

Mechanism and Origin of Enantioselectivity for Diels-Alder Reaction Catalyzed by Chiral Phosphoric Acids in Synthesising 1-trifluoroacetamido cyclohex-1-ene

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Table of contents

1. Investigation of stepwise diradical mechanism	3
2. Reaction mechanisms for pathways II, III and IV.....	5
3. Reaction pathways for the reaction involving other substrate and the substituent effect.....	7
4. QTAIM analyses of transition states	9
5. The distortion/interaction analyses	17
6. The truncation model calculations of TSI-2 and TSII-2	18
7. The energy decomposition analysis (EDA) based on SAPT theory	20
8. Calculated Gibbs free energy correction (GFEC), energy (E) and Gibbs free energy (G) of all optimized structures, and imaginary frequencies (ν_i s) of all transition states (TSs).	22
9. Cartesian coordinates	24

1. Investigation of stepwise diradical mechanism

In terms of Ma and coworkers' work, the D–A reaction may take place via a stepwise diradical mechanism. Accordingly, the stepwise diradical mechanism was proposed, as displayed in Fig. S1. Firstly, CPA interacts with **R1** and **R2** to form the complex **COM-1**. After going through the transition state **TS-1**, a C–C bond forms in the diradical intermediate **INT-2**. Then the single electron transfers occur and lead to the transition state **TS-2**. After the intramolecular radical coupling, a new C–C bond forms and a six-membered ring structure is yielded, ultimately generating the product **P**. To confirm the existence the diradical intermediate, the structure of diradical intermediate **INT-2** formed in Fig. S1 was constructed for geometry optimization at the M06-2X/6-31G(d,p) level of theory., and the spin density calculation for **INT-2** was also carried out. As shown in Fig. S2, no spin density distribution for unpaired electrons was found for **INT-2**. Therefore, the stepwise diradical mechanism can be ruled out.

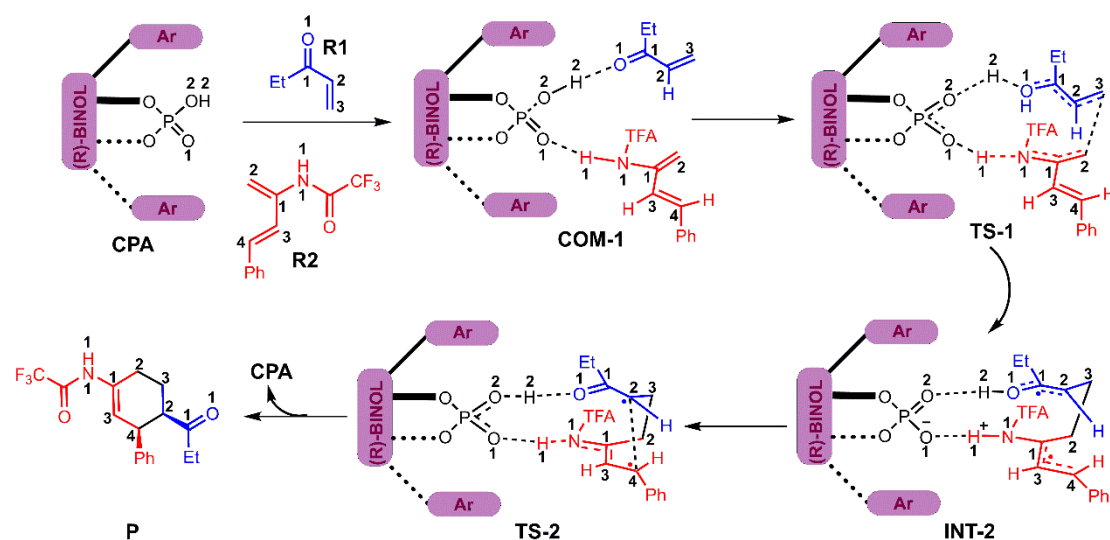


Fig. S1 Proposed stepwise diradical mechanism for the synthesis of **P** via D–A reaction between **R1** and **R2** catalyzed by CPA.

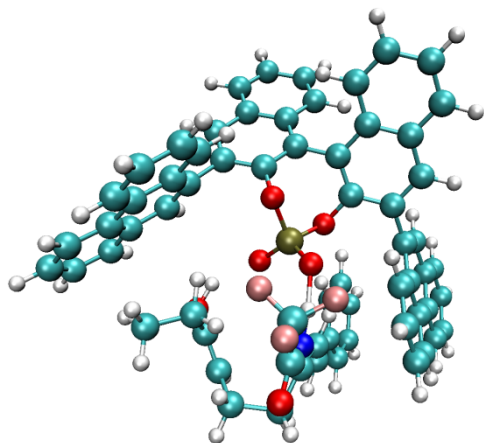


Fig. S2 Spin density distribution for INT-2.

2. Reaction mechanisms for pathways II, III and IV.

For pathway **II** shown in Fig. 4, **CPA** interacts with **R1** and **R2** to form the ternary complex **COMII-1** which needs to absorb an energy of $3.8 \text{ kcal}\cdot\text{mol}^{-1}$. Within this complex, an $\text{O2-H2}\cdots\text{O1}$ hydrogen bond forms between **R1** and **CPA** with the $\text{H2}\cdots\text{O1}$ distance of $1.43 \text{ \AA}$ (Fig. 7). In addition, the N1 atom of **R2** interacts with the O atom of P=O group in **CPA** as a $\text{N1-H1}\cdots\text{O1}$ hydrogen bond with the $\text{H1}\cdots\text{O1}$ distance of $1.83 \text{ \AA}$. The ternary complex **COMII-1** absorbs an energy of $16.7 \text{ kcal}\cdot\text{mol}^{-1}$ to form the transition state **TSII-1**, and then leading to the formation of the imine-enol intermediate **INTII-2**. In **TSII-1**, the H2 atom of **CPA** transfers to O1 atom of **R1**, resulting in the formation of an O1-H2 bond with a length of $1.05 \text{ \AA}$. The $\text{O2-H2}\cdots\text{O1}$ hydrogen bond transforms into the $\text{O1-H2}\cdots\text{O2}$ hydrogen bond with the $\text{H2}\cdots\text{O2}$ distance of $1.42 \text{ \AA}$. Concurrently, the $\text{N1-H1}\cdots\text{O1}$ hydrogen bond is present with the $\text{H1}\cdots\text{O1}$ distance of $1.71 \text{ \AA}$. The distance between C2 atom of **R2** and C3 atom of **R1** is $2.13 \text{ \AA}$. In **INTII-2**, the C2 atom of **R2** forms a bond with the C3 atom of **R1**, exhibiting a bond length of $1.56 \text{ \AA}$. The $\text{H2}\cdots\text{O2}$ distance of the $\text{O1-H2}\cdots\text{O2}$ hydrogen bond increases to $1.87 \text{ \AA}$, while the $\text{H1}\cdots\text{O1}$ distance in $\text{N1-H1}\cdots\text{O1}$ hydrogen bond becomes $1.65 \text{ \AA}$. The energy barrier for the reaction from **COMII-1** to **INTII-2** is reduced to $16.7 \text{ kcal}\cdot\text{mol}^{-1}$. Then **INTII-2** surmounts an energy barrier of $14.8 \text{ kcal}\cdot\text{mol}^{-1}$ and goes through the transition state **TSII-2** to achieve the intramolecular Michael addition cyclization reaction. In **TSII-2**, the $\text{H2}\cdots\text{O2}$ distance of $\text{O1-H2}\cdots\text{O2}$ hydrogen bond is $1.96 \text{ \AA}$, and the $\text{H1}\cdots\text{O1}$ distance of $\text{N1-H1}\cdots\text{O1}$ hydrogen bond is $2.00 \text{ \AA}$. Additionally, the distance between the C2 atom of **R1** and C4 atom of **R2** is $3.25 \text{ \AA}$, indicating that a new C-C bond is on the verge of formation, ultimately leading to the production of the (1R, 6S) byproduct **P_{II}**. Simultaneously, **CPA** dissociates from the reaction system to participate in the subsequent catalytic cycle.

With respect to pathway **III** (or **IV**), the Gibbs free energy profile is shown in Fig. 5 (or Fig. 6). Firstly, the ternary complex **COMIII-1** (or **COMIV-1**) forms among **CPA**, **R1** and **R2**, which needs to absorb an energy of $3.9 \text{ kcal}\cdot\text{mol}^{-1}$ (or $4.0 \text{ kcal}\cdot\text{mol}^{-1}$). In **COMIII-1** (or **COMIV-1**), the $\text{H2}\cdots\text{O1}$ distance of $\text{O2-H2}\cdots\text{O1}$ hydrogen bond between **R1** and **CPA** is $1.44 \text{ \AA}$ (or $1.44 \text{ \AA}$). Meanwhile, the N1-H1 bond of **R2** interacts with the O atom of P=O group of **CPA** to form a $\text{N1-H1}\cdots\text{O1}$ hydrogen bond with $\text{H1}\cdots\text{O1}$ distance of $1.81 \text{ \AA}$ in **COMIII-1** (or $1.82 \text{ \AA}$ in **COMIV-1**). After absorbing an energy of $18.7 \text{ kcal}\cdot\text{mol}^{-1}$ (or $18.7 \text{ kcal}\cdot\text{mol}^{-1}$), **COMIII-1** (or **COMIV-1**) is

converted into the transition state **TSIII-1** (or **TSIV-1**) which then form the imine-enol intermediate **INTIII-2** (or **INTIV-2**). During the process from **COMIII-1** (or **COMIV-1**) to **TSIII-1** (or **TSIV-1**), the H2 atom of **CPA** transfers to O1 atom of **R1** which results in the formation of an O1-H2 bond with bond length of 1.05 Å (or 1.04 Å). Accordingly, the O2-H2...O1 hydrogen bond transforms into a new O1-H2...O2 hydrogen bond. While the H1...O1 distance of N1-H1...O1 hydrogen bond becomes 1.79 Å (or 1.76 Å). The distance between C2 atom of **R2** and C3 atom of **R1** becomes 2.12 Å (or 2.16 Å) in **TSIII-1** (or **TSIV-1**), indicative of the bonding process between C2 and C3 atoms. From **TSIII-1** (or **TSIV-1**) to **INTIII-2** (or **INTIV-2**), an energy of 11.3 kcal·mol⁻¹ (or 14.7 kcal·mol⁻¹) is released. In **INTIII-2** (or **INTIV-2**), the C2 atom of **R2** forms a bond with the C3 atom of **R1**, resulting in a C-C bond length of 1.58 Å (or 1.57 Å). Simultaneously, the H2...O2 distance of O1-H2...O2 hydrogen bond increases to 1.80 Å (or 1.78 Å), and the H1...O1 distance of N1-H1...O1 hydrogen bond becomes 1.43 Å (or 1.49 Å). After going through the transition states **TSIII-2** (or **TSIV-2**) and overcoming an energy barrier of 18.6 kcal·mol⁻¹ (or 4.7 kcal·mol⁻¹), the intramolecular addition and cyclization reactions finish. In **TSIII-2** (or **TSIV-2**), the H2...O2 distance of O1-H2...O2 hydrogen bond is found to be 1.72 Å (or 1.70 Å), and the H1...O1 distance of N1-H1...O1 hydrogen bond is 1.98 Å (is 1.74 Å). The distance between the C2 atom of **R1** and C4 atom of **R2** is approximately 2.68 Å (or 2.47 Å), indicating that a new C-C bond is about to form. Finally, after the dissociation of **CPA** from the reaction system, the (1R, 6R) or (1S, 6S) byproduct is generated.

3. Reaction pathways for the reaction involving other substrate and the substituent effect

To assess the substituent effect on the reaction, the reactions in Scheme S1 was also theoretically investigated. The reaction pathways for the reaction shown in Scheme S1 are displayed in Figs. S3 and S4. To evaluate the theoretical ee values for D–A reaction between **R1** and **R2ad** in synthesising the product catalyzed by **CPA**, the activation Gibbs free energy (i.e., ΔG_{act}) for the rate-determining step in each pathway was selected. For pathways **adI** and **adII**, the activation Gibbs free energies for their rate-determining steps are 25.9 and 30.9 kcal·mol⁻¹, respectively (Figs. S3 and S4). The ee value can be calculated in terms of the activation Gibbs free energies for the rate-determining steps of pathways **adI** and **adII**. Their relative rate ratio (**rrel**) can be calculated as follows.

$$\mathbf{rrel(adI): rrel(adI)} = \exp\left(-\frac{\Delta G_{\text{act}}(\text{adI})}{RT}\right) : \exp\left(-\frac{\Delta G_{\text{act}}(\text{adII})}{RT}\right) = 5.37 \times 10^3 : 1$$

Here $R = 1.986 \times 10^{-3}$ kcal (mol K)⁻¹ and $T = 293.15$ K.

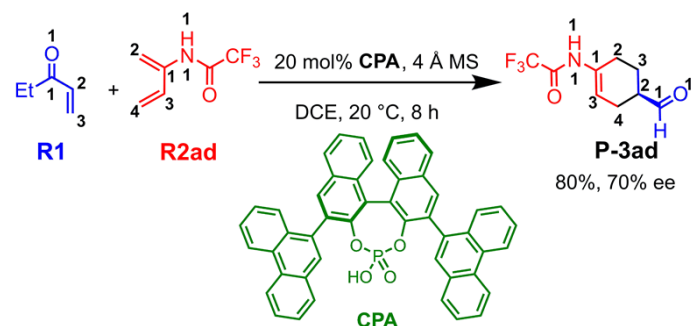
Correspondingly, the ee value is calculated by the following equations. The enantiomeric ratio (**er**) is calculated as:

$$\mathbf{er = \frac{rrel(adI)}{rrel(adII)} = 5.37 \times 10^3}$$

Thereby, the ee value is calculated as:

$$\mathbf{ee = \frac{er - 1}{er + 1} \times 100\% = 99\%}$$

With regard to the reaction shown in Scheme S1, its calculated er value is 5.37×10^3 . Evidently, when the phenyl group is replaced by a hydrogen atom, the er value significantly decreases from 6.14×10^6 to 5.37×10^3 . It should be noted that the reaction in Scheme S1 using 20 mol% **CPA** proceeded 8h which takes a even longer time than the reaction in Scheme 1 using 5 mol% **CPA** (i.e., 4h), indicating the presence of phenyl group in **R2** is important in providing higher ee value. In addition, compared to the reaction in Scheme S1, the less amount of the catalyst **CPA** used suggests that **R2** is more reactive than the substrate without phenyl group.



Scheme S1. Synthesis of **P-3ad** via D–A reaction between **R1** and **R2ad** catalyzed by **CPA**.

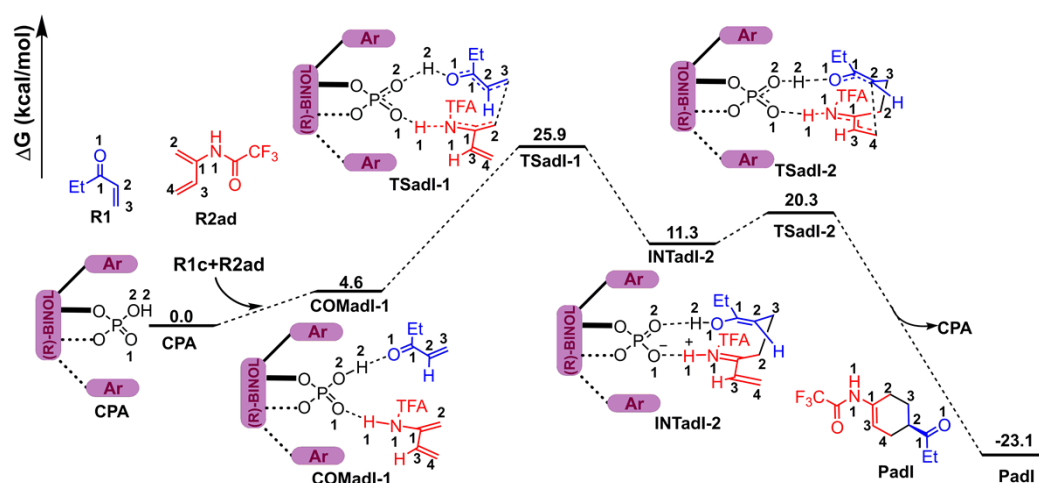


Fig. S3 Gibbs free energy profile for pathway **adI** involving **CPA**-catalyzed reaction of **R1** and **R2ad** to form product **PadI**.

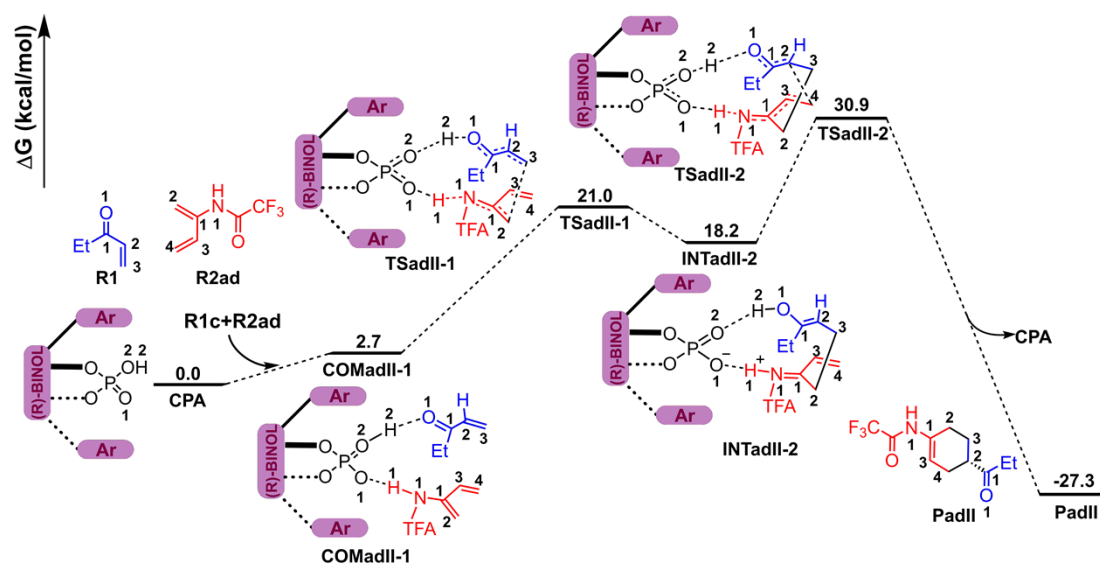


Fig. S4 Gibbs free energy profile for pathway **adII** involving **CPA**-catalyzed reaction of **R1** and **R2ad** to form product **PadII**.

