-142.8	126.1	-121	-2.1	57.5	-86.9	-128.9	60.1	11.9	-81.2	-178.3
1318.inp	19.54	-216.5	57.59	-140.5	105	-122.5	-0.1	88	-51.8	-68.6	-48.2	70.5	173.9	-179.5
1319.inp	20.13	-215.91	58.18	-139.1	105.2	-119.7	-0.9	91.3	-47.1	-65	-147.3	72.3	76.7	-178.7
1320.inp	17.58	-218.46	55.63	-141.3	115.4	-122.1	-1.1	73.6	-60.5	166.2	-129.2	-62.5	99.9	-178.6
1320a.inp	17.58	-218.46	55.63	-141.3	116.9	-121	-3.3	65.5	-68.8	131.1	-168.9	-98.1	59.8	-178.3
1321.inp	16.12	-219.91	54.17	-141.7	116.1	-120.7	-0.8	70.1	-65.1	159.7	-41.3	-67.1	-174	-178.3
1322.inp	19.68	-216.36	57.73	-139.6	130.5	-119.9	-2.8	52.9	-86.6	152.2	70.2	-70.9	-67.7	-178.2
1323.inp	5.43	-230.61	43.48	-74.6	125.2	120.1	-177.2	-143.3	95.3	59.5	-66.9	179.7	173.4	178.4
1324.inp	5.93	-230.11	43.98	-70.4	135.7	120	-176.5	-155.1	80.9	64	59.3	-174.5	-62.3	178.8
1325.inp	6.06	-230.48	44.11	-68.3	134.9	120.2	-176.6	-154.4	82.7	57.2	-173.4	176.9	66.5	178.9
1326.inp	8.43	-227.61	46.48	-77.3	149	120.4	178.7	-150.8	82.1	-63.9	31.5	60.5	-92.1	178.4
1326a.inp	8.65	-227.29	46.7	-69.9	146	119.3	178.8	-148.2	84.2	-34.5	60	89.5	-64.2	178.8
1327.inp	6.06	-230.48	44.11	-73.3	140.9	121.1	-179.9	-133.9	102	-58.1	-67.8	63.2	171.1	178.5
1328.inp	6.88	-229.16	44.93	-70.2	146.4	120.9	-177.7	-142.3	92.1	-62.7	-179	58.2	59.8	178.7
1329.inp	8.13	-227.9	46.18	-70.3	146.3	120	179.4	-151.3	84.8	176.5	-142.6	-63.6	98.1	178.7
1329a.inp	8.03	-228	46.08	-70.2	146.2	120.8	177.4	-146.6	89.5	142.5	-177.6	-98	62.7	178.7
1330.inp	6.06	-229.98	44.11	-74.8	141.4	120.3	178.5	-136.6	100.6	171.1	-62.2	-68.8	178.6	178.4
1331.inp	6.58	-229.46	44.63	-69.3	143.9	120.5	-179.9	-150.8	83.7	177.6	60	-61.2	60.8	178.6
1332.inp	7.13	-228.91	45.18	-81.9	125.9	120.3	-178.4	58.4	-70.4	51.5	-65.5	178.4	166.8	178.6
1333.inp	8.48	-227.56	46.53	-77.1	141.2	119.9	-177.6	52.2	-81.4	54.4	76.5	-174.1	-55.7	178.4
1334.inp	7.16	-228.88	45.21	-78.1	140	119.8	179.9	62.7	-66.9	51.3	-169.8	177.9	62.8	178.5
1335.inp	13.5	-222.54	51.55	-68.5	133.7	120.1	179.8	72.4	-69.1	-53.1	84.4	86.2	-55.1	178.7
1335a.inp	13.68	-222.36	51.73	-69.6	143.5	120.5	-170.7	59.5	-81.1	-103.7	59.4	34.1	-78	178.6
1336.inp	9.44	-226.6	47.49	-70.3	126.6	120.6	-168.4	77.9	-55.1	-70.4	-55	61.7	174.3	178.2
1337.inp	9.41	-226.63	47.46	-68.5	138.1	120.8	-175.8	80.9	-53	-71.6	-165.4	59.7	64	178.3
1338.inp	9.13	-226.91	47.18	-68.4	140.1	120.1	-175.9	68.6	-60.5	171.4	-138.1	-62.7	96.8	178.8
1338a.inp	9.04	-227	47.09	-69.3	141.9	120.4	-177.8	59.4	-70.2	140.3	-173.7	-94.4	60.5	178.6
1339.inp	7.93	-228.11	45.98	-68.9	130.3	119.7	-174.4	57.6	-71.6	159.5	-66.1	-74	167.4	179
1340.inp	9.14	-226.89	47.19	-68.5	136.6	119.6	-176.4	52.1	-82.3	166.3	79	-62.5	-52.5	178.9
1341.inp	5.77	-230.25	43.82	-78.9	117	-2.2	-179.1	-135.1	103.1	60.9	-64.9	-179.3	175.7	179.7
1342.inp	6.72	-229.3	44.77	-74	129.4	-1.5	-178.9	-147.9	87.8	64.3	59.3	-174.4	-61.9	179.7
1343.inp	6.83	-229.21	44.88	-71.4	128.4	-1.5	-178.7	-145	91.8	58.5	-173.3	177.9	67.1	179.8
1344.inp	9.64	-226.4	47.69	-73.2	127.5	-0.7	-179.2	-145.5	87.5	-31.4	62.8	92	-61.2	179.9
1344a..inp	9.29	-226.75	47.34	-91.5	125	-1.2	-179.8	-153.1	80.1	-64.9	29.7	59.3	-93.7	-179.8
1345.inp	6.96	-229.06	45.01	-76.1	120.7	0	-178.3	-134.2	101.7	-61.2	-68.4	60.1	170.6	179.3
1346.inp	7.73	-228.31	45.78	-70.1	127	-1.5	-176.8	-148	86.5	-64.9	-179	56.2	59.8	179.7
1347.inp	9.12	-226.91	47.17	-69.7	124.6	1	-177	-147.3	88.9	146.7	-178.3	-94.6	62.4	179.6
1347a.inp	9.01	-227.03	47.06	-71	125.4	0.7	-177.2	-151.9	84.5	177.1	-143.3	-63.3	97.6	179.6
1348.inp	6.83	-229.21	44.88	-80.5	122.4	1	-179.8	-133.9	103.2	172.1	-62.1	-68.1	178.8	179.6
1349.inp	7.43	-228.61	45.48	-73.1	125.9	0.2	-178.4	-148.7	85.8	178	64	-60.7	-57	179.7
1350.inp	7.25	-228.78	45.3	-85.5	118.3	-1.3	179.7	63.5	-65.1	53	-53	180	179.8	179.8
1351.inp	9.71	-226.33	47.76	-80	122.7	0.4	179.7	50.5	-82.5	51.6	65.9	-177.6	-65.9	179.7
1352.inp	8.12	-227.92	46.17	-85.9	119.2	0	179.9	63.3	-66.1	49.8	-166.6	176.3	66.3	179.6
1353.inp	14.32	-221.72	52.37	-74.8	120.9	-0.9	-177.8	82.8	-56.2	-54.3	108	81.7	-27.5	179.2
1353a.inp	14.59	-221.45	52.64	-70	132.6	0	-177.1	55.6	-83.5	-107	53.8	28.8	-82.4	179.2
1354.inp	9.57	-226.47	47.62	-70.1	123.9	-0.9	-175.6	80.4	-52.7	-66.4	-51.9	65.3	177.4	179
1355.inp	10.33	-225.71	48.38	-69.5	124.4	0.9	-173.6	81.3	-52.5	-70.8	-164.6	60.5	65	178.9
1356.inp	10.14	-225.9	48.19	-70	123.6	0.2	-176.1	67.8	-61.6	171.1	-140	-63.1	94.9	179.7
1356a.inp	10.18	-225.86	48.23	-70.2	127.4	-1.3	-177.3	60	-69.5	140.1	-171.2	-94.6	63.1	179.3
1357.inp	8.13	-227.91	46.18	-70	125.9	-2.4	-178.9	64.2	-65.2	165.7	-51	-67.5	-177.5	179.7
1358.inp	10.65	-225.39	48.7	-71.1	130.2	-3.1	179.4	51.4	-82.6	164.8	70.8	-64.5	-60.5	179.9
1359.inp	5.18	-230.86	43.23	-70.6	143.4	119.4	-169.8	-99.7	138.6	75.4	-59	-165.5	-179.3	178.9
1360.inp	6.32	-229.72	44.37	-71.2	144.2	119.7	-171.8	-97.7	138.7	78.5	62.4	-161.1	-59.2	179
1361.inp	6.54	-229.5	44.59	-71.9	146.8	119.2	-170.8	-97.7	138.9	75.8	-167.1	-165.5	72.8	179
1362.inp	8.57	-227.47	46.62	-70.9	141.5	117.9	-175.6	-94.1	138.4	-67.1	32.3	57.1	-91.7	178.9
1363.inp	5.61	-230.43	43.66	-70.4	139.8	117.9	-175.8	-93.2	142	-65.5	-63.8	56	174.4	178.8
1364.inp	6.46	-229.58	44.51	-70.8	139.8	117.5	-176.4	-91.3	142.9	-67.2	-177.5	54	60.9	179.1
1365.inp	7.99	-228.05	46.04	-71.1	142.5	120.1	-177.7	-88.3	147.8	178.7	-146.6	-61.8	94.3	179

1365a.inp	8.03	-228.01	46.08	-71.6	146.7	119	-176	-80.6	155.6	144.9	-176.9	-95.9	63	178.9
1366.inp	5.53	-230.51	43.58	-71.4	146.4	119.3	-176.7	-87.7	149.1	174.4	-58	-65.9	-177.8	178.8
1367.inp	6.44	-229.6	44.49	-71.8	145.5	119.7	-178.1	-84.1	150.5	178.5	64.9	-60.3	-56.5	178.8
1368.inp	7.74	-228.31	45.79	-75.4	145.6	119.3	-168.5	64.9	-63.8	59.5	-57.8	-172.5	175.4	178.5
1369.inp	8.47	-227.57	46.52	-76.7	145.3	119.4	-176.7	52.7	-80.9	54.5	74.9	-173.8	-57.2	178.4
1370.inp	7.12	-228.92	45.17	-75.8	146.5	118.1	-178.2	64.2	-65.3	52.7	-167.9	179.4	65.1	178.4
1371.inp	13.49	-222.55	51.54	-69	133.8	121.2	180	72.2	-69.5	-52.9	82.8	86.5	-56.8	178.7
1371a.inp	13.69	-222.35	51.74	-69.4	142.4	119.9	-170.7	59.4	-81.1	-103.6	59.3	34.2	-78.2	178.6
1372.inp	9.46	-226.58	47.51	-73.1	135.5	119.8	-167.8	80.3	-52.4	-70.2	-52.4	62	177.1	178.4
1373.inp	9.42	-226.62	47.47	-68.8	137.5	119	-175.6	80.5	-53.5	-71.7	-165.6	59.7	63.8	178.5
1374.inp	9.13	-226.91	47.18	-68.6	140.5	119.7	-176	68.7	-60.5	171.3	-138.2	-62.8	96.7	178.9
1374a.inp	9.04	-227	47.09	-69.1	142.2	120.7	-177.7	59.6	-70	140.4	-173.7	-94.2	60.5	178.8
1375.inp	7.93	-228.11	45.98	-69.1	130.2	119.7	-174.2	57.7	-71.5	159.6	-66	-73.9	167.5	179.1
1376.inp	9.14	-226.89	47.19	-68.5	136.9	120	-176.4	52	-82.4	166.2	78.8	-62.6	-52.7	178.8
1377.inp	5.91	-230.13	43.96	-75.9	137.4	-0.6	-178.3	-103.5	134.7	63.2	-60.7	-177.2	179.2	179.6
1378.inp	7.29	-228.75	45.34	-75.2	136.7	-0.2	-179	-102.7	133	66.7	60.2	-172.2	-61.2	179.9
1379.inp	7.09	-228.95	45.14	-74.7	136.7	0	-177.6	-103.6	133.5	60.5	-172.2	179.6	67.9	179.9
1380.inp	9.42	-226.61	47.47	-73.9	129.9	-0.6	-179.7	-82.4	150.6	-31.5	64.9	92	-59.2	-180
1380a.inp	9.83	-226.2	47.88	-72.7	128.4	0.2	-178	-89	144.1	-61.4	30.4	62.3	-93	179.9
1381.inp	6.74	-229.3	44.79	-72.7	130.8	0	-178.3	-84.3	151.6	-54.4	-63	66.7	175.6	179.7
1382.inp	7.69	-228.35	45.74	-72.8	131.2	0	-179.2	-82.8	151.8	-60.4	-178	60.5	60.8	179.7
1383.inp	9.27	-226.77	47.32	-73.1	129.5	-1	-179.3	-91	145.2	178.2	-146.6	-62.5	94.5	180
1383a.inp	9.13	-226.91	47.18	-73.3	127.5	-0.4	-178.5	-85.2	151.1	142.8	-176.7	-98	63.4	-180
1384.inp	6.73	-229.31	44.78	-73.6	129	-0.8	-177.9	-88.9	148	173.6	-57.4	-66.6	-177.1	179.7
1385.inp	7.86	-228.18	45.91	-73.6	127.2	0.3	-178.9	-86.8	147.7	179.2	64.8	-56.4	-56.4	-179.9
1386.inp	5.7	-230.34	43.75	-73.2	-12.3	3.4	178.9	-102.7	135.9	64.9	-60.2	-176.1	-179.8	177.9
1387.inp	6.64	-229.39	44.69	-70.8	-12.9	3.9	176.9	-100.2	136.3	68.4	59	-171.3	-61.7	176.1
1388.inp	6.95	-229.09	45	-73.9	-15.3	5.1	179.1	-102.6	134.7	63.2	-171.6	-178	68.9	177.8
1389.inp	8.79	-227.25	46.84	-84.3	-11	4.7	179.9	-80.3	153.4	-29	63.2	93.7	-60.6	176.8
1390.inp	6.33	-229.7	44.38	-79.3	-15.9	4.1	-178.3	-85.1	150.7	-57.7	-62.4	64.4	176	178
1391.inp	7.34	-228.7	45.39	-76.7	-18.3	3	-179.5	-83.7	150.9	-62.8	-178.1	58	60.5	179
1392.inp	8.71	-227.33	46.76	-100	125.8	119.3	-176.8	-142.8	95.8	59.7	-65.3	179.8	175	-0.6
1393.inp	9.6	-226.44	47.65	-89.9	144.4	124.9	-178.1	-154.1	81.8	64	67.2	-174.1	-54.9	1.2
1394.inp	9.17	-226.87	47.22	-89.2	139.5	118.5	-178.2	-156.2	81.1	56.9	-173.4	176.9	66.5	0.5
1395.inp	11.56	-224.48	49.61	-86	151.7	120.2	178.1	-147	85.3	-36	63.5	88.3	-61	0.8
1396.inp	9.45	-226.59	47.5	-93.3	137.9	120.7	178.4	-138.4	97.7	-60	-71.9	61.5	167.3	-0.5
1397.inp	9.76	-226.28	47.81	-86.5	147.6	121.7	-179	-148.2	86.3	-63.4	-179.6	57.7	59.3	0.3
1398.inp	10.96	-225.08	49.01	-85.9	150.4	120.4	178	-147.9	88.2	142.4	-177.9	-98.2	62.3	0.2
1398a.inp	11.16	-224.88	49.21	-88.5	151.9	120	177.2	-153.4	82.7	176	-142.5	-63.7	98.1	0.5
1399.inp	9.47	-226.57	47.52	-95.8	141.6	119.9	176.4	-138.9	98.4	168.7	-67.4	-71.2	173.6	-0.1
1400.inp	9.55	-226.49	47.6	-86.3	152.4	119.3	180	-148.3	86.3	178	63.6	-60.7	-57.5	0.8
1401.inp	10.43	-225.61	48.48	-111.3	123.9	117.2	-176.8	59	-69.8	50.4	-63.7	177.4	168.9	-0.7
1402.inp	12.05	-223.99	50.1	-108.2	136.6	119.1	-178.1	51.8	-81.8	52.7	78	-175.9	-54.1	-0.2
1403.inp	10.67	-225.37	48.72	-109.2	134.5	118.1	179.1	61.6	-68	47.9	-170.8	174.5	61.7	-0.4
1404.inp	16.82	-219.22	54.87	-90.3	150.3	120.6	-172.9	60.3	-80.4	-103.1	59.6	34.9	-78.2	0.5
1404a.inp	16.71	-219.33	54.76	-92.5	138.9	119.3	179.6	79.2	-60.7	-56.3	103.4	80.9	-33.7	-0.1
1405.inp	12.84	-223.2	50.89	-95.5	135.3	120.2	-169.5	80.1	-52.6	-68.3	-53.1	63.9	176.2	-0.3
1406.inp	12.53	-223.51	50.58	-88.8	144.4	120.5	-177.1	80.9	-53.2	-74.4	-166.2	57.1	62.8	0
1407.inp	12.03	-224.01	50.08	-86.4	150.9	121.1	-177	70.1	-58.9	171.8	-136.2	-62.2	98.6	0.3
1407a.inp	12.24	-223.8	50.29	-88.9	151.7	121.5	-178.5	60.2	-69.3	140.3	-173.6	-94.2	60.5	0.3
1408.inp	11.25	-224.79	49.3	-93.5	128.3	120.3	-176	57	-72.2	159.1	-65.9	-74.5	167.5	0.2
1409.inp	12.24	-223.8	50.29	-88.6	141.4	120.3	-176.7	51.6	-82.7	166.6	78.3	-62.2	-53.3	0.5
1410.inp	8.84	-227.2	46.89	-107	115.9	-3.8	-177.9	-131.3	106.8	61.3	-62.6	-179.1	178	0.1
1411.inp	10.1	-225.94	48.15	-91.7	143.6	1.6	-179.4	-136.3	99.3	64.1	61	-174.7	-60.1	1.5
1412.inp	10.1	-225.94	48.15	-92.1	142.9	1.7	-179.8	-135.6	101.1	57.9	-174.4	177.3	66.1	1.1
1413.inp	12.98	-223.06	51.03	-91	146	0.4	-179	-140.4	92.3	-32.5	64.3	91.2	-59.9	1.2
1414.inp	10.11	-225.93	48.16	-106.1	121.9	-0.3	-178.6	-126.6	109.1	-60	-66.4	61.1	172.6	0.4
1415.inp	10.88	-225.15	48.93	-95.9	131.3	-1.6	-177.5	-146.7	87.8	-64.7	-178.7	56.4	60.1	0.8
1416.inp	12.35	-223.69	50.4	-96.6	130.4	-1.7	-178.7	-145	91.1	146.5	-177.9	-94.6	62.7	0.8
1416a.inp	12.22	-223.82	50.27	-97.8	129	0.8	-179	-152.1	84.3	176.8	-143.6	-63.4	97.4	0.8
1417.inp	9.88	-226.16	47.93	-107.3	116.3	-1.2	-178	-132.9	104.3	172.7	-60.1	-67.7	-179.2	0.2
1418.inp	10.87	-225.17	48.92	-95.3	142.6	-0.9	-179.8	-143.8	90.5	177.7	66	-60.8	-55.1	1.8
1419.inp	10.23	-225.81	48.28	-116.1	119.3	-4.9	-177.8	64.3	-64.4	52.1	-52.7	179.3	-179.6	0.5
1420.inp	12.87	-223.17	50.92	-105.4	118.8	-0.5	-178.6	51	-82.3	51.5	65.9	-177.5	-65.9	0.3
1421.inp	11.06	-224.98	49.11	-116.6	118.5	-4.5	-177.1	64.1	-65.4	49.8	-166.3	176.4	66.9	0.5
1422.inp	17.58	-218.46	55.63	-99.9	126.6	-1.7	-177.2	83.8	-55	-53.8	108.2	82.1	-27	0.2
1422a.inp	17.83	-218.21	55.88	-96.9	126	-1	-177.7	54.2	-84.7	-107.4	53.3	28.1	-82.7	1
1423.inp	12.89	-223.15	50.94	-97	129.1	-0.4	-176.8	81.2	-51.8	-65	-51.9	66.8	177.3	0.6
1424.inp	13.69	-222.35	51.74	-96.4	130.4	0.1	-175.9	82.2	-51.5	-68.5	-163.7	62.7	65.9	0.7
1425.inp	13.4	-222.63	51.45	-96.4	131.4	-1.5	-178.3	68.9	-60.5	171.9	-140.1	-62.3	94.7	0.9
1425a.inp	13.43	-222.61	51.48	-95.4	133.5	-2.4	-178.4	60.4	-69.1	139.6	-171.1	-95	63	0.8
1426.inp	11.37	-224.67	49.42	-96.1	131.8	-0.9	-178.7	65.1	-64.3	167	-50.7	-66.1	-177.2	1
1427.inp	13.87	-222.17	51.92	-92.3	137.3	-2.7	179.4	51.7	-82.3	164.9	71	-64.4	-60.3	1
1428.inp	12.94	-223.1	50.99	-100.3	116.2	-4.2	-4.3	-134.6	104.4	62.9	-63.9	-177.7	177.5	-179.2
1429.inp	13.56	-222.48	51.61	-75	125.2	-0.2	-2.1	-153.4	83.1	64.7	54.1	-174	-66.5	179.6
1430.inp	13.42	-222.62	51.47	-76.2	124.7	0	-2.9	-152.2	85.2	60.7	-170	-179.7	70.7	179.6
1431.inp	16.12	-219.92	54.17	-79.8	126.8	-0.4	-2.7	-153.7	80.1	-65.3	30.5	58.8	-92.5	-179.9
1431a.inp	16.99	-219.05	55.04	-80.1	126	-0.2	-3.1	-151.5	82.2	-31.7	61	91.9	-62.7	-180
1432.inp	14.61	-221.43	52.66	-90	116.6	-1.1	-3	-131.5	104.8	-60.9	-66.9	60.3	172.5	-179.3