4. QTAIM analyses of transition states

Table S1 Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (d , in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (V , in a.u.), the Electronic Kinetic Energy Density (G , in a.u.) and the Electronic Energy Density (H , in a.u.) at the BCPs of **TSI-1**, **TSII-1**, **TSIII-1** and **TSIV-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSI-1	1	O-H...O	1.41	0.0943	0.1099	0.0712	-0.1149	-0.0437
	2	lp-lp	2.08	0.0667	0.0489	0.0269	-0.0416	-0.0147
	3	N-H...O	1.85	0.0285	0.1191	0.0277	-0.0256	0.0021
	4	C-H...O	2.26	0.0153	0.0613	0.0130	-0.0107	0.0023
	5	C-H...O	2.71	0.0068	0.0241	0.0044	-0.0035	0.0009
	6	C-H...O	2.43	0.0125	0.0480	0.0099	-0.0078	0.0021
	7	p- π	3.29	0.0055	0.0188	0.0037	-0.0027	0.0010
	8	π - π	3.32	0.0069	0.0203	0.0042	-0.0034	0.0008
	9	C-H... π	2.82	0.0068	0.0222	0.0047	-0.0038	0.0009
	10	C-H... π	2.77	0.0080	0.0260	0.0055	-0.0045	0.0010
	11	C-H... π	3.38	0.0023	0.0076	0.0014	-0.0010	0.0005
TSII-1	1	O-H...O	1.42	0.0892	0.1246	0.0699	-0.1086	-0.0387
	2	lp-lp	2.13	0.0616	0.0530	0.0255	-0.0377	-0.0122
	3	N-H...O	1.71	0.0419	0.1419	0.0391	-0.0428	-0.0037
	4	C-H...O	2.27	0.0156	0.0634	0.0136	-0.0113	0.0023
	5	C-H...O	2.58	0.0098	0.0361	0.0074	-0.0058	0.0016
	6	p- π	3.67	0.0037	0.0112	0.0021	-0.0015	0.0007
	7	π - π	3.50	0.0054	0.0161	0.0033	-0.0025	0.0008
	8	C-H... π	2.83	0.0065	0.0187	0.0039	-0.0032	0.0008
	9	C-H... π	3.11	0.0047	0.0147	0.0029	-0.0022	0.0007
	10	C-H... π	2.97	0.0055	0.0175	0.0035	-0.0027	0.0008
TSIII-1	1	O-H...O	1.44	0.0882	0.1126	0.0670	-0.1058	-0.0388
	2	lp-lp	2.12	0.0630	0.0518	0.0258	-0.0387	-0.0129
	3	N-H...O	1.79	0.0335	0.1282	0.0319	-0.0318	0.0001
	4	C-H...O	2.10	0.0195	0.0826	0.0179	-0.0151	0.0028
	5	C-H...O	2.52	0.0111	0.0408	0.0084	-0.0067	0.0018
	6	p- π	3.29	0.0072	0.0242	0.0050	-0.0039	0.0011
	7	C-H... π	2.86	0.0066	0.0204	0.0043	-0.0035	0.0008
	8	C-H... π	2.71	0.0080	0.0249	0.0053	-0.0043	0.0010
	9	C-H... π	3.29	0.0027	0.0088	0.0017	-0.0012	0.0005
	10	C-H... π	3.00	0.0048	0.0146	0.0029	-0.0022	0.0007
	11	C-H... π	3.70	0.0010	0.0033	0.0006	-0.0003	0.0002
TSIV-1	1	O-H...O	1.45	0.0815	0.1422	0.0671	-0.0987	-0.0316
	2	lp-lp	2.16	0.0585	0.0554	0.0245	-0.0352	-0.0107
	3	N-H...O	1.76	0.0367	0.1354	0.0344	-0.0349	-0.0005
	4	C-H...O	2.50	0.0110	0.0400	0.0083	-0.0066	0.0017
	5	C-H...O	2.62	0.0077	0.0267	0.0055	-0.0043	0.0012
	6	C-H...O	2.52	0.0103	0.0394	0.0081	-0.0064	0.0017

7	C-H $\cdots$ O	2.40	0.0118	0.0436	0.0090	-0.0070	0.0019
8	p- π	3.92	0.0017	0.0054	0.0010	-0.0007	0.0003
9	C-H $\cdots\pi$	2.88	0.0061	0.0191	0.0040	-0.0031	0.0008
10	C-H $\cdots\pi$	2.85	0.0061	0.0192	0.0040	-0.0031	0.0008

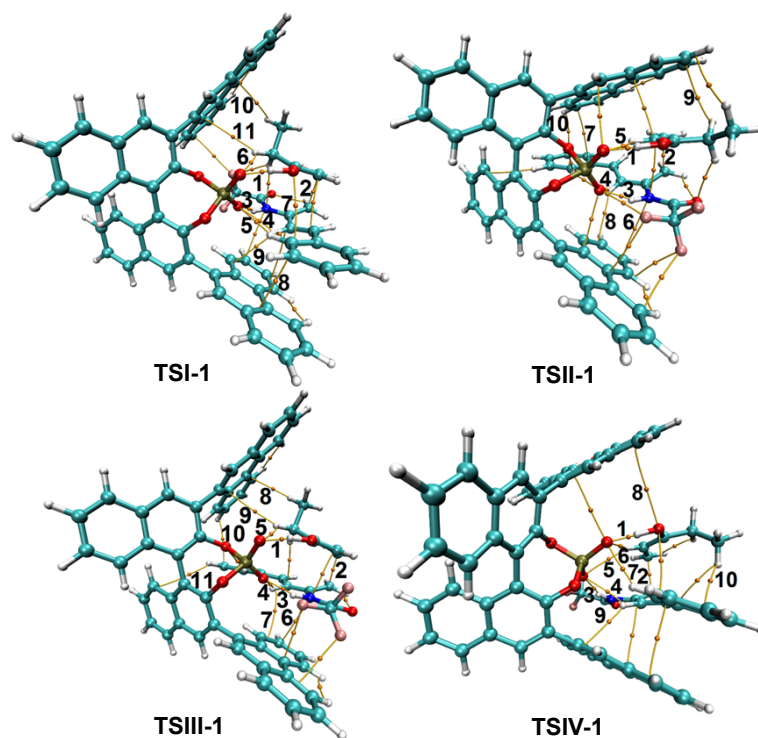


Fig. S5 The interacting atoms numbered with dotted lines in which the bond paths and BCPs appeared for **TSI-1**, **TSII-1**, **TSIII-1** and **TSIV-1**.

In **TSI-1**, after hydrogen atom transfer, the newly formed O1-H1 bond in **R1** forms an O1-H2 $\cdots$ O2 hydrogen bond with P=O2 of **CPA**. The distance between H2 $\cdots$ O2 is 1.41 Å, the electron density is 0.0943 a.u., and the Laplace value of the electron density is 0.1099 a.u. (Table S1 and Fig. S5). Concurrently, the hydrogen bond N1-H1 $\cdots$ O1 forms between N1 from **R2** and O1 from **CPA**, where the distance between H1 and O1 measures 1.85 Å, with an electron density of 0.0285 a.u. and a Laplacian value of 0.1191 a.u.. Additionally, the critical interactions formed at the transition state involve the C3 atom from **R1** and the C2 atom from **R2**, exhibiting a bond length of 2.08 Å, which provides favorable structural conditions for molecular vibrations. Notably, this distance is the shortest among the four reaction pathways, with an electron density of 0.0667 a.u. and a Laplacian value of 0.0489 a.u..

In contrast, in **TSII-1**, the O1-H2 $\cdots$ O2 hydrogen bond exhibits a distance of 1.42 Å between H2 and O2, with an electron density of 0.0892 a.u. and a Laplacian value of 0.1246 a.u.. Meanwhile, the N1-H1 $\cdots$ O1 hydrogen bond has a distance of 1.71 Å between H1 and O1, with an electron density of 0.0419 a.u. and a Laplacian value of 0.1419 a.u.. The distance between C3 of **R1** and C2 of **R2** is 2.13 Å, with an electron density of 0.0616 a.u. and a Laplacian value of 0.0480 a.u.. In

TSIII-1 (or **TSIV-1**), the O1-H2...O2 hydrogen bond shows the distance of 1.44 Å (or 1.45 Å), with corresponding electron density of 0.0882 a.u. (or 0.0815 a.u.) and Laplacian value of 0.1126 a.u. (or 0.1422 a.u.). The N1-H1...O1 hydrogen bond has distances of 1.79 Å (or 1.76 Å) between H1 and O1, with the electron density of 0.0335 a.u. (or 0.0367 a.u.) and corresponding Laplacian value of 0.1282 a.u. (or 0.1354 a.u.). Additionally, the distance between C3 of **R1** and C2 of **R2** is 2.12 Å (or 2.16 Å), with electron density of 0.0630 a.u. (or 0.0585 a.u.) and Laplacian value of 0.0518 a.u. (or 0.0554 a.u.).

Table S2 Intermolecular Bond Critical Points (BCPs) and the Corresponding Distances between Atoms (d , in Å), Classifications of the Intermolecular Interactions, Electron Density (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the Electronic Potential Energy Density (V , in a.u.), the Electronic Kinetic Energy Density (G , in a.u.) and the Electronic Energy Density (H , in a.u.) at the BCPs of **TSI-2**, **TSII-2**, **TSIII-2**, and **TSIV-2**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSI-2	1	O-H...O	1.74	0.0377	0.1271	0.0347	-0.0376	-0.0029
	2	lp-lp	2.42	0.0336	0.0574	0.0165	-0.0186	-0.0021
	3	N-H...O	1.84	0.0290	0.1157	0.0274	-0.0258	0.0016
	4	C-H...O	2.47	0.0112	0.0425	0.0089	-0.0071	0.0017
	5	C-H...O	2.52	0.0120	0.0461	0.0098	-0.0081	0.0017
	6	C-H...O	2.38	0.0126	0.0470	0.0097	-0.0077	0.0020
	7	C-H...O	2.21	0.0166	0.0636	0.0134	-0.0109	0.0025
	8	C-H...O	2.42	0.0124	0.0453	0.0095	-0.0076	0.0019
	9	lp- π	3.19	0.0083	0.0254	0.0054	-0.0045	0.0009
	10	lp- π	3.23	0.0070	0.0221	0.0046	-0.0037	0.0009
	11	π - π	3.37	0.0066	0.0196	0.0041	-0.0032	0.0008
	12	C-H... π	2.86	0.0064	0.0207	0.0043	-0.0034	0.0009
	13	C-H... π	2.78	0.0070	0.0216	0.0045	-0.0037	0.0009
TSII-2	1	O-H...O	1.96	0.0253	0.0898	0.0213	-0.0201	0.0012
	2	lp-lp	2.29	0.0460	0.0583	0.0202	-0.0258	-0.0056
	3	N-H...O	2.00	0.0204	0.0866	0.0186	-0.0156	0.0030
	4	C-H...O	2.18	0.0181	0.0745	0.0162	-0.0137	0.0025
	5	C-H...O	2.40	0.0125	0.0476	0.0099	-0.0080	0.0020
	6	C-H...O	2.38	0.0113	0.0422	0.0086	-0.0067	0.0019
	7	C-H...O	2.40	0.0135	0.0521	0.0111	-0.0091	0.0020
	8	C-H...O	2.53	0.0096	0.0372	0.0078	-0.0061	0.0016
	9	p- π	3.12	0.0075	0.0301	0.0061	-0.0046	0.0015
	10	π - π	3.36	0.0063	0.0191	0.0040	-0.0031	0.0008
	11	C-H... π	2.89	0.0056	0.0169	0.0035	-0.0028	0.0007
	12	C-H... π	2.81	0.0064	0.0185	0.0039	-0.0031	0.0007
TSIII-2	1	O-H...O	1.72	0.0427	0.1129	0.0354	-0.0426	-0.0072
	2	lp-lp	2.25	0.0517	0.0536	0.0208	-0.0281	-0.0074
	3	N-H...O	1.98	0.0224	0.0898	0.0199	-0.0173	0.0026
	4	C-H...O	2.22	0.0171	0.0695	0.0151	-0.0128	0.0023
	5	C-H...O	2.57	0.0090	0.0319	0.0066	-0.0053	0.0013
	6	C-H...O	2.25	0.0144	0.0558	0.0115	-0.0091	0.0024
	7	C-H...O	2.39	0.0125	0.0474	0.0098	-0.0078	0.0020
	8	p- π	3.11	0.0078	0.0308	0.0062	-0.0048	0.0015
	9	C-H... π	2.98	0.0048	0.0144	0.0029	-0.0023	0.0007
	10	C-H... π	2.73	0.0078	0.0243	0.0051	-0.0041	0.0010
TSIV-2	1	O-H...O	1.70	0.0405	0.1357	0.0379	-0.0420	-0.0040
	2	lp-lp	2.47	0.0342	0.0529	0.0156	-0.0180	-0.0024
	3	N-H...O	1.74	0.0386	0.1367	0.0362	-0.0383	-0.0021
	4	C-H...O	2.26	0.0154	0.0601	0.0127	-0.0104	0.0023

5	C-H...O	2.61	0.0100	0.0360	0.0074	-0.0060	0.0015
6	C-H...O	2.44	0.0116	0.0428	0.0089	-0.0071	0.0018
7	C-H...O	2.21	0.0140	0.0587	0.0120	-0.0093	0.0027
8	lp- π	3.52	0.0054	0.0189	0.0038	-0.0028	0.0010
9	π - π	3.23	0.0068	0.0212	0.0045	-0.0036	0.0008
10	p- π	3.74	0.0024	0.0078	0.0015	-0.0010	0.0005
11	π - π	3.39	0.0078	0.0254	0.0053	-0.0044	0.0010

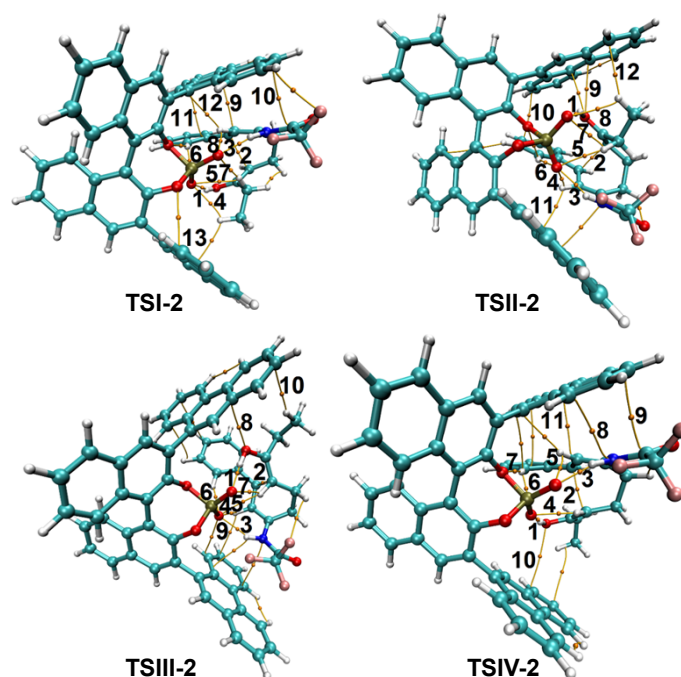


Fig. S6 The interacting atoms numbered with dotted lines in which the bond paths and BCPs appeared for **TSI-2**, **TSII-2**, **TSIII-2**, and **TSIV-2**.

In **TSI-2**, the O1-H2 bond formed in **R1** after proton transfer forms an O1-H2 $\cdots$ O2 hydrogen bond with O2 in P=O2 of **CPA**. The distance between H1 $\cdots$ O2 is 1.74 Å, the electron density is 0.0377 a.u., and the Laplace value of the electron density is 0.1271 a.u. (Table S2 and Fig. S6).. The N1-H1 of **R2** forms a hydrogen bond with the O1 of **CPA**, namely the N1-H1 $\cdots$ O1 hydrogen bond. The distance between H1 $\cdots$ O1 is 1.84 Å, the electron density is 0.0290 a.u., and the Laplace value of the electron density is 0.1157 a.u.. Additionally, the distance between C2 of **R1** and C4 of **R2** is measured at 2.42 Å, with an electron density of 0.0336 a.u. and a Laplacian value of 0.0574 a.u.. For **TSII-2**, multiple hydrogen bonds and π - π interactions significantly influence the stability and spatial arrangement of the molecule. Specifically, in the O1-H2 $\cdots$ O2 hydrogen bond, the distance between H1 and O2 is 1.96 Å, with an electron density of 0.0253 a.u. and a Laplacian value of 0.0898 a.u.. In the N1-H1 $\cdots$ O1 hydrogen bond, the distance between H1 and O1 is 2.00 Å, with an electron density of 0.0204 a.u. and a Laplacian value of 0.0866 a.u.. Additionally, the distance between C2 in **R1** and C4 in **R2** is 2.29 Å, with an electron density of 0.0460 a.u. and a Laplacian value of 0.0583 a.u.. The hydrogen bonding and π - π interactions in the **TSII-2** transition state collaboratively stabilize the molecular system. However, the cooperativity of these interactions results in a more compact molecular arrangement, leading to increased steric hindrance. In **TSIII-2**, the molecule

exhibits significant internal torsion, leading to a dense concentration of interaction points and the formation of multiple π - π and C-H $\cdots$ O interactions. This tightly packed molecular arrangement substantially enhances steric hindrance. In contrast, **TSIV-2** features particularly pronounced π - π stacking between the aromatic rings, along with multiple interwoven hydrogen bonds, resulting in an overall tighter structure. This transition state structure encompasses the highest number of π - π interactions and hydrogen bonds, consequently exhibiting the strongest steric hindrance.

5. The distortion/interaction analyses

Table S3 The distortion/interaction energy analyses of **TSI-2**, **TSII-2**, **TSIII-2** and **TSIV-2** Including distortion energy (ΔE_{dist} , kcal·mol⁻¹), interaction energy (ΔE_{int} , kcal·mol⁻¹), activation energy (ΔE_{act} , kcal·mol⁻¹), activated Gibbs free energy (ΔG , kcal·mol⁻¹), and relative activated Gibbs free energy ($\Delta\Delta G$, kcal·mol⁻¹)

	TSI-2	TSII-2	TSIII-2	TSIV-2
$\Delta E_{\text{dist}}(\text{CPA})^{\text{a}}$	-1.96	-0.65	0.59	-0.24
$\Delta E_{\text{dist}}(\text{P})^{\text{b}}$	0.99	10.11	8.62	-0.79
$\Delta E_{\text{dist}}(\text{total})^{\text{c}}$	-0.97	9.46	9.21	-1.03
$\Delta E_{\text{int}}(\text{TSX})^{\text{d}}$	-131.61	-123.07	-127.05	-128.45
$\Delta E_{\text{int}}^{\text{e}}$	-132.57	-113.61	-117.83	-129.48
ΔG	3.60	17.41	18.55	4.73
$\Delta\Delta G^{\text{f}}$	0.00	13.81	14.95	1.13

^a $\Delta E_{\text{dist}}(\text{CPA})$ is the energy difference between the transition state of the **CPA** fragment and the optimized **CPA**. ^b $\Delta E_{\text{dist}}(\text{P})$ is the energy difference between the transition state of the **P** fragment and the optimized **P**. ^c $\Delta E_{\text{dist}}(\text{total})$ is the sum of $\Delta E_{\text{dist}}(\text{CPA})$ and $\Delta E_{\text{dist}}(\text{P})$. ^d $\Delta E_{\text{int}}(\text{TSX})$ is the interaction energy of **TSX-2** (**X** = **I**, **II**, **III**, **IV**). ^e ΔE_{int} is the sum of $\Delta E_{\text{dist}}(\text{total})$ and ΔE_{int} . ^f $\Delta\Delta G$ is the difference between the activation Gibbs free energy of **TSX-2** (**X** = **I**, **II**, **III**, **IV**) and that of **TSI-2**.

6. The truncation model calculations of TSI-2 and TSII-2

Table S4 The interaction energies (ΔE_{int} , in kcal·mol⁻¹) for the fragments A, B and C in **TSI-2** and **TSII-2**, and the energy difference ($\Delta\Delta E_{int}$, in kcal·mol⁻¹) between the fragments.