1433.inp	14.66	-221.38	52.71	-80	125.9	-1.7	-2	-152.8	82.3	-65.5	-178.3	55.8	60.9	-179.9
1434.inp	15.28	-220.75	53.33	-82.7	126.3	-0.9	-3.4	-157.5	79.6	176.3	-142.3	-63.7	98.9	-179.9
1434a.inp	15.91	-220.13	53.96	-83	125.7	-0.7	-3.8	-152.3	84.5	145.2	-177.2	-95.7	63.7	-179.9
1435.inp	14.19	-221.84	52.24	-89.6	117.3	-0.8	-4	-132.2	105.4	171.3	-61.5	-69.1	179.9	-179.3
1436.inp	14.47	-221.57	52.52	-82.6	125.8	-1	-2.9	-153.6	81.8	177.6	60.4	-61.1	-59.9	-179.8
1437.inp	15.96	-220.08	54.01	-76.4	124.7	122.8	-7.6	-141.5	97.4	61.7	-111.5	-178.5	-178.5	178.8
1438.inp	13.58	-222.46	51.63	-72.8	126.4	121.5	-6.3	-149.4	87.2	64.5	54	-173.9	-173.9	178.9
1439.inp	14.16	-221.88	52.21	-73.1	126.1	122.2	-8.6	-148.8	88.4	59.1	-177.2	179.1	179.1	179.1
1440.inp	17.02	-219.02	55.07	-74.5	123.3	121	-2	-143.4	88.7	-64.5	39.6	59.9	59.9	179.2
1440a.inp	17.01	-219.03	55.06	-74.3	126.7	121.4	-8	-147.5	86	-32.9	58.2	91.2	91.2	179.2
1441.inp	17.27	-218.77	55.32	-73.6	125.4	122.9	-11.8	-136.4	100.9	-59.4	-104.1	62	62	179.2
1442.inp	15.2	-220.84	53.25	-75.1	126.7	121.4	-8.1	-150	85	-65.4	178.1	56.4	57.3	179.3
1443.inp	16.57	-219.47	54.62	-75.4	126.6	121.8	-9.7	-148.8	87.7	145.4	-178.6	-95	59.5	179.4
1443a.inp	16.47	-219.56	54.52	-77.6	125.5	122.3	-7.5	-152.1	84.8	176.1	-141.4	-63.6	99.7	179.3
1445.inp	14.59	-221.45	52.64	-75.9	126.8	122.9	-7.9	-150.1	85.2	176.7	58.2	-61.6	-62.2	179.2
1446.inp	5.67	-230.37	43.72	-161.1	151	121.7	-169.8	-99.2	139.2	75.6	-59.9	-165.3	179.6	-178.5
1447.inp	6.51	-229.53	44.56	-161.6	151	120.2	-171.3	-97.3	139.1	77.2	62.3	-162.3	-59.6	-178.8
1448.inp	6.8	-229.24	44.85	-161.3	152.4	120.8	-170.1	-97.9	139.6	74.7	-167.3	-166.5	72.3	-178.87
1449.inp	8.92	-227.12	46.97	-161.6	144.8	118.7	-175.8	-100	132.5	-66.8	32.5	57.5	-91.4	-178.9
1450.inp	6.19	-229.85	44.24	-161.8	143.9	118.8	-176.4	-99.3	136	-65.1	-64.5	56.3	173.9	-178.8
1451.inp	6.82	-229.22	44.87	-162	143.4	119	-177.6	-96.6	137.6	-67	-177.8	54.3	60.7	-178.6
1452.inp	8.2	-227.83	46.25	-162.6	147.8	118.2	-177.9	-88.9	147.2	178.3	-146.6	-62.1	94.3	-178.8
1452a.inp	8.14	-227.9	46.19	-162.6	152.7	120.7	-176	-80.5	155.7	145.5	-177	-95.4	62.8	-178.7
1453.inp	5.87	-230.17	43.92	-161.9	149.9	120.2	-177	-87.9	149.9	173.6	-58.5	-66.7	-178.3	178.7
1454.inp	6.58	-229.46	44.63	-162.4	152.1	119.1	-177.5	-84.8	149.7	177.8	65	-61	-56.6	178.7
1455.inp	7.63	-228.41	45.68	-160.9	131.1	117.4	-174.6	58.6	-70.3	51.6	-66.8	178.7	165.8	-179
1456.inp	8.95	-227.09	47	-161.6	144.3	119.8	-175.6	51.9	-81.8	53.6	74.8	-174.9	-57.3	-178.9
1457.inp	7.54	-228.5	45.59	-162.6	146.6	118.6	-177.3	63	-66.6	50.3	-169.3	177	63.6	-179
1458.inp	14.14	-221.89	52.19	-162.3	141	119.3	-179.4	73.2	-68.3	-52.7	84.3	86.7	-55.1	-179
1459.inp	10.3	-225.73	48.35	-160.9	151	119.8	-165.7	84	-47.8	-64.8	-52	67.4	178.3	-178.9
1460.inp	9.91	-226.13	47.96	-162.3	152.8	119.5	-177.5	83.1	-50.6	-70.1	-163.2	61.2	66.3	-178.9
1461.inp	9.27	-226.76	47.32	-161.8	156.5	120.2	-176.8	70.8	-58.1	171.6	-136	-62.4	98.9	-178.9
1461a.inp	9.5	-226.54	47.55	-161.8	155.6	119.3	-177.6	60.5	-69.1	140.3	-173.5	-94.1	60.6	-178.7
1462.inp	8.58	-227.46	46.63	-161.9	133.7	118.6	-175.9	57.1	-72.2	158.5	-68.2	-75	165.1	-178.5
1463.inp	9.52	-226.52	47.57	-161.9	144.3	119.3	-176.7	52	-82.4	166.1	78.3	-62.4	-53.4	-178.2
1464.inp	5.41	-230.63	43.46	-156	146	-2.6	179.7	-128.4	109.7	61.1	-62.2	-179.1	178.2	-175.5
1465.inp	6.35	-229.69	44.4	-154.9	152.8	-3.2	179.3	-147	88.7	63.2	56.2	-175.4	-64.9	-175.4
1466.inp	6.26	-229.78	44.31	-155.3	151.4	-3.7	178.1	-143.1	93.6	57.8	-173.7	177.5	66.6	-175.3
1467.inp	8.98	-227.05	47.03	-153.6	154	-4.9	-179.1	-149.9	83.1	-64.8	30.9	59.2	-92.6	-175.3
1467a.inp	9.37	-226.67	47.42	-155	151.2	-4.1	178.5	-143.6	89.4	-31	62	92.6	-61.9	-175.2
1468.inp	6.75	-229.29	44.8	-155.3	144.8	-3.4	179.3	-130.2	105.6	-60.5	-66.3	60.9	172.6	-175.4
1469.inp	7.36	-228.68	45.41	-153.6	154.7	-4.4	-179.8	-143.8	90.5	-64.8	-178.9	56.5	59.8	-175.3
1470.inp	8.73	-227.31	46.78	-154.4	151.3	-3.9	179.8	-143.8	92.3	146.4	-178.2	-94.6	62.4	-175.3
1470a.inp	8.59	-227.45	46.64	-154.5	150.8	-4.5	179.6	-150.6	85.6	176.7	-142.8	-63.4	97.9	-175.3
1471.inp	6.51	-229.53	44.56	-155.3	141.2	-4.1	179.2	-131.8	105.2	172.7	-59.7	-67.5	-178.8	-175.3
1472.inp	7.17	-228.87	45.22	-154.2	149.3	-3.5	-179.6	-148	86.6	178.2	61.6	-60.5	-59.3	-175.3
1473.inp	6.83	-229.21	44.88	-155.7	144.5	-3.8	-179.5	64.1	-64.6	53.3	-54.6	-179.6	178.3	-175.3
1474.inp	9.4	-226.64	47.45	-154.8	150.3	-3.3	178.3	52.1	-81	52.4	66.8	-176.6	-65.1	-175.4
1475.inp	7.72	-228.32	45.77	-155.2	143.6	-3.7	-179.4	64.6	-64.9	51	-165.9	177.5	67.2	-175.5
1476.inp	14.05	-221.98	52.1	-154.8	148.8	-4.7	-179.8	55.6	-83.5	-107.4	54.4	28.3	-81.9	-175.3
1476a.inp	14.1	-221.94	52.15	-155.8	137.6	-3.3	179.7	83.7	-55.2	-53.6	107.6	82.5	-28	-175.5
1477.inp	9.38	-226.66	47.43	-155.6	138.8	-2.8	-178.3	81.4	-51.8	-67.1	-52.9	64.9	176.1	-175.4
1478.inp	10.15	-225.89	48.2	-155.3	139.4	-2.4	-177.8	82.1	-51.9	-71.3	-165.2	60.1	64.1	-175.5
1479.inp	9.65	-226.39	47.7	-155.7	137.5	-3.1	179.7	68.9	-60.5	171.4	-139.9	-62.8	94.8	-175.3
1479a.inp	9.67	-226.37	47.72	-154.5	142.1	-3.1	-179.5	60.8	-68.7	140.1	-171.2	-94.6	62.9	-175.4
1480.inp	7.6	-228.44	45.65	-156	138.4	-3.3	179.9	64.6	-64.8	165.1	-52.3	-68	-178.9	-175.4
1481.inp	10.04	-226	48.09	-156	144.1	-3.1	177.4	52.3	-81.6	165.1	71.1	-64.3	-60.2	-175.5
1482.inp	6.15	-229.88	44.2	-161.1	130.4	117.5	-175.8	-142.8	95.9	60.1	-63.1	-179.8	177	-178.9
1483.inp	6.58	-229.46	44.63	-161.9	137.2	118.4	-178.2	-159.1	77.2	62.9	54.1	-175.5	-67.4	-178.8
1484.inp	6.57	-229.47	44.62	-161.8	137.8	118.2	-178.8	-156.5	80.8	56.8	-173.5	176.7	66.3	-178.9
1485.inp	8.7	-227.34	46.75	-162.7	152.3	120.1	-179.9	-152.1	81.1	-63.5	30.7	60.5	-92.7	-178.8
1485a.inp	8.99	-227.05	47.04	-163	153	118.8	177.1	-149.5	82.9	-35.3	61.1	89.1	-63.3	-178.8
1486.inp	6.42	-229.62	44.47	-162.8	148.2	120.2	-178.1	-131.2	104.6	-57.5	-65.4	63.9	173.4	-178.8
1487.inp	7.06	-228.98	45.11	-162.6	152.6	119.8	180	-149.2	85.4	-63.4	-179.2	58	59.5	-178.8
1488.inp	8.35	-227.69	46.4	-163.2	151.2	117.7	176.3	-154.5	81.6	175.8	-141.7	-63.8	98.7	-178.9
1488a.inp	8.17	-227.87	46.22	-163	155.3	117.8	176.1	-149.5	86.7	141.9	-177.5	-98.4	62.6	-178.9
1489.inp	6.5	-229.54	44.55	-163	145.9	118.5	179.7	-136.9	100.3	171.6	-60.1	-68.4	-179.4	-178.9
1490.inp	6.97	-229.07	45.02	-163	151.2	118.1	178.3	-151.8	82.8	177.5	61.2	-61	-59.9	-178.9
1491.inp	5.43	-230.61	43.48	-154.3	126.9	-1.6	-178.9	-114.6	123.4	61.7	-61.4	-178.7	179	-175.5
1492.inp	6.65	-229.39	44.7	-154.4	129.4	-1.3	-179.7	-115.4	120.2	64.7	59	-174.1	-62.1	-175.5
1493.inp	6.42	-229.62	44.47	-154.7	129.5	-2.4	179.7	-113.4	123.5	58.4	-173.6	177.7	66.8	-175.4
1494.inp	9.33	-226.71	47.38	-154	129.8	-3.5	-179.3	-90.8	142.3	-61.8	31	62.1	-92.4	-175.4
1494a.inp	8.77	-227.27	46.82	-155.7	132.0	-2.1	179.3	-82.9	150	-31.8	64.9	91.8	-59.2	-175.2
1495.inp	6.39	-229.65	44.44	-154	129.0	-3.5	-179.7	-89.8	146	-56.4	-63.9	64.7	174.8	-175.4
1496.inp	7.05	-228.99	45.1	-154.3	131.2	-3.6	179.2	-86	148.7	-60.9	-178.4	59.9	60.5	-175.3
1497.inp	8.63	-227.41	46.68	-155.2	134.6	-2.7	179.5	-89.4	146.8	178.3	-146.8	-62.4	94.4	-175.2
1497a.inp	8.47	-227.56	46.52	-155.6	137.4	-2.7	-180	-84.2	152.1	142.8	-176.8	-97.9	63.3	-175.3
1498.inp	6.35	-229.69	44.4	-155.1	135.3	-2.5	179.8	-91.3	145.6	174.1	-58.4	-66.3	-177.7	-175.3
1499.inp	7.24	-228.8	45.29	-154.7	136.4	-4.8	179.6	-87.5	146.9	178.9	65	-59.9	-56.3	-175.2