	Fragment A	Fragment B	Fragment C
$\Delta E_{int}(\text{TSI-2})$	-116.58	-18.38	-6.18
$\Delta E_{int}(\text{TSII-2})$	-113.08	-11.72	-9.73
$\Delta\Delta E_{int}$	3.50	6.67	-3.55

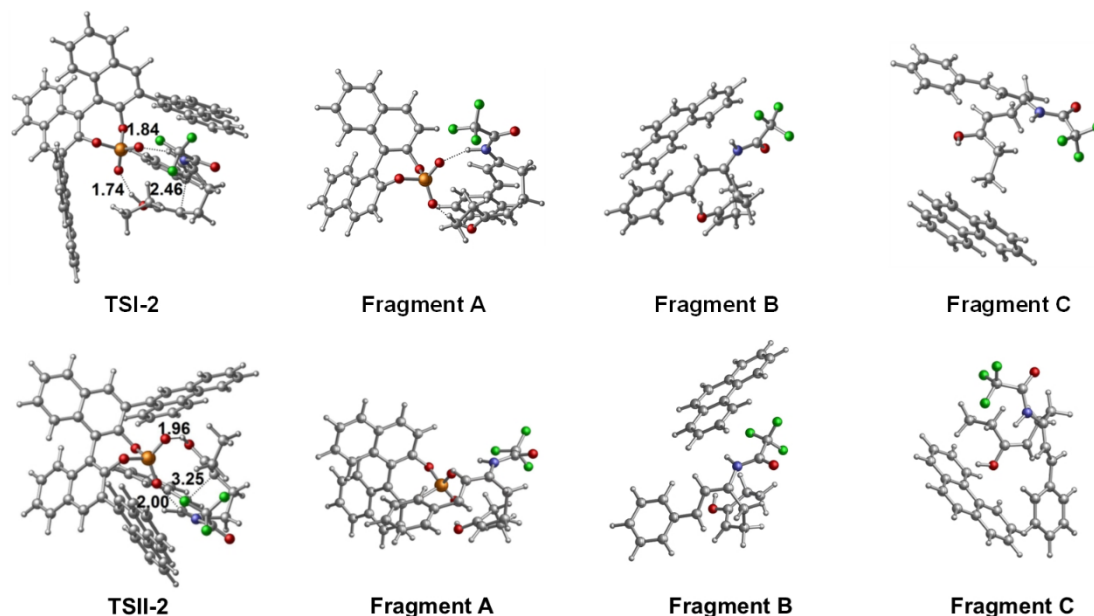


Fig. S7 The truncation models for **TSI-2** and **TSII-2** composed of the phosphate main skeleton (fragment A) and the two anthracene groups (fragments B and C). In fragment A, the 3,3' -anthracene group is replaced by a hydrogen atom, while in fragments B and C, the main skeleton and functional groups are removed

To elucidate the influence of steric effects and intermolecular interactions on the reaction selectivity and stability, we further performed the truncation model calculations for the transition states **TSI-2** and **TSII-2** in pathways **I** and **II**, respectively (Table S4). In the transition state **TSI-2** or **TSII-2**, the catalyst is divided into three independent components by cutting the C-C bond connecting the bulky substituents to the phosphate backbone (Fig. S7). This results in the formation of three segments: the phosphate backbone (fragment A), and the two bulky substituents (fragments B and C). Subsequently, hydrogen atoms are added to complete the molecular structure, followed by optimization to ensure the rationality of the truncated model in terms of electronic structure and geometry. It presents the entire **TSI-2** structure, along with the separately extracted fragments A, B, and C. By calculating the interaction energies between the substrate and fragments A, B, and C, the

contributions of the different parts of the catalyst to the reaction stability and selectivity can be quantified. The phosphate backbone is the core structure of the catalyst, providing key hydrogen bonding and electrostatic interactions. The interaction energy of **TSI-2** ($-116.58 \text{ kcal}\cdot\text{mol}^{-1}$) is more negative than that of **TSII-2** ($-113.08 \text{ kcal}\cdot\text{mol}^{-1}$), indicating that **TSI-2** has a stronger binding ability between the catalyst and the substrate, and thus higher stability. The energy difference between the two is $3.50 \text{ kcal}\cdot\text{mol}^{-1}$, suggesting that fragment A contributes more to the stability of the **TSI-2** transition state due to stronger interactions. Fragment B primarily affects the spatial arrangement and steric hindrance in the transition state, while also influencing stability through van der Waals forces and π - π interactions. In **TSII-2**, the interaction energy of fragment B is relatively weak at $-11.72 \text{ kcal}\cdot\text{mol}^{-1}$, whereas in **TSI-2**, the interaction energy is significantly stronger, reaching $-18.38 \text{ kcal}\cdot\text{mol}^{-1}$. The energy difference between these two values ($6.67 \text{ kcal}\cdot\text{mol}^{-1}$) indicates that **TSI-2** is more favorable for the reaction due to the stronger interactions of fragment B, which contributes significantly to the stability of the transition state. This suggests that fragment B plays a more prominent role in stabilizing the transition state in **TSI-2**, potentially by reducing unfavorable spatial effects and further optimizing the reaction pathway. Fragment C also influences spatial hindrance, but its contribution is smaller compared to that of fragment B. The interaction energy of fragment C ($-3.55 \text{ kcal}\cdot\text{mol}^{-1}$) suggests that in **TSI-2**, fragment C may help reduce the adverse steric effects in the transition state, thereby enhancing reaction activity. Overall, **TSI-2** is the more optimal transition state due to stronger interactions between the catalyst and the substrate and the smaller unfavorable steric effects.

7. The energy decomposition analysis (EDA) based on SAPT theory

Table S5 Energy decomposition analyses (EDA) of the transition states **TSI-2**, **TSII-2**, **TSIII-2** and **TSIV-2**. Interaction energy (ΔE_{int} , kcal·mol⁻¹), electrostatic interaction energy (ΔE_{els} , kcal·mol⁻¹), exchange repulsion energy (ΔE_{xrep} , kcal·mol⁻¹), orbital interaction energy (ΔE_{orb} , kcal·mol⁻¹), and dispersion correction energy (ΔE_{disp} , kcal·mol⁻¹).

	TSI-2	TSII-2	TSIII-2	TSIV-2
ΔE_{int}	-132.82	-123.89	-128.11	-130.22
ΔE_{els}	-125.60	-121.24	-121.54	-123.39
ΔE_{xrep}	102.21	106.25	99.78	96.71
ΔE_{orb}	-44.26	-41.51	-42.65	-45.11
ΔE_{disp}	-59.26	-60.84	-57.80	-53.54

The interaction energy (ΔE_{int}) is the sum of all attractive and repulsive terms (i.e., $\Delta E_{\text{int}} = \Delta E_{\text{els}} + \Delta E_{\text{xrep}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$). A more negative value of ΔE_{int} indicates a more stable transition state. It can be seen from Table S5 that the order of ΔE_{int} is **TSI-2** (-132.82 kcal/mol) > **TSIV-2** (-130.22 kcal/mol) > **TSIII-2** (-128.11 kcal/mol) > **TSII-2** (-123.89 kcal/mol). Because **TSI-2** and **TSII-2** represent the competing pathways for a pair of enantiomers, the major product will be determined by the pathway **I**. **TSI-2** is the most stable transition state, while **TSII-2** is the least stable. The difference in interaction energy between the least stable (**TSII-2**) and the most stable (**TSI-2**) transition states is approximately 8.93 kcal/mol. This difference primarily originates from variations in the following components. The significantly negative ΔE_{els} value for **TSI-2** or **TSII-2** indicates that the electrostatic attraction plays an extremely important role in stabilizing the transition state. The electrostatic attraction in **TSI-2** is about 4.36 kcal/mol stronger than in **TSII-2**, and it is one of the key factors leading to the enantioselectivity. The exchange repulsion energy ΔE_{xrep} is significantly positive for **TSI-2** or **TSII-2** which is a major contributor to the energy barrier. The most stable **TSI-2** has a lower ΔE_{xrep} energy (102.21 kcal/mol), while the less stable **TSII-2** has the higher ΔE_{xrep} energy (106.25 kcal/mol). The difference between them is 4.04 kcal/mol. A lower exchange repulsion energy means that the steric hindrance in **TSI-2** is smaller when the reactants approach each other, so the resultant geometry is more favorable. This is often related to the "shape complementarity" provided by the cavity of the chiral catalyst. The difference in exchange repulsion energy is another core factor determining enantioselectivity, potentially as important as the electrostatic interaction. The negative orbital interaction energy ΔE_{orb} for **TSI-2** or **TSII-2** contributes to its stabilization. The orbital interaction in **TSI-2** (-44.26 kcal/mol) is stronger than

that in **TSII-2** (-41.51 kcal/mol) by 2.75 kcal/mol, meaning that the key orbitals in **TSI-2** overlap more effectively, which further stabilizes it. The negative dispersion correction energy (ΔE_{disp}) are very important stabilizing forces. It is noteworthy that both the more stable **TSI-2** and the less stable **TSII-2** have strong dispersion interactions, but **TSII-2**'s dispersion correction energy (ΔE_{disp}) is even stronger (by 1.58 kcal/mol compared to **TSI-2**). The orbital and dispersion interactions are very important but they are not the primary determinant of enantioselectivity because they are not stronger than the electrostatic interaction energy ΔE_{els} . Compared **TSII-2** with **TSI-2**, it is evident that **TSII-2** has the stronger dispersion interaction but the weaker electrostatic interaction and the higher repulsion energy. This reveals that a strong dispersion attraction alone is not sufficient. **TSII-2** might adopt a conformation that is unfavorable both electrostatically and sterically in order to maximize dispersion contacts, but the stabilization gain does not offset the stabilization loss. In contrast, in **TSI-2**, electrostatic complementarity, minimized steric hindrance, and good orbital interaction achieve a perfect synergistic balance. Even though its dispersion interaction is not the strongest, its overall stability is higher. Therefore, the high enantioselectivity of this reaction is primarily driven by the combined effects of differences in electrostatic complementarity and spatial repulsion (steric hindrance) in the transition states. The favored transition state (**TSI-2**) simultaneously achieves the optimal electrostatic alignment (more negative ΔE_{els}), the smoothest spatial approach (smaller ΔE_{xrep} and effective orbital overlap (reasonably negative ΔE_{orb}), and this cooperative effect overcomes its minor disadvantage in dispersion interaction, resulting in the lower interaction energy and making it the dominant reaction pathway.

8. Calculated Gibbs free energy correction (GFEC), energy (E) and Gibbs free energy (G) of all optimized structures, and imaginary frequencies (ν_i s) of all transition states (TSs).

Table S6 GFEC, E, G, relative Gibbs free energies (ΔG) of all optimized structures and imaginary frequencies (ν_i s) of all TSs.

	GFEC/a.u.	E/a.u.	G/a.u.	$\Delta G/(\text{kcal}\cdot\text{mol}^{-1})$	vis of TS
R1	0.089627	-270.533776	-270.444149		
R2	0.157465	-892.821218	-892.663753		
CPA	0.568490	-2489.030284	-2488.461794		
CPA+R1	0.681202	-2759.586148	-3651.568699	0.6	
COMI-1	0.865010	-3652.427738	-3651.562728	4.4	
TSI-1	0.870026	-3652.403829	-3651.533803	22.5	-450.68
INTI-2	0.874409	-3652.426725	-3651.552316	10.9	
TSI-2	0.875416	-3652.422023	-3651.546607	14.5	-156.20
P_I	0.877244	-3652.473028	-3651.595784	-16.4	
II(CPA+R1)	0.681202	-2759.586148	-3651.568699	0.6	
COMII-1	0.866248	-3652.429964	-3651.563716	3.8	
TSII-1	0.871717	-3652.408803	-3651.537086	20.5	-340.70
INTII-2	0.877214	-3652.420102	-3651.542888	16.8	
TSII-2	0.877108	-3652.396396	-3651.519288	31.6	-289.06
P_{II}	0.877943	-3652.468250	-3651.590307	-12.9	
III(CPA+R1)	0.681985	-2759.586608	-3651.568376	0.8	
COMIII-1	0.865406	-3652.428833	-3651.563427	3.9	
TSIII-1	0.870238	-3652.403950	-3651.533712	22.6	-365.41
INTIII-2	0.874907	-3652.426535	-3651.551628	11.3	
TSIII-2	0.876421	-3652.398490	-3651.522069	29.9	-264.84
P_{III}	0.875722	-3652.476182	-3651.60046	-19.3	
IV(CPA+R1)	0.680416	-2759.585194	-3651.568531	0.7	
COMIV-1	0.867963	-3652.431239	-3651.563276	4.0	
TSIV-1	0.873742	-3652.407284	-3651.533542	22.7	-320.47
INTIV-2	0.870038	-3652.427036	-3651.556998	8.0	
TSIV-2	0.874271	-3652.423727	-3651.549456	12.7	-137.93
P_{IV}	0.874260	-3652.475827	-3651.601567	-20.0	
R2ad	0.082703	-661.76721	-661.684507		
COMadI-1	0.786086	-3421.369175	-3420.583089	4.7	
TSadI-1	0.794185	-3421.343392	-3420.549207	25.9	
INTadI-1	0.795887	-3421.36834	-3420.572453	11.3	
TSadI-2	0.79843	-3421.356554	-3420.558124	20.3	
PadI	0.801585	-3421.428872	-3420.627287	-23.1	
COMadII-1	0.787087	-3421.373163	-3420.586076	2.7	
TSadII-1	0.793058	-3421.349984	-3420.556926	21.0	
INTadII-1	0.796522	-3421.35798	-3420.561458	18.2	
TSadII-2	0.799968	-3421.341163	-3420.541195	30.9	

PadII	0.799213	-3421.433113	-3420.6339	-27.3
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9. Cartesian coordinates

R1

C	1.67608900	-0.99037500	-0.47756600
O	0.12813300	1.89220400	-0.13922200
C	1.04026500	-0.16495700	0.64878800
C	-0.06769300	0.71392200	0.10678300
C	-1.40494200	0.12503400	-0.18008700
C	-1.75391800	-1.13353500	0.08694600
H	2.50222500	-1.59030600	-0.08863400
H	0.94943600	-1.66564200	-0.93700000
H	2.07019900	-0.33356800	-1.25814500
H	1.78461000	0.49954400	1.09351900
H	0.65687200	-0.82496700	1.43223200
H	-2.10838500	0.81785200	-0.63624500
H	-2.74963600	-1.49882200	-0.14573800
H	-1.06918300	-1.84225600	0.54460500

R2

C	3.44188300	-0.98348600	-0.63220000
C	4.70491400	-1.56257900	-0.62246400
C	5.75867100	-0.94534800	0.05324600
C	5.53992600	0.25920000	0.71713100
C	4.27436900	0.83836200	0.70928100
C	3.20508000	0.22360300	0.04366900
C	1.88538200	0.87031200	0.08387300
C	0.72565400	0.31815300	-0.29760500
C	-0.56442000	1.03107100	-0.27391500
N	-1.65041900	0.15784500	-0.01939400
C	-0.69663800	2.34740300	-0.48860000
C	-2.96255700	0.45801700	-0.08986600
C	-3.90116100	-0.73099500	0.19184000
O	-3.47296500	1.53054000	-0.34620000
F	-3.24664500	-1.87589000	0.43173400
F	-4.66555100	-0.46369200	1.25141200
F	-4.70306100	-0.92701500	-0.85517800
H	2.63846300	-1.46637200	-1.18019100
H	4.87174200	-2.49600600	-1.15104600
H	6.74477100	-1.39889600	0.05502700
H	6.35466700	0.74985200	1.24030200
H	4.10382700	1.77819800	1.22779400
H	1.87316200	1.88292900	0.48523300
H	0.69147100	-0.71774900	-0.63294800
H	-1.41000700	-0.79709700	0.21995300

H	-1.64893600	2.85299200	-0.43682100
H	0.18819000	2.92000100	-0.73999600

CPA

C	-1.57559200	1.02730900	-0.17918700
C	-2.92683600	0.91558000	-0.60498700
C	-3.42415800	1.90784600	-1.41402400
C	-2.61592400	2.99369900	-1.83908400
C	-1.26176400	3.08099000	-1.40723700
C	-0.75244500	2.08035100	-0.51340700
C	-3.13594600	3.98415700	-2.71499300
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C	-0.98430300	5.07158700	-2.77082800
C	-0.45680900	4.13695900	-1.91538800
C	0.64202900	2.10811800	0.00666000
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C	2.51725700	3.17218100	1.18896400
C	3.31779000	2.04105200	0.89156500
C	2.81204900	0.95161500	0.22237400
C	1.45773900	1.01562100	-0.19914400
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C	0.89877400	5.35466700	1.87236900
C	2.26008200	5.33293800	2.26183700
C	3.04818400	4.26215600	1.93109000
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O	-1.08194300	0.00792100	0.62908100
P	-0.04232400	-1.04939300	-0.00847400
O	0.55833400	-1.90508900	1.01536500
O	-0.79221200	-1.84126100	-1.15654600
C	-3.74486000	-0.27326600	-0.23926700
C	3.65733300	-0.23462200	-0.08847900
C	-4.19344000	-1.08796200	-1.23069800
C	-4.96881500	-2.26405900	-0.95706100
C	-5.28858800	-2.59940400	0.38055100
C	-4.84265000	-1.71761100	1.45298500
C	-4.07895200	-0.56195400	1.14286400
C	4.28141800	-1.00454300	0.97303500
C	5.15452600	-2.07542600	0.64089600
C	5.39535800	-2.40633700	-0.75795500
C	4.73032800	-1.65946300	-1.75987400
C	3.86821900	-0.57657900	-1.38701900
C	-5.15939800	-1.96833000	2.80691100
C	-4.74851100	-1.11627100	3.80956000
C	-4.00500500	0.03405500	3.49748700

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C	-6.44346400	-4.57692100	-0.43663000
C	-6.03337300	-3.77761400	0.61067500
C	4.01526500	-0.73275100	2.33528200
C	4.60959400	-1.46614700	3.33852300
C	5.49585000	-2.50571800	3.01294400
C	5.75466400	-2.80395800	1.69241100
C	6.25700400	-3.44902900	-1.16739400
C	6.44332800	-3.73593900	-2.50376900
C	5.77610000	-2.99259200	-3.49459300
C	4.93375500	-1.96888100	-3.12337200
H	-4.45631600	1.85719800	-1.74984500
H	-4.17473200	3.90667900	-3.02321700
H	-2.74407800	5.75631200	-3.83904700
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H	4.35373400	2.03319300	1.22068300
H	-0.68659400	4.34914300	0.86450900
H	0.27287800	6.19373700	2.15881800
H	2.67015200	6.15948000	2.83289800
H	4.08939900	4.21915800	2.23782800
H	-1.13390500	-1.29183600	-1.88379100
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H	3.39171200	-0.00725200	-2.18131800
H	-5.74129000	-2.84305900	3.07273900
H	-5.00582900	-1.33351000	4.84127600
H	-3.68905600	0.70988300	4.28548900
H	-3.11455600	1.19816200	1.94702500
H	-5.13909100	-2.81509700	-3.03341500
H	-6.45381000	-4.86925100	-2.58160200
H	-7.01348900	-5.47765200	-0.23215700
H	-6.29071300	-4.07273700	1.62137700
H	3.31898700	0.05835600	2.59036200
H	4.38677900	-1.24427300	4.37718600
H	5.96915200	-3.08413100	3.79988800
H	6.42775300	-3.62265500	1.46630900
H	6.78664900	-4.04109500	-0.43004000
H	7.11017400	-4.54260900	-2.79125200
H	5.92737300	-3.22566500	-4.54367700
H	4.41137100	-1.38069200	-3.87295000

COMI-1

C	-2.80610900	0.97836000	-0.71485800
C	-3.82516800	0.15653700	-1.26552800
C	-4.79598000	0.76129000	-2.02401500
C	-4.78053400	2.15897100	-2.27158900
C	-3.76084500	2.96758400	-1.69371100
C	-2.77323400	2.34862600	-0.85766900
C	-5.76437400	2.76251700	-3.09932600
C	-5.72825700	4.10685900	-3.36478700
C	-4.69656800	4.90641600	-2.81817000
C	-3.73880500	4.35425300	-2.00501000
C	-1.68846400	3.11397900	-0.18497100
C	-1.94780800	4.15956100	0.75900000
C	-0.84390400	4.81672000	1.37451600
C	0.47832500	4.39988500	1.07881600
C	0.73245900	3.36380500	0.21191000
C	-0.38021200	2.74249200	-0.40890900
C	-3.26237400	4.54178700	1.14372900
C	-3.46241200	5.54680500	2.05554200
C	-2.36396500	6.22517000	2.63695500
C	-1.08483300	5.86215000	2.30691200
O	-0.13653700	1.68548800	-1.27904400
O	-1.81314900	0.34334400	0.02214400
P	-0.34682800	0.21811100	-0.63874800
O	0.66187800	-0.15527900	0.37619500
O	-0.46920200	-0.68698500	-1.89321000
C	-3.82255100	-1.31037900	-1.01962400
C	2.12404400	2.91190700	-0.07025600
C	-3.65173800	-2.16498600	-2.06165000
C	-3.63386700	-3.58842400	-1.87882300
C	-3.80015400	-4.13312500	-0.58231400
C	-3.99653600	-3.22753300	0.54304800
C	-4.01864600	-1.82698800	0.32147200
C	2.92680400	2.31572100	0.98101900
C	4.29131300	2.00831100	0.73268200
C	4.85824000	2.25293100	-0.58741000
C	4.02214400	2.77696900	-1.60268500
C	2.65686100	3.10147500	-1.30520000
C	-4.16540300	-3.69895500	1.86462400
C	-4.37381300	-2.83174800	2.91453200
C	-4.43310700	-1.44723800	2.68473600
C	-4.25361300	-0.95829600	1.41116800
C	-3.41289100	-4.44432200	-2.97970500
C	-3.35730000	-5.81006400	-2.81115500

C	-3.52615500	-6.35764200	-1.52681400
C	-3.74260400	-5.53707300	-0.43892800
C	2.36806500	2.00374500	2.24289400
C	3.13670400	1.45234400	3.24486600
C	4.49639700	1.18445000	3.01522500
C	5.05392000	1.44830400	1.78272800
C	6.20184400	1.96543400	-0.91416800
C	6.68901900	2.18606900	-2.18489100
C	5.85466600	2.70812900	-3.18963600
C	4.54106100	3.00001000	-2.89775200
H	-5.59440600	0.15909100	-2.44971500
H	-6.54169400	2.13335300	-3.52419600
H	-6.48134600	4.55977400	-4.00150600
H	-4.66030200	5.96628100	-3.04922100
H	-2.94695600	4.97705200	-1.60275200
H	1.30844100	4.90206700	1.56983500
H	-4.11381800	4.02328900	0.71704100
H	-4.47323800	5.82194000	2.33950600
H	-2.54003300	7.02187200	3.35245800
H	-0.23159200	6.36011500	2.75921400
H	0.24135900	-1.44603700	-1.95076600
H	-3.49168500	-1.77064000	-3.06198700
H	2.04914800	3.53616900	-2.09535500
H	-4.13691000	-4.76312700	2.06899300
H	-4.49727700	-3.22105300	3.92014000
H	-4.60768500	-0.76570500	3.51100100
H	-4.29635200	0.11199000	1.23671800
H	-3.28125500	-4.00394100	-3.96446900
H	-3.18415900	-6.46129300	-3.66193500
H	-3.48425200	-7.43340300	-1.38777600
H	-3.86432700	-5.99303700	0.53704400
H	1.31138300	2.18467500	2.41003000
H	2.68765000	1.20874100	4.20284700
H	5.10240300	0.74133700	3.79894300
H	6.09670900	1.20121400	1.62106400
H	6.87031900	1.55332400	-0.16683500
H	7.72370100	1.94926200	-2.41175300
H	6.24558700	2.87898600	-4.18776000
H	3.88202200	3.40637100	-3.66063500
C	4.12513100	-0.90359500	-1.40931000
C	4.63065700	-0.61845800	-2.67152800
C	5.78826100	-1.24920200	-3.12552800
C	6.43317800	-2.17732000	-2.31064800
C	5.92257300	-2.46916000	-1.04977100

C	4.77097100	-1.82884100	-0.57580400
C	4.23216600	-2.18917200	0.74566400
C	3.35865800	-1.44154500	1.42931800
C	2.74653000	-1.81959800	2.71649500
N	1.41739500	-1.34259800	2.78711000
C	3.35240900	-2.52569500	3.67913600
C	0.45621800	-1.73308300	3.64370600
C	-0.92736000	-1.20169900	3.20853100
O	0.55734700	-2.45425100	4.61739800
F	-1.33765300	-1.85346200	2.11182400
F	-1.81973200	-1.38704000	4.17515300
F	-0.88500400	0.10394600	2.91369700
H	3.20756200	-0.42272600	-1.07680200
H	4.12171800	0.10402700	-3.30210100
H	6.18170100	-1.02096100	-4.11147600
H	7.33070800	-2.67920000	-2.65953200
H	6.41808000	-3.20362700	-0.41949800
H	4.56763900	-3.13992500	1.16055400
H	3.00997300	-0.49889300	1.00941300
H	1.12053000	-0.74769900	2.00736000
H	2.84978900	-2.80119800	4.59480900
H	4.38517000	-2.82133200	3.53494700
C	-0.62169600	-3.75807500	-0.27818900
O	1.28583500	-2.43262100	-2.13333300
C	0.85606000	-3.44253100	-0.01900100
C	1.62141400	-3.28687100	-1.30449400
C	2.76932500	-4.14167600	-1.65845200
C	3.18520800	-5.18867000	-0.94351800
H	-1.13800400	-3.90299700	0.67239400
H	-1.11480800	-2.93339200	-0.80093100
H	-0.74601700	-4.66521500	-0.87810100
H	1.31146500	-4.19519900	0.62536500
H	0.92982900	-2.47958000	0.49660600
H	3.26710200	-3.85561300	-2.58159700
H	4.03168300	-5.78097000	-1.27716400
H	2.71114700	-5.50183500	-0.01878500

TSI-1

C	-2.33736800	1.76154500	-0.50453500
C	-3.55598500	1.36925100	-1.12367300
C	-4.26484900	2.32305000	-1.81228100
C	-3.79925600	3.65878100	-1.92435600
C	-2.59042400	4.03997500	-1.27661100
C	-1.87609000	3.06100000	-0.50950800

C	-4.51946700	4.61971800	-2.68337400
C	-4.05164600	5.90142400	-2.81665500
C	-2.83323200	6.27425500	-2.20026700
C	-2.12140600	5.37086500	-1.45099800
C	-0.63421600	3.38460400	0.24298300
C	-0.60551900	4.37961300	1.27451400
C	0.62664300	4.65592600	1.93209400
C	1.78987700	3.92918500	1.57327900
C	1.75285000	2.93613700	0.62562900
C	0.51469800	2.66358100	-0.01426600
C	-1.76863000	5.07942400	1.70121800
C	-1.69693900	6.02016700	2.69750200
C	-0.46288100	6.31741900	3.32516500
C	0.67104400	5.64444800	2.95216100
O	0.47587200	1.65652600	-0.95952200
O	-1.61593000	0.79463200	0.16415500
P	-0.23210500	0.24700700	-0.51882200
O	0.52839200	-0.44584300	0.55753300
O	-0.53878500	-0.45510000	-1.82076100
C	-4.04240100	-0.03469800	-1.04845500
C	2.99119500	2.19611800	0.24723600
C	-4.20212600	-0.73758300	-2.20064700
C	-4.70881000	-2.07964200	-2.21105500
C	-5.07737300	-2.70250900	-0.99517100
C	-4.88960900	-1.97240700	0.25266400
C	-4.38453500	-0.64540200	0.22409900
C	3.52696500	1.16346000	1.11157500
C	4.74197600	0.51606400	0.76156200
C	5.41189000	0.86719700	-0.48411800
C	4.87461500	1.90612200	-1.28078600
C	3.65427100	2.54766100	-0.88515000
C	-5.18637400	-2.55177100	1.50787100
C	-5.01072600	-1.85101800	2.68186200
C	-4.54239000	-0.52691900	2.64804600
C	-4.23946300	0.06102300	1.44009400
C	-4.83363000	-2.78240500	-3.43052300
C	-5.31848000	-4.07109600	-3.45410400
C	-5.70239500	-4.68997200	-2.25000600
C	-5.58574600	-4.02011000	-1.04965100
C	2.86093300	0.79154000	2.30242500
C	3.39291000	-0.16102900	3.14445900
C	4.61271100	-0.77923600	2.81909400
C	5.26546800	-0.45141500	1.64938400
C	6.56122700	0.19459900	-0.95586900

C	7.16356900	0.55963100	-2.14236100
C	6.64947000	1.62259100	-2.90791100
C	5.51781100	2.28099400	-2.48102400
H	-5.20350900	2.05282100	-2.28870500
H	-5.44468200	4.31139100	-3.16232600
H	-4.60507300	6.62918600	-3.40125000
H	-2.45529900	7.28384500	-2.32668800
H	-1.18265700	5.66718700	-0.99570500
H	2.72733500	4.15828400	2.07399500
H	-2.72384800	4.85365600	1.24007500
H	-2.59706200	6.53849800	3.01253900
H	-0.42277200	7.06807700	4.10785200
H	1.62360800	5.84625700	3.43425000
H	-0.11084700	-1.78088600	-2.01763400
H	-3.92737400	-0.28567300	-3.15034300
H	3.25954800	3.33609800	-1.52164200
H	-5.55793200	-3.56873700	1.55997900
H	-5.24115900	-2.32268100	3.63185400
H	-4.41446500	0.03043700	3.57043800
H	-3.88135400	1.08483400	1.41989700
H	-4.53653100	-2.28417300	-4.34932000
H	-5.40880300	-4.60626700	-4.39390400
H	-6.09205500	-5.70295100	-2.26373700
H	-5.88730700	-4.52847200	-0.14084800
H	1.91373000	1.26192300	2.54381400
H	2.86612400	-0.43510400	4.05335000
H	5.03853900	-1.52384900	3.48445700
H	6.20227200	-0.94595200	1.41883200
H	6.97783800	-0.63354500	-0.39373100
H	8.04097300	0.02104500	-2.48646600
H	7.13468900	1.90904200	-3.83562200
H	5.08976800	3.08837700	-3.06933300
C	3.17824300	-1.05033400	-2.02232300
C	3.50626000	-0.39937600	-3.20373600
C	4.39891500	-0.98287400	-4.10381100
C	4.95334000	-2.23240700	-3.82657800
C	4.61480100	-2.89445100	-2.65254300
C	3.73810700	-2.30569100	-1.72843200
C	3.38809100	-3.03526200	-0.51484900
C	2.77782500	-2.47166800	0.55535300
C	2.20013600	-3.22456400	1.62931500
N	1.28014700	-2.46753300	2.35108600
C	2.32912500	-4.59811500	1.75402500
C	0.52741200	-2.85704000	3.40982900

C	-0.49800900	-1.76990000	3.79769600
O	0.55532500	-3.91315000	4.00392700
F	-1.51169000	-1.76331500	2.92304300
F	-0.98748500	-2.00113200	5.00844800
F	0.05603500	-0.55051100	3.78434200
H	2.48316500	-0.58604200	-1.32638700
H	3.06279200	0.56749700	-3.42102500
H	4.65676700	-0.46541800	-5.02284200
H	5.64307100	-2.69060000	-4.52815500
H	5.03437600	-3.87330600	-2.43587300
H	3.65061000	-4.09050900	-0.50485900
H	2.57306600	-1.40582000	0.55252700
H	1.06631600	-1.54987800	1.93894400
H	1.92745700	-5.09971400	2.62306500
H	3.20624500	-5.04397700	1.30015500
C	-2.14261200	-4.26820100	-0.43893500
O	0.34955300	-2.73236300	-2.09608100
C	-1.06096800	-3.20359200	-0.19294500
C	0.14010900	-3.48063600	-1.06428500
C	0.96347000	-4.60035600	-0.85898200
C	0.95562200	-5.30358200	0.34842000
H	-2.99484400	-4.07295200	0.21512600
H	-2.49201400	-4.23360400	-1.47540400
H	-1.77094900	-5.27489600	-0.23557600
H	-0.77466300	-3.19471000	0.85897200
H	-1.46769800	-2.22029200	-0.43350300
H	1.68694000	-4.82890200	-1.63448000
H	1.43669300	-6.27613400	0.38334700
H	0.11625000	-5.19139300	1.02740600

INTI-2

C	-1.52528200	2.37430200	-0.26008500
C	-2.69333100	2.40542000	-1.06823300
C	-2.86097100	3.47575900	-1.91140300
C	-1.89629900	4.51358300	-1.99492000
C	-0.73369700	4.46698000	-1.17380700
C	-0.57886600	3.37384500	-0.25536300
C	-2.06874900	5.58969400	-2.90591100
C	-1.11801300	6.57054800	-3.02129900
C	0.05554000	6.50760400	-2.23318400
C	0.24470200	5.48628100	-1.33535600
C	0.61911200	3.24484400	0.61928300
C	0.99133100	4.26501300	1.55500200
C	2.24122000	4.16505900	2.22692400

C	3.10067200	3.07268200	1.93929900
C	2.71497300	2.05581000	1.10172700
C	1.42267300	2.12669200	0.50550700
C	0.14500400	5.36631400	1.85866400
C	0.53167200	6.31804100	2.76906200
C	1.78507900	6.22721700	3.42095100
C	2.61905000	5.17189400	3.15457900
O	1.02956000	1.08595500	-0.30714500
O	-1.34905500	1.29372000	0.57677900
P	-0.26982100	0.15902100	0.11360900
O	0.03279400	-0.57809500	1.39505500
O	-0.66465700	-0.55575100	-1.12813000
C	-3.70368500	1.31230000	-1.02073500
C	3.69552800	1.00602900	0.68736300
C	-3.90983200	0.55078600	-2.12799900
C	-4.95621700	-0.43022800	-2.19343700
C	-5.81732500	-0.61505000	-1.08580000
C	-5.55472500	0.13169200	0.13820600
C	-4.51274700	1.09668800	0.16493800
C	3.70814700	-0.32083000	1.26890000
C	4.65561000	-1.27939200	0.81637300
C	5.62053700	-0.91145400	-0.21338600
C	5.62612900	0.41863500	-0.69678200
C	4.63610900	1.34890100	-0.23259000
C	-6.31054000	-0.07418700	1.31458700
C	-6.06375300	0.64934000	2.46179000
C	-5.05021500	1.62182700	2.47694600
C	-4.29370500	1.84025300	1.34676400
C	-5.15118900	-1.18563000	-3.37113000
C	-6.19647100	-2.07714600	-3.47012600
C	-7.08258800	-2.23236000	-2.38766600
C	-6.89372800	-1.52095400	-1.22107900
C	2.82269800	-0.66030400	2.31525600
C	2.85508900	-1.91227000	2.89278900
C	3.77441600	-2.86984100	2.43395900
C	4.65370200	-2.55747900	1.41725100
C	6.56743700	-1.81621700	-0.74263300
C	7.49143400	-1.41065800	-1.68490600
C	7.50691300	-0.08134800	-2.14337800
C	6.58044200	0.81607200	-1.65805000
H	-3.74797000	3.53238000	-2.53671200
H	-2.96805900	5.61052300	-3.51525000
H	-1.25476600	7.38756800	-3.72228700
H	0.81773100	7.27241700	-2.34428400

H	1.15702200	5.44718100	-0.75103800
H	4.08813800	3.04736900	2.39258900
H	-0.82273000	5.44044100	1.37344300
H	-0.13195900	7.14634800	2.99619700
H	2.07767600	6.99020800	4.13498900
H	3.58050900	5.08173900	3.65251900
H	-1.78991400	-1.60233300	-2.20182500
H	-3.28605800	0.69591100	-3.00682900
H	4.64359400	2.35309800	-0.64947600
H	-7.09704600	-0.82001000	1.32744400
H	-6.65537200	0.46640200	3.35313900
H	-4.86023600	2.19784500	3.37683000
H	-3.51307400	2.59362200	1.36302600
H	-4.46327000	-1.04251100	-4.19974600
H	-6.34323600	-2.65060600	-4.37979800
H	-7.91769100	-2.92117700	-2.46770800
H	-7.59091500	-1.66678300	-0.40373600
H	2.10429400	0.07661000	2.65650000
H	2.16889700	-2.15607200	3.69734800
H	3.80055100	-3.85736300	2.88467700
H	5.36547500	-3.30798000	1.09245400
H	6.57794000	-2.84903500	-0.41261700
H	8.20929000	-2.12537900	-2.07506600
H	8.23877800	0.23126100	-2.88139800
H	6.56519500	1.84356900	-2.01181600
C	2.78335500	-1.20134700	-2.22115500
C	3.55302600	-0.43853900	-3.08544200
C	4.52539500	-1.04644300	-3.88335300
C	4.71168800	-2.42818400	-3.83913800
C	3.92864100	-3.20210300	-2.99311600
C	2.97347600	-2.59513600	-2.16036000
C	2.20207500	-3.43210500	-1.26570800
C	1.53947600	-2.96505400	-0.17274000
C	0.71455100	-3.76855700	0.66142100
N	0.11253800	-3.09553600	1.65025100
C	0.41236600	-5.20583700	0.39785100
C	-0.63255800	-3.63373600	2.69060600
C	-1.23162300	-2.52559100	3.58542100
O	-0.82397700	-4.79415300	2.94467100
F	-2.11736900	-1.80201400	2.89972300
F	-1.83964000	-3.06808700	4.63083400
F	-0.27134000	-1.70619000	4.02316500
H	2.00683300	-0.72562600	-1.62985200
H	3.39829300	0.63468900	-3.13561000

H	5.13223600	-0.44059100	-4.54915100
H	5.46245700	-2.89741000	-4.46635300
H	4.05868900	-4.27998600	-2.95483800
H	2.18756000	-4.49282200	-1.50454400
H	1.64602700	-1.92349200	0.11374700
H	0.14299100	-1.98861400	1.57752400
H	0.48100100	-5.78395100	1.31968300
H	1.12796800	-5.60558100	-0.31897800
C	-4.21430000	-3.45505000	-0.32781800
O	-2.01600800	-2.50783200	-2.48917400
C	-2.83390000	-2.80087200	-0.22821100
C	-1.94377200	-3.27048500	-1.35359400
C	-1.21496900	-4.39307900	-1.36316800
C	-1.02926600	-5.30935000	-0.18814900
H	-4.89977900	-3.04457300	0.41956200
H	-4.64575600	-3.28445000	-1.31885100
H	-4.13791800	-4.53598900	-0.17121900
H	-2.39312100	-3.02178900	0.74594000
H	-2.92434700	-1.70959100	-0.29323700
H	-0.64597200	-4.60987000	-2.26549900
H	-1.17520800	-6.35714000	-0.46931500
H	-1.75101200	-5.08886100	0.60231700

TSI-2

C	2.99886300	0.97510500	0.08413300
C	4.08778100	0.17618100	0.53157400
C	5.04711200	0.77252300	1.31194500
C	4.95081700	2.13701300	1.69149800
C	3.84732200	2.91939900	1.24520500
C	2.87089100	2.31583700	0.38510400
C	5.92868300	2.72560400	2.53749200
C	5.80944800	4.02800100	2.94851600
C	4.69435400	4.79646300	2.53698200
C	3.73948800	4.25900800	1.71015000
C	1.68185500	3.05234500	-0.12884900
C	1.78910500	4.23108800	-0.93583600
C	0.59763800	4.87924500	-1.37104000
C	-0.66523700	4.33120800	-1.03128700
C	-0.77384800	3.16932000	-0.30549000
C	0.42466900	2.54103900	0.13137500
C	3.03911600	4.76225200	-1.35920400
C	3.09640700	5.89212900	-2.13569200
C	1.91105800	6.55635400	-2.53471200
C	0.69064900	6.05544200	-2.16366900

O	0.32180300	1.37147700	0.85123800
O	2.03873700	0.36928300	-0.69466900
P	0.61750300	-0.02703700	0.02572500
O	-0.36833000	-0.19212000	-1.08690100
O	0.81842500	-1.05995900	1.08943000
C	4.13314700	-1.27796800	0.21651700
C	-2.10230300	2.59771700	0.05440000
C	4.07280700	-2.17035000	1.23952800
C	4.07015900	-3.58747800	1.01510300
C	4.14077400	-4.09176500	-0.30621200
C	4.24482800	-3.14787600	-1.41272900
C	4.24005800	-1.75270200	-1.15016400
C	-3.02418000	2.14535200	-0.97290000
C	-4.31588300	1.67753400	-0.60546800
C	-4.69026900	1.62399600	0.80215300
C	-3.75591300	2.05647100	1.77371000
C	-2.46700000	2.53330300	1.36251400
C	4.35216800	-3.57780900	-2.75490600
C	4.45869700	-2.67525000	-3.79133900
C	4.46798500	-1.29537800	-3.52660900
C	4.36202600	-0.84758000	-2.22867800
C	3.94945800	-4.47821500	2.10449900
C	3.89741900	-5.83912100	1.89931400
C	3.96569900	-6.34638500	0.58910500
C	4.08475000	-5.49184200	-0.48826100
C	-2.65241100	2.13428500	-2.33625200
C	-3.53361400	1.72079600	-3.31281000
C	-4.81915500	1.28119000	-2.95564700
C	-5.19347400	1.25135000	-1.62806300
C	-5.93194000	1.11990300	1.25187000
C	-6.23460200	1.06810600	2.59755500
C	-5.31141300	1.52473900	3.55660700
C	-4.09025200	2.01030700	3.14588400
H	5.89349400	0.18841100	1.66370000
H	6.76821200	2.11493000	2.85821300
H	6.55882800	4.46901100	3.59784300
H	4.59057000	5.81970200	2.88395500
H	2.88384900	4.85623500	1.41451600
H	-1.56416600	4.83948800	-1.37181000
H	3.95464600	4.25664200	-1.07159300
H	4.05997000	6.27805700	-2.45308300
H	1.97367100	7.45219800	-3.14396100
H	-0.22952100	6.54133800	-2.47637800
H	0.14927100	-2.46960300	1.85390900