1500.inp	5.94	-230.09	43.99	-149.7	-2.3	0.7	179.9	-127.7	110.5	61.1	-62.6	-179.4	178.1	-175.8
1501.inp	6.63	-229.41	44.68	-149	-2.4	-0.6	-179.3	-149.1	86.9	63.2	56.5	-175.8	-64.4	-176.2
1502.inp	6.91	-229.13	44.96	-148.8	-4.5	0	178.9	-145.8	91.2	57.5	-173.9	176.8	66.7	-176.2
1503.inp	9.13	-226.9	47.18	-147.1	-4.8	-1.4	-179.7	-145	88.7	-29.7	60.9	93.1	-62.3	-176.7
1503a.inp	8.99	-227.05	47.04	-147	3.0	4.6	177.8	-152.7	80.9	-63.7	29	60.4	-94	-176.7
1504.inp	6.84	-229.2	44.89	-148.6	-4.2	-0.1	-179.5	-125.7	110.2	-58.1	-65	62.8	174.3	-176.4
1505.inp	7.61	-228.43	45.66	-149.4	-3.2	0.3	-179.5	-148	86.7	-63.7	-179.5	57.3	59.7	-176
1506.inp	9.33	-226.71	47.38	-149.6	-4.0	0.4	179.7	-146.6	89.6	146.4	-178.4	-94.8	62.4	-175.8
1506a.inp	9.18	-226.86	47.23	-150.2	-2.4	1.6	-179.4	-151.7	84.8	177	-143.1	-63.3	97.9	-175.8
1507.inp	6.92	-229.12	44.97	-148.9	-4.2	-0.1	-179.4	-129.8	107.4	173.2	-60.2	-67.3	-179.2	-175.8
1508.inp	7.41	-228.63	45.46	-148.5	-2.8	-1.2	-178	-150	84.8	178.5	60.8	-60.7	-59.7	-175.9
1509.inp	7.54	-228.5	45.59	-149.4	-1.7	1.2	179.9	64.8	-64.1	53.4	-53.3	-179.3	179.3	-175.8
1510.inp	10.18	-225.86	48.23	-149.5	-2.7	0.6	-179.3	52.2	-81.4	51.5	67.3	-177.1	-64.8	-175.5
1511.inp	8.37	-227.67	46.42	-149.7	-3.6	2.8	179.5	64.8	-64.8	50.5	-165.8	177.3	67	-175.5
1512.inp	14.83	-221.21	52.88	-149.3	-4.2	-1.3	-176.2	85.3	-53.3	-52.6	108.5	83.3	-26.4	-175.5
1512a.inp	15.14	-220.9	53.19	-150.8	-4.7	1.4	-179.3	55.5	-83.6	-108.1	54	27.7	-82.3	-175.6
1513.inp	10.29	-225.75	48.34	-148.9	-4.9	-1.5	-177.2	81.7	-51.5	-65.5	-52	66.5	177	-175.5
1514.inp	10.96	-225.08	49.01	-149.6	-4.8	-1.2	-175.9	82.7	-51.2	-69.2	-163.7	62.2	65.8	-175.5
1515.inp	10.55	-225.49	48.6	-150.3	-4.9	2	-179.1	69.1	-60.5	171.2	-140	-62.8	94.7	-175.5
1515a.inp	10.58	-225.46	48.63	-151.7	-3.8	1.3	-179.3	60.9	-68.8	139.7	-171.1	-94.8	63	-175.4
1516.inp	8.62	-227.42	46.67	-149.6	-2.7	1.6	179.2	65.2	-64.3	166.1	-50.9	-66.8	-177.6	-175.7
1517.inp	11.17	-224.87	49.22	-150.5	-4.7	2.8	178.3	52.6	-81.7	165.1	72.2	-63.9	-59.4	-175.6
1518.inp	6.4	-229.64	44.45	-147	58.9	-3.7	-178.6	-128.2	109.9	61.6	-61.4	-178.9	179.1	-176.8
1519.inp	7.07	-228.97	45.12	-147.3	57.9	-2.1	-177.9	-152	84.1	63.8	55	-175.1	-65.9	-177.2
1529.inp	7.45	-228.59	45.5	-147.4	57.9	-3.3	-179.7	-147.9	89.1	58.4	-173.7	177.8	66.7	-176.5
1521.inp	9.43	-226.61	47.48	-146.5	60.0	-1.5	179.4	-153.2	80.3	-64.5	29.9	59.5	-93.3	-177.5
1521a.inp	9.91	-226.12	47.96	-146.4	63.7	-3.2	-178.5	-148.8	84.6	-30.9	59.9	92.2	-63.7	-177.5
1522.inp	7.52	-228.51	45.57	-146.5	58.5	-3.9	-177.9	-129.4	106.4	-59.7	-64.7	61.4	174.3	-176.8
1523.inp	8.2	-227.84	46.25	-146.7	57.3	-3.8	-179.3	-149.9	84.8	-64.6	-179.3	56.5	59.7	-176.7
1524.inp	9.61	-226.43	47.66	-146.5	56.3	-4	-179.7	-152.9	832.5	176.8	-142.8	-63.3	98	-176.5
1524a.inp	9.75	-226.29	47.8	-147.2	59.1	-4.2	179	-148.1	88.1	146	-178.4	-94.9	62.3	-176.2
1525.inp	7.35	-228.69	45.4	-147.3	60.2	-3.4	-178.8	-131.7	105.4	173.1	-58.9	-67.3	-178	-176.8
1526.inp	7.79	-228.25	45.84	-147.2	60.4	-3.5	-177.6	-151.3	83.7	178.3	59.9	-60.9	-60.6	-177.2
1527.inp	7.88	-228.15	45.93	-147.5	57.0	-3.3	-179.4	64.3	-64.6	52.9	-53.6	-179.8	179.1	-176.6
1528.inp	10.57	-225.47	48.62	-147.9	56.3	-5.5	-179.4	52.2	-81.3	51.6	67.1	-177	-65	-176.4
1529.inp	8.65	-227.38	46.7	-147.6	56.9	-3.8	-178.7	64.6	-65	50.8	-165.9	177.7	67	-176.6
1530.inp	15.47	-220.56	53.52	-148.2	58.6	-4.5	-179.6	55.3	-83.8	-108.4	53.8	27.4	-82.4	-176
1530a.inp	15.19	-220.85	53.24	-147.6	56.3	-3.6	-177.5	84.4	-54.3	-52.8	108.6	83.1	-26.5	-176.4
1531.inp	10.67	-225.37	48.72	-147.6	57.7	-3.5	-176.9	81.4	-51.8	-65.4	-52	66.6	177.1	-176.4
1532.inp	11.33	-224.71	49.38	-148	56.6	-3.7	-176.2	82.2	-51.7	-69.5	-163.9	62	65.6	-176.3
1533.inp	10.93	-225.11	48.98	-147.7	57.2	-4	-179.4	69	-60.6	171.2	-139.9	-62.8	94.6	-176.1
1533a.inp	10.92	-225.12	48.97	-147.7	57.5	-4.1	-179.2	60.4	-69.2	139.7	-171.4	-94.7	62.7	-176.1
1534.inp	9.01	-227.03	47.06	-147.8	57.2	-2.6	179.9	64.7	-64.9	165.1	-51.5	-67.8	-178.2	-176.3
1535.inp	11.53	-224.5	49.58	-147.7	57.2	-2.9	178.5	52	-82.2	164.5	71.8	-64.5	-59.8	-176.1
1536.inp	9.48	-226.55	47.53	-153.3	61.1	118.1	-179.4	-127.1	111	61.4	-61.8	-179	178.7	179.8
1537.inp	10.2	-225.83	48.25	-152.6	60.5	120	-179.2	-152.3	83.8	63.8	55.5	-175	65.5	179.7
1538.inp	10.52	-225.52	48.57	-154.8	60.4	120	179.6	-150.1	87	58.3	-173.6	177.8	66.8	-179.7
1539.inp	12.59	-223.45	50.64	-149.9	59.1	119.1	178.8	-152.3	81.1	-64.4	29.7	59.6	-93.4	179.1
1539a.inp	13.03	-223	51.08	-151.9	59.7	119.4	-178.9	-148.2	85.2	-30.8	60.4	92.2	-63.1	179.3
1540.inp	10.66	-225.38	48.71	-153.1	59.9	119.6	-178.8	-130.7	105.1	-59.9	-65	61.2	174	180
1541.inp	11.32	-224.72	49.37	-153.8	59.4	119.9	-179.3	-150.3	84.4	-64.4	-179.3	56.4	59.7	179.9
1542.inp	12.7	-223.34	50.75	-155.2	59.1	121.3	179.5	-154.1	82.3	176.6	-142.3	-63.4	98.5	-179.5
1542a.inp	12.84	-223.2	50.89	-154.9	60.5	119.4	-180	-149	87.3	146.3	-178.4	-94.8	62.3	-179.7
1543.inp	10.49	-225.55	48.54	-153.4	59.6	120.3	-179.4	-132.3	104.8	172.9	-59.5	-67.4	-178.6	-179.9
1544.inp	10.94	-225.1	48.99	-153.8	58.1	120.5	-179.1	-151.1	83.7	178.1	60.5	-60.9	-60.2	180
1545.inp	10.92	-225.12	48.97	-152.7	59.7	120.6	179.7	64.3	-64.7	53	-53.3	-179.7	179.3	-179.9
1546.inp	13.5	-222.54	51.55	-154.7	59.6	120.4	179.7	52	-81.6	51.2	66.4	-177.5	-65.7	-179.7
1547.inp	11.73	-224.31	49.78	-153.4	59.5	120.1	-179.4	64.7	-65	50.9	-165.8	177.8	67	180
1548.inp	18.34	-217.7	56.39	-155.2	60.0	120.6	178.4	54	-84.8	-108.9	53.5	26.4	-82.6	-179.4
1548a.inp	18.16	-217.87	56.21	-155.2	59.8	120.4	-179.2	83.5	-55.5	-53.6	108.5	82.6	-27.1	-179.5
1549.inp	13.62	-222.42	51.67	-154.9	60.6	119.5	-178.4	81.3	-52.1	-65.7	-51.3	66.4	177.6	-179.6
1550.inp	14.34	-221.7	52.39	-155.1	60.0	120.4	-177	81.9	-52.2	-69.7	-163.6	61.9	65.7	-179.6
1551.inp	13.96	-222.07	52.01	-154.2	58.9	119.7	-179.8	69.2	-60.5	170.9	-139.7	-63	94.8	-179.6
1551a.inp	13.94	-222.1	51.99	-155.6	59.9	120.5	-179.4	60.3	-69.3	139.5	-171.5	-95	62.5	-179.5
1552.inp	12.01	-224.03	50.06	-153	60.1	119.7	179.4	64.8	-64.9	164.5	-50.9	-68.4	-177.7	-179.9
1553.inp	14.48	-221.55	52.53	-155	58.7	121.5	178.3	51.8	-82.4	163.5	70.6	-65.5	-61	-179.3
1554.inp	5.31	-230.72	43.36	-152.4	-52.2	-4.7	178.6	-136.4	102.2	60.9	-65.3	-179.5	175.6	-176.2
1555.inp	5.87	-230.17	43.92	-152.9	-48.7	-5.5	178.1	-150.3	85.6	63.2	57.6	-175.3	-63.3	-176
1556.inp	6.14	-229.9	44.19	-152	-47.9	-6.1	179	-149.3	87.8	58.2	-173.9	177.6	66.8	-176
1557.inp	8.43	-227.61	46.48	-152.8	-48.9	-5.9	178.4	-147.5	85.6	-31.9	62	91.7	-61.8	-175.7
1558.inp	6.24	-229.8	44.29	-152.3	-51.0	-6.9	179.5	-132.9	103.3	-57.9	-68.2	63	171.4	-175.6
1559.inp	6.95	-229.09	45	-152.1	-45.5	-6.6	-179.1	-146.7	87.9	-63	-179.6	57.8	59.6	-175.5
1560.inp	8.67	-227.37	46.72	-153.5	-46.5	-6.6	179.8	-150.9	85.6	177.1	-144.1	-63.4	97.2	-175.6
1560a.inp	8.76	-227.28	46.81	-150.8	-46.5	-6.7	179.4	-146.7	89.6	146.4	-178.6	-94.9	62.4	-175.9
1561.inp	6.62	-229.42	44.67	-152.7	-51.5	-4.5	178	-135.1	102.3	171.4	-63.3	-68.9	178	-175.8
1562.inp	6.9	-229.14	44.95	-152.8	-47.8	-6	179	-150.3	84.4	178.2	61.9	-60.5	-58.8	-175.6
1563.inp	6.97	-229.07	45.02	-150.9	-49.3	-5.4	175.9	64.8	-64.1	55.5	-53.3	-177.5	179.2	-176.6
1564.inp	9.82	-226.22	47.87	-150.8	-48.1	-5.5	177.1	51.5	-81.7	52.7	66.7	-176.4	-65.4	-176.1
1565.inp	8.11	-227.93	46.16	-151.3	-47.3	-5.8	177	65.6	-63.9	54.3	-164.9	-179.2	67.9	-175.9

1566.inp	14.49	-221.54	52.54	-151.3	-50.4	-7.2	-179.5	83	-56.2	-54.3	107.4	82	-28.4	-175.7
1566a.inp	14.56	-221.48	52.61	-150.8	-50.9	-6.1	178.7	53.4	-85.3	-107.9	52.8	27.3	-83.1	-175.9
1567.inp	9.7	-226.34	47.75	-150.9	-49.2	-6.7	179.6	81.1	-52.4	-66.8	-52.4	65.1	176.4	-175.9
1568.inp	10.5	-225.54	48.55	-151.1	-47.9	-7	-177.9	81.8	-52.3	-71.4	-165	60.1	64.3	-175.7
1569.inp	10.1	-225.93	48.15	-150.7	-50.1	-6.3	-179.5	68.1	-61.5	171	-139.9	-63.2	94.6	-175.6
1569a.inp	10.11	-225.93	48.16	-152.2	-46.5	-5.8	-179.4	60.3	-69.3	139.9	-171.4	-94.7	62.8	-175.6
1570.inp	7.88	-228.16	45.93	-151.3	-50.1	-5.5	178.9	64.2	-65.4	165.3	-51.2	-67.9	-177.8	-176.4
1571.inp	10.63	-225.41	48.68	-151.1	-48.4	-6.2	177.4	51.3	-82.7	164.5	70.7	-64.8	-60.8	-176
1572.inp	5.91	-230.12	43.96	-158.6	-37.6	121.7	170.1	-139.5	99	61.9	-74.7	-177.7	166.2	-179.4
1573.inp	6.53	-229.51	44.58	-161.9	-34.1	122.9	174.5	-130.9	104.4	63.4	65.9	-175.1	-55.3	-179.5
1574.inp	6.07	-229.97	44.12	-162.5	-39.7	124	176.5	-148.5	88.4	59.1	-172.4	179	67.9	-179
1575.inp	9.14	-226.9	47.19	-159.7	-33.6	124.7	177.1	-129.1	103.6	-31.4	66.8	92.4	-57.5	-178.8
1576.inp	6.73	-229.31	44.78	-161	-39.5	122.5	169.8	-137.4	99	-60.8	-75.7	61	164	-178.9
1577.inp	6.89	-229.15	44.94	-162.6	-41.1	121.8	176.5	-149.1	85.4	-64.1	-177.6	57.5	61.3	-178.8
1578.inp	8.67	-227.37	46.72	-163	-39.6	123.2	176	-146.9	89.2	145.9	-177.1	-94.7	63.5	-179
1578a.inp	8.54	-227.5	46.59	-162.5	-43.1	122.1	175.3	-156.5	79.7	176.8	-145	-62.8	96	-179
1579.inp	7.25	-228.79	45.3	-161.8	-41.6	122.8	168.7	-138.6	98.9	167.6	-72.9	-72	168.5	-179
1580.inp	7.4	-228.64	45.45	-162.5	-33.3	124.3	175.7	-135.8	98.4	177.4	68.3	-61.1	-52.8	-179.1
1581.inp	8.57	-227.47	46.62	-158.7	-33.0	123.1	168.2	68.1	-60.8	62.4	-53	-170.5	179.2	-180
1582.inp	10.79	-225.25	48.84	-160.2	-40.9	119.6	164.9	47.2	-84.6	52.5	64.4	-178.1	-67.7	-179.6
1583.inp	9.99	-226.05	48.04	-159.6	-41.1	121	162.4	60.1	-69	47.3	-168.7	173.2	62.6	-179.3
1584.inp	14.32	-221.72	52.37	-162.9	-44.1	120.2	178.2	52.2	-86.3	-108.5	52.6	26.2	-83.2	-179.1
1584a.inp	14.77	-221.27	52.82	-161.3	-38.6	119.6	171.3	81.1	-59.5	-58.5	103.9	79.1	-34	-179.2
1585.inp	9.58	-226.46	47.63	-161.3	-40.6	119.7	173.3	81.3	-52.5	-72.8	-53.3	59.3	174.6	-179.5
1586.inp	10.36	-225.68	48.41	-161.5	-38.0	120.4	174.7	82.2	-52.3	-77.2	-166.3	54.6	61.9	-179.2
1587,inp	10.06	-225.98	48.11	-161.8	-40.3	121.3	177.1	69.6	-60	173.7	-140.1	-60.4	94.2	-179.2
1587a.inp	9.77	-226.27	47.82	-162.8	-42.1	120.8	177.2	58.8	-70.3	134.7	-170.7	-99.9	63.1	-179.1
1588.inp	7.88	-228.15	45.93	-161.7	-42.9	121.5	175.4	64.6	-65	166.3	-51.1	-66.9	-178	-179.6
1589.inp	10.39	-225.65	48.44	-162.4	-44.3	120	177.8	48.9	-84.7	161.9	69	-67.8	-62.3	-179.2
1590.inp	8.97	-227.06	47.02	-140.3	128.9	118.1	-174.4	-140.1	98.4	60.6	-62.2	-179.4	177.8	0.3
1591.inp	9.42	-226.62	47.47	-142.6	134.0	119.1	-177.6	-157.8	78.5	63.1	57.8	-175.5	-67.6	0.6
1592.inp	9.47	-226.57	47.52	-143.8	133.5	120.2	-178.8	-154.9	82.3	57	-173.4	176.9	66.5	0.8
1593.inp	11.62	-224.42	49.67	-142.8	148.5	121.2	-179.1	-151.3	81.9	-63.6	30.5	60.2	-92.8	0.9
1593a.inp	11.94	-224.1	49.99	-144.5	149.3	119.7	177.5	-148.3	84.1	-34.8	61.2	89.5	-63.2	1
1594.inp	9.38	-226.66	47.43	-143.5	144.2	120	-177.6	-127.6	108.1	-57.3	-64.7	64	174	0.8
1595.inp	10.19	-225.84	48.24	-143.8	148.4	120	-177.2	-127.1	107.2	-61.3	-178.8	59.6	59.9	1
1596.inp	11.35	-224.68	49.4	-145.1	148.4	120.3	176.8	-153.4	82.7	175.8	-141.9	-63.9	98.6	1
1596a.inp	11.18	-224.86	49.23	-145.4	150.1	119.8	175.9	-148.8	87.3	142.5	-177.6	-97.8	62.6	1
1597.inp	9.44	-226.6	47.49	-144.5	142.1	120	-179.6	-135.3	101.8	172.3	-59.4	-67.8	-178.7	0.9
1598.inp	9.93	-226.11	47.98	-144.2	149.4	120	178.8	-150.8	83.8	177.6	61	-61	-60	1
1599.inp	10.4	-225.64	48.45	-141.3	126.3	119.6	-174	59.4	-69.5	51.8	-64.9	179	167.9	0.4
1600.inp	11.9	-224.14	49.95	-142.6	140.9	120.3	-175.6	52.5	-81.3	53.4	75.9	-174.9	-56.2	0.7
1601.inp	10.48	-225.56	48.53	-143.4	138.6	120.2	-177.6	62.6	-67.1	49.8	-170	176.6	62.8	0.7
1602.inp	17.13	-218.91	55.18	-144.3	132.9	119.1	178.2	73.4	-68.1	-53.6	87.2	85.6	-52.3	0.5
1602a.inp	17.16	-218.88	55.21	-142.5	146.4	121	-171.6	59.7	-81	-104.2	60.2	33.7	-77.5	0.9
1603.inp	13.42	-222.62	51.47	-141.1	121.6	119.1	-171.7	77.2	-56.1	-69.4	-58.5	62.8	170.3	0.3
1604.inp	12.92	-223.62	50.97	-143.9	151.3	120.9	-177.5	83.3	-50.4	-70.3	-163.3	61	66.2	1
1605.inp	12.45	-223.59	50.5	-143.7	149.4	120.2	-177.9	60.1	-69.5	140.3	-173.8	-94.1	60.3	1
1605a.inp	12.32	-223.72	50.37	-143.6	153.5	121.9	-177.1	70.9	-58	171.3	-135.6	-62.6	99.2	1.3
1606.inp	11.4	-224.64	49.45	-143	124.9	121.2	-176.5	58.2	-71.1	159.6	-65.1	-73.9	168.2	0.7
1607.inp	12.52	-223.51	50.57	-143.8	141.8	119.1	-176.8	52.5	-81.9	166.3	78.9	-62.3	-52.8	0.6
1608.inp	8.79	-227.24	46.84	-130.7	125.9	-4.2	-178.2	-105.2	132.9	62.4	-60.4	-178.2	179.7	1.5
1609.inp	10.09	-225.94	48.14	-130.5	125.5	-4	-179.7	-103.4	132.4	65.9	59.9	-173.1	-61.5	1.5
1610.inp	9.92	-226.12	47.97	-131.6	125.7	-2.8	-179.1	-104	133	59.3	-172.7	178.5	67.5	1.6
1611.inp	12.26	-223.78	50.31	-132.3	121.0	-3.3	178.8	-81.6	151.6	-30.7	64.6	92.6	-59.3	1.5
1611a.inp	12.69	-223.35	50.74	-131.4	123.2	-3	-178.6	-86.4	146.7	-61.7	31	62.2	-92.6	1.4
1612.inp	9.72	-226.32	47.77	-129.8	120.7	-2.4	-178.6	-84.6	151.2	-55	-62.9	66.1	175.7	1.3
1613.inp	10.58	-225.45	48.63	-131.3	124.7	-3.9	-179.4	-82.9	151.8	-60.8	-178	60	60.7	1.5
1614.inp	12.16	-223.88	50.21	-131	124.3	-3	-178.4	-88	148.2	178.2	-146	-62.5	95	1.5
1614a.inp	12.02	-224.02	50.07	-132.1	122.7	-3.8	-179.2	-83.3	152.9	142.6	-176.7	-98.1	63.3	1.5
1615.inp	9.71	-226.33	47.76	-130.5	124.6	-3.9	-177.7	-89.3	147.6	173.6	-57.9	-66.8	-177.6	1.4
1616.inp	10.73	-225.31	48.78	-131.2	123.8	-3.3	-179.8	-85.2	149.3	179.1	64.9	-59.7	-56.4	1.5
1617.inp	10.23	-225.81	48.28	-128.1	128.2	-3.6	-177.6	64.7	-64	52.9	-52.7	-180	-179.6	1.4
1618.inp	12.86	-223.18	50.91	-124	122.7	-3.9	-178.2	51.9	-81.5	52	66.4	-176.8	-65.4	1.1
1619.inp	11.09	-224.94	49.14	-122.7	123.9	-3.8	-178.1	64.4	-65.1	50.2	-166.1	176.8	67.1	1
1620.inp	17.59	-218.45	55.64	-126.3	123.0	-4	-178.4	84.4	-54.3	-52.9	108	83	-27.1	1.2
1620a.inp	17.66	-218.38	55.71	-126.5	124.3	-4.3	-178.8	55.9	-83.2	-107.2	53.7	28.5	-82.5	1.6
1621.inp	12.92	-223.11	50.97	-126.4	124.0	-3.9	-177.8	81.8	-51.3	-65.8	-51.9	66.1	177.2	1.3
1622.inp	13.69	-222.35	51.74	-127.2	124.3	-3.9	-176.9	82.7	-51.2	-69.9	-164.2	61.4	65.2	1.3
1623.inp	13.23	-222.81	51.28	-129	122.7	-4.1	-179	69	-60.4	171.5	-140	-62.8	94.8	1.4
1623a.inp	13.22	-222.82	51.27	-131.9	124.2	-3.1	-179.1	60.9	-68.5	139.9	-171.1	-94.7	63.1	1.6
1624.inp	11.16	-224.88	49.21	-132.8	124.6	-3.8	179.3	65.1	-64.3	165.9	-50.8	-67.2	-177.3	1.6
1625.inp	13.63	-222.41	51.68	-134.1	124.5	-3.8	178.5	51.9	-82.1	165	71.1	-64.2	-60.3	1.6
1626.inp	11.59	-224.45	49.64	-154.9	152.0	-2.1	4.5	-111.2	128	64.1	-62.8	-177	177.9	-175.6
1627.inp	13.08	-222.95	51.13	-153.7	154.9	-3.7	5	-114.3	121.8	67.1	60.1	-172.3	-61	-175.6
1628.inp	12.72	-223.31	50.77	-153.6	156.2	-4.1	5.1	-115.3	122.1	61.8	-171.5	-179.5	69	-175.5
1629.inp	15.39	-220.85	53.44	-153.9	151.6	-4.7	5.3	-90.7	143.6	-25.7	64.7	96.8	-59.1	-175.3
1629a.inp	15.8	-220.24	53.85	-151.8	151.7	-6.9	5.7	-97.6	135.8	-62.9	31.3	60.7	-92.2	-175.2
1630.inp	12.48	-223.56	50.53	-152.2	152.7	-4.7	4	-98.2	137.7	-57.4	-65	63.4	173.7	-175.4

1631.inp	13.4	-222.64	51.45	-153.1	152.3	-6.1	4.2	-96.1	138.7	-62.8	-178.2	57.8	60.6	-175.2
1632.inp	14.15	-221.89	52.2	-152.9	150.7	-4.8	5.7	-90.6	146	142.8	-176.3	-98.2	63.7	-175.2
1632a.inp	14.69	-221.35	52.74	-152.4	152.1	-6.5	4.9	-98.2	138.2	176.8	-145.2	-64	95.7	-175.3
1633.inp	12.19	-223.85	50.24	-152.5	152.3	-6.5	4.3	-99.2	137.8	171.2	-60.3	-69.4	-179.8	-175.2
1634.inp	13.5	-222.54	51.55	-153	151.9	-5.6	3.9	-96.4	138.3	177.9	65.2	-61.1	-56	-175.3
1635.inp	15.37	-220.67	53.42	-148.4	128.8	-4.3	-0.7	64.7	-70.1	47.3	-45.5	-179.4	-179	-175.3
1636.inp	18.74	-217.3	56.79	-150.9	130.4	-5.7	-2.9	56.1	-84	48.5	71.6	-173.9	-67.7	-175.4
1637.inp	16.17	-219.87	54.22	-150.2	128.9	-4.7	-1.3	64.5	-71.1	45.3	-163.9	178	62.7	-175.1
1638.inp	22.41	-213.63	60.46	-152.2	128.2	-3.6	-2.2	58	-86	-132.9	59.6	7.2	-81.2	-175.7
1638a.inp	22.58	-213.46	60.63	-147.8	111.0	-3.8	0.6	86.7	-57.3	-58.4	136.8	82.2	-3.3	-175.4
1639.inp	18.88	-217.14	56.93	-146.3	108.3	-4.2	1.4	85.7	-54.4	-69.8	-45.5	69.6	176.4	-176.8
1640.inp	19.65	-216.39	57.7	-147.5	107.7	-3.6	-0.3	89.1	-49.8	-67.2	-146.6	70.3	77	-175.6
1641.inp	17.51	-218.53	55.56	-149.9	128.5	-4.9	-1.9	60.6	-73.7	132	-169.8	-97.4	58.9	-175.1
1641a.inp	17.48	-218.56	55.53	-149.4	126.4	-4.9	0.9	69.1	-64.9	166.7	-128	-62.2	101.2	-175.3
1642.inp	16.17	-219.86	54.22	-148.3	126.6	-5.5	0.9	66	-69.2	162.8	-39.6	-64	-172.3	-175.5
1643.inp	19.2	-216.84	57.25	-150.3	132.3	-5.4	-1.6	51.6	-87.6	149.8	69.4	-73.7	-68.2	-175.5
1644.inp	13.56	-222.48	51.61	-154.5	130.7	116.7	2.4	-98.7	142.1	64.7	-62.8	-177.4	178.3	-179.4
1645.inp	14	-222.03	52.05	-159.4	146.2	121.1	4.7	-106.3	131.2	68.3	61.6	-171.8	-59	-178.8
1646.inp	13.32	-222.72	51.37	-159.8	146.7	120.8	6.3	-108.2	130.8	63	-166.5	-179.1	74.4	-178.9
1647.inp	15.54	-220.5	53.59	-161.6	147.9	120.7	2.9	-90	144.4	-25.9	64.6	96.4	-58.9	-178.9
1647a.inp	15.98	-220.05	54.03	-162.1	151.0	119.6	2.1	-95.5	139.2	-62	25.1	61	-97.2	-178.6
1648.inp	13.52	-222.53	51.57	-160.2	137.1	118.4	2	-86.6	151.3	-55	-65.4	64.9	174	-178.8
1649.inp	13.63	-222.41	51.68	-161.8	149.5	120.7	3.8	-94.9	140.2	-62.5	-175.4	58	63.4	-178.7
1650.inp	14.39	-221.65	52.44	-161.6	149.8	121	3.8	-91.9	144.6	143	-174.4	-98	65.7	-178.7
1650a.inp	14.86	-221.17	52.91	-161.5	150.3	119.5	1.5	-94.6	142.1	175.6	-152.2	-66	89.7	-178.8
1651.inp	13.09	-222.95	51.14	-159.9	139.5	120.3	2.5	-86.5	152.7	164.4	-62.2	-77	178.9	-178.7
1652.inp	13.83	-222.21	51.88	-162.1	148.7	120.5	2.6	-93.9	141.2	177.7	65.7	-61.5	-55.3	-178.9
1653.inp	17.06	-218.98	55.11	-146	119.5	116	-0.1	70.9	-64.2	59.5	-41	-166.7	-174	-179.5
1654.inp	21.68	-214.36	59.73	-156.2	126.9	117.2	-3.5	62.8	-78.7	64.9	79.5	-155.6	-60.4	-178.8
1655.inp	18.09	-217.95	56.14	-154.5	123.2	115.6	-1.2	70.9	-63.9	60.6	-149.1	-166.8	78.7	-178.7
1656.inp	25.88	-210.15	63.93	-153.1	107.4	122.1	-6.2	92.1	-52.8	-62.2	132.5	79.7	-9.1	-179.5
1657.inp	21.17	-214.87	59.22	-148.8	113.0	117.1	-5.2	86.5	-54.7	-86.2	-44.8	53.8	175.8	-180
1658.inp	22.02	-214.02	60.07	-150.1	113.8	117.2	-5.6	86.8	-54.8	-88.7	-157.4	50.6	63.6	-178.8
1659.inp	18.94	-217.1	56.99	-151.1	122.3	119.8	-2.8	72.9	-61.4	168.3	-128.8	-60.4	100.2	-179
1659a.inp	19.44	-216.59	57.49	-152.9	121.8	117	-6.6	65.5	-68.7	130.4	-168.9	-98.9	59.6	-178.8
1660.inp	17.59	-218.45	55.64	-150.4	122.3	116.5	-2.6	70.7	-65.1	167.7	-39.4	-58.7	-172.5	-179.5
1661.inp	21.28	-214.76	59.33	-155.4	130.6	121.1	-7.5	57.1	-82.7	154.8	72.7	-68.1	-65.7	-179.2
1662.inp	8.37	-227.67	46.42	53	56.5	121.1	179.4	-98.6	139.9	63.2	-60.8	-177.2	179.2	179.1
1663.inp	8.49	-227.54	46.54	53.3	24.7	122.3	-176.5	-102	133.9	66.7	62.2	-172.5	-59.2	179.7
1664.inp	8.66	-227.38	46.71	54.6	19.1	122.3	-176.6	-104.2	133	59.7	-173.8	178.6	66.4	-178.6
1665.inp	10.58	-225.46	48.63	56.2	14.4	123.5	-177	-83.8	149.5	-30.6	64	92.4	-59.8	-179
1666.inp	8.78	-227.26	46.83	57	23.6	123.4	176.2	-79.7	157	-56.5	-69.9	64.6	169.1	-179.7
1667.inp	9.19	-226.85	47.24	54.6	17.7	123	-175.6	-86.7	147.9	-61.3	-178.5	59.2	60.4	-178.6
1668.inp	10.61	-225.43	48.66	54.6	16.9	122.2	-175.4	-85.8	150.5	143.3	-177	-97.7	63.1	-178.7
1668a.inp	10.77	-225.27	48.82	55.5	16.8	122.8	-175.9	-89.2	147	178.4	-145.8	-62.4	95.2	-179.2
1669.inp	9	-227.04	47.05	57.6	24.5	122.5	175.6	-82	155.5	170.7	-64.2	-69.2	176.4	179.3
1670.inp	8.94	-227.1	46.99	55.6	16.5	123.6	-176.5	-88.9	145.6	179.3	64.4	-59.9	-56.6	-179.3
1671.inp	9.93	-226.11	47.98	54.1	57.8	120.3	178.1	67.7	-61.3	58.8	-51.8	-173.7	-179.3	179.9
1672.inp	12.58	-223.46	50.63	56.7	60.4	121.1	177.1	54.1	-79.5	54.2	67.7	-174.3	-64.6	-178.5
1673.inp	10.83	-225.21	48.88	54.9	56.8	120.9	178.1	68.6	-61.1	58.1	-161.8	-175	71.1	179.8
1674.inp	17.34	-218.7	55.39	57	59.8	120.2	177.8	85.4	-54.1	-55.5	108.1	81.1	-28.1	-178.6
1675.inp	6.77	-229.27	44.82	63	-0.6	123.9	-178.7	-135.4	103	60.8	-64.5	-179.5	176.4	-178.6
1676.inp	8.74	-227.3	46.79	64.1	3.2	122.5	177	-141.3	93.8	64.2	69.5	-173.8	-52.1	-178.2
1677.inp	8.16	-227.88	46.21	60	2.0	121.6	-175.8	-153.6	83.8	58.1	-173.2	177.2	67.6	-178.7
1678.inp	10.94	-225.1	48.99	64.2	2.6	122.5	176.6	-139.2	93	-33.9	70.1	90.5	-54.3	-178.5
1679.inp	7.43	-228.61	45.48	62.8	-0.8	121.9	-177	-135.1	101.1	-58.4	-67.2	62.7	172.1	-178.8
1680.inp	8.73	-227.31	46.78	60.3	3.6	121.8	-174	-151.6	83.1	-63.4	-178.7	57.6	60.2	178.7
1681.inp	10.57	-225.47	48.62	60.4	2.6	121.8	-175.4	-150.8	85.6	146.7	-177.6	-94.8	63.3	-179.2
1681a.inp	10.32	-225.72	48.37	59.5	2.9	121.8	-173.8	-156.8	80	177.3	-143	-63.3	98.3	-179.1
1682.inp	7.79	-228.25	45.84	62.9	-0.1	123.3	-178.9	-136.1	101.2	172.2	-62.5	-68.2	178.7	-178.7
1683.inp	9.38	-226.66	47.43	63.8	4.5	122.8	177.3	-143.7	90.3	176.7	70.4	-61.2	-51	-178.3
1684.inp	8.41	-227.63	46.46	57.7	-122.8	121.5	-176.3	-140.8	98.1	59.2	-60.3	179.2	179.5	-179.4
1685.inp	9.01	-227.04	47.06	56.2	-121.0	121.3	176.3	-154.5	81.2	67.3	55.7	-170.2	-66.3	-179.4
1686.inp	8.87	-227.17	46.92	59.6	-109.6	121.9	-178.3	-158.2	79.3	56.3	-173	176.3	66.6	-179.5
1687.inp	14.05	-221.99	52.1	50.8	68.0	5.4	-0.2	-129.2	110.4	64.5	-63.9	-176.6	177.4	176.3
1688.inp	14.85	-221.19	52.9	47.7	65.8	5.1	1.5	-137.5	98.8	67	58.2	-172.1	-62.6	177.3
1689.inp	14.62	-221.42	52.67	47.2	66.2	5.4	1	-137.9	99.4	62.2	-171.1	-178.7	69.7	177.3
1690.inp	18.14	-217.9	56.19	43.9	64.7	4.2	1.5	-139.3	94.3	-64.5	28.8	59.2	-94.1	177.9
1691.inp	15.28	-220.75	53.33	46.3	61.0	5.6	-0.2	-116.6	119.3	-58.7	-65.9	62.1	173.1	177.2
1692.inp	16.08	-219.96	54.13	46.5	60.4	6.1	0.2	-115.8	118.7	-63.4	-178.9	57.2	60.1	177.2
1693.inp	17.12	-218.92	55.17	44.4	64.4	1.2	-0.1	-143.3	93.1	176.3	-142.7	-63.9	98.2	178.3
1693a.inp	16.62	-219.42	54.67	47.8	59.6	6.1	0.6	-110.6	125.8	147.6	-177.8	-94	63	175.5
1694.inp	14.66	-221.38	52.71	46.4	59.2	5.1	-0.8	-115.4	121.8	166.3	-61.8	-74.2	179	178.4
1695.inp	15.95	-220.09	54	44.8	60.2	5.8	0.2	-121.4	112.8	176.5	63.4	-62.4	-57.5	178.4
1696.inp	19.35	-216.69	57.4	47.2	81.4	2.3	2.2	70.7	-64	41.8	-49	175.7	177.4	178.8
1697.inp	25.68	-210.36	63.73	51.7	89.8	4.9	-9.4	51.2	-88.3	47	66.2	-175	-73.9	177.6
1698.inp	20.25	-215.79	58.3	44.5	78.8	3.8	5	73.7	-60.6	44.8	-154	177.7	73.6	178.3
1699.inp	29.16	-206.88	67.21	52.1	87.8	5.8	-8.9	53.7	-91.7	-111.4	57.5	31.5	-87.1	177.5
1699a.inp	27.29	-208.75	65.34	47.7	82.6	5.6	4.8	88.5	-56.7	-61	118.4	82.2	-23.8	178.2

1700.inp	22.92	-213.12	60.97	49.1	82.1	4.8	6.9	85.4	-54.2	-71.6	-54.1	67.5	168.3	178.3
1701.inp	23.26	-212.78	61.31	46.6	77.8	1.7	7.7	88.8	-49.9	-70.4	-156.9	67.1	67.3	178.2
1702.inp	21.88	-214.16	59.93	47.5	80.5	2.2	4.8	75.5	-59.4	168	-138.2	-60.1	90.8	178.4
1702a.inp	21.77	-214.26	59.82	44.7	80.5	3.2	4.7	68.1	-65.7	127.9	-158.1	-100.4	70.8	178.4
1703.inp	20.12	-215.92	58.17	48.6	82.0	3.3	4.7	71.3	-63.7	156.7	-48.5	-69.8	178.9	178.8
1704.inp	25.33	-210.71	63.38	56	79.9	3.4	-19.7	40.3	-96.2	166.6	69	-59.9	-67.9	175.8
1705.inp	16.69	-219.35	54.74	55.6	70.5	120.5	-2.3	-127.3	112.1	64.3	-63.6	-176.8	177.8	179.1
1706.inp	17.62	-218.42	55.67	52.6	68.5	121.1	0.04	-135.5	100.6	66.7	57.9	-172.4	-62.7	-179.5
1707.inp	17.41	-218.63	55.46	52.2	68.3	120.6	0	-136.2	101	62.4	-171.4	-178.6	69.5	-179.6
1708.inp	20.89	-215.15	58.94	51.4	69.2	121.2	-0.3	-141.1	92.9	-64.5	27.4	59.1	-95.2	-178.7
1709.inp	18.14	-219.9	56.19	50.5	60.8	122.4	-0.3	-115.1	120.9	-58.3	-65.8	62.5	173.3	-179.7
1710.inp	18.99	-217.05	57.04	51.8	60.2	122.8	0.1	-113.5	121.2	-63.1	-178.9	57.4	60.2	-179.7
1711.inp	19.99	-216.05	58.04	50.1	68.6	122.7	-1.6	-144.2	92.4	176.4	-142.8	-63.8	98.3	-178.5
1711a.inp	19.62	-216.42	57.67	52	60.2	122.2	0.7	-108.1	128.4	147.7	-177.7	-94.1	63.3	177.4
1712.inp	17.56	-218.48	55.61	50	58.9	123.3	-0.9	-114.4	122.9	166.8	-61.7	-73.8	179.2	-179
1713.inp	18.86	-217.18	56.91	50.4	58.4	123.5	-0.1	-115.3	119.3	175.6	63.7	-63.4	-57.1	-179.1
1727.inp	5.55	-230.49	43.6	-68.6	-16.3	125.1	176.1	-94.1	144.9	67	-59.1	-173.6	-179	177.4
1728.inp	5.8	-230.24	43.85	-65.4	-25.2	124.4	179	-98.6	138	70.4	58.4	-169.3	-62.4	176
1729.inp	6.13	-229.91	44.18	-69.5	-26.8	126.2	-179.4	-100.2	137.3	64.9	-170.2	-176.2	70.1	177.3
1730.inp	8.05	-227.99	46.1	-66.5	-28.5	126.8	-175.6	-82.5	150.4	-63.1	32.7	60.7	-91.4	177.8
1730a.inp	8.03	-228.01	46.08	-76.1	-30.8	126.3	-175.8	-79.7	153.7	-29.9	63.4	93.3	-61	176.6
1731.inp	5.95	-230.09	44	-73.7	-24.0	126.1	-179.7	-79.5	156.5	-59.4	-62.9	62.3	175.1	178.2
1732.inp	6.35	-229.68	44.4	-67.6	-32.7	127.2	-177.4	-82.9	151.6	-62.9	-177.6	58.2	60.7	179.8
1733.inp	8.09	-227.95	46.14	-62.3	-31.2	126.7	-179.6	-82.6	153.8	142.8	-176.5	-98.1	63.6	178.1
1733a.inp	7.91	-228.13	45.96	-60.3	-34.0	126.3	-179.8	-88.4	148	177.9	-142.6	-62.6	98.3	177.9
1734.inp	6.05	-229.99	44.1	-63.2	-25.8	127.1	175.2	-82.1	155.4	174.1	-56.7	-66.1	-176.1	177.8
1735.inp	6.34	-229.7	44.39	-59.7	-29.8	126.5	176.5	-83.7	151.3	179.9	62.9	-59.7	-57.6	176.2
1736.inp	7.44	-228.6	45.49	-78	-16.3	125.9	177.6	69.9	-59.1	66.2	-52.1	-166	-179.3	177.4
1737.inp	9.59	-226.44	47.64	-67.1	-26.8	126.9	167.3	52	-80.8	52.2	70.4	-177.3	-62	178
1738.inp	8.38	-227.65	46.43	-66.1	-23.4	124.7	171.7	69.9	-59.5	62	-161.6	-171.5	71.5	178.8
1739.inp	13.85	-222.19	51.9	-62.7	-26.8	125.5	177.2	71.2	-70.9	-76.2	54.4	63.8	-85.6	178.4
1740.inp	8.68	-227.36	46.73	-74.4	-28.3	125.7	177.6	81.6	-52.2	-75.7	-54.2	56.7	174.1	177.3
1741.inp	9.37	-226.67	47.42	-64	-28.5	125.6	175.6	83	-51.5	-77.3	-166.2	54.3	62.4	178.8
1742.inp	9.23	-226.81	47.28	-63.2	-31.5	126.5	176.9	70.4	-59.3	173.9	-140.1	-60.3	94.4	178.7
1743.inp	7.22	-228.82	45.27	-75.3	-34.9	127	179.7	65	-64.7	167.9	-52.6	-64.8	-179.4	177.8
1744.inp	9.46	-226.58	47.51	-62	-35.2	126.1	175.4	51.3	-82.6	164.1	72.1	-65.4	-59.3	178.1

Appendix II. A structure tree of 3'-pentyl formiate

					HCOC3				
			t				e		
			COC3C2				COC3C2		
		g-	g+	t-		g-	g+	t-	
ω2,3; ω3,4									
τ τ		1.plu	10.plu	37.plu		19.plu	28.plu	46.plu	
	Rel. E	0	5.98	0		16.32	21.21	16.32	
	(KJ/mol)								
tg-		2.plu	11.plu	38.plu		20.plu	29.plu	47.plu	
	Rel. E	4.64	16.4	3.35		20.92	30.42	19.66	
tg+		3.plu	12.plu	39.plu		21.plu	30.plu	48.plu	
	Rel. E	1.22	8.66	2.68		19.71	23.89	19.04	
g+g-		4.plu	13.plu	40.plu		22.plu	31.plu	49.plu	
		4a.plu	13a.plu	40a.plu		22a.plu	31a.plu	49a.plu	
	Rel. E	13.97	35.44	13.97		31.92	47.15	30.29	
		15.61	35.44	15.61		30.29	47.15	31.92	
g+t		5.plu	14.plu	41.plu		23.plu	32.plu	50.plu	
	Rel. E	3.35	16.4	4.64		19.66	30.42	20.92	
g+g+		6.plu	15.plu	42.plu		24.plu	33.plu	51.plu	
	Rel. E	5.65	18.33	6.11		21.97	32.26	22.43	
g-g+		7.plu	16.plu	43.plu		25.plu	34.plu	52.plu	
		7a.plu	16a.plu	43a.plu		25a.plu	34a.plu	52a.plu	
	Rel. E	11.17	16.15	11.17		27.99	31.8	27.7	
		11.63	16.15	11.63		27.7	31.8	27.99	
g-t		8.plu	17.plu	44.plu		26.plu	35.plu	53.plu	
	Rel. E	2.72	8.66	1.22		19.04	23.89	19.71	
g-g-		9.plu	18.plu	45.plu		27.plu	36.plu	54.plu	
	Rel. E	6.11	18.33	5.65		22.43	32.26	21.97	