H	3.98023300	-1.81338400	2.26198900
H	-1.77462200	2.86187600	2.13423000
H	4.35777700	-4.63688800	-2.98458700
H	4.54037100	-3.03347100	-4.81261600
H	4.55926300	-0.58422800	-4.34126600
H	4.37505100	0.21833200	-2.02454900
H	3.88924900	-4.06603300	3.10810600
H	3.80013200	-6.51751600	2.74082700
H	3.92120900	-7.41788900	0.42150600
H	4.12822900	-5.91587700	-1.48506600
H	-1.65157600	2.44688000	-2.61269500
H	-3.22738500	1.72460800	-4.35350100
H	-5.51246400	0.94789500	-3.72166700
H	-6.18616700	0.89607400	-1.37643700
H	-6.66653300	0.76068900	0.54020600
H	-7.19470300	0.67471600	2.91657500
H	-5.55741000	1.48280400	4.61298300
H	-3.35534000	2.34974300	3.87132400
C	-1.56390100	-0.30785200	3.15440100
C	-1.10447200	0.15082800	4.38134000
C	-1.80525000	-0.15484400	5.54930500
C	-2.96373400	-0.93338900	5.49603200
C	-3.42240100	-1.39975900	4.27284600
C	-2.73781400	-1.07801400	3.08652900
C	-3.29580500	-1.52805300	1.83329900
C	-2.95484800	-1.03668900	0.56629000
C	-3.42109900	-1.69196500	-0.55153200
N	-2.87971700	-1.30359200	-1.76620800
C	-4.27604800	-2.90231200	-0.40888700
C	-3.36511500	-1.60408800	-3.00147100
C	-2.40622600	-1.25544000	-4.15666200
O	-4.41615400	-2.13936400	-3.27990500
F	-1.86065400	-2.38506500	-4.61985200
F	-3.08591800	-0.69158000	-5.15548700
F	-1.41805700	-0.43672300	-3.79612900
H	-1.00596700	-0.07749500	2.25569400
H	-0.19780300	0.74548300	4.42629300
H	-1.44421000	0.20912800	6.50626300
H	-3.50188200	-1.17319500	6.40696500
H	-4.32629800	-2.00114700	4.21757300
H	-4.20725200	-2.10988700	1.93009800
H	-2.23608300	-0.22972900	0.45450000
H	-2.02080500	-0.73281300	-1.70277400
H	-4.65275400	-3.24363300	-1.36814000

H	-5.13758200	-2.63624800	0.20897500
C	0.69690700	-3.91571600	-0.29542400
O	-0.51272700	-3.12789200	2.18684400
C	-0.72570300	-3.35087700	-0.20661500
C	-1.30838400	-3.45973500	1.17229800
C	-2.60234600	-3.84585500	1.41505100
C	-3.55443800	-4.14595600	0.30368400
H	1.03964900	-3.87429200	-1.33277500
H	1.39268900	-3.32614400	0.30459600
H	0.73666600	-4.95701400	0.03868600
H	-1.37338800	-3.85475400	-0.92548700
H	-0.70417200	-2.29301600	-0.49069300
H	-2.90085400	-4.00260200	2.44687400
H	-4.37445700	-4.76507000	0.67286500
H	-3.06489000	-4.70974600	-0.49207900
P_I			
C	-2.38345900	-1.48507900	-0.61786900
C	-3.45264300	-2.13142100	-1.23844800
C	-4.68414900	-2.22334000	-0.59568100
C	-4.84102200	-1.66725400	0.67347500
C	-3.77272100	-1.02306400	1.28974800
C	-2.53152200	-0.92287200	0.65296700
C	-1.41058800	-0.15025400	1.33056000
C	-0.04065600	-0.62894000	0.93107100
C	1.01513200	0.16921700	0.73857500
N	2.26328600	-0.43340400	0.44006100
C	0.96284400	1.66703600	0.86626000
C	3.35750200	0.16745200	-0.06492400
C	4.56484400	-0.77511200	-0.23800900
O	3.50857700	1.33359000	-0.37524400
F	5.01919200	-0.70228800	-1.48888000
F	5.55031200	-0.39861100	0.57989500
F	4.27938500	-2.05840600	0.02510500
H	-1.42526900	-1.42086800	-1.12758900
H	-3.31907700	-2.56407000	-2.22540100
H	-5.51591200	-2.72714000	-1.07786500
H	-5.79621600	-1.73785100	1.18467300
H	-3.89800400	-0.59069500	2.27984700
H	-1.51344000	-0.33402800	2.40972200
H	0.08819900	-1.70692600	0.84154600
H	2.30828100	-1.43946000	0.56110300
H	1.07699600	2.12055300	-0.12218500
H	1.82901300	2.00590600	1.44220700

C	-2.08527800	1.58549500	-2.73737600
O	-3.29325000	2.16574200	-0.31011500
C	-1.27489200	1.64336100	-1.45013000
C	-2.15008100	1.76103200	-0.21851500
C	-1.60089900	1.38509800	1.15695600
C	-0.31902800	2.12841200	1.56628100
H	-1.42507400	1.52383600	-3.60571200
H	-2.74219200	0.71034100	-2.73884100
H	-2.71331400	2.47265800	-2.83948100
H	-0.61848400	2.52501900	-1.44963100
H	-0.61505600	0.77624100	-1.34561200
H	-2.40119800	1.68500500	1.84003100
H	-0.19671900	1.97090400	2.64369000
H	-0.44845300	3.20491000	1.41722000

COMII-1

C	2.56676900	0.15010500	-1.13795000
C	3.04054200	1.36657700	-1.69461800
C	4.14220800	1.31240600	-2.50828600
C	4.77480700	0.07381700	-2.80454700
C	4.28916600	-1.13351500	-2.22307300
C	3.16936900	-1.07425300	-1.32911400
C	5.88497700	0.02149100	-3.68883300
C	6.47696900	-1.17473500	-4.00307800
C	5.97493700	-2.37743900	-3.45165900
C	4.91009200	-2.35919500	-2.58575600
C	2.60056700	-2.26206100	-0.62994500
C	3.35936900	-3.07202800	0.27749300
C	2.70458300	-4.14023900	0.95781200
C	1.31471500	-4.35677700	0.76923900
C	0.56941500	-3.55310900	-0.05859400
C	1.25316300	-2.52486500	-0.75976300
C	4.72675400	-2.81687700	0.57732000
C	5.40814000	-3.60395400	1.47178700
C	4.76633200	-4.68925500	2.11575500
C	3.44380900	-4.94620800	1.86577200
O	0.50453200	-1.71251400	-1.60452300
O	1.43306100	0.23885800	-0.34481400
P	0.04061100	-0.30948600	-0.96395600
O	-0.95290200	-0.38452400	0.12358200
O	-0.30190600	0.51243500	-2.23118200
C	2.32203800	2.62599700	-1.34624400
C	-0.90824500	-3.68748300	-0.21230300
C	1.44424300	3.17976200	-2.22111700

C	0.66454000	4.33593000	-1.87620900
C	0.83932000	4.95835400	-0.61721000
C	1.77994200	4.37526900	0.33048800
C	2.50413700	3.20888300	-0.03043700
C	-1.79630900	-3.34846500	0.88606400
C	-3.20270800	-3.40996500	0.69381200
C	-3.73986600	-3.83768700	-0.59163200
C	-2.83883900	-4.15887500	-1.63487200
C	-1.42540900	-4.06249800	-1.41078500
C	1.96971000	4.90819000	1.62611400
C	2.83336900	4.31803900	2.52469800
C	3.55242100	3.16720600	2.16125600
C	3.38700600	2.62494300	0.90594300
C	-0.32409900	4.81305300	-2.76647500
C	-1.11618400	5.88944700	-2.42954400
C	-0.92514800	6.53103500	-1.19165000
C	0.03352300	6.07720400	-0.30877200
C	-1.29347200	-2.91054700	2.13281600
C	-2.14096000	-2.55562000	3.16040900
C	-3.53186200	-2.61071200	2.97104200
C	-4.04664600	-3.02648900	1.76139400
C	-5.12496000	-3.93853600	-0.85377400
C	-5.58813500	-4.33581900	-2.09101100
C	-4.68733400	-4.65118600	-3.12463100
C	-3.33257500	-4.56387300	-2.89498600
H	4.53955000	2.22455600	-2.94513600
H	6.24878900	0.95168500	-4.11609500
H	7.32279200	-1.20501600	-4.68222800
H	6.43355100	-3.32359900	-3.72067000
H	4.52570100	-3.28848000	-2.17845600
H	0.82943800	-5.15568700	1.32412600
H	5.22880600	-1.98070200	0.10318600
H	6.44908900	-3.38942700	1.69164900
H	5.32119800	-5.30488100	2.81613600
H	2.93003300	-5.76144100	2.36732700
H	-1.12194500	1.15939400	-2.15029500
H	1.28088900	2.71883300	-3.19154700
H	-0.76028000	-4.29157400	-2.23983500
H	1.42801900	5.79594700	1.93196200
H	2.95616200	4.74386500	3.51572100
H	4.22889900	2.69996700	2.86950800
H	3.94260100	1.73437200	0.62823700
H	-0.45455400	4.30588500	-3.71895000
H	-1.87826100	6.24599400	-3.11565600

H	-1.53841500	7.38659000	-0.92639100
H	0.14597900	6.58635300	0.64156200
H	-0.22020200	-2.83718100	2.27554700
H	-1.73178700	-2.21526100	4.10677300
H	-4.20245000	-2.31671500	3.77235300
H	-5.12223600	-3.04827100	1.63270000
H	-5.84597500	-3.70527200	-0.07909600
H	-6.65701100	-4.40499000	-2.26668900
H	-5.06032600	-4.96133600	-4.09545400
H	-2.62004900	-4.80213700	-3.67996200
C	1.65127300	0.05620900	2.89928100
C	2.95745600	-0.37620900	3.09921800
C	3.70393900	0.10860700	4.17447000
C	3.13848800	1.04419800	5.03905100
C	1.83415100	1.48697300	4.83251900
C	1.06600500	0.98592600	3.77334800
C	-0.32196500	1.44603400	3.59841000
C	-1.24644800	0.75476000	2.91930500
C	-2.64858000	1.15914700	2.70795700
N	-3.18142700	0.55934800	1.54362500
C	-3.32833300	1.99167100	3.51152200
C	-4.40915600	0.75665800	1.03709500
C	-4.69401000	-0.02348600	-0.26239900
O	-5.30594500	1.45700400	1.47557700
F	-3.61871700	-0.62539500	-0.77401400
F	-5.62541600	-0.95582800	-0.03499600
F	-5.17799800	0.81371500	-1.18677300
H	1.09148700	-0.30383400	2.04036800
H	3.39838700	-1.08977500	2.40796600
H	4.72239000	-0.23421400	4.32904500
H	3.71443500	1.43358200	5.87310800
H	1.39608900	2.21974500	5.50543200
H	-0.57997900	2.39285000	4.07201800
H	-0.96512800	-0.18346600	2.45042300
H	-2.52147300	0.00967100	0.98620800
H	-4.34760100	2.28653200	3.31449200
H	-2.83773000	2.36436700	4.40338100
C	-4.47287900	3.51985400	-2.71103700
O	-2.27414700	2.00327400	-2.15626500
C	-3.81306600	3.61059500	-1.34367400
C	-2.54949200	2.79583000	-1.24678400
C	-1.65964700	2.93254000	-0.08331300
C	-1.93305900	3.72587300	0.95598400
H	-5.38931300	4.11365500	-2.72440300

H	-3.80419500	3.89968400	-3.48850500
H	-4.72238400	2.48700200	-2.95852400
H	-4.48564500	3.25370000	-0.55177800
H	-3.56714000	4.64703400	-1.08991900
H	-0.73540100	2.35865800	-0.10820900
H	-1.23657300	3.80172100	1.78609500
H	-2.84291100	4.31603600	1.01967300

TSII-1

C	2.46577400	0.36671800	-1.19345000
C	2.79341400	1.62092100	-1.77572300
C	3.85367100	1.67643200	-2.64233200
C	4.59608700	0.50799000	-2.96736600
C	4.26064300	-0.73945000	-2.36459100
C	3.18181200	-0.79017200	-1.42160100
C	5.66604100	0.56464200	-3.89967900
C	6.36386000	-0.56605200	-4.23906900
C	6.01197300	-1.81072300	-3.66489000
C	4.98837700	-1.89665000	-2.75426600
C	2.75884900	-2.02850000	-0.70714100
C	3.62529200	-2.75949100	0.16971700
C	3.10338100	-3.88429700	0.87295000
C	1.73425800	-4.23271700	0.73493500
C	0.88536400	-3.50416300	-0.06181200
C	1.43573500	-2.41348700	-0.79099300
C	4.97184500	-2.37277700	0.41922900
C	5.76016800	-3.08795200	1.28616000
C	5.25091200	-4.22867700	1.95259600
C	3.95061400	-4.61247000	1.75162800
O	0.58947200	-1.67267000	-1.59358700
O	1.38539300	0.34363900	-0.34051900
P	-0.01043800	-0.32899800	-0.88469600
O	-0.78545600	-0.65429700	0.34388100
O	-0.59567300	0.48908200	-2.00336500
C	1.96116800	2.79915000	-1.40229700
C	-0.57641200	-3.78515100	-0.15837500
C	1.01558700	3.26547800	-2.25661500
C	0.11905500	4.32372700	-1.88507100
C	0.23200500	4.93323800	-0.61237800
C	1.25171800	4.45117600	0.31000100
C	2.10234200	3.38538500	-0.08340700
C	-1.45280500	-3.54344600	0.97452200
C	-2.85256600	-3.73440300	0.83135300
C	-3.39301600	-4.20914600	-0.43595100

C	-2.50386600	-4.43764600	-1.51315200
C	-1.09966800	-4.20211800	-1.34024600
C	1.40620200	4.98800100	1.60942800
C	2.35759600	4.49793000	2.47955300
C	3.20289800	3.44770200	2.08275000
C	3.07296900	2.90363200	0.82441100
C	-0.91973700	4.71021900	-2.76104200
C	-1.82686100	5.68088900	-2.39422000
C	-1.70592300	6.30567800	-1.13892600
C	-0.69613400	5.94272800	-0.27083600
C	-0.94992400	-3.06010100	2.20478200
C	-1.78979100	-2.77732200	3.25962000
C	-3.17659400	-2.96002800	3.11821800
C	-3.69159500	-3.42736600	1.92823900
C	-4.77040800	-4.44376500	-0.64820000
C	-5.23830800	-4.88255600	-1.86949000
C	-4.34949300	-5.10613200	-2.93699200
C	-3.00235200	-4.88607200	-2.75674800
H	4.13332800	2.62211300	-3.09898100
H	5.91340100	1.52507400	-4.34350500
H	7.17813100	-0.51309900	-4.95452000
H	6.55317000	-2.70662500	-3.95230600
H	4.71928400	-2.85824000	-2.32968300
H	1.34923200	-5.07411200	1.30587400
H	5.37113300	-1.49278100	-0.07313800
H	6.78316500	-2.77323800	1.46662900
H	5.88857000	-4.78668000	2.63053200
H	3.53741300	-5.47254800	2.27119500
H	-1.78227200	1.27193200	-2.00345800
H	0.88435200	2.79758700	-3.22832600
H	-0.44726100	-4.35610900	-2.19620800
H	0.77025600	5.80240800	1.93833200
H	2.45343200	4.92572400	3.47287100
H	3.94713600	3.05660900	2.76940400
H	3.72421900	2.08968300	0.52109900
H	-0.99837100	4.21449100	-3.72497100
H	-2.62692100	5.96785900	-3.06968500
H	-2.41198200	7.07809200	-0.84983900
H	-0.63468800	6.43846800	0.69144300
H	0.11601800	-2.88657300	2.30702700
H	-1.38080600	-2.39962100	4.19188300
H	-3.84359500	-2.72900600	3.94283800
H	-4.76426200	-3.55174300	1.83738600
H	-5.48114600	-4.28386000	0.15430700

H	-6.30103000	-5.05613100	-2.00624900
H	-4.72582800	-5.44939800	-3.89533300
H	-2.29951100	-5.05076600	-3.56887400
C	1.78958800	0.17542400	2.94432200
C	3.10593300	-0.20355800	3.18174800
C	3.81887700	0.35649100	4.24323200
C	3.21334800	1.31015700	5.06071400
C	1.90018400	1.70192500	4.81744100
C	1.16761400	1.12611200	3.77084100
C	-0.21688500	1.55057200	3.53130000
C	-1.11178600	0.77559900	2.89322600
C	-2.45675200	1.17365000	2.49828600
N	-2.98452700	0.34472900	1.52939600
C	-3.04527900	2.37701600	2.82829000
C	-4.21815500	0.46011100	0.96560700
C	-4.45883700	-0.44914100	-0.25725400
O	-5.13952900	1.16428300	1.32565600
F	-3.34204600	-0.98432100	-0.74667000
F	-5.29328000	-1.43888300	0.07307400
F	-5.03815100	0.27232000	-1.21941400
H	1.25408000	-0.23031900	2.08900300
H	3.58273700	-0.92977800	2.52881500
H	4.84665400	0.05749000	4.42443700
H	3.76653100	1.75417800	5.88244300
H	1.42883900	2.45321100	5.44590600
H	-0.48742100	2.54175800	3.89374700
H	-0.81248000	-0.21444100	2.56582200
H	-2.29214900	-0.26908300	1.05435800
H	-4.08921000	2.55075800	2.61970600
H	-2.59930700	2.95548300	3.62908200
C	-4.86681100	3.31463500	-2.50825600
O	-2.66971700	1.82500000	-2.08610200
C	-4.24103900	3.30665600	-1.11915200
C	-2.93049500	2.56935400	-1.05796000
C	-2.03704600	2.66932100	0.01166300
C	-2.25559900	3.43395300	1.15775500
H	-5.79783700	3.88554600	-2.49114800
H	-4.19262500	3.77354300	-3.23661800
H	-5.08687600	2.30063300	-2.84630300
H	-4.92034500	2.83588000	-0.39520700
H	-4.07609400	4.32882600	-0.76541000
H	-1.10299800	2.11879500	-0.06512400
H	-1.38160600	3.69072000	1.75153400
H	-3.07692300	4.14431200	1.19305200

INTII-2

C	-2.24924100	1.16980100	-1.01071700
C	-3.40763900	0.47998000	-1.46422800
C	-4.34143700	1.18900400	-2.17797300
C	-4.16834500	2.56498900	-2.47575600
C	-3.01739900	3.24670500	-1.99137800
C	-2.06423100	2.52479600	-1.20445100
C	-5.12052500	3.27468200	-3.25292600
C	-4.93430600	4.59723300	-3.55733200
C	-3.77619100	5.26859200	-3.10134500
C	-2.84268000	4.61303100	-2.34018200
C	-0.85819500	3.15305300	-0.60190300
C	-0.94357000	4.20882700	0.36191700
C	0.25268600	4.67705400	0.97654700
C	1.48887200	4.06474300	0.65414000
C	1.57217000	3.02029100	-0.23532600
C	0.37523000	2.59540500	-0.87634300
C	-2.18102200	4.77518400	0.77975400
C	-2.21698500	5.76725900	1.72680800
C	-1.02343300	6.25160900	2.31197200
C	0.18092000	5.71401400	1.94453700
O	0.43402700	1.55583700	-1.77796000
O	-1.29413700	0.44966200	-0.32631200
P	0.09296000	0.08007100	-1.14876200
O	1.10493400	-0.19175400	-0.06777200
O	-0.17083300	-0.88134200	-2.25064700
C	-3.60115100	-0.96685200	-1.17586600
C	2.86622800	2.33202300	-0.49439400
C	-3.64519700	-1.85095300	-2.20498600
C	-3.86032400	-3.25381000	-1.99461600
C	-4.04093000	-3.74793700	-0.68114800
C	-4.00903700	-2.80991400	0.43344300
C	-3.79193000	-1.43044500	0.18509600
C	3.55271900	1.63515700	0.57949500
C	4.80894400	1.02324000	0.33021700
C	5.41394600	1.12848600	-0.99090000
C	4.68555800	1.76529600	-2.02281900
C	3.40663000	2.34726200	-1.73876100
C	-4.18133300	-3.22735100	1.76996700
C	-4.15237000	-2.32866100	2.81592300
C	-3.95941000	-0.96276000	2.56335100
C	-3.78123900	-0.52801400	1.26878900
C	-3.86877200	-4.14309600	-3.08828300