Appendix II. Energies and Parameters of all stable conformations in 3-pentyl formiate

Force field energies and geometries with PCMODEL Version 4 (without Pi): files *.inp

files *.inp	Rel. E	δ Hf	MMXE	HCOC3	HC3OC	COC3C2	COC3C4	OC3C2C1	OC3C4C5	ω 2',3'	ω 3',4'
1.inp	0	-113.19	2.91	-179.2	12.3	-107.6	130.5	62.8	-61.5	-177.4	178.5
2.inp	1.11	-112.08	4.02	-179.3	12.4	-106.5	129.1	66.5	61.7	-172.1	-60
3.inp	0.82	-112.38	3.73	-179.2	14.1	-105.7	131.3	60.1	-172.3	179.5	67.7
4.inp	3.34	-109.86	6.25	-179	36.8	-81.9	150.8	-32.1	65.8	91.8	-58.8
4a.inp	3.73	-109.47	6.64	-179.3	31	-85.5	147.2	-62.6	32.6	61.8	-91.5
5.inp	0.8	-112.39	3.71	-179.4	34.9	-84.2	151.6	-57.3	-64.4	64.2	173.9
6.inp	1.35	111.84	4.26	-179.4	34.4	-84.3	150.2	-62.3	-178.2	58.9	60.3
7.inp	2.67	110.52	5.58	-178.9	35.4	-84.5	151.6	142.5	-176.6	-98	63.2
7a.inp	2.78	-110.41	5.69	-179.1	30.8	-88.3	147.8	178.1	-146.1	-62.4	94.7
8.inp	0.65	-112.55	3.56	-179.1	31	-88.5	148.4	172.8	-58.8	-67.3	-178.6
9.inp	1.46	-111.74	4.37	-179.2	32.4	-86	148.3	178.6	65.8	-59.9	-55.9
10.inp	1.43	-111.77	4.34	-180	-180	64.3	-64.3	54.5	-54.4	-178.5	178.6
11.inp	3.92	-109.27	6.83	179.4	165.5	51.9	-81.3	53.4	67.7	-175.6	-64.1
12.inp	2.07	-111.13	4.98	179.8	-179.9	64.5	-64.8	51.6	-166.6	178.1	66.5
13.inp	8.47	-104.72	11.38	-180	-165.4	83.9	-54.9	-53.7	107.1	82.5	-28.5
13a.inp	8.47	-104.72	11.38	179.9	165.3	54.9	-84	-107	53.7	28.6	-82.4
14.inp	3.92	-109.27	6.83	-179.4	-165.6	81.1	-52	-67.7	-53.5	64.1	175.4
15.inp	4.38	-108.81	7.29	-179.6	-165.1	81.9	-52.1	-72.7	-166	58.6	63.1
16.inp	3.86	-109.34	6.77	-179.2	-176.1	69	-60.4	171.9	-140.5	-62.3	94.3
16a.inp	3.86	-109.34	6.77	179.2	176.1	60.4	-68.9	140.5	-171.7	-94.3	62.5
17.inp	2.07	-111.13	4.98	-179.8	179.8	64.7	-64.6	166.3	-52	-66.8	-178.5
18.inp	4.38	-108.81	7.29	179.6	165.1	52.1	-81.8	166.1	72.6	-63.1	-58.7
19.inp	3.9	-109.29	6.81	0.8	8.7	-111	127.2	62.7	-61.9	-177.6	178.3
20.inp	5	-108.2	7.91	0.8	5.5	-112.9	122.7	65.8	60.6	-172.8	-60.8
21.inp	4.71	-108.49	7.62	0.8	6.6	-112.6	124.3	59.4	-173.4	178.6	66.8
22.inp	7.63	-105.56	10.54	0.2	21.7	-94.6	138.2	-63.3	31.9	60.9	-91.8
22a.inp	7.24	-105.95	10.15	1.4	36.2	-82.5	150.3	-31.8	65.6	92	-58.9
23.inp	4.7	-108.5	7.61	0.6	33	-86	149.8	-57.3	-64.6	64	173.9
24.inp	5.25	-107.95	8.16	0.9	32.7	-86	148.5	-62.3	-178.3	58.8	60.2
25.inp	6.69	-106.51	9.6	1	28.8	-90.2	146	178.7	-146.6	-61.9	94.3
25a.inp	6.62	-106.58	9.53	1.4	33	-86.8	149.4	144.2	-177	-96.7	63
26.inp	4.55	-108.65	7.46	1	27.9	-91.4	145.5	174	-58.8	-66.1	-178.4
27.inp	5.36	-107.83	8.27	1	31.7	-86.7	147.7	179.3	65.5	-59.3	-56
28.inp	5.07	-108.13	7.98	0	-179.9	64	-63.8	55.1	-54.9	-178.6	178.8
29.inp	7.27	-105.93	10.18	-1.5	166.3	52.1	-80	55.5	68.5	-174.6	-62.1
30.inp	5.71	-107.48	8.62	-0.1	-179.4	64.6	-64	52.9	-166.2	178.7	67.7
31.inp	11.27	-101.92	14.18	-0.1	-166.2	82	-55.4	-50.4	96.6	84.6	-38
31a.inp	11.27	-101.92	14.18	0.1	166.1	55.3	-82.2	-96.7	50.4	37.8	-84.5
32.inp	7.27	-105.93	10.18	1.6	-166.4	79.9	-52.2	-68.5	-55.4	62.1	174.7
33.inp	7.71	-105.48	10.62	1.6	-166.4	80.2	-52.9	-74.3	-168.5	55.9	61.7
34.inp	7.6	-105.59	10.51	0.7	-176.6	68.2	-60.7	171.5	-141.6	-63.3	93.8
34a.inp	7.6	-105.59	10.51	-0.9	176.5	60.6	-68.2	141.3	-171.7	-94	63.1
35.inp	5.71	-107.48	8.62	0.1	179.3	63.9	-64.7	165.8	-52.9	-68.1	-178.7
36.inp	7.71	-105.48	10.62	-1.5	166.1	52.6	-80.4	168.4	74.2	-61.9	-56
37.inp	0	-113.19	2.91	179.2	-13.4	-131.5	106.6	61.1	-62.7	-178.3	177.5
38.inp	0.8	-112.39	3.71	179.2	-33.5	-150.2	85.5	64.7	58	-173.6	-63.4
39.inp	0.64	-112.55	3.55	179.1	-30.6	-148	88.8	58.9	-173	178.7	67.1
40.inp	3.34	-109.86	6.25	179	-36.8	-150.8	81.9	-65.8	32.1	58.8	-91.8
40a.inp	3.73	-109.47	6.64	179.3	-30.8	-147	85.7	-32.4	62.8	91.6	-61.7
41.inp	1.11	-112.08	4.02	179.2	-14.1	-130.7	104.9	-61.9	-66.7	59.8	171.9
42.inp	1.46	-111.74	4.37	179.1	-32.1	-147.9	86.3	-65.7	-178.7	55.9	59.7
43.inp	2.67	-110.52	5.58	178.9	-35.8	-152.1	84.1	176.6	-142.5	-63.2	98
43a.inp	2.78	-110.41	5.69	179.1	-31.2	-148.2	87.9	145.9	-178.1	-94.8	62.3
44.inp	0.82	-112.38	3.73	179.1	-13.8	-131	106	172.4	-59.9	-67.6	-179.3
45.inp	1.35	-111.84	4.26	179.3	-34.1	-149.9	84.6	178	62.6	-60.4	-58.6
46.inp	3.9	-109.29	6.81	-1	-8.2	-126.7	111.4	61.8	-62.7	-178.3	177.6
47.inp	4.7	-108.5	7.61	-0.5	-32.7	-149.5	86.3	64.3	57.4	-174.1	-64
48.inp	4.55	-108.65	7.46	-1.1	-28.3	-145.9	91.1	58.4	-174.2	178	66.1
49.inp	7.24	-105.95	10.15	-1.2	-36.2	-150.3	82.5	-65.4	31.8	59	-92
49a.inp	7.62	-105.57	10.53	-0.6	-24.2	-140.7	92.1	-31.8	63.1	92	-61.1
50.inp	5	-108.2	7.91	-0.9	-8.5	-125.6	110.1	-60.9	-66.3	60.6	172.4
51.inp	5.36	-107.83	8.27	-0.9	-31.5	-147.5	86.8	-65.4	-179.2	56.2	59.4
52.inp	6.62	-106.58	9.53	-1.2	-31.6	-148	88.2	177.1	-144.6	-63	96.3
52a.inp	6.69	-106.51	9.6	-0.9	-27.5	-144.7	91.5	146.5	-178.5	-94.5	62.1
53.inp	4.71	-108.49	7.62	-0.9	-7.7	-125.3	111.7	173.4	-59.7	-66.8	-178.9
54.inp	5.25	-107.95	8.16	-0.4	-32.2	-148.1	86.4	178.4	62.4	-60.2	-58.7

Appendix III. A structure tree of N-TFA-L-Phe-O-3'-pentyl ester (subtree 1)

										Φ																Φ							
										g-																g+							
								Ψ								$C_FC_ONC^*$		$C^*C_OOC_3$						Ψ								$C_FC_ONC^*$	
			t+		t-		t		e		g+		g-			e		e		t+		t-		t		e		g+		g-		e	
			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O	
		t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
ω2ə,3ə, ω3ə,4ə																																	
tt		t0001.inp	t0010.inp	t0073.inp	t0082.inp	t0037.inp	t0046.inp	t0019.inp	t0028.inp	o. sol.	o. sol	t0055.inp	t0064.inp	t0091.inp	t0100.inp	t0109.inp	t0118.inp	t1714.inp	o. sol	t0865.inp	t0874.inp	o. sol	o. sol	t0847.inp	t0856.inp	t0811.inp	t0820.inp	t0883.inp	t0829.inp	t0892.inp	t0901.inp		
	Rel. E	0.00	6.99	15.56	21.51	2.76	12.34	5.86	12.84			7.66	18.49	13.56	20.25	33.10	44.43	21.59		7.82	15.65			12.55	22.18	10.46	16.99	19.12	22.09	29.92	38.99		
	KJ/mo																																
tg-		t0002.inp	t0011.inp	t0074.inp	t0083.inp	t0038.inp	t0047.inp	t0020.inp	t0029.inp	o. sol.	o. sol	t0056.inp	t0065.inp	t0092.inp	t0101.inp	t0110.inp	t0119.inp	t1715.inp	o. sol	t0866.inp	t0875.inp	o. sol	o. sol	t0848.inp	t0857.inp	t0812.inp	t0821.inp	t0884.inp	t0830.inp	t0893.inp	t0902.inp		
	Rel. E	4.02	18.74	17.78	32.01	6.57	18.95	11.46	23.85			10.46	26.07	22.76	31.88	35.98	66.78	25.40		8.95	23.10			14.31	31.67	17.82	28.16	18.45	32.13	36.57	53.35		
tg+		t0003.inp	t0012.inp	t0075.inp	t0084.inp	t0039.inp	t0048.inp	t0021.inp	t0030.inp	o. sol.	o. sol	t0057.inp	t0066.inp	t0093.inp	t0102.inp	t0111.inp	t0120.inp	t1716.inp	o. sol	t0867.inp	t0876.inp	o. sol	o. sol	t0849.inp	t0858.inp	t0813.inp	t0822.inp	t0885.inp	t0831.inp	t0894.inp	t0903.inp		
	Rel. E	3.72	11.84	20.08	25.52	8.54	11.88	12.43	16.95			9.08	19.16	16.99	24.98	37.03	48.74	26.19		11.05	16.90			14.43	25.65	16.90	21.59	20.46	25.48	35.52	46.02		
+g-		t0004.inp	t0013.inp	t0076.inp	t0085.inp	t0040.inp	t0049.inp	t0022.inp	t0031.inp	o. sol.	o. sol	t0058.inp	t0067.inp	t0094.inp	t0103.inp	t0112.inp	t0121.inp	t1717.inp	o. sol	t0868.inp	t0877.inp	o. sol	o. sol	t0850.inp	t0859.inp	t0814.inp	t0823.inp	t0886.inp	t0832.inp	t0895.inp	t0904.inp		
		t0004a.inp	t0013a.inp	t0076a.inp	t0085a.inp	no. sol.	0049a.inp	t0022a.inp	t0031a.inp	o. sol.	o. sol	no. sol.	no. sol.	no. sol.	0103a.inp	t0112a.inp	no. sol.	no. sol.	o. sol	t0868a.inp	t0877a.inp	o. sol	o. sol	t0850a.inp	t0859a.inp	t0814a.inp	t0823a.inp	t0886a.inp	t0832a.inp	t0895a.inp	t0904a.inp		
	Rel. E	15.02	38.41	32.93	55.40	14.60	37.91	21.67	43.26			19.83	45.19	28.20	52.38	46.48	81.09	36.65		23.10	46.69			25.52	48.99	25.98	48.28	27.61	56.74	48.16	68.74		
		15.23	39.41	32.76	46.11		39.71	20.88	44.89						52.72	49.71				23.68	44.27			26.99	47.86	24.85	48.58	30.50	58.45	46.11	76.69		
g+t		t0005.inp	t0014.inp	t0077.inp	t0086.inp	t0041.inp	t0050.inp	t0023.inp	t0032.inp	o. sol.	o. sol	t0059.inp	t0068.inp	t0095.inp	t0104.inp	t0113.inp	t0122.inp	t1718	o. sol	t0869.inp	t0878.inp	o. sol	o. sol	t0851.inp	t0860.inp	t0815.inp	t0824.inp	t0887.inp	t0833.inp	t0896.inp	t0905.inp		
	Rel. E	4.56	18.16	19.79	37.45	2.72	19.41	9.00	23.60			11.17	22.47	17.78	33.22	41.30	65.52	22.09		9.96	26.11			15.36	30.84	14.27	27.95	24.89	36.44	35.40	54.18		
+g+		t0006.inp	t0015.inp	t0078.inp	t0087.inp	t0042.inp	t0051.inp	t0024.inp	t0033.inp	o. sol.	o. sol	t0060.inp	t0069.inp	t0096.inp	t0105.inp	t0114.inp	t0123.inp	no. sol.	o. sol	t0870.inp	t0879.inp	o. sol	o. sol	t0852.inp	t0861.inp	t0816.inp	t0825.inp	t0888.inp	t0834.inp	t0897.inp	t0906.inp		
	Rel. E	7.95	21.30	21.13	36.28	6.07	21.38	13.43	26.40			12.47	25.90	20.25	34.94	42.84	67.03			15.19	29.16			16.86	30.84	18.37	30.96	25.36	39.41	39.50	56.44		
-g+		t0007.inp	t0016.inp	t0079.inp	t0088.inp	t0043.inp	t0052.inp	t0025.inp	t0034.inp	o. sol.	o. sol	t0061.inp	t0070.inp	t0097.inp	t0106.inp	t0115.inp	t0124.inp	t1719.inp	o. sol	t0871.inp	t0880.inp	o. sol	o. sol	t0853.inp	t0862.inp	t0817.inp	t0826.inp	t0889.inp	t0835.inp	t0898.inp	t0907.inp		
		t0007a.inp	t0016a.inp	t0079a.inp	no. sol.	0043a.inp	t0052a.inp	t0025a.inp	t0034a.inp	o. sol.	o. sol	0061a.inp	t0070.inp	0097a.inp	t0106a.inp	t0115a.inp	t0124a.inp	1719a.inp	o. sol	t0871a.inp	t0880a.inp	o. sol	o. sol	0853a.inp	t0862a.inp	t0817a.inp	t0826a.inp	t0889a.inp	t0835a.inp	t0898a.inp	t0907a.inp		
	Rel. E	15.19	20.17	26.90	34.60	14.64	20.67	20.84	24.64			20.46	25.44	27.87	32.76	43.26	56.44	32.59		21.05	27.91			24.02	29.20	26.44	30.29	30.29	37.28	45.77	52.51		
		14.35	19.41	29.33		15.23	19.66	20.67	24.98			19.87	24.81	26.61	33.81	47.24	56.65	31.92		21.63	27.11			23.93	29.33	24.52	29.75	32.38	38.99	45.73	54.22		
g-t		t0008.inp	t0017.inp	t0080.inp	t0089.inp	t0044.inp	t0053.inp	t0026.inp	t0035.inp	o. sol.	o. sol	t0062.inp	t0071.inp	t0098.inp	t0107.inp	t0116.inp	t0125.inp	t1720.inp	o. sol	t0872.inp	t0881.inp	o. sol	o. sol	t0854.inp	t0863.inp	t0818.inp	t0827.inp	t0890.inp	t0836.inp	t0899.inp	t0908.inp		
	Rel. E	6.23	11.42	18.33	24.60	4.10	11.34	9.50	16.23			13.72	16.61	19.54	25.27	38.70	50.21	22.47		10.67	23.26			17.11	21.42	14.10	21.21	18.49	28.74	36.23	42.01		
g-g-		t0009.inp	t0018.inp	t0081.inp	t0090.inp	t0045.inp	t0054.inp	t0027.inp	t0036.inp	o. sol.	o. sol	t0063.inp	t0072.inp	t0099.inp	t0108.inp	t0117.inp	t0126.inp	t1721.inp	o. sol	t0873.inp	t0882.inp	o. sol	o. sol	t0855.inp	t0864.inp	t0819.inp	t0828.inp	t0891.inp	t0837.inp	t0900.inp	t0909.inp		
	Rel. E	8.12	21.09	25.82	38.70	7.45	21.25	13.51	25.94			12.30	26.36	21.38	33.68	39.50	66.07	24.85		14.90	29.54			16.61	31.42	19.62	31.97	23.10	40.67	40.29	52.55		

Caption:

1. **no. sol. = no solution found for these parameters, not stable conformation**
2. **Rel. E = relative energy (kJ/mol)**
3. **Rel. E is below 10KJ/mol or 2.40Kcal/mol respectively, marked in green colour in Table(Tree); over 15KJ/mol or 3.60 Kcal/mol marked in red colour; between of these is marked black colour.**
4. **Because of steric hindrance, only a few conformations are in the low energy range marked in green colour.**
5. **Torsion angle χ = NC*CC_{Ph}; Φ = CNC*C_O; Ψ = NC*C_OO**

Appendix III. A structure tree of N-TFA-L-Phe-O-3'-pentyl ester (subtree 2)

										Φ																Φ							
										g-																g+							
								Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$						Ψ								$C_FC_ONC^*$
			t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e
			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O
		t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
ω2,3, ω3,4																																	
tt		t0127.plu	t0136.plu	t0199.plu	t0208.plu	t0163.plu	t0172.plu	t0145.plu	t0154.plu	t0217.plu	t0226.plu	t0181.plu	t0190.plu	t0235.plu	t0244.plu	t0253.plu	t0262.plu	t0946.plu	t0955.plu	t0964.plu	t0973.plu	o. sol	o. sol	t0982.plu	t0991.plu	t0928.plu	t0937.plu	o. sol	o. sol	t1000.plu	t1009.plu		
	Rel. E	6.65	13.18	18.74	24.94	7.03	13.22	7.70	14.31	9.87	15.65	6.95	13.56	19.00	25.15	37.74	49.71	22.72	28.62	10.29	17.49			7.49	16.48	7.66	14.52			31.97	39.20		
tg-		t0128.plu	t0137.plu	t0200.plu	t0209.plu	t0164.plu	t0173.plu	t0146.plu	t0155.plu	t0218.plu	t0227.plu	t0182.plu	t0191.plu	t0236.plu	t0245.plu	t0254.plu	t0263.plu	t0947.plu	t0956.plu	t0965.plu	t0974.plu	o. sol	o. sol	t0983.plu	t0992.plu	t0929.plu	t0938.plu	o. sol	o. sol	t1001.plu	t1010.plu		
	Rel. E	10.59	23.60	23.43	36.36	13.81	24.89	11.21	25.56	12.38	27.61	10.42	24.56	24.27	36.65	38.83	64.85	27.82	39.66	13.05	26.74			9.33	25.52	11.42	26.57			38.91	55.40		
tg+		t0129.plu	t0138.plu	t0201.plu	t0210.plu	t0165.plu	t0174.plu	t0147.plu	t0156.plu	t0219.plu	t0228.plu	t0183.plu	t0192.plu	t0237.plu	t0246.plu	t0255.plu	t0264.plu	t0948.plu	t0957.plu	t0966.plu	t0975.plu	o. sol	o. sol	t0984.plu	t0993.plu	t0930.plu	t0939.plu	o. sol	o. sol	t1002.plu	t1011.plu		
	Rel. E	10.67	16.99	22.64	28.79	12.84	17.70	12.55	18.54	14.23	19.37	11.05	17.91	23.39	28.87	37.82	52.68	26.86	32.47	12.84	20.13			9.83	19.75	11.92	18.20			37.70	42.93		
+g-		t0130.plu	t0139.plu	t0202.plu	t0211.plu	t0166.plu	t0175.plu	t0148.plu	t0157.plu	t0220.plu	t0229.plu	t0184.plu	t0193.plu	t0238.plu	t0247.plu	t0256.plu	t0265.plu	t0949.plu	t0958.plu	t0967.plu	t0976.plu	o. sol	o. sol	t0985.plu	t0994.plu	t0931.plu	t0940.plu	o. sol	o. sol	t1003.plu	t1012.plu		
		t0130a.plu	t0139a.plu	t0202a.plu	t0211a.plu	t0166a.plu	t0175a.plu	t0148a.plu	t0157a.plu	t0220a.plu	t0229a.plu	t0184a.plu	t0193a.plu	t0238a.plu	t0247a.plu	t0256a.plu	t0265a.plu	t0949a.plu	t0958a.plu	t0967a.plu	t0976a.plu	o. sol	o. sol	t0985a.plu	t0994a.plu	t0931a.plu	t0940a.plu	o. sol	o. sol	t1003a.plu	t1012a.plu		
	Rel. E	22.47	43.51	33.93	55.65	24.39	43.72	20.88	45.06	21.21	48.24	20.46	44.85	35.73	55.65	52.97	78.41	38.91	59.29	23.85	47.61			20.38	43.93	21.97	47.61			45.90	70.50		
		21.76	42.63	31.55	53.26	22.38	44.10	20.00	45.77	23.01	47.66	21.67	45.48	34.56	56.32	49.33	79.66	36.74	58.95	24.85	47.24			22.68	43.89	20.25	44.60			46.99	72.30		
g+t		t0131.plu	t0140.plu	t0203.plu	t0212.plu	t0167.plu	t0176.plu	t0149.plu	t0158.plu	t0221.plu	t0230.plu	t0185.plu	t0194.plu	t0239.plu	t0248.plu	t0257.plu	t0266.plu	t0950.plu	t0959.plu	t0968.plu	t0977.plu	o. sol	o. sol	t0986.plu	t0995.plu	t0932.plu	t0941.plu	o. sol	o. sol	t1004.plu	t1013.plu		
	Rel. E	11.46	22.80	21.88	36.53	11.38	23.68	10.67	25.31	13.97	29.20	10.63	25.69	24.52	36.53	43.14	63.09	26.36	39.50	15.27	29.50			10.75	23.43	10.33	24.31			35.06	50.96		
+g+		t0132.plu	t0141.plu	t0204.plu	t0213.plu	t0168.plu	t0177.plu	t0150.plu	t0159.plu	t0222.plu	t0231.plu	t0186.plu	t0195.plu	t0240.plu	t0249.plu	t0258.plu	t0267.plu	t0951.plu	t0960.plu	t0969.plu	t0978.plu	o. sol	o. sol	t0987.plu	t0996.plu	t0933.plu	t0942.plu	o. sol	o. sol	t1005.plu	t1014.plu		
	Rel. E	14.48	25.69	25.06	39.71	14.81	27.07	13.81	29.54	17.03	31.00	13.47	29.00	27.36	39.96	42.93	66.02	29.46	42.89	17.36	31.00			12.18	25.90	14.14	26.36			39.58	53.05		
-g+		t0133.plu	t0142.plu	t0205.plu	t0214.plu	t0169.plu	t0178.plu	t0151.plu	t0160.plu	t0223.plu	t0232.plu	t0187.plu	t0196.plu	t0241.plu	t0250.plu	t0259.plu	t0268.plu	t0952.plu	t0961.plu	t0970.plu	t0979.plu	o. sol	o. sol	t0988.plu	t0997.plu	t0934.plu	t0943.plu	o. sol	o. sol	t1006.plu	t1015.plu		
		t0133a.plu	t0142a.plu	t0205a.plu	t0214a.plu	t0169a.plu	t0178a.plu	t0151a.plu	t0160a.plu	t0223a.plu	t0232a.plu	t0187a.plu	t0196a.plu	t0241a.plu	t0250a.plu	t0259a.plu	t0268a.plu	t0952a.plu	t0961a.plu	t0970a.plu	t0979a.plu	o. sol	o. sol	t0988a.plu	t0997a.plu	t0934a.plu	t0943a.plu	o. sol	o. sol	t1006a.plu	t1015a.plu		
	Rel. E	20.33	25.31	31.80	37.20	22.05	26.19	21.51	27.45	23.56	29.41	21.13	26.82	32.72	38.16	45.31	57.74	36.32	40.67	23.64	28.66			19.37	24.64	20.46	24.94			46.36	50.12		
		19.96	25.06	29.54	35.40	21.13	25.82	21.00	27.24	24.02	29.16	21.05	26.36	33.18	38.12	47.91	57.20	35.69	40.63	23.81	28.07			19.20	24.81	19.92	25.23			44.81	51.09		
g-t		t0134.plu	t0143.plu	t0206.plu	t0215.plu	t0170.plu	t0179.plu	t0152.plu	t0161.plu	t0224.plu	t0233.plu	t0188.plu	t0197.plu	t0242.plu	t0251.plu	t0260.plu	t0269.plu	t0953.plu	t0962.plu	t0971.plu	t0980.plu	o. sol	o. sol	t0989.plu	t0998.plu	t0935.plu	t0944.plu	o. sol	o. sol	t1007.plu	t1016.plu		
	Rel. E	11.17	16.65	21.71	29.04	11.55	17.36	11.46	18.58	13.97	21.38	11.92	17.82	23.39	29.83	41.09	52.76	26.65	32.09	15.02	21.46			11.92	16.99	10.25	18.70			34.48	42.13		
g-g-		t0135.plu	t0144.plu	t0207.plu	t0216.plu	t0171.plu	t0180.plu	t0153.plu	t0162.plu	t0225.plu	t0234.plu	t0189.plu	t0198.plu	t0243.plu	t0252.plu	t0261.plu	t0270.plu	t0954.plu	t0963.plu	t0972.plu	t0981a.plu	o. sol	o. sol	t0990.plu	t0999.plu	t0936.plu	t0945.plu	o. sol	o. sol	t1008.plu	t1017.plu		
	Rel. E	14.18	27.32	24.77	39.33	15.77	28.37	13.26	29.83	15.61	31.46	14.14	27.45	27.32	40.25	42.68	65.61	30.42	42.68	18.16	29.50			16.02	27.36	13.26	29.54			39.33	53.22		

Appendix III. A structure tree of N-TFA-L-Phe-O-3'-pentyl ester (subtree 3)

										Φ															Φ								
										g-															g+								
								Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$						Ψ							$C_FC_ONC^*$		
			t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		
			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O	
		t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t
ω2,3, ω3,4																																		
tt		t0271.plu	t0280.plu	o. sol.	o. sol.	t0307.plu	t0316.plu	t0289.plu	t0298.plu	t0361.plu	t0370.plu	t0325.plu	t0334.plu	t0379.plu	t0388.plu	t0397.plu	t0406.plu	o. sol.	o. sol.	t1054.plu	t1063.plu	o. sol.	o. sol.	t1072.plu	t1081.plu	t1036.plu	t1045.plu	no. sol.	no. sol.	t1090.plu	t1099.plu	t1108.plu		
	Rel. E	7.11	12.22			11.72	23.43	1.72	10.38	13.85	20.25	7.32	20.38	20.46	27.07	43.39	53.30			12.30	19.00			8.62	18.49	11.34	18.74			43.10	51.80	46.40		
tg-		t0272.plu	t0281.plu	o. sol.	o. sol.	t0308.plu	t0317.plu	t0290.plu	t0299.plu	t0362.plu	t0371.plu	t0326.plu	t0335.plu	t0380.plu	t0389.plu	t0398.plu	t0407.plu	o. sol.	o. sol.	t1055.plu	t1064.plu	o. sol.	o. sol.	t1073.plu	t1082.plu	t1037.plu	t1046.plu	no. sol.	no. sol.	t1091.plu	t1100.plu	t1109.plu		
	Rel. E	10.59	23.68			16.11	23.39	3.64	23.81	20.04	31.51	3.26	27.15	22.55	38.99	42.22	67.78			14.43	30.46			13.56	27.20	12.30	31.63			43.76	65.65	48.95		
tg+		t0273.plu	t0282.plu	o. sol.	o. sol.	t0309.plu	t0318.plu	t0291.plu	t0300.plu	t0363.plu	t0372.plu	t0327.plu	t0336.plu	t0381.plu	t0390.plu	t0399.plu	t0408.plu	o. sol.	o. sol.	t1056.plu	t1065.plu	o. sol.	o. sol.	t1074.plu	t1083.plu	t1038.plu	t1047.plu	no. sol.	no. sol.	t1092.plu	t1101.plu	t1110.plu		
	Rel. E	10.96	15.65			16.95	15.73	7.28	14.48	20.29	22.93	6.32	23.97	22.97	30.67	42.47	55.94			15.48	23.56			12.22	21.92	13.26	22.43			43.56	55.94	47.95		
+g-		t0274.plu	t0283.plu	o. sol.	o. sol.	t0310.plu	t0319.plu	t0292.plu	t0301.plu	t0364.plu	t0373.plu	t0328.plu	t0337.plu	t0382.plu	t0391.plu	t0400.plu	t0409.plu	o. sol.	o. sol.	t1057.plu	t1066.plu	o. sol.	o. sol.	t1075.plu	t1084.plu	t1039.plu	t1048.plu	no. sol.	no. sol.	t1093.plu	t1102.plu	t1111.plu		
		t0274a.plu	t0283a.plu	o. sol.	o. sol.	no. sol.	t0319a.plu	t0292a.plu	t0301a.plu	no. sol.	t0373a.plu	t0328a.plu	t0337a.plu	t0382a.plu	t0391a.plu	t0400a.plu	no. sol.	o. sol.	o. sol.	no. sol.	t1066a.plu	o. sol.	o. sol.	t1075a.plu	t1084a.plu	t1039a.plu	t1048a.plu	no. sol.	no. sol.	t1093a.plu	no. sol.	t1111a.plu		
	Rel. E	23.39	42.26			22.01	43.76	13.26	41.30	33.01	50.71	15.31	42.34	35.65	59.58	52.38	84.01			29.46	52.05			23.81	44.27	22.68	47.24			50.84	77.11	61.84		
		22.51	45.94				46.32	14.90	43.89		52.80	15.82	43.35	35.82	56.40	56.82					51.92			25.23	46.07	23.60	47.15			50.79		60.54		
g+t		t0275.plu	t0294.plu	o. sol.	o. sol.	t0311.plu	t0320.plu	t0293.plu	t0302.plu	t0365.plu	t0374.plu	t0329.plu	t0338.plu	t0383.plu	t0392.plu	t0401.plu	t0410.plu	o. sol.	o. sol.	t1058.plu	t1067.plu	o. sol.	o. sol.	t1076.plu	t1085.plu	t1040.plu	t1049.plu	no. sol.	no. sol.	t1094.plu	t1103.plu	t1112.plu		
	Rel. E	13.14	22.97			10.00	29.25	3.81	21.00	17.91	31.88	7.57	21.92	26.69	37.11	33.93	70.46			22.55	30.75			11.51	24.23	13.01	24.18			44.22	56.61	50.00		
+g+		t0276.plu	t0285.plu	o. sol.	o. sol.	t0312.plu	t0321.plu	t0294.plu	t0303.plu	t0366.plu	t0375.plu	t0330.plu	t0339.plu	t0384.plu	t0393.plu	t0402.plu	t0411.plu	o. sol.	o. sol.	t1059.plu	t1068.plu	o. sol.	o. sol.	t1077.plu	t1086.plu	t1041.plu	t1050.plu	no. sol.	no. sol.	t1095.plu	t1104.plu	t1113.plu		
	Rel. E	15.48	25.69			13.05	26.78	8.08	24.10	22.93	34.27	6.57	24.27	28.12	39.12	47.70	73.51			22.43	35.31			14.02	27.11	15.69	26.74			44.10	58.41	53.14		
-g+		t0277.plu	t0286.plu	o. sol.	o. sol.	t0313.plu	t0322.plu	t0295.plu	t0304.plu	t0367.plu	t0376.plu	t0331.plu	t0340.plu	t0385.plu	t0394.plu	t0403.plu	t0412.plu	o. sol.	o. sol.	t1060.plu	t1069.plu	o. sol.	o. sol.	t1078.plu	t1087.plu	t1042.plu	t1051.plu	no. sol.	no. sol.	t1096.plu	t1105.plu	t1114.plu		
		t0277a.plu	t0286a.plu	o. sol.	o. sol.	t0313a.plu	t0322a.plu	t0295a.plu	t0304a.plu	t0367a.plu	t0376a.plu	t0331a.plu	t0340a.plu	t0385a.plu	t0394a.plu	t0403a.plu	t0412a.plu	o. sol.	o. sol.	t1060a.plu	t1069a.plu	o. sol.	o. sol.	t1078a.plu	t1087a.plu	t1042a.plu	t1051a.plu	no. sol.	no. sol.	t1096a.plu	t1105a.plu	t1114a.plu		
	Rel. E	20.71	24.60			21.05	24.69	15.52	21.76	29.33	33.22	15.98	22.30	33.89	38.24	50.58	61.59			26.57	32.09			21.80	27.07	22.09	26.99			50.50	56.61	57.78		
		21.25	24.10			20.84	24.35	15.77	22.51	28.91	32.34	15.15	21.51	33.97	37.49	53.01	62.72			26.07	31.51			21.63	27.20	21.59	27.45			49.71	53.93	55.77		
g-t		t0278.plu	t0287.plu	o. sol.	o. sol.	t0314.plu	t0323.plu	t0296.plu	t0305.plu	t0368.plu	t0377.plu	t0332.plu	t0341.plu	t0386.plu	t0395.plu	t0404.plu	t0413.plu	o. sol.	o. sol.	t1061.plu	t1070.plu	o. sol.	o. sol.	t1079.plu	t1088.plu	t1043.plu	t1052.plu	no. sol.	no. sol.	t1097.plu	t1106.plu	t1115.plu		
	Rel. E	12.59	15.98			10.59	15.98	4.48	13.35	13.81	24.52	10.84	13.93	26.57	29.54	46.44	55.86			17.70	22.84			13.10	23.51	15.94	19.08			43.93	49.12	47.28		
g-g-		t0279.plu	t0288.plu	o. sol.	o. sol.	t0315.plu	t0324.plu	t0297.plu	t0306.plu	t0369.plu	t0378.plu	t0333.plu	t0342.plu	t0387.plu	t0396.plu	t0405.plu	t0414.plu	o. sol.	o. sol.	t1062.plu	t1071.plu	o. sol.	o. sol.	t1080.plu	t1089.plu	t1044.plu	t1053.plu	no. sol.	no. sol.	t1098.plu	t1107.plu	t1116.plu		
	Rel. E	14.02	26.36			14.90	26.36	7.15	23.77	18.37	35.52	1.43	22.97	26.90	39.58	46.53	68.87			19.20	32.93			15.48	29.54	15.02	29.96			44.35	54.85	52.34		

Appendix III. A structure tree of N-TFA-L-Phe-O-3'-pentyl ester (subtree 4)

																																		χ		
																																		t-		
										Φ																Φ										
										g-																g+										
								Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$							Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$			
			t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e		t+	
			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O	
		t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t
ω2,3, ω3,4																																				
tt		t1130.plu	t1139.plu	o. sol.	o. sol.	t1251.plu	t1260.plu	t1233.plu	t1242.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1148.plu	t1157.plu	t1269.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1278.plu	o. sol.	o. sol.
	Rel. E	23.18	30.25			22.22	28.87	24.48	31.00					35.4	42.0	52.0																		25.36		
tg-		t1131.plu	t1140.plu	o. sol.	o. sol.	t1252.plu	t1261.plu	t1234.plu	t1243.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1149.plu	t1158.plu	t1270.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1279.plu	o. sol.	o. sol.
	Rel. E	26.53	40.12			27.45	40.17	28.07	41.25					40.2	52.8	54.4																		28.66		
tg+		t1132.plu	t1141.plu	o. sol.	o. sol.	t1253.plu	t1262.plu	t1235.plu	t1244.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1150.plu	t1159.plu	t1271.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1280.plu	o. sol.	o. sol.
	Rel. E	26.65	34.35			27.11	33.51	29.46	34.98					39.0	46.2	53.2																		28.49		
+g-		t1133.plu	t1142.plu	o. sol.	o. sol.	t1254.plu	t1263.plu	t1236.plu	t1245.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1151.plu	t1160.plu	t1272.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1281.plu	o. sol.	o. sol.
		t1133a.plu	no. sol.	o. sol.	o. sol.	no. sol.	1263a.plu	1236a.plu	1245a.plu	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	1160a.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	o. sol.	o. sol.
	Rel. E	37.66	64.27			37.45	59.45	38.12	61.46					51.3	72.7	64.5																		36.28		
		36.99					60.08	37.24	62.38						72.2																					
g+t		t1134.plu	t1143.plu	o. sol.	o. sol.	t1255.plu	t1264.plu	t1237.plu	t1246.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1152.plu	t1161.plu	t1273.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1282.plu	o. sol.	o. sol.
	Rel. E	27.61	38.83			26.57	38.83	27.74	42.05					39.7	51.5	59.8																		27.28		
+g+		t1135.plu	t1144.plu	o. sol.	o. sol.	t1256.plu	t1265.plu	t1238.plu	t1247.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1153.plu	t1162.plu	t1274.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1283.plu	o. sol.	o. sol.
	Rel. E	30.50	43.01			30.38	42.97	30.88	45.90					41.5	56.1	59.3																		29.41		
-g+		t1136.plu	t1145.plu	o. sol.	o. sol.	t1257.plu	t1266.plu	t1239.plu	t1248.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1154.plu	t1163.plu	t1275.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1284.plu	o. sol.	o. sol.
		t1136a.plu	1145a.plu	o. sol.	o. sol.	1257a.plu	1266a.plu	1239a.plu	1248a.plu	o. sol.	o. sol.	o. sol.	o. sol.	1154a.plu	1163a.plu	1275a.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	1284a.plu	o. sol.	o. sol.
	Rel. E	36.44	41.88			36.90	41.63	38.20	43.64					49.2	54.5	59.4																		36.23		
		36.90	41.63			37.36	41.51	37.95	43.47					49.2	54.6	64.3																		37.24		
g-t		t1137.plu	t1146.plu	o. sol.	o. sol.	t1258.plu	t1267.plu	t1240.plu	t1249.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1155.plu	t1164.plu	t1276.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1285.plu	o. sol.	o. sol.
	Rel. E	28.16	33.10			26.65	32.43	28.16	35.15					36.4	46.3	57.9																		27.53		
g-g-		t1138.plu	t1147.plu	o. sol.	o. sol.	t1259.plu	t1268.plu	t1241.plu	t1250.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1156.plu	t1165.plu	t1277.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1286.plu	o. sol.	o. sol.
	Rel. E	29.62	43.85			30.33	43.30	30.38	44.64					37.6	55.9	58.7																		30.04		