C	-4.05143800	-5.49451600	-2.89898800
C	-4.23231100	-5.99108800	-1.59855100
C	-4.22667800	-5.13555600	-0.51657500
C	2.96884200	1.49958700	1.85984200
C	3.59230300	0.79013300	2.86273900
C	4.83031800	0.17612400	2.61616500
C	5.41976600	0.29319100	1.37558300
C	6.68763200	0.60603300	-1.30127100
C	7.20689200	0.69995800	-2.57439200
C	6.47263500	1.32104700	-3.59869100
C	5.23199800	1.84659000	-3.32131900
H	-5.23779500	0.68261200	-2.52590900
H	-5.99885900	2.74268100	-3.60767200
H	-5.66674400	5.12985100	-4.15483900
H	-3.62273000	6.31091500	-3.36136000
H	-1.95161800	5.13242700	-2.00370100
H	2.39019600	4.40921000	1.15532200
H	-3.10431200	4.40721300	0.34669500
H	-3.17163700	6.18366300	2.03190000
H	-1.06776600	7.03956200	3.05631600
H	1.10474100	6.06312700	2.39718600
H	-0.94896900	-2.28772100	-1.37649100
H	-3.48506100	-1.49819700	-3.22063200
H	2.87045900	2.83235300	-2.54997200
H	-4.34224500	-4.27618900	1.99092800
H	-4.29001100	-2.67969700	3.83415600
H	-3.94392500	-0.24875700	3.38173200
H	-3.62956900	0.52944600	1.07649100
H	-3.72002900	-3.74038500	-4.08649900
H	-4.05281700	-6.17222000	-3.74646800
H	-4.37360100	-7.05555300	-1.44084000
H	-4.36181900	-5.55329600	0.47425000
H	1.99907200	1.95027700	2.04335100
H	3.11761300	0.69642300	3.83477100
H	5.32457100	-0.39245200	3.39739900
H	6.36711700	-0.20284400	1.20219800
H	7.28055400	0.12387700	-0.53293200
H	8.18941200	0.29051500	-2.78515700
H	6.88505200	1.38784900	-4.60000100
H	4.65208600	2.33541300	-4.09895300
C	-1.16137800	0.96381600	3.01113200
C	-1.97510600	2.02827600	3.36922900
C	-2.60260600	2.04317000	4.61655400
C	-2.43084200	0.98314000	5.50558200

C	-1.62326400	-0.08845500	5.14941900
C	-0.96280100	-0.10118000	3.91128400
C	-0.09694400	-1.22099800	3.58813200
C	0.81856400	-1.17209700	2.58839100
C	1.69510400	-2.22886300	2.20074100
C	1.69035900	-3.58255400	2.83776800
C	3.52638300	-2.70955900	0.68061100
C	4.11674200	-2.26922500	-0.67962900
O	4.03208300	-3.64564700	1.24276100
F	3.49615400	-1.21289200	-1.19462900
F	5.40858700	-1.98708500	-0.52087700
F	4.02572900	-3.28203100	-1.54255400
H	-0.72508800	0.93356000	2.01500200
H	-2.12812000	2.84625600	2.67157200
H	-3.23602800	2.88093200	4.89013000
H	-2.92780500	0.99230200	6.46958000
H	-1.48664200	-0.92011000	5.83527400
H	-0.20769900	-2.10713200	4.20937600
H	0.91305700	-0.26313700	2.01103900
H	2.70106000	-3.88564300	3.11435700
H	1.08098100	-3.54492100	3.74010100
C	0.58711200	-4.15590600	-2.49986700
O	-1.17844500	-2.86624000	-0.61939600
C	1.05267500	-3.60080900	-1.15102400
C	-0.07636900	-3.49679300	-0.15921700
C	-0.09754500	-3.99068400	1.09059900
C	1.07230700	-4.59209400	1.81768200
H	1.44650000	-4.29874200	-3.15984200
H	0.07735800	-5.11535200	-2.37598100
H	-0.09719100	-3.46050500	-2.99105000
H	1.45788700	-2.59584100	-1.32525400
H	1.85195600	-4.23043100	-0.75283700
H	-1.01149700	-3.81854800	1.65673600
H	0.78233900	-5.48153700	2.38628900
H	1.85907400	-4.90676600	1.12986800
N	2.45618900	-1.94532300	1.13660500
H	2.05935000	-1.12601800	0.52318800
P_{II}			
C	-2.34192700	-1.37923000	0.69321400
C	-3.40946500	-2.01256200	1.32662300
C	-4.57991800	-2.28761500	0.62174100
C	-4.67479400	-1.93075600	-0.72227600
C	-3.60645200	-1.29676200	-1.35292500

C	-2.43139700	-1.00966000	-0.65304900
C	-1.32105800	-0.22660000	-1.33205800
C	0.05041900	-0.66929600	-0.89526700
C	1.08883900	0.15674300	-0.72628100
C	1.02182000	1.64253800	-0.94363500
C	3.44383700	0.23080000	0.05856600
C	4.61832800	-0.71133100	0.39074200
O	3.63823900	1.42538900	0.17872500
F	4.31503900	-2.01122200	0.25980800
F	5.64797100	-0.44849900	-0.41665900
F	5.01962900	-0.50810300	1.64620500
H	-1.43551400	-1.15426600	1.24959600
H	-3.32620700	-2.29012000	2.37310600
H	-5.41127300	-2.78084100	1.11547200
H	-5.58005900	-2.14803800	-1.28098500
H	-3.68301900	-1.01605600	-2.40092400
H	-1.41436000	-0.40974000	-2.41186000
H	0.18782700	-1.73737500	-0.73080600
H	1.11522500	2.14493400	0.02198600
H	1.87961900	1.95881600	-1.54378700
C	-3.55911500	2.07027100	2.11728900
O	-0.98912700	1.62463800	1.17550500
C	-3.28715200	1.95826000	0.62678900
C	-1.84395300	1.63210000	0.30991600
C	-1.51715200	1.30488100	-1.14329800
C	-0.27435400	2.04674000	-1.65064200
H	-4.60667000	2.31902000	2.30247800
H	-3.33612000	1.12427800	2.61908900
H	-2.93306200	2.84222100	2.57094700
H	-3.52228000	2.89430500	0.10060200
H	-3.91525900	1.19134700	0.15537500
H	-2.38204900	1.59688400	-1.74927700
H	-0.18079700	1.83158300	-2.72123500
H	-0.41771500	3.12722100	-1.55331800
N	2.32965300	-0.41021400	-0.34135000
H	2.35844200	-1.42361900	-0.31773500

COMIII-1

C	-1.47299000	2.48500200	-0.32137900
C	-2.74661200	2.50514900	-0.94787300
C	-3.15907000	3.68206900	-1.51993100
C	-2.33567700	4.83923300	-1.50510900
C	-1.06978900	4.80148500	-0.85361400
C	-0.65684600	3.58824700	-0.20742900

C	-2.75631000	6.03569600	-2.14471600
C	-1.94862200	7.14337600	-2.16089300
C	-0.67589700	7.09678000	-1.54406600
C	-0.24637500	5.95876700	-0.90795000
C	0.63103400	3.46530600	0.53059400
C	0.96059800	4.30143300	1.64779500
C	2.22813800	4.14175000	2.27787300
C	3.12439400	3.14314400	1.81728400
C	2.78972200	2.29983300	0.78689300
C	1.52295200	2.47626600	0.17285600
C	0.05646800	5.26074900	2.18218300
C	0.41104600	6.03718300	3.25644100
C	1.68557700	5.90171100	3.85807200
C	2.57017700	4.97053800	3.38054400
O	1.19300600	1.62138200	-0.87031500
O	-1.05781000	1.27450000	0.21566300
P	0.10356200	0.47005800	-0.57552800
O	0.54297100	-0.64373800	0.29464600
O	-0.36560900	0.18255000	-2.02124700
C	-3.59269900	1.27946800	-0.96970100
C	3.71533200	1.23400800	0.30395700
C	-3.84130000	0.65469400	-2.15042000
C	-4.68942200	-0.50179000	-2.23289900
C	-5.26990500	-1.03633600	-1.05774800
C	-4.98361500	-0.39750900	0.22194500
C	-4.16232300	0.75983900	0.26121900
C	3.87633100	0.00861600	1.06074600
C	4.78027200	-0.98651400	0.60215700
C	5.48667900	-0.79173000	-0.65754700
C	5.29741200	0.41949000	-1.36719200
C	4.40932800	1.41990200	-0.84809600
C	-5.48292700	-0.90783800	1.44084700
C	-5.19672000	-0.29934000	2.64476900
C	-4.40459900	0.86001600	2.67766800
C	-3.90052100	1.37770700	1.50456700
C	-4.95857800	-1.09549500	-3.48609900
C	-5.79592200	-2.18479600	-3.58425200
C	-6.36977700	-2.72576200	-2.41980500
C	-6.10640100	-2.16886900	-1.18446700
C	3.14251500	-0.21993400	2.24719900
C	3.32135200	-1.37149100	2.98334700
C	4.24723100	-2.33795500	2.55471500
C	4.95260600	-2.15053000	1.38524800
C	6.33473100	-1.77115700	-1.22177300

C	6.97231300	-1.55163600	-2.42525100
C	6.78971900	-0.34235500	-3.11998900
C	5.96220100	0.62591700	-2.59558900
H	-4.13214700	3.73490400	-2.00071700
H	-3.72951400	6.04838300	-2.62729800
H	-2.27539600	8.05256600	-2.65498300
H	-0.03031500	7.96851200	-1.57951100
H	0.73712300	5.93363200	-0.45171800
H	4.08797300	3.03509900	2.30865700
H	-0.92824700	5.36734500	1.74040500
H	-0.29517800	6.75918300	3.65383400
H	1.95174100	6.52761500	4.70360000
H	3.54543300	4.83966200	3.84098000
H	-0.86695800	-0.68811900	-2.30750200
H	-3.39713000	1.03307900	-3.06770100
H	4.28517200	2.33939000	-1.41505200
H	-6.09726400	-1.80075700	1.44293900
H	-5.58594700	-0.71862300	3.56722800
H	-4.18692700	1.34587700	3.62348500
H	-3.28992400	2.27447900	1.53382400
H	-4.49548300	-0.66891800	-4.37179100
H	-6.00503100	-2.63027700	-4.55182800
H	-7.02503900	-3.58840800	-2.49016400
H	-6.56842900	-2.60813300	-0.30768800
H	2.42706600	0.52643700	2.57631600
H	2.74718400	-1.53154800	3.89094500
H	4.39294900	-3.24478100	3.13317500
H	5.64587200	-2.92022200	1.06560400
H	6.48296600	-2.71978700	-0.71889200
H	7.61453000	-2.32171900	-2.84071100
H	7.29329000	-0.17835800	-4.06735900
H	5.80068200	1.56239800	-3.12257000
C	-1.19418200	-2.38146400	3.78683000
C	-2.21631300	-1.99103100	4.64273700
C	-3.07173600	-2.94211400	5.20211900
C	-2.89414000	-4.28947800	4.89898000
C	-1.87217900	-4.68089400	4.03836700
C	-1.00998000	-3.73671800	3.46492900
C	0.03187900	-4.20312200	2.53721000
C	0.84424500	-3.41141300	1.82332100
C	1.88178900	-3.89341200	0.89101100
N	2.13314100	-2.94152100	-0.12268300
C	2.50597500	-5.07583300	0.99419400
C	2.91605700	-3.10713600	-1.20612700

C	2.71461300	-1.98465400	-2.24657300
O	3.64586800	-4.04195800	-1.47592100
F	2.58540500	-0.77748500	-1.68058700
F	3.72469500	-1.94211200	-3.10505700
F	1.58474600	-2.21726800	-2.93721100
H	-0.53777100	-1.62521300	3.36487300
H	-2.34583100	-0.93879100	4.87636300
H	-3.86816800	-2.63219800	5.87148500
H	-3.55195800	-5.03738200	5.33073200
H	-1.73687300	-5.73251700	3.79923700
H	0.10762900	-5.28410200	2.42449800
H	0.73566200	-2.32995400	1.87298800
H	1.64587100	-2.04251900	-0.02501600
H	3.25309700	-5.39926900	0.28522200
H	2.25949000	-5.72171100	1.82887500
C	-2.19995300	-2.22389100	0.09606600
O	-1.62561100	-1.74723600	-2.92233100
C	-1.33664300	-2.98741600	-0.91680900
C	-1.89008700	-2.78224100	-2.29789300
C	-2.80933200	-3.74788800	-2.91772700
C	-3.36608400	-4.75391700	-2.23960800
H	-1.71340100	-2.21364200	1.07361100
H	-2.34368200	-1.18612400	-0.22358500
H	-3.18699500	-2.68471400	0.19287100
H	-1.27979200	-4.04748000	-0.66381000
H	-0.32161000	-2.58303400	-0.91592000
H	-3.06953600	-3.54164300	-3.95172100
H	-4.09136300	-5.40862400	-2.71301300
H	-3.13431000	-4.95073300	-1.19669800

TSIII-1

C	-2.31308100	1.47484200	-0.84178600
C	-3.52497900	1.00646000	-1.41831500
C	-4.33587900	1.91534700	-2.05204500
C	-3.98220400	3.28627000	-2.14752800
C	-2.77756400	3.74476400	-1.54372500
C	-1.95258000	2.80684400	-0.84121900
C	-4.80994300	4.20722900	-2.84373500
C	-4.45092900	5.52545200	-2.95648400
C	-3.23829300	5.97764900	-2.38276600
C	-2.42285000	5.11338000	-1.69581500
C	-0.69354200	3.20217100	-0.15563400
C	-0.66429200	4.14548600	0.92193300
C	0.58421100	4.44383400	1.53829300

C	1.76027100	3.78563600	1.09765300
C	1.72871400	2.84121200	0.09942500
C	0.47641300	2.56609000	-0.51258100
C	-1.83831000	4.76042300	1.43895500
C	-1.76417700	5.64582700	2.48493000
C	-0.51676200	5.96845700	3.07232100
C	0.62941500	5.37635100	2.60988500
O	0.41878900	1.58844200	-1.49297800
O	-1.49597900	0.54947200	-0.22393400
P	-0.07838400	0.13211200	-0.94712900
O	0.80428800	-0.37554800	0.14313700
O	-0.34729200	-0.72288500	-2.16018600
C	-3.91050200	-0.42860400	-1.33185700
C	2.96706400	2.15349400	-0.35727300
C	-3.95249300	-1.18010300	-2.46212600
C	-4.36448400	-2.55517900	-2.44477200
C	-4.77842900	-3.15130000	-1.22971800
C	-4.74757000	-2.35455600	-0.00929400
C	-4.29846600	-1.00899600	-0.05916600
C	3.73861200	1.32184700	0.54854500
C	4.96117000	0.75006200	0.10299900
C	5.44887300	1.04044800	-1.23910100
C	4.63393900	1.80095700	-2.10965200
C	3.39111000	2.33566900	-1.63533000
C	-5.13780900	-2.88664000	1.24090200
C	-5.08248200	-2.13011700	2.39203700
C	-4.63858500	-0.79841600	2.33917100
C	-4.25795700	-0.25098600	1.13357800
C	-4.35235300	-3.31576500	-3.63501800
C	-4.73910500	-4.63752000	-3.63008100
C	-5.15577600	-5.23452200	-2.42614000
C	-5.17522700	-4.50740400	-1.25372600
C	3.28322900	1.03593300	1.85647400
C	4.00946300	0.22648400	2.70451800
C	5.20766100	-0.35601000	2.25984200
C	5.66406800	-0.10580800	0.98205600
C	6.69796200	0.58814500	-1.72020700
C	7.10498400	0.85998000	-3.00939700
C	6.28006900	1.59855600	-3.87816700
C	5.06477100	2.06416900	-3.42945200
H	-5.27089500	1.58183600	-2.49437900
H	-5.72977400	3.83990200	-3.29026600
H	-5.08661700	6.22270800	-3.49254600
H	-2.94819600	7.01776100	-2.49276500

H	-1.49021200	5.47036900	-1.27217500
H	2.70450900	4.02377600	1.58135300
H	-2.80183100	4.51475200	1.00556400
H	-2.67140300	6.10071400	2.86970000
H	-0.47513000	6.67492500	3.89501300
H	1.59261700	5.59877400	3.06065500
H	0.13581000	-2.06889200	-2.01654100
H	-3.65239900	-0.74523300	-3.41198800
H	2.79873700	2.93683500	-2.32073300
H	-5.48770000	-3.91052700	1.30671900
H	-5.38498600	-2.56483000	3.33933400
H	-4.59417800	-0.20262100	3.24525100
H	-3.92533700	0.78152900	1.09417000
H	-4.02621500	-2.83624100	-4.55386100
H	-4.72313900	-5.21711700	-4.54742700
H	-5.46180300	-6.27582900	-2.41723000
H	-5.49485900	-4.99958900	-0.34207800
H	2.33662500	1.45025000	2.18782200
H	3.63862900	0.01887100	3.70360800
H	5.76859700	-1.01619600	2.91399700
H	6.57765100	-0.58590600	0.64999600
H	7.35691300	0.01894600	-1.07415900
H	8.06917600	0.50104800	-3.35526300
H	6.60536200	1.80409200	-4.89295700
H	4.41812700	2.64606800	-4.08045600
C	-0.92539500	-0.10432100	3.46908900
C	-1.85532500	0.79330600	3.97744100
C	-2.27460700	0.69862300	5.30609700
C	-1.76380700	-0.30813900	6.12317300
C	-0.82665000	-1.20502400	5.61952200
C	-0.38092700	-1.10509800	4.29457400
C	0.63839800	-2.04023000	3.80355400
C	1.34148400	-1.80178000	2.68229100
C	2.31374500	-2.68192200	2.04869700
N	2.76814700	-2.18529900	0.84699900
C	2.58454800	-3.97811800	2.44238700
C	3.73714700	-2.75164200	0.06829600
C	3.83991100	-2.18280200	-1.36070700
O	4.49643400	-3.64691200	0.36778700
F	3.08570500	-1.09892800	-1.55479700
F	5.11073000	-1.87724500	-1.62215100
F	3.46554100	-3.11946100	-2.23600800
H	-0.63919100	-0.03953900	2.42136800
H	-2.26148600	1.56544800	3.33022300

H	-3.00326100	1.40145400	5.69795100
H	-2.09364900	-0.39344400	7.15371800
H	-0.42233900	-1.98661600	6.25724700
H	0.80449400	-2.93696300	4.39893800
H	1.17144100	-0.87280900	2.15189700
H	2.26240700	-1.36532900	0.47094100
H	3.47551200	-4.47644400	2.09510700
H	2.17115300	-4.31015900	3.38833200
C	-1.79859800	-4.31188700	-0.00415500
O	0.65524900	-2.96785700	-1.84814300
C	-0.81022900	-3.13527200	0.06988700
C	0.44748500	-3.48824700	-0.68126300
C	1.34247000	-4.46498200	-0.21846000
C	1.29540700	-4.96565200	1.08501300
H	-2.70985800	-4.05702100	0.54042200
H	-2.06667700	-4.52221700	-1.04369100
H	-1.37650400	-5.22085700	0.42954600
H	-0.57188300	-2.89448400	1.10885000
H	-1.27363900	-2.25477000	-0.38015400
H	2.13384800	-4.77091200	-0.89496000
H	1.83029100	-5.88405900	1.30424200
H	0.41771100	-4.78916000	1.69970100

INTIII-2

C	-2.00673400	2.12871900	-0.36310300
C	-3.25386800	1.91762700	-1.01097500
C	-3.89719300	3.00626900	-1.54472000
C	-3.33499900	4.30805600	-1.47009700
C	-2.09642500	4.50506600	-0.79539700
C	-1.44660400	3.37759500	-0.19277700
C	-3.98849700	5.41809900	-2.06899900
C	-3.43001300	6.66940700	-2.02353000
C	-2.18336400	6.86170500	-1.38150000
C	-1.53350500	5.81063000	-0.78387700
C	-0.17053800	3.48678700	0.56600900
C	-0.03935000	4.30524900	1.73525700
C	1.21643300	4.35389200	2.40522400
C	2.29650600	3.56795400	1.92852300
C	2.15875400	2.73985400	0.84190200
C	0.90236100	2.70936800	0.17607200
C	-1.12469000	5.04363200	2.28442700
C	-0.95534900	5.81171800	3.40889200
C	0.30444000	5.88695600	4.05103600
C	1.36324800	5.16819100	3.56077100