Appendix III. A structure tree of N-TFA-L-Phe-O-3'-pentyl ester (subtree 5)

										Φ							
										g-							
								Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$
			t+		t-		t		e		g+		g-		e		e
			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O
		t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
ω2,3, ω3,4																	
tt		t1323.plu	t1332.plu	o. sol.	o. sol.	t1359.plu	t1368.plu	t1727.inp	t1736.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1392.plu	t1401.plu	t1437.plu	o. sol.
	Rel. E	22.72	29.83			21.67	32.38	23.22	31.13					36.44	43.64	66.78	
tg-		t1324.plu	t1333.plu	o. sol.	o. sol.	t1360.plu	t1369.plu	t1728.inp	t1737.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1393.plu	t1402.plu	t1438.plu	o. sol.
	Rel. E	24.81	35.48			26.44	35.44	24.27	40.12					40.17	50.42	56.82	
tg+		t1325.plu	t1334.plu	o. sol.	o. sol.	t1361.plu	t1370.plu	t1729.inp	t1738.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1394.plu	t1403.plu	t1439.plu	o. sol.
	Rel. E	25.36	29.96			27.36	29.79	25.65	35.06					38.37	44.64	59.25	
+g-		t1326.plu	t1335.plu	o. sol.	o. sol.	t1362.plu	t1371.plu	t1730.inp	t1739.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1395.plu	t1404.plu	t1440.plu	o. sol.
		t1326a.plu	335a.plu	o. sol.	o. sol.	no. sol.	371a.plu	730a.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	404a.plu	440a.plu	o. sol.
	Rel. E	35.27	56.48			35.86	56.44	33.68	57.95					48.37	70.37	71.21	
		36.19	57.24				57.28	33.60							69.91	71.17	
g+t		t1327.plu	t1336.plu	o. sol.	o. sol.	t1363.plu	t1372.plu	t1731.inp	t1740.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1396.plu	t1405.plu	t1441.plu	o. sol.
	Rel. E	25.36	39.50			23.47	39.58	24.89	36.32					39.54	53.72	72.26	
+g+		t1328.plu	t1337.plu	o. sol.	o. sol.	t1364.plu	t1373.plu	t1732.inp	t1741.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1397.plu	t1406.plu	t1442.plu	o. sol.
	Rel. E	28.79	39.37			27.03	39.41	26.57	39.20					40.84	52.43	63.60	
-g+		t1329.plu	t1338.plu	o. sol.	o. sol.	t1365.plu	t1374.plu	t1733.inp	t1742.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1398.plu	t1407.plu	t1443.plu	o. sol.
		t1329a.plu	338a.plu	o. sol.	o. sol.	365a.plu	374a.plu	733a.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	398a.plu	407a.plu	443a.plu	o. sol.
	Rel. E	34.02	38.20			33.43	38.20	33.85	38.62					45.86	50.33	69.33	
		33.60	37.82			33.60	37.82	33.10						46.69	51.21	68.91	
g-t		t1330.plu	t1339.plu	o. sol.	o. sol.	t1366.plu	t1375.plu	t1734.inp	t1743.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1399.plu	t1408.plu	no. sol.	o. sol.
	Rel. E	25.36	33.18			23.14	33.18	25.31	30.21					39.62	47.07		
g-g-		t1331.plu	t1340.plu	o. sol.	o. sol.	t1367.plu	t1376.plu	t1735.inp	t1744.inp	o. sol.	o. sol.	o. sol.	o. sol.	t1400.plu	t1409.plu	t1445.plu	o. sol.
	Rel. E	27.53	38.24			26.94	38.24	26.53	39.58					39.96	51.21	61.04	

										Φ							
										g+							
								Ψ							$C_FC_ONC^*$		C^*C_OO
			t+		t-		t		e		g+		g-		e		e
			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC
		t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
ω2,3, ω3,4																	
tt		o. sol.	o. sol.	t1684.plu	o. sol.	o. sol.	o. sol.	t1675.plu	o. sol.	t1662.plu	t1671.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1705.plu	o. sol.
	Rel. E			35.19				28.33		35.02	41.55					69.83	
tg-		o. sol.	o. sol.	t1685.plu	o. sol.	o. sol.	o. sol.	t1676.plu	o. sol.	t1663.plu	t1672.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1706.plu	o. sol.
	Rel. E			37.70				36.57		35.52	52.63					73.72	
tg+		o. sol.	o. sol.	t1686.plu	o. sol.	o. sol.	o. sol.	t1677.plu	o. sol.	t1664.plu	t1673.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1707.plu	o. sol.
	Rel. E			37.11				34.14		36.23	45.31					72.84	
+g-		o. sol.	o. sol.	t1209.inp	o. sol.	o. sol.	o. sol.	t1678.plu	o. sol.	t1665.plu	t1674.plu	o. sol.	o. sol.	o. sol.	o. sol.	t1708.plu	o. sol.
		o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	no. sol.	o. sol.	no. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	o. sol.
	Rel. E			57.91				45.77		44.27	72.55					87.40	
g+t		o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	t1679.plu	o. sol.	t1666.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1709.plu	o. sol.
	Rel. E							31.09		36.74						75.90	
+g+		o. sol.	o. sol.	t1210.inp	o. sol.	o. sol.	o. sol.	t1680.plu	o. sol.	t1667.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1710.plu	o. sol.
	Rel. E			52.76				36.53		38.45						79.45	
-g+		o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	t1681.plu	o. sol.	t1668.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1711.plu	o. sol.
		o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	681a.plu	o. sol.	668a.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	711a.plu	o. sol.
	Rel. E							44.22		44.39						83.64	
								43.18		45.06						82.09	
g-t		o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	t1682.plu	o. sol.	t1669.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1712.plu	o. sol.
	Rel. E							32.59		37.66						73.47	
g-g-		o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	t1683.plu	o. sol.	t1670.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1713.plu	o. sol.
	Rel. E							39.25		37.40						78.91	

Appendix III. A structure tree of N-TFA-L-Phe-O-3'-pentyl ester (subtree 6)

																																		χ
																																		e
										Φ																Φ								
										g-																g+								
								Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$							Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$	
			t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e	
			HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O	
		t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t
ω2,3, ω3,4																																		
tt		t1341.plu	t1350.plu	o. sol.	o. sol.	t1377.plu	no. sol.	t1386.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1410.plu	t1419.plu	t1428.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1229.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1687.plu	t1696.plu	t1491.plu
	Rel. E	24.14	30.33			24.73		23.85						36.99	42.80	54.14										25.02						58.79	80.96	22.72
tg-		t1342.plu	t1351.plu	o. sol.	o. sol.	t1378.plu	no. sol.	t1387.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1411.plu	t1420.plu	t1429.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1230.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1688.plu	t1697.plu	t1492.plu
	Rel. E	28.12	40.63			30.50		27.78						42.26	53.85	56.74										27.70						62.13	107.45	27.82
tg+		t1343.plu	t1352.plu	o. sol.	o. sol.	t1379.plu	no. sol.	t1388.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1412.plu	t1421.plu	t1430.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1231.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1689.plu	t1698.plu	t1493.plu
	Rel. E	28.58	33.97			29.66		29.08						42.26	46.28	56.15										26.57						61.17	84.73	26.86
g+g-		t1344.plu	t1353.plu	o. sol.	o. sol.	t1380.plu	no. sol.	t1389.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1413.plu	t1422.plu	t1431.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1232.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1690.plu	t1699.plu	t1494.plu
		t1344a.plu	353a.plu	o. sol.	o. sol.	380a.plu	no. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	422a.plu	431a.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	699a.plu	494a.plu
	Rel. E	40.33	59.91			39.41		36.78						54.31	73.55	67.45										38.12						75.90	122.01	39.04
		38.87	61.04			41.13									74.60	71.09																	114.18	36.69
g+t		t1345.plu	t1354.plu	o. sol.	o. sol.	t1381.plu	no. sol.	t1390.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1414.plu	t1423.plu	t1432.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1722.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1691.plu	t1700.plu	t1495.plu
	Rel. E	29.12	40.04			28.20		26.48						42.30	53.93	61.13										27.28						63.93	95.90	26.74
g+g+		t1346.plu	t1355.plu	o. sol.	o. sol.	t1382.plu	no. sol.	t1391.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1415.plu	t1424.plu	t1433.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1723.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1692.plu	t1701.plu	t1496.plu
	Rel. E	32.34	43.22			32.17		30.71						45.52	57.28	61.34										30.25						67.28	97.32	29.50
g-g+		t1347.plu	t1356.plu	o. sol.	o. sol.	t1383.plu	no. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1416.plu	t1425.plu	t1434.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1724.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1693.plu	t1702.plu	t1497.plu
		t1347a.plu	356a.plu	o. sol.	o. sol.	383a.plu	no. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	416a.plu	425a.plu	434a.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	724a.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	693a.plu	702a.plu	497a.plu
	Rel. E	38.16	42.43			38.79								51.67	56.07	63.93										36.11						71.63	91.55	36.11
		37.70	42.59			38.20								51.13	56.19	66.57										36.48						69.54	91.09	35.44
g-t		t1348.plu	t1357.plu	o. sol.	o. sol.	t1384.plu	no. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1417.plu	t1426.plu	t1435.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1725.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1694.plu	t1703.plu	t1498.plu
	Rel. E	28.58	34.02			28.16								41.34	47.57	59.37										27.15						61.34	84.18	26.57
g-g-		t1349.plu	t1358.plu	o. sol.	o. sol.	t1385.plu	no. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1418.plu	t1427.plu	t1436.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1726.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t1695.plu	t1704.plu	t1499.plu
	Rel. E	31.09	44.56			32.89								45.48	58.03	60.54										29.08						66.73	105.98	30.29

							Φ														Φ								
							t-														t+								
					Ψ								$C_FC_ONC^*$		$C^*C_OOC_3$							Ψ						$C_FC_ONC^*$		$C^*C_OOC_3$
t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e
HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O
e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
o. sol.	o. sol.	o. sol.	t1464.plu	t1473.plu	t1500.plu	t1509.plu	t1518.plu	t1527.plu	t1554.plu	t1563.plu	t1608.plu	t1617.plu	t1626.plu	t1635.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			22.64	28.58	24.85	31.55	26.78	32.97	22.22	29.16	36.78	42.80	48.49	64.31																
o. sol.	o. sol.	o. sol.	t1465.plu	t1474.plu	t1501.plu	t1510.plu	t1519.plu	t1528.plu	t1555.plu	t1564.plu	t1609.plu	t1618.plu	t1627.plu	t1636.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			26.57	39.33	27.74	42.59	29.58	44.22	24.56	41.09	42.22	53.81	54.73	78.41																
o. sol.	o. sol.	o. sol.	t1466.plu	t1475.plu	t1502.plu	t1511.plu	t1520.plu	t1529.plu	t1556.plu	t1565.plu	t1610.plu	t1619.plu	t1628.plu	t1637.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			26.19	32.30	28.91	35.02	31.17	36.19	25.69	33.93	41.51	46.40	53.22	67.66																
o. sol.	o. sol.	o. sol.	t1467.plu	t1476.plu	t1503.plu	t1512.plu	t1521.plu	t1530.plu	t1557.plu	t1566.plu	t1611.plu	t1620.plu	t1629.plu	t1638.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
o. sol.	o. sol.	o. sol.	467a.plu	476a.plu	503a.plu	512a.plu	521a.plu	530a.plu	no. sol.	566a.plu	611a.plu	620a.plu	629a.plu	638a.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			37.57	58.79	38.20	62.05	39.46	64.73	35.27	60.63	51.30	73.60	64.39	93.76																
			373.92	58.99	37.61	63.35	41.46	63.55		60.92	53.09	73.89	66.11	94.47																
o. sol.	o. sol.	o. sol.	t1468.plu	t1477.plu	t1504.plu	t1513.plu	t1522.plu	t1531.plu	t1558.plu	t1567.plu	t1612.plu	t1621.plu	t1630.plu	t1639.plu	o. sol.	o. sol.	o. sol.	o. sol.	no.sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no.sol.	o. sol.	o. sol.	
			28.24	39.25	28.62	43.05	31.46	44.64	26.11	40.58	40.67	54.06	52.22	78.99																
o. sol.	o. sol.	o. sol.	t1469.plu	t1478.plu	t1505.plu	t1514.plu	t1523.plu	t1532.plu	t1559.plu	t1568.plu	t1613.plu	t1622.plu	t1631.plu	t1640.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			30.79	42.47	31.84	45.86	34.31	47.40	29.08	43.93	44.27	57.28	56.07	82.22																
o. sol.	o. sol.	o. sol.	t1470.plu	t1479.plu	t1506.plu	t1515.plu	t1524.plu	t1533.plu	t1560.plu	t1569.plu	t1614.plu	t1623.plu	t1632.plu	t1641.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
o. sol.	o. sol.	o. sol.	470a.plu	479a.plu	506a.plu	515a.plu	524a.plu	533a.plu	560a.plu	569a.plu	614a.plu	623a.plu	632a.plu	641a.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			36.53	40.38	39.04	44.14	40.21	45.73	36.28	42.26	50.88	55.35	59.20	73.26																
			35.94	40.46	38.41	44.27	40.79	45.69	36.65	42.30	50.29	55.31	61.46	73.14																
o. sol.	o. sol.	o. sol.	t1471.plu	t1480.plu	t1507.plu	t1516.plu	t1525.plu	t1534.plu	t1561.plu	t1570.plu	t1615.plu	t1624.plu	t1633.plu	t1642.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			27.24	31.80	28.95	36.07	30.75	37.70	27.70	32.97	40.63	46.69	51.00	67.66																
o. sol.	o. sol.	o. sol.	t1472.plu	t1481.plu	t1508.plu	t1517.plu	t1526.plu	t1535.plu	t1562.plu	t1571.plu	t1616.plu	t1625.plu	t1634.plu	t1643.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
			30.00	42.01	31.00	46.74	32.59	48.24	28.87	44.48	44.89	57.03	56.48	80.33																

χ																																
t+																																
								Φ																Φ								
								t-																t+								
C_3						Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$						Ψ						$C_FC_ONC^*$		$C^*C_OOC_3$		
	t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e	
o	HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O	
t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	
t1482.plu	o. sol	o. sol	o. sol	t1446.plut	1455.plu	o. sol	o. sol	t1536.plut	1545.plut	1572.plut	1581.plut	1590.plut	1599.plut	1644.plut	1653.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
25.73				23.72	31.92			39.66	45.69	24.73	35.86	37.53	43.51	56.74	71.38																		
t1483.plu	o. sol	o. sol	o. sol	t1447.plut	1456.plu	o. sol	o. sol	t1537.plut	1546.plut	1573.plut	1582.plut	1591.plut	1600.plut	1645.plut	1654.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
27.53				27.24	37.45			42.68	56.48	27.32	45.15	39.41	49.79	58.58	90.71																		
t1484.plu	o. sol	o. sol	o. sol	t1448.plut	1457.plu	o. sol	o. sol	t1538.plut	1547.plut	1574.plut	1583.plut	1592.plut	1601.plut	1646.plut	1655.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
27.49				28.45	31.55			44.02	49.08	25.40	41.80	39.62	43.85	55.73	75.69																		
t1485.plu	o. sol	o. sol	o. sol	t1449.plut	1458.plu	o. sol	o. sol	t1539.plut	1548.plut	1575.plut	1584.plut	1593.plut	1602.plut	1647.plut	1656.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
485a.plu	o. sol	o. sol	o. sol	no. sol.	no. sol.	o. sol	o. sol	539a.plu	548a.plu	no. sol.	584a.plu	593a.plu	602a.plu	647a.plu	no. sol.	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
36.40				37.32	59.16			52.68	76.73	38.24	59.91	48.62	71.67	65.02	108.28																		
37.61								54.52	75.98		61.80	49.96	71.80	66.86																		
t1486.plu	o. sol	o. sol	o. sol	t1450.plut	1459.plu	o. sol	o. sol	t1540.plut	1549.plut	1576.plut	1585.plut	1594.plut	1603.plut	1648.plut	1657.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
26.86				25.90	43.10			44.60	56.99	28.16	40.08	39.25	56.15	56.57	88.58																		
t1487.plu	o. sol	o. sol	o. sol	t1451.plut	1460.plu	o. sol	o. sol	t1541.plut	1550.plut	1577.plut	1586.plut	1595.plut	1604.plut	1649.plut	1658.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
29.54				28.53	41.46			47.36	60.00	28.83	43.35	42.63	54.14	57.03	92.13																		
t1488.plu	o. sol	o. sol	o. sol	t1452.plut	1461.plu	o. sol	o. sol	t1542.plut	1551.plut	1578.plut	1587.plut	1596.plut	1605.plut	1650.plut	1659.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
488a.plu	o. sol	o. sol	o. sol	452a.plu	461a.plu	o. sol	o. sol	542a.plu	551a.plu	578a.plu	587a.plu	596a.plu	605a.plu	650a.plu	659a.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
34.94				34.31	38.79			53.14	58.41	36.28	42.09	47.49	52.09	60.21	79.24																		
34.18				34.06	39.75			53.72	58.32	35.73	40.88	46.78	51.55	62.17	81.34																		
t1489.plu	o. sol	o. sol	o. sol	t1453.plut	1462.plu	o. sol	o. sol	t1543.plut	1552.plut	1579.plut	1588.plut	1597.plut	1606.plut	1651.plut	1660.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
27.20				24.56	35.90			43.89	50.25	30.33	32.97	39.50	47.70	54.77	73.60																		
t1490.plu	o. sol	o. sol	o. sol	t1454.plut	1463.plu	o. sol	o. sol	t1544.plut	1553.plut	1580.plut	1589.plut	1598.plut	1607.plut	1652.plut	1661.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
29.16				27.53	39.83			45.77	60.58	30.96	43.47	41.55	52.38	57.86	89.04																		

					Φ																Φ							
					t-																t+							
			Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$							Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$
t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e
HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O
e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
o. sol	t1211.plu	t1220.plu	t1175.plu	t1184.plu	t1287.plu	t1296.plu	t1166.plu	no. sol.	t1193.plu	t1200.plu	t1305.plu	t1314.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	22.7	29.1	28.5	34.7	28.6	35.0	26.2		35.56	41.97	53.35	63.60																
o. sol	t1212.plu	t1221.plu	t1176.plu	t1185.plu	t1288.plu	t1297.plu	t1167.plu	no. sol.	t1194.plu	t1201.plu	t1306.plu	t1315.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	50.5	40.7	32.9	45.9	34.2	46.2	29.6		40.29	53.68	56.19	82.42																
o. sol	t1213.plu	t1222.plu	t1177.plu	t1186.plu	t1289.plu	t1298.plu	t1168.plu	no. sol.	t1195.plu	t1202.plu	t1307.plu	t1316.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	26.8	33.6	33.1	38.2	33.9	38.8	30.0		40.25	46.53	52.89	67.86																
o. sol	t1214.plu	t1223.plu	t1178.plu	t1187.plu	t1290.plu	t1299.plu	t1169.plu	no. sol.	t1196.plu	t1203.plu	t1308.plu	t1317.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
o. sol.	no. sol.	1223a.plu	1178a.plu	1187a.plu	no. sol.	no. sol.	1169a.plu	no. sol.	no.sol.	1203a.plu	1308a.plu	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	39.8	60.0	43.0	65.7	42.8	65.7	41.4		49.50	74.06	65.44	95.10																
		60.8	41.4	65.2			41.7			65.48	67.99																	
o. sol	t1215.plu	t1224.plu	t1179.plu	t1188.plu	t1291.plu	t1300.plu	t1170.plu	no. sol.	no. sol.	t1204.plu	t1309.plu	t1318.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	28.5	39.9	31.2	45.9	31.2	46.4	30.9			53.22	54.73	81.76																
o. sol	t1216.plu	t1225.plu	t1180.plu	t1189.plu	t1292.plu	t1301.plu	t1171.plu	no. sol.	no. sol.	t1205.plu	t1310.plu	t1319.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	31.3	44.1	34.3	48.7	35.3	49.2	34.3			57.49	56.32	84.22																
o. sol	t1217.plu	t1226.plu	t1181.plu	t1190.plu	t1293.plu	t1302.plu	t1172.plu	no. sol.	t1197.plu	t1206.plu	t1311.plu	t1320.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
o. sol	1217a.plu	1226a.plu	1181a.plu	1190a.plu	1293a.plu	1302a.plu	1172a.plu	no. sol.	1197a.plu	1206a.plu	1311a.plu	1320a.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	36.0	41.8	42.1	46.9	41.3	46.9	40.2		50.58	55.31	58.07	73.55																
	36.7	41.8	41.5	46.9	41.8	47.0	40.6		49.92	55.35	61.42	73.55																
o. sol	t1218.plu	t1227.plu	t1182.plu	t1191.plu	t1294.plu	t1303.plu	t1173.plu	no. sol.	t1198.plu	t1207.plu	t1312.plu	t1321.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	27.0	32.6	32.0	49.2	31.3	38.8	31.4		40.12	57.11	52.38	67.45																
o. sol	t1219.plu	t1228.plu	t1183.plu	t1192.plu	t1295.plu	t1304.plu	t1174.plu	no. sol.	t1199.plu	t1208.plu	t1313.plu	t1322.plu	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.
	29.4	43.3	35.2	38.7	34.7	49.3	33.6		43.51	45.98	57.61	82.34																

	χ																														
	g+																														
									Φ															Φ							
									t-															t+							
C*C$_O$OC$_3$								Ψ							$C_FC_ONC^*$		C*C$_O$OC$_3$						Ψ					$C_FC_ONC^*$		C*C$_O$OC$_3$	
e		t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e	
HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$		HC$_3$OC$_O$	
e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
t1117.plu	t0685.plu	t0694.plu	t0343.plu	t0352.plu	t0721.plu	t0730.plu	t0703.plu	t0712.plu	o. sol	t0766.plu	t0739.plu	t0748.plu	t0775.plu	t0784.plu	t0793.plu	t0802.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
70.37	6.53	12.72	9.71	18.87	10.54	12.84	4.48	11.46		11.46	7.66	19.41	26.79	33.10	34.98	52.47																
t1118.plu	t0686.plu	t0695.plu	t0344.plu	t0353.plu	t0722.plu	t0731.plu	t0704.plu	t0713.plu	o. sol	t767.plu	t0740.plu	t0749.plu	t0776.plu	t0785.plu	t0794.plu	t0803.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
97.53	9.67	23.47	13.05	25.44	14.56	23.64	6.19	24.14		23.93	17.78	27.61	30.12	44.27	41.13	67.74																
t1119.plu	t0687.plu	t0696.plu	t0345.plu	t0354.plu	t0723.plu	t0732.plu	t0705.plu	t0714.plu	o. sol	t0768.plu	t0741.plu	t0750.plu	t0777.plu	t0786.plu	t0795.plu	t0804.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
73.72	9.29	15.94	13.85	20.50	14.98	16.11	9.92	14.48		14.64	8.91	23.81	29.79	36.57	39.62	56.23																
t1120.plu	t0688.plu	t0697.plu	t0346.plu	t0355.plu	t0724.plu	t0733.plu	t0706.plu	t0715.plu	o. sol	t0769.plu	t0742.plu	t0751.plu	t0778.plu	t0787.plu	t0796.plu	t0805.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
no. sol.	0688a.plu	0697a.plu	0346a.plu	0355a.plu	0724a.plu	0733a.plu	0706a.plu	0715a.plu	o. sol	0769a.plu	0742a.plu	0751a.plu	0778a.plu	0787a.plu	0796a.plu	0805a.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
111.88	21.59	43.93	29.37	45.27	21.71	45.40	17.45	44.56		44.64	25.48	45.19	42.09	66.61	50.88	86.57																
	22.89	45.44	31.63	44.77	21.25	43.43	16.48	44.69		43.39	25.19	45.31	38.87	57.57	52.17	83.35																
t1121.plu	t0689.plu	t0698.plu	t0347.plu	t0356.plu	t0725.plu	t0734.plu	t0707.plu	t0716.plu	o. sol	t0770.plu	t0743.plu	t0752.plu	t0779.plu	t0788.plu	t0797.plu	t0806.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
85.06	12.68	25.23	16.40	29.00	9.04	25.23	12.26	25.69		25.06	9.29	24.35	33.10	38.66	37.95	70.84																
t1122.plu	t0690.plu	t0699.plu	t0348.plu	t0357.plu	t0726.plu	t0735.plu	t0708.plu	t0717.plu	o. sol	t0771.plu	t0744.plu	t0753.plu	t0780.plu	t0789.plu	t0798.plu	t0807.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
85.44	14.52	26.69	20.71	29.75	11.84	26.57	12.05	27.61		27.74	9.92	27.49	35.10	47.20	42.47	86.11																
t1123.plu	t0691.plu	t0700.plu	t0349.plu	t0358.plu	t0727.plu	t0736.plu	t0709.plu	t0718.plu	o. sol	t0772.plu	t0745.plu	t0754.plu	t0781.plu	t0790.plu	t0799.plu	t0808.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
1123a.plu	t0691a.plu	t0700a.plu	t0349a.plu	t0358a.plu	t0727a.plu	t0736a.plu	t0709a.plu	t0718a.plu	o. sol	no. sol.	t0745a.plu	t0754a.plu	t0781a.plu	t0790a.plu	t0799a.plu	t0808a.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
80.58	19.96	24.85	26.57	26.40	19.71	23.81	19.58	24.69		25.56	19.12	25.73	40.54	44.31	47.91	62.09																
78.91	20.21	23.77	22.01	28.37	19.87	24.81	19.50	25.44			19.29	25.86	40.96	45.27	46.15	62.89																
t1124.plu	t0692.plu	t0701.plu	t0350.plu	t0359.plu	t0728.plu	t0737.plu	t0710.plu	t0719.plu	o. sol	t0773.plu	t0746.plu	t0755.plu	t0782.plu	t0791.plu	t0800.plu	t0809.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
73.43	11.63	16.40	16.11	22.76	10.25	16.61	14.85	16.69		16.61	13.39	17.15	32.17	36.90	36.69	56.23																
t1125.plu	t0693.plu	t0702.plu	t0351.plu	t0360.plu	t0729.plu	t0738.plu	t0711.plu	t0720.plu	o. sol	t0774.plu	t0747.plu	t0756.plu	t0783.plu	t0792.plu	t0801.plu	t0810.plu	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol	o. sol
95.06	14.06	25.69	19.66	28.16	13.51	25.52	9.16	27.78		28.07	22.68	28.28	34.69	46.36	42.89	68.91																

		χ																															
		g-																															
										Φ																Φ							
										t-																t+							
	$C^*C_OOC_3$							Ψ							$C_FC_ONC^*$		$C^*C_OOC_3$							Ψ							$C_FC_ONC^*$		C^*C_OO
	e		t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e
	HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC
t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e
t1018.plu	t1027.plu	t0541.plu	t0550.plu	t0613.plu	t0622.plu	t0577.plu	t0586.plu	t0559.plu	t0568.plu	t0631.plu	t0640.plu	t0595.plu	t0604.plu	t0649.plu	t0658.plu	t0667.plu	t0676.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
39.50	62.84	9.50	15.15	16.23	22.68	9.00	15.40	11.13	17.74	9.46	15.61	10.33	16.82	18.95	25.10	32.47	49.33																
t1019.plu	t1028.plu	t0542.plu	t0551.plu	t0614.plu	t0623.plu	t0578.plu	t0587.plu	t0560.plu	t0569.plu	t0632.plu	t0641.plu	t0596.plu	t0605.plu	t0650.plu	t0659.plu	t0668.plu	t0677.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
43.64	86.90	12.97	25.94	20.79	34.31	13.51	26.02	14.23	29.20	12.59	26.78	13.85	28.83	24.64	36.07	37.66	65.14																
t1020.plu	t1029.plu	t0543.plu	t0552.plu	t0615.plu	t0624.plu	t0579.plu	t0588.plu	t0561.plu	t0570.plu	t0633.plu	t0642.plu	t0597.plu	t0606.plu	t0651.plu	t0660.plu	t0669.plu	t0678.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
42.63	63.51	12.80	18.83	20.29	26.65	13.10	18.79	14.69	21.38	13.93	18.74	13.93	21.17	24.02	28.83	35.90	53.76																
t1021.plu	t1030.plu	t0544.plu	t0553.plu	t0616.plu	t0625.plu	t0580.plu	t0589.plu	t0562.plu	t0571.plu	t0634.plu	t0643.plu	t0598.plu	t0607.plu	t0652.plu	t0661.plu	t0670.plu	t0679.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
1021a.plu	t1030.plu	0544a.plu	0553a.plu	0616a.plu	0625a.plu	0580a.plu	0589a.plu	0562a.plu	0571a.plu	0634a.plu	0643a.plu	0598a.plu	0607a.plu	0652a.plu	0661a.plu	0670a.plu	0679a.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
57.82	102.72	23.30	45.44	31.21	53.56	24.43	45.23	23.35	49.37	22.47	47.20	24.60	49.12	32.55	57.15	49.25	78.70																
55.06	94.98	25.23	46.02	28.79	53.93	25.23	45.73	24.56	48.74	24.06	46.32	25.40	48.66	35.19	56.78	52.01	65.77																
t1022.plu	t1031.plu	t0545.plu	t0554.plu	t0617.plu	t0626.plu	t0581.plu	t0590.plu	t0563.plu	t0572.plu	t0635.plu	t0644.plu	t0599.plu	t0608.plu	t0653.plu	t0662.plu	t0671.plu	t0680.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
45.44	76.57	14.73	26.36	19.29	34.18	14.27	25.77	15.15	29.46	14.02	27.24	15.36	29.04	24.02	37.24	41.05	62.80																
t1023.plu	t1032.plu	t0546.plu	t0555.plu	t0618.plu	t0627.plu	t0582.plu	t0591.plu	t0564.plu	t0573.plu	t0636.plu	t0645.plu	t0600.plu	t0609.plu	t0654.plu	t0663.plu	t0672.plu	t0681.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
48.79	78.32	16.78	29.46	22.80	37.61	17.32	28.95	17.66	32.34	17.32	29.96	18.24	32.43	26.90	40.12	42.01	65.77																
t1024.plu	t1033.plu	t0547.plu	t0556.plu	t0619.plu	t0628.plu	t0583.plu	t0592.plu	t0565.plu	t0574.plu	t0637.plu	t0646.plu	t0601.plu	t0610.plu	t0655.plu	t0664.plu	t0673.plu	t0682.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
1024a.plu	1033a.plu	0547a.plu	0556a.plu	no.sol.	0628a.plu	0583a.plu	0592a.plu	0565a.plu	0574a.plu	0637a.plu	0646a.plu	0601a.plu	0610a.plu	0655a.plu	0664a.plu	0673a.plu	0682a.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
53.43	73.72	17.07	27.28	29.33	35.31	22.13	26.99	24.23	30.08	23.01	28.12	24.31	30.17	33.01	38.37	43.64	58.53																
50.84	74.43	22.59	27.11		35.48	22.64	26.90	24.73	29.92	23.39	28.16	24.69	30.04	33.35	38.24	46.02	58.37																
t1025.plu	t1034.plu	t0548.plu	t0557.plu	t0620.plu	t0629.plu	t0584.plu	t0593.plu	t0566.plu	t0575.plu	t0638.plu	t0647.plu	t0602.plu	t0611.plu	t0656.plu	t0665.plu	t0674.plu	t0683.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
42.84	66.61	7.20	18.58	16.74	26.36	13.64	18.41	15.56	21.71	13.60	20.33	15.44	21.00	23.26	30.00	38.70	53.05																
t1026.plu	t1035.plu	t0549.plu	t0558.plu	t0621.plu	t0630.plu	t0585.plu	t0594.plu	t0567.plu	t0576.plu	t0639.plu	t0648.plu	t0603.plu	t0612.plu	t0657.plu	t0666.plu	t0675.plu	t0684.plu	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol	no. sol
48.16	86.11	8.79	28.91	20.92	37.24	16.78	28.70	17.49	32.47	15.40	30.54	17.82	32.13	27.03	40.38	41.67	65.81																

		χ																																			
		t																																		
											Φ														Φ											
											t-														t+											
	$C^*C_OOC_3$								Ψ								$C_FC_ONC^*$		$C^*C_OOC_3$						Ψ						$C_FC_ONC^*$		C^*C_OO	
	e		t+		t-		t		e		g+		g-		e		e		t+		t-		t		e		g+		g-		e		e	
	HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC_O		HC_3OC	
t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	t	e	
t0910.inp	t0919.inp	t0415.inp	t0424.inp	t0487.inp	t0496.inp	t0451.inp	t0460.inp	t0433.inp	t0442.inp	t0757.inp	o. sol.	t0469.inp	t0478.inp	t0505.inp	t0514.inp	t0523.inp	t0532.inp	t1126.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0838.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
41.42	61.21	3.77	10.21	11.55	18.49	5.56	16.53	15.44	21.80	11.72		9.92	19.54	14.77	20.88	33.76	44.27	21.42										22.59								
t0911.inp	t0920.inp	t0416.inp	t0425.inp	t0488.inp	t0497.inp	t0452.inp	t0461.inp	t0434.inp	t0443.inp	t0758.inp	o. sol.	t0470.inp	t0479,inp	t0506.inp	t0515.inp	t0524.inp	t0533.inp	t1127.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0839.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
47.03	88.99	7.03	21.09	15.27	29.83	7.49	21.76	19.79	32.89	14.90		12.22	28.33	18.16	33.56	38.45	66.82	24.56										23.89								
t0912.inp	t0921.inp	t0417.inp	t0426.inp	t0489.inp	t0498.inp	t0453.inp	t0462.inp	t0435.inp	t0444.inp	t0759.inp	o. sol.	t0471.inp	t0480.inp	t0507.inp	t0516.inp	t0525.inp	t0534.inp	t1128.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0840.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
46.11	66.36	6.74	14.18	16.82	22.84	10.13	15.94	20.42	20.96	16.11		12.18	23.81	18.24	25.77	35.06	48.83	24.52										24.27								
t0913.inp	t0922.inp	t0418.inp	t0427.inp	t0490.inp	t0499.inp	t0454.inp	t0463.inp	t0436.inp	t0445.inp	t0760.inp	o. sol.	t0472.inp	t0481.inp	t0508.inp	t0517.inp	t0526.inp	t0535.inp	t1129.inp	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0841.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
0913a.inp	no. sol.	0418a.inp	0427a.inp	0490a.inp	0499a.inp	0454a.inp	0463a.inp	0436a.inp	0445a.inp	0760a.inp	o. sol.	no. sol.	0481a.inp	0508a.inp	0517a.inp	0526a.inp	no. sol	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
60.21	105.10	17.45	42.26	29.00	54.14	21.63	43.39	30.04	52.89	25.15		23.56	45.86	30.75	53.68	47.07	81.17	35.82										34.98								
62.38		17.91	42.26	29.79	54.06	20.96	42.13	28.74	51.80	27.07			46.61	29.83	54.06	48.87																				
t0914.inp	t0923.inp	t0419.inp	t0428.inp	t0491.inp	t0500.inp	t0455.inp	t0464.inp	t0437.inp	t0446.inp	t0761.inp	o. sol.	t0473.inp	t0482.inp	t0509.inp	t0518.inp	t0527.inp	t0536.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0842.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
48.99	79.50	6.95	43.22	16.57	33.97	6.19	25.15	18.83	32.76	17.61		14.73	24.73	18.95	33.22	35.48	65.35											27.74								
t0915.inp	t0924.inp	t0420.inp	t0429.inp	t0492.inp	t0501.inp	t0456.inp	t0465.inp	t0438.inp	t0447.inp	t0762.inp	o. sol.	t0474.inp	t0483.inp	t0510.inp	t0519.inp	t0528.inp	t0537.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0843.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
53.30	80.00	9.79	25.31	18.74	34.35	8.87	26.11	22.55	35.65	19.71		16.19	28.24	22.22	36.78	38.24	67.03											28.74								
t0916.inp	t0925.inp	t0421.inp	t0430.inp	t0493.inp	t0502.inp	t0457.inp	t0466.inp	t0439.inp	t0448.inp	t0763.inp	o. sol.	t0475.inp	t0484.inp	t0511.inp	t0520.inp	t0529.inp	t0538.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0844.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
0916a.inp	0925a.inp	0421a.inp	0430a.inp	0493a.inp	0502a.inp	0457a.inp	0466a.inp	0439a.inp	0448a.inp	0763a.inp	o. sol.	0475a.inp	0484a.inp	0511a.inp	0520a.inp	0529a.inp	0538a.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	0844a.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
56.57	77.82	17.07	23.01	23.72	32.59	17.07	23.26	29.37	34.18	25.36		23.14	28.37	29.25	33.72	41.00	56.69											35.98								
57.32	74.48	15.94	21.92	26.28	28.70	17.07	23.01	28.91	34.27	25.69		22.68	28.20	28.12	34.85	43.30	56.19											36.44								
t0917.inp	t0926.inp	t0422.inp	t0431.inp	t0494.inp	t0503.inp	t0458.inp	t0467.inp	t0440.inp	t0449.inp	t0764.inp	o. sol.	t0476.inp	t0485.inp	t0512.inp	t0521.inp	t0530.inp	t0539.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0845.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
46.90	69.50	8.62	14.10	15.82	22.89	7.20	19.71	18.87	26.07	16.69		15.56	19.29	20.46	24.98	34.10	50.04											29.33								
t0918.inp	t0927.inp	t0423.inp	t0432.inp	t0495.inp	t0504.inp	t0459.inp	t0468.inp	t0441.inp	t0450.inp	t0765.inp	o. sol.	t0477.inp	t0486.inp	t0513.inp	t0522.inp	t0531.inp	t0540.inp	no. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	o. sol.	t0846.inp	o. sol.	o. sol.	o. sol.	o. sol.	no. sol.		
52.59	89.91	10.84	23.22	19.46	37.66	8.79	23.77	22.34	36.57	17.99		15.69	30.00	24.60	35.90	39.62	65.98											28.49								

My academic teachers were the following professors and lecturers:

B. Koppenhoefer, E. Bayer, K-P. Zeller, W. Voelter, G. Häfelinger, K. E. Geckeler, T-H. Tang, I. G. Csizmadia, F-M. Miao, B-L. Qin, X-T. Zhang, J-H. Zhao, Y-L. Bo, Y. Li, S-Q. Su, D-Y. Yan, S-J. Sun, S-L. Zhuang, J-K. Hao

Curriculum Vitae

Mrs. Wei Zhou

21 March, 1964	Born in Tianjin, VR. China
Sept. 1971 - July 1976	Chengdudao elementary school in Tianjin
Sept. 1976 - July 1982	ShiYan high school in Tianjin
Sept. 1982 - July 1986	Studies at Department of Chemistry in Tianjin Normal University
July 1986	Bachelor of Science
Sept. 1986 - June 1989	Experimental part for Master of Science, under the guidance of Prof. Ting-Hua Tang, "A theoretical study of Markovnikov and anti-Markovnikov protonation of olefines by He-$H^{(+)}$" at Department of Chemistry in Tianjin Normal University
June 1989	Master of Science
June 1989 - June 1991	Lecturer at Department of Chemistry in Tianjin Normal University
July 1991 - Dec. 1995	Assistant professor at Department of Chemistry in Tianjin Normal University
Jan. 1996 - May 1997	Scientific work under the guidance of Prof. Dr. K. E. Geckeler, Institut fuer Organische Chemie der Universitaet Tuebingen (DFG Project)
June 1997 – Oct. 2000	Experimental part of thesis: "Factors Governing Chiral Recognition Phenomena – A Multiple Appoach" at Institut fuer Organische Chemie der Universitaet Tuebingen under the guidance of Prof. Dr. Bernhard Koppenhoefer
May 1990	Married to Guang-Wen Meng

This thesis „**Factors Governing Chiral Recognition Phenomena – A Multiple Approach**“ was published in 2001 by Wei Zhou, Fichtenweg 9/203-204, D-72076 Tuebingen