O	0.76208400	1.88706800	-0.92241700
O	-1.35421800	1.02216300	0.13714700
P	-0.05839300	0.48179100	-0.71401600
O	0.66929300	-0.38673100	0.28522900
O	-0.42987300	-0.01799200	-2.06476500
C	-3.83640800	0.55061400	-1.10070700
C	3.29630000	1.90480900	0.35691800
C	-3.97353000	-0.04122500	-2.31570500
C	-4.58786900	-1.32986300	-2.46860100
C	-5.09138300	-2.00921800	-1.33393800
C	-4.89204400	-1.41812300	-0.01657400
C	-4.28063800	-0.14154700	0.09589200
C	3.67621100	0.69661600	1.06286600
C	4.76940200	-0.08021300	0.59348500
C	5.48209300	0.33182800	-0.60900600
C	5.08137900	1.52128800	-1.26550600
C	3.98730200	2.29058800	-0.74658800
C	-5.27832400	-2.08575100	1.16830600
C	-5.09000000	-1.51382100	2.40859100
C	-4.51674100	-0.23541600	2.51421900
C	-4.12162600	0.43430300	1.37706300
C	-4.70661900	-1.91420900	-3.74941800
C	-5.33276400	-3.13009800	-3.91328700
C	-5.87074600	-3.79100500	-2.79337100
C	-5.75070100	-3.24302800	-1.53320500
C	2.97279500	0.27053900	2.21395700
C	3.34368100	-0.86757500	2.89477700
C	4.43447500	-1.63122700	2.44106000
C	5.12783300	-1.24414800	1.31493100
C	6.54390400	-0.41501700	-1.16790100
C	7.17647100	0.00155700	-2.32042100
C	6.77580300	1.18479400	-2.96736500
C	5.74356000	1.93099800	-2.44372200
H	-4.85555900	2.87506100	-2.04018300
H	-4.93727500	5.24969700	-2.57102500
H	-3.93343200	7.51157100	-2.48718800
H	-1.73437200	7.84979700	-1.36708400
H	-0.57255300	5.96961800	-0.30638200
H	3.24814300	3.61223600	2.45241900
H	-2.09904200	4.98671300	1.81159200
H	-1.79747100	6.36353800	3.81443300
H	0.42277100	6.50358600	4.93613500
H	2.33255200	5.19892900	4.05073700
H	-0.65133400	-1.61784500	-2.84907200

H	-3.61053900	0.46422600	-3.20682900
H	3.70115800	3.19559200	-1.27694500
H	-5.72483300	-3.07198000	1.11215700
H	-5.38828700	-2.05199900	3.30287300
H	-4.38387900	0.22463700	3.48832000
H	-3.68012200	1.42161000	1.46459900
H	-4.29666200	-1.38161600	-4.60316100
H	-5.42036900	-3.57269100	-4.90031400
H	-6.38015300	-4.74109800	-2.92005200
H	-6.17144400	-3.77971800	-0.69042000
H	2.12098500	0.85056800	2.55173700
H	2.78781600	-1.17942600	3.77414200
H	4.73010700	-2.52833000	2.97636000
H	5.96193700	-1.85165100	0.98340600
H	6.87036100	-1.33680300	-0.70057900
H	7.98632400	-0.59180700	-2.73291600
H	7.27629500	1.50352800	-3.87610800
H	5.41602900	2.84446200	-2.93255900
C	-0.92286900	-2.44571300	3.76248500
C	-1.78525800	-2.23946500	4.82949500
C	-1.95481600	-3.23065400	5.79900700
C	-1.26779800	-4.43911300	5.69472900
C	-0.40883100	-4.65384500	4.62415600
C	-0.21455400	-3.65683000	3.65466300
C	0.70007700	-3.92651900	2.55582600
C	1.16554200	-2.98436800	1.69947800
C	1.99071700	-3.28446200	0.56494300
N	2.31679300	-2.24046700	-0.19353200
C	2.21971600	-4.67642200	0.10028200
C	3.23166300	-2.27571500	-1.25120600
C	2.98016700	-1.20387000	-2.33205200
O	4.15799500	-3.03236500	-1.37075600
F	2.60280400	-0.04718400	-1.78517400
F	4.08631700	-1.00352600	-3.03786100
F	2.01995200	-1.61100200	-3.15771900
H	-0.82174400	-1.67914600	2.99924800
H	-2.33380300	-1.30646000	4.90449600
H	-2.63129900	-3.06206400	6.63094200
H	-1.40582600	-5.21216500	6.44331100
H	0.12717600	-5.59442400	4.53068400
H	1.01370700	-4.96329000	2.45087700
H	0.90843000	-1.93992700	1.83563900
H	1.70158500	-1.32291100	-0.02962700
H	3.11966800	-4.76054200	-0.50041300

H	2.29669200	-5.36205000	0.94386400
C	-2.46626400	-4.05801900	-1.02428900
O	-0.51109000	-2.55290600	-3.11320500
C	-1.32671900	-3.04229300	-0.88715300
C	-0.29571400	-3.26026500	-1.97165700
C	0.69334200	-4.17041300	-1.92820500
C	0.96281300	-5.07438200	-0.76317600
H	-3.23031300	-3.89165600	-0.25987100
H	-2.94013300	-3.96735800	-2.00697800
H	-2.09047300	-5.08088200	-0.92052800
H	-0.87618300	-3.11229100	0.10595200
H	-1.72662600	-2.02627700	-0.98803900
H	1.34469200	-4.24865900	-2.79646300
H	1.16897000	-6.09234800	-1.10878700
H	0.09961500	-5.12527000	-0.09379600

TSIII-2

C	-1.39192500	2.33689800	-0.39551200
C	-2.64146100	2.30561500	-1.07495500
C	-3.00520500	3.40854700	-1.81071800
C	-2.16616800	4.54484800	-1.92654900
C	-0.91539000	4.56038600	-1.24969000
C	-0.55385000	3.43362600	-0.44293400
C	-2.54580700	5.65627100	-2.72630000
C	-1.70966100	6.73268700	-2.86986600
C	-0.44864500	6.73620600	-2.22544700
C	-0.05976000	5.68136000	-1.43844600
C	0.74015000	3.36584800	0.28454500
C	1.09498700	4.30544200	1.30374500
C	2.35915100	4.17943100	1.94408700
C	3.22547000	3.12278100	1.56942500
C	2.87010500	2.19212600	0.62176700
C	1.59869400	2.32197400	-0.00226700
C	0.21800100	5.33959900	1.73565000
C	0.59650100	6.21289900	2.72373800
C	1.86880000	6.10441700	3.33719100
C	2.72710000	5.10609300	2.95715500
O	1.19444600	1.37740600	-0.93101500
O	-0.99871700	1.23757300	0.34291800
P	0.13912400	0.25497000	-0.35057200
O	-0.50418900	-0.45785500	-1.50430300
C	-3.56527700	1.13582100	-1.03301000
C	3.84120600	1.12519800	0.24114000
C	-3.76886300	0.41678300	-2.16744900

C	-4.76331700	-0.61530800	-2.24711500
C	-5.55360100	-0.92164900	-1.11312300
C	-5.34414600	-0.16175400	0.11432600
C	-4.36313100	0.86498900	0.14723800
C	4.10119200	0.00686300	1.12720500
C	5.11405700	-0.93365500	0.79632400
C	5.86601600	-0.77691000	-0.44239300
C	5.55991800	0.31304600	-1.29302900
C	4.54768800	1.25543500	-0.91121300
C	-6.13485100	-0.36818000	1.26650200
C	-5.99054800	0.42162400	2.38801400
C	-5.03167800	1.44732400	2.41051800
C	-4.22665000	1.65427900	1.31114500
C	-4.98292200	-1.29656500	-3.46454200
C	-5.96766000	-2.25540500	-3.56959400
C	-6.74990200	-2.57092800	-2.44439300
C	-6.54237100	-1.92281900	-1.24277000
C	3.35531500	-0.17322100	2.31543500
C	3.60691400	-1.23311400	3.15981700
C	4.62091900	-2.15436000	2.84477600
C	5.35501900	-2.00568500	1.68790100
C	6.87068600	-1.68255000	-0.85149900
C	7.53273600	-1.51661400	-2.04982900
C	7.22048600	-0.43547800	-2.89411100
C	6.24991700	0.46535700	-2.51584000
H	-3.95996500	3.40897400	-2.32987500
H	-3.50960600	5.62780600	-3.22707200
H	-2.00328000	7.57750200	-3.48450400
H	0.22003700	7.58037700	-2.36106700
H	0.91476900	5.69294900	-0.96262300
H	4.19457700	3.04355900	2.05598900
H	-0.76383200	5.42699500	1.28282200
H	-0.08755200	6.99261100	3.04350100
H	2.15412200	6.80651900	4.11391100
H	3.70067800	4.99825300	3.42735900
H	-1.83076000	-1.33374700	-0.84747100
H	-3.18267800	0.63497800	-3.05634000
H	4.35461100	2.09583700	-1.57358900
H	-6.88619800	-1.14949000	1.27500700
H	-6.62333300	0.24943600	3.25324900
H	-4.91960100	2.07078200	3.29237800
H	-3.48433700	2.44652800	1.32741700
H	-4.36489600	-1.04065700	-4.32100100
H	-6.13638800	-2.76764800	-4.51151000

H	-7.52274900	-3.32971400	-2.51856300
H	-7.16578300	-2.18796800	-0.39635100
H	2.55909100	0.52610200	2.54328000
H	3.02033200	-1.35678600	4.06494400
H	4.82375100	-2.98835200	3.50922400
H	6.12534100	-2.73454900	1.46349300
H	7.12819400	-2.53149900	-0.22878500
H	8.29721300	-2.22861400	-2.34431500
H	7.74277700	-0.31412900	-3.83773500
H	5.99550400	1.30707800	-3.15422900
C	-1.63872300	-1.40063000	2.74717000
C	-2.61603400	-0.71103600	3.45253200
C	-3.67661000	-1.39960700	4.04249900
C	-3.77515900	-2.78380900	3.91018000
C	-2.80448900	-3.48005200	3.19916400
C	-1.71526900	-2.79839700	2.63582100
C	-0.67650400	-3.57187100	1.95517500
C	0.67455100	-3.13700300	1.92442600
C	1.51090600	-3.74317000	1.02412400
N	2.41161100	-2.91158300	0.37602000
C	1.09962700	-5.02729100	0.39620400
C	3.24751300	-3.31078300	-0.63267500
C	3.22787300	-2.35631500	-1.84148800
O	3.83275700	-4.36488200	-0.71621900
F	2.93457500	-1.09945300	-1.50094100
F	4.37294700	-2.37684100	-2.50917800
F	2.25896500	-2.78762100	-2.66477200
H	-0.82382100	-0.86466600	2.26718800
H	-2.55494000	0.36889100	3.53583000
H	-4.43307100	-0.85366400	4.59769900
H	-4.60443900	-3.31827100	4.36200600
H	-2.86785700	-4.56026000	3.09637600
H	-0.89921300	-4.63244900	1.85886900
H	0.90991000	-2.13573200	2.26313600
H	1.90301600	-5.50125700	-0.16152100
H	0.78080100	-5.71621100	1.17883300
C	-3.86824100	-4.51024600	-1.49569300
O	-2.56043200	-1.92074100	-0.48943700
C	-3.26154600	-4.14215500	-0.13552300
C	-2.15357300	-3.16167600	-0.32228700
C	-0.80520700	-3.44855200	-0.28731600
C	-0.12911900	-4.74574500	-0.57152800
H	-4.75642600	-5.13204200	-1.36063300
H	-4.15726400	-3.60583400	-2.03653000

H	-3.14682800	-5.06183800	-2.10518200
H	-2.89022400	-5.03307600	0.37937300
H	-4.01775400	-3.66408000	0.49730700
H	-0.17580500	-2.57281800	-0.43344400
H	0.27474500	-4.69256600	-1.58767300
H	-0.81482100	-5.59622200	-0.52387300
O	0.79836400	-0.51096600	0.75083000
H	2.17018600	-1.91099000	0.43796300
P_{III}			
C	1.53564900	1.90286900	1.02595700
C	2.12278200	3.12910900	1.32067100
C	2.99311400	3.72648500	0.40830600
C	3.26555000	3.09144000	-0.79977200
C	2.67475600	1.86200200	-1.09184300
C	1.81036300	1.25083400	-0.18169500
C	1.17267800	-0.09487100	-0.48896700
C	-0.33695600	0.02162900	-0.49332700
C	-1.14183900	-0.90876600	0.03491900
C	-0.64724500	-2.19200700	0.65358400
C	-3.30921700	0.25031400	-0.27744400
C	-4.82128300	0.04348300	-0.06672000
O	-2.94546900	1.31496000	-0.73912600
F	-5.12252500	-1.14713600	0.47172100
F	-5.29941200	0.99189500	0.73926000
F	-5.45771400	0.13793000	-1.23541600
H	0.84916100	1.44620700	1.73524100
H	1.89963300	3.62198900	2.26200600
H	3.45167000	4.68315000	0.63817000
H	3.93610300	3.55156800	-1.51909200
H	2.88197400	1.37312700	-2.04090600
H	1.49309200	-0.38552100	-1.49985900
H	-0.75661200	0.91393200	-0.94009300
H	-0.77479400	-2.13680700	1.74246100
H	-1.27309200	-3.02234600	0.30538100
C	5.13386200	-2.33341100	-0.86873800
O	3.77152400	-1.64327900	1.43920700
C	3.74630600	-1.71481900	-0.94438100
C	3.12290800	-1.50587100	0.42022200
C	1.63908400	-1.17723800	0.50284200
C	0.81241200	-2.45719700	0.30185000
H	5.55772000	-2.45095600	-1.86874200
H	5.80472400	-1.70431500	-0.27959900
H	5.09729300	-3.31659000	-0.39217900

H	3.06406500	-2.32029600	-1.55396200
H	3.78620700	-0.73234900	-1.43309600
H	1.46890300	-0.81926300	1.52545300
H	1.20397800	-3.26467100	0.92749500
H	0.88762300	-2.77928700	-0.74345800
N	-2.55216500	-0.80388400	0.08177300
H	-3.04163500	-1.61195200	0.44883300

COMIV-1

C	-1.52528200	2.37430200	-0.26008500
C	-2.69333100	2.40542000	-1.06823300
C	-2.86097100	3.47575900	-1.91140300
C	-1.89629900	4.51358300	-1.99492000
C	-0.73369700	4.46698000	-1.17380700
C	-0.57886600	3.37384500	-0.25536300
C	-2.06874900	5.58969400	-2.90591100
C	-1.11801300	6.57054800	-3.02129900
C	0.05554000	6.50760400	-2.23318400
C	0.24470200	5.48628100	-1.33535600
C	0.61911200	3.24484400	0.61928300
C	0.99133100	4.26501300	1.55500200
C	2.24122000	4.16505900	2.22692400
C	3.10067200	3.07268200	1.93929900
C	2.71497300	2.05581000	1.10172700
C	1.42267300	2.12669200	0.50550700
C	0.14500400	5.36631400	1.85866400
C	0.53167200	6.31804100	2.76906200
C	1.78507900	6.22721700	3.42095100
C	2.61905000	5.17189400	3.15457900
O	1.02956000	1.08595500	-0.30714500
O	-1.34905500	1.29372000	0.57677900
P	-0.26982100	0.15902100	0.11360900
O	0.03279400	-0.57809500	1.39505500
O	-0.66465700	-0.55575100	-1.12813000
C	-3.70368500	1.31230000	-1.02073500
C	3.69552800	1.00602900	0.68736300
C	-3.90983200	0.55078600	-2.12799900
C	-4.95621700	-0.43022800	-2.19343700
C	-5.81732500	-0.61505000	-1.08580000
C	-5.55472500	0.13169200	0.13820600
C	-4.51274700	1.09668800	0.16493800
C	3.70814700	-0.32083000	1.26890000
C	4.65561000	-1.27939200	0.81637300
C	5.62053700	-0.91145400	-0.21338600

C	5.62612900	0.41863500	-0.69678200
C	4.63610900	1.34890100	-0.23259000
C	-6.31054000	-0.07418700	1.31458700
C	-6.06375300	0.64934000	2.46179000
C	-5.05021500	1.62182700	2.47694600
C	-4.29370500	1.84025300	1.34676400
C	-5.15118900	-1.18563000	-3.37113000
C	-6.19647100	-2.07714600	-3.47012600
C	-7.08258800	-2.23236000	-2.38766600
C	-6.89372800	-1.52095400	-1.22107900
C	2.82269800	-0.66030400	2.31525600
C	2.85508900	-1.91227000	2.89278900
C	3.77441600	-2.86984100	2.43395900
C	4.65370200	-2.55747900	1.41725100
C	6.56743700	-1.81621700	-0.74263300
C	7.49143400	-1.41065800	-1.68490600
C	7.50691300	-0.08134800	-2.14337800
C	6.58044200	0.81607200	-1.65805000
H	-3.74797000	3.53238000	-2.53671200
H	-2.96805900	5.61052300	-3.51525000
H	-1.25476600	7.38756800	-3.72228700
H	0.81773100	7.27241700	-2.34428400
H	1.15702200	5.44718100	-0.75103800
H	4.08813800	3.04736900	2.39258900
H	-0.82273000	5.44044100	1.37344300
H	-0.13195900	7.14634800	2.99619700
H	2.07767600	6.99020800	4.13498900
H	3.58050900	5.08173900	3.65251900
H	-1.78991400	-1.60233300	-2.20182500
H	-3.28605800	0.69591100	-3.00682900
H	4.64359400	2.35309800	-0.64947600
H	-7.09704600	-0.82001000	1.32744400
H	-6.65537200	0.46640200	3.35313900
H	-4.86023600	2.19784500	3.37683000
H	-3.51307400	2.59362200	1.36302600
H	-4.46327000	-1.04251100	-4.19974600
H	-6.34323600	-2.65060600	-4.37979800
H	-7.91769100	-2.92117700	-2.46770800
H	-7.59091500	-1.66678300	-0.40373600
H	2.10429400	0.07661000	2.65650000
H	2.16889700	-2.15607200	3.69734800
H	3.80055100	-3.85736300	2.88467700
H	5.36547500	-3.30798000	1.09245400
H	6.57794000	-2.84903500	-0.41261700

H	8.20929000	-2.12537900	-2.07506600
H	8.23877800	0.23126100	-2.88139800
H	6.56519500	1.84356900	-2.01181600
C	2.78335500	-1.20134700	-2.22115500
C	3.55302600	-0.43853900	-3.08544200
C	4.52539500	-1.04644300	-3.88335300
C	4.71168800	-2.42818400	-3.83913800
C	3.92864100	-3.20210300	-2.99311600
C	2.97347600	-2.59513600	-2.16036000
C	2.20207500	-3.43210500	-1.26570800
C	1.53947600	-2.96505400	-0.17274000
C	0.71455100	-3.76855700	0.66142100
N	0.11253800	-3.09553600	1.65025100
C	0.41236600	-5.20583700	0.39785100
C	-0.63255800	-3.63373600	2.69060600
C	-1.23162300	-2.52559100	3.58542100
O	-0.82397700	-4.79415300	2.94467100
F	-2.11736900	-1.80201400	2.89972300
F	-1.83964000	-3.06808700	4.63083400
F	-0.27134000	-1.70619000	4.02316500
H	2.00683300	-0.72562600	-1.62985200
H	3.39829300	0.63468900	-3.13561000
H	5.13223600	-0.44059100	-4.54915100
H	5.46245700	-2.89741000	-4.46635300
H	4.05868900	-4.27998600	-2.95483800
H	2.18756000	-4.49282200	-1.50454400
H	1.64602700	-1.92349200	0.11374700
H	0.14299100	-1.98861400	1.57752400
H	0.48100100	-5.78395100	1.31968300
H	1.12796800	-5.60558100	-0.31897800
C	-4.21430000	-3.45505000	-0.32781800
O	-2.01600800	-2.50783200	-2.48917400
C	-2.83390000	-2.80087200	-0.22821100
C	-1.94377200	-3.27048500	-1.35359400
C	-1.21496900	-4.39307900	-1.36316800
C	-1.02926600	-5.30935000	-0.18814900
H	-4.89977900	-3.04457300	0.41956200
H	-4.64575600	-3.28445000	-1.31885100
H	-4.13791800	-4.53598900	-0.17121900
H	-2.39312100	-3.02178900	0.74594000
H	-2.92434700	-1.70959100	-0.29323700
H	-0.64597200	-4.60987000	-2.26549900
H	-1.17520800	-6.35714000	-0.46931500
H	-1.75101200	-5.08886100	0.60231700

TSIV-1

C	3.03103500	-0.96499500	-0.14722500
C	4.09994400	-0.10049200	-0.51394400
C	5.05205300	-0.58414700	-1.37708600
C	4.96177100	-1.89196400	-1.92259000
C	3.86693000	-2.73194800	-1.56848700
C	2.90024300	-2.25269600	-0.62354800
C	5.93095000	-2.36155100	-2.84933400
C	5.81026100	-3.59999700	-3.42525700
C	4.70194300	-4.41974200	-3.10526300
C	3.75607200	-3.99887900	-2.20432200
C	1.70922900	-3.05032500	-0.21568800
C	1.80999100	-4.33677600	0.40652200
C	0.61524700	-5.04483100	0.72207500
C	-0.64451300	-4.45319900	0.45252500
C	-0.74880700	-3.19287500	-0.08611300
C	0.45329100	-2.50520300	-0.40497600
C	3.05649200	-4.92458500	0.75835000
C	3.10733200	-6.15858900	1.35645600
C	1.91919000	-6.87603900	1.63665100
C	0.70175100	-6.32660100	1.33022400
O	0.35338800	-1.23459200	-0.93398800
O	2.08298900	-0.47839900	0.72720600
P	0.64840400	0.00431800	0.10626800
O	-0.32008300	0.00483500	1.23793200
O	0.84508700	1.20017600	-0.77882500
C	4.09962700	1.31489000	-0.05179700
C	-2.07735800	-2.58195800	-0.37464000
C	3.95578000	2.29672800	-0.98022700
C	3.85582900	3.68055700	-0.61580200
C	3.91973100	4.05532500	0.74745700
C	4.10657800	3.01712000	1.75365200
C	4.19898300	1.65858900	1.35391000
C	-3.03167300	-2.32906100	0.69184300
C	-4.32265700	-1.82220200	0.37655900
C	-4.68061500	-1.56947900	-1.01395200
C	-3.71732000	-1.81572800	-2.02088200
C	-2.41886900	-2.30883400	-1.66221200
C	4.20236700	3.31981700	3.13056900
C	4.38584600	2.32951000	4.07169500
C	4.48800300	0.98669400	3.67182800
C	4.39635500	0.66219400	2.33641800
C	3.66454800	4.66617500	-1.60968000

C	3.53992200	5.99513600	-1.26952200
C	3.60706500	6.37386400	0.08325200
C	3.79254300	5.42518800	1.06804400
C	-2.69692200	-2.55653200	2.04532800
C	-3.60926600	-2.32991000	3.05437300
C	-4.88559000	-1.83250300	2.74628400
C	-5.22644900	-1.57591600	1.43451800
C	-5.94604300	-1.07970400	-1.40814400
C	-6.24165200	-0.85909700	-2.73765000
C	-5.28470000	-1.12090100	-3.73542400
C	-4.04194800	-1.59280600	-3.37762700
H	5.88324200	0.05119100	-1.67176000
H	6.76498700	-1.71117400	-3.09890700
H	6.55286900	-3.95029100	-4.13498200
H	4.59553400	-5.38920100	-3.58193600
H	2.90595100	-4.63332300	-1.97933600
H	-1.54631400	-5.00926700	0.69733700
H	3.97416400	-4.38095800	0.56020100
H	4.06815800	-6.58765000	1.62340500
H	1.97812500	-7.85323400	2.10519400
H	-0.22037900	-6.85549400	1.55524000
H	0.32023900	2.48269100	-1.19126700
H	3.85936700	2.03613000	-2.03121600
H	-1.70412500	-2.48878900	-2.46217200
H	4.13184200	4.34852000	3.46494800
H	4.45391200	2.59018600	5.12325600
H	4.63680600	0.20733000	4.41226200
H	4.47757100	-0.37520000	2.02670700
H	3.61100200	4.35208700	-2.64864400
H	3.39139000	6.74663500	-2.03842800
H	3.51055900	7.41994700	0.35707600
H	3.83679500	5.75096400	2.10098900
H	-1.69961700	-2.90325200	2.29251300
H	-3.33311400	-2.52329200	4.08551000
H	-5.60103600	-1.63954700	3.53969800
H	-6.21315200	-1.18075800	1.22186400
H	-6.70826600	-0.87477800	-0.66518000
H	-7.22214600	-0.48457700	-3.01495800
H	-5.52392400	-0.94495000	-4.77961200
H	-3.28491300	-1.78893100	-4.13212600
C	-1.59737000	0.73388500	-2.96549600
C	-1.21102700	0.40893900	-4.26043200
C	-1.97736200	0.82916400	-5.34832700
C	-3.12628600	1.59141000	-5.13765000

C	-3.50735700	1.92762800	-3.84374600
C	-2.75825400	1.48790100	-2.74189400
C	-3.21403800	1.83906100	-1.39813400
C	-2.89701100	1.18126400	-0.25907800
C	-3.30653500	1.62730000	1.05504200
N	-2.77290100	0.87309200	2.09884400
C	-3.91213200	2.84464700	1.28453100
C	-3.16121800	0.94694600	3.39752500
C	-2.18606500	0.29488200	4.39722200
O	-4.13510500	1.50932800	3.85319800
F	-1.52192400	1.26677500	5.03517200
F	-2.86420400	-0.40055200	5.31201600
F	-1.28931300	-0.50917600	3.82817600
H	-0.98223500	0.42327300	-2.12912000
H	-0.30479700	-0.16783800	-4.41964000
H	-1.67383100	0.57295800	-6.35875400
H	-3.72141400	1.92512200	-5.98188500
H	-4.40361500	2.51952700	-3.67375800
H	-3.90475500	2.67988200	-1.35657400
H	-2.27338500	0.29074900	-0.29813500
H	-1.93512700	0.31564200	1.86511600
H	-4.28265400	3.09690600	2.26733700
H	-4.35433000	3.37357800	0.44979500
O	-0.03804100	3.38301300	-1.55632700
C	-1.44652100	5.24016800	-1.28522500
C	-0.86458500	3.96833300	-0.74396500
C	-1.08144800	3.47211900	0.54232200
C	-2.05300000	3.92873600	1.42790700
H	-2.19203000	5.64116200	-0.59760400
H	-0.51404900	2.58712300	0.82199400
H	-1.96355200	3.62602200	2.46800300
H	-2.57311200	4.86666200	1.25725300
C	-2.02591900	5.08803800	-2.69157800
H	-2.92438100	4.46602400	-2.68049600
H	-2.30012400	6.06826000	-3.08821400
H	-1.29977300	4.63110400	-3.36728000
H	-0.61336000	5.95523200	-1.30845300

INTIV-2

C	3.03103500	-0.96499500	-0.14722500
C	4.09994400	-0.10049200	-0.51394400
C	5.05205300	-0.58414700	-1.37708600
C	4.96177100	-1.89196400	-1.92259000
C	3.86693000	-2.73194800	-1.56848700

C	2.90024300	-2.25269600	-0.62354800
C	5.93095000	-2.36155100	-2.84933400
C	5.81026100	-3.59999700	-3.42525700
C	4.70194300	-4.41974200	-3.10526300
C	3.75607200	-3.99887900	-2.20432200
C	1.70922900	-3.05032500	-0.21568800
C	1.80999100	-4.33677600	0.40652200
C	0.61524700	-5.04483100	0.72207500
C	-0.64451300	-4.45319900	0.45252500
C	-0.74880700	-3.19287500	-0.08611300
C	0.45329100	-2.50520300	-0.40497600
C	3.05649200	-4.92458500	0.75835000
C	3.10733200	-6.15858900	1.35645600
C	1.91919000	-6.87603900	1.63665100
C	0.70175100	-6.32660100	1.33022400
O	0.35338800	-1.23459200	-0.93398800
O	2.08298900	-0.47839900	0.72720600
P	0.64840400	0.00431800	0.10626800
O	-0.32008300	0.00483500	1.23793200
O	0.84508700	1.20017600	-0.77882500
C	4.09962700	1.31489000	-0.05179700
C	-2.07735800	-2.58195800	-0.37464000
C	3.95578000	2.29672800	-0.98022700
C	3.85582900	3.68055700	-0.61580200
C	3.91973100	4.05532500	0.74745700
C	4.10657800	3.01712000	1.75365200
C	4.19898300	1.65858900	1.35391000
C	-3.03167300	-2.32906100	0.69184300
C	-4.32265700	-1.82220200	0.37655900
C	-4.68061500	-1.56947900	-1.01395200
C	-3.71732000	-1.81572800	-2.02088200
C	-2.41886900	-2.30883400	-1.66221200
C	4.20236700	3.31981700	3.13056900
C	4.38584600	2.32951000	4.07169500
C	4.48800300	0.98669400	3.67182800
C	4.39635500	0.66219400	2.33641800
C	3.66454800	4.66617500	-1.60968000
C	3.53992200	5.99513600	-1.26952200
C	3.60706500	6.37386400	0.08325200
C	3.79254300	5.42518800	1.06804400
C	-2.69692200	-2.55653200	2.04532800
C	-3.60926600	-2.32991000	3.05437300
C	-4.88559000	-1.83250300	2.74628400
C	-5.22644900	-1.57591600	1.43451800

C	-5.94604300	-1.07970400	-1.40814400
C	-6.24165200	-0.85909700	-2.73765000
C	-5.28470000	-1.12090100	-3.73542400
C	-4.04194800	-1.59280600	-3.37762700
H	5.88324200	0.05119100	-1.67176000
H	6.76498700	-1.71117400	-3.09890700
H	6.55286900	-3.95029100	-4.13498200
H	4.59553400	-5.38920100	-3.58193600
H	2.90595100	-4.63332300	-1.97933600
H	-1.54631400	-5.00926700	0.69733700
H	3.97416400	-4.38095800	0.56020100
H	4.06815800	-6.58765000	1.62340500
H	1.97812500	-7.85323400	2.10519400
H	-0.22037900	-6.85549400	1.55524000
H	0.32023900	2.48269100	-1.19126700
H	3.85936700	2.03613000	-2.03121600
H	-1.70412500	-2.48878900	-2.46217200
H	4.13184200	4.34852000	3.46494800
H	4.45391200	2.59018600	5.12325600
H	4.63680600	0.20733000	4.41226200
H	4.47757100	-0.37520000	2.02670700
H	3.61100200	4.35208700	-2.64864400
H	3.39139000	6.74663500	-2.03842800
H	3.51055900	7.41994700	0.35707600
H	3.83679500	5.75096400	2.10098900
H	-1.69961700	-2.90325200	2.29251300
H	-3.33311400	-2.52329200	4.08551000
H	-5.60103600	-1.63954700	3.53969800
H	-6.21315200	-1.18075800	1.22186400
H	-6.70826600	-0.87477800	-0.66518000
H	-7.22214600	-0.48457700	-3.01495800
H	-5.52392400	-0.94495000	-4.77961200
H	-3.28491300	-1.78893100	-4.13212600
C	-1.59737000	0.73388500	-2.96549600
C	-1.21102700	0.40893900	-4.26043200
C	-1.97736200	0.82916400	-5.34832700
C	-3.12628600	1.59141000	-5.13765000
C	-3.50735700	1.92762800	-3.84374600
C	-2.75825400	1.48790100	-2.74189400
C	-3.21403800	1.83906100	-1.39813400
C	-2.89701100	1.18126400	-0.25907800
C	-3.30653500	1.62730000	1.05504200
N	-2.77290100	0.87309200	2.09884400
C	-3.91213200	2.84464700	1.28453100

C	-3.16121800	0.94694600	3.39752500
C	-2.18606500	0.29488200	4.39722200
O	-4.13510500	1.50932800	3.85319800
F	-1.52192400	1.26677500	5.03517200
F	-2.86420400	-0.40055200	5.31201600
F	-1.28931300	-0.50917600	3.82817600
H	-0.98223500	0.42327300	-2.12912000
H	-0.30479700	-0.16783800	-4.41964000
H	-1.67383100	0.57295800	-6.35875400
H	-3.72141400	1.92512200	-5.98188500
H	-4.40361500	2.51952700	-3.67375800
H	-3.90475500	2.67988200	-1.35657400
H	-2.27338500	0.29074900	-0.29813500
H	-1.93512700	0.31564200	1.86511600
H	-4.28265400	3.09690600	2.26733700
H	-4.35433000	3.37357800	0.44979500
O	-0.03804100	3.38301300	-1.55632700
C	-1.44652100	5.24016800	-1.28522500
C	-0.86458500	3.96833300	-0.74396500
C	-1.08144800	3.47211900	0.54232200
C	-2.05300000	3.92873600	1.42790700
H	-2.19203000	5.64116200	-0.59760400
H	-0.51404900	2.58712300	0.82199400
H	-1.96355200	3.62602200	2.46800300
H	-2.57311200	4.86666200	1.25725300
C	-2.02591900	5.08803800	-2.69157800
H	-2.92438100	4.46602400	-2.68049600
H	-2.30012400	6.06826000	-3.08821400
H	-1.29977300	4.63110400	-3.36728000
H	-0.61336000	5.95523200	-1.30845300

TSIV-2

C	-3.00475000	0.86214600	-0.07746100
C	-4.01043300	-0.08683000	-0.41245700
C	-4.97380400	0.28277300	-1.31675200
C	-4.95706700	1.56223300	-1.93264600
C	-3.92688800	2.49133100	-1.60758900
C	-2.94840000	2.12870100	-0.62228300
C	-5.93615200	1.91360300	-2.90017800
C	-5.88660000	3.12359800	-3.54290400
C	-4.84106200	4.03180500	-3.25199100
C	-3.88752100	3.72554600	-2.31319000
C	-1.81360000	3.02000600	-0.24921400
C	-1.99272800	4.33426600	0.29148900

C	-0.84318000	5.12713200	0.57391700
C	0.45247500	4.59763900	0.34251900
C	0.63161900	3.31785000	-0.12371200
C	-0.52659900	2.53918500	-0.39714100
C	-3.27450300	4.87045600	0.59617800
C	-3.40267600	6.13362000	1.11662000
C	-2.26021700	6.93311200	1.36342200
C	-1.01007800	6.43625200	1.10164000
O	-0.34828900	1.25061900	-0.84586300
O	-2.04883000	0.48070300	0.83726000
P	-0.57837300	0.03868800	0.25408100
O	0.37037700	0.18042000	1.39769700
O	-0.67185500	-1.20577200	-0.56722200
C	-3.94360300	-1.46136700	0.15560400
C	1.98708500	2.75565400	-0.38910700
C	-3.65976000	-2.49995400	-0.67201100
C	-3.50227800	-3.83965000	-0.18255200
C	-3.66461300	-4.10983300	1.19779700
C	-4.00781300	-3.01136300	2.09295400
C	-4.14020400	-1.69751500	1.57221400
C	2.93055200	2.53048300	0.69125500
C	4.22760000	2.02357000	0.40140400
C	4.59151500	1.71599700	-0.97626900
C	3.63791500	1.93611800	-1.99901400
C	2.34300400	2.45763500	-1.66747700
C	-4.21404000	-3.20820500	3.47705900
C	-4.53653800	-2.15859200	4.31067500
C	-4.66962000	-0.85977400	3.79110400
C	-4.47517700	-0.63863400	2.44575900
C	-3.15620300	-4.88334900	-1.06934100
C	-2.97480700	-6.16857000	-0.60830300
C	-3.13778000	-6.44370800	0.76157700
C	-3.47514900	-5.43719000	1.64314900
C	2.57378000	2.77730000	2.03607100
C	3.47156400	2.56854300	3.06077500
C	4.75775700	2.07930900	2.77754700
C	5.12073600	1.80681200	1.47494000
C	5.84299600	1.16868800	-1.33952600
C	6.12964200	0.85578200	-2.65231200
C	5.18029000	1.08415500	-3.66590200
C	3.95521300	1.62114600	-3.33982500
H	-5.75707000	-0.42046200	-1.58724000
H	-6.71983500	1.19548100	-3.12526400
H	-6.63682100	3.38274000	-4.28294300

H	-4.78947100	4.97805600	-3.78123500
H	-3.08531300	4.42685700	-2.11223200
H	1.31808000	5.22061500	0.55469700
H	-4.15690800	4.26358000	0.42297400
H	-4.38934200	6.52273900	1.34731000
H	-2.37893500	7.93217900	1.77013300
H	-0.12201600	7.02955300	1.30139700
H	-0.26869600	-2.55221600	-1.51526000
H	-3.49319800	-2.31836400	-1.73070400
H	1.63311100	2.61200100	-2.47718600
H	-4.12101600	-4.20130200	3.90150800
H	-4.68914500	-2.33825000	5.37015200
H	-4.92533200	-0.03367000	4.44680400
H	-4.58360800	0.36347400	2.04258200
H	-3.02933100	-4.64835800	-2.12272900
H	-2.70570400	-6.96478700	-1.29523400
H	-2.99494400	-7.45454300	1.13039400
H	-3.58774400	-5.68094800	2.69337300
H	1.57178700	3.12576900	2.26068300
H	3.17659800	2.76488400	4.08611100
H	5.46131200	1.90004600	3.58468800
H	6.11351400	1.41621800	1.28269900
H	6.59659800	0.98148700	-0.58341800
H	7.09636600	0.43084600	-2.90353600
H	5.41176300	0.83395300	-4.69644200
H	3.20469300	1.79582400	-4.10616900
C	1.35668000	-0.52775300	-2.98278000
C	0.93859900	-0.21957800	-4.27048500
C	1.58703600	-0.78112600	-5.37160200
C	2.64720700	-1.67031300	-5.18718600
C	3.05649600	-1.99673200	-3.90123200
C	2.42971300	-1.41261700	-2.78521700
C	2.93515000	-1.74065400	-1.46861900
C	2.81876500	-0.92707000	-0.32828800
C	3.24029100	-1.41546600	0.88890600
N	2.85238900	-0.72713600	2.02450000
C	3.77984200	-2.79735500	0.99050200
C	3.44573500	-0.83575000	3.24344000
C	2.61082000	-0.28491300	4.41454700
O	4.51424300	-1.34836300	3.49905800
F	2.14662600	-1.31600300	5.12916500
F	3.37842100	0.45243000	5.21886100
F	1.56884000	0.44881300	4.02515400
H	0.84146900	-0.10024500	-2.13259800

H	0.10472300	0.46000500	-4.41499400
H	1.26081300	-0.53182700	-6.37656500
H	3.14677800	-2.10930300	-6.04430200
H	3.88201600	-2.68633000	-3.74563300
H	3.68001400	-2.53189500	-1.46294800
H	2.27373800	0.01159900	-0.37405100
H	1.99152500	-0.15605400	1.91895200
H	4.18119500	-3.00601900	1.97769000
H	4.58674900	-2.93235500	0.26814500
C	0.85318000	-6.12764400	-2.40401000
O	0.08675000	-3.30802300	-2.04963200
C	1.78949000	-4.92285200	-2.25332900
C	1.14859100	-3.84044700	-1.44668600
C	1.55895100	-3.37787000	-0.22761600
C	2.63949100	-3.86792100	0.66548400
H	1.32576800	-6.90274200	-3.01157500
H	0.61101900	-6.55370100	-1.42636000
H	-0.07973100	-5.82935300	-2.88795000
H	2.01192300	-4.50476200	-3.24308100
H	2.73306000	-5.22474500	-1.79334600
H	0.92185600	-2.60709100	0.19765100
H	2.18874000	-4.12399800	1.62884400
H	3.13801500	-4.75988600	0.28042700
P_{IV}			
C	-1.89702000	1.96068300	0.95068400
C	-2.66952700	3.07001100	1.27937000
C	-3.68511300	3.49520400	0.42237100
C	-3.91766700	2.80642900	-0.76452300
C	-3.14126600	1.69449700	-1.09089000
C	-2.12824800	1.25577600	-0.23618800
C	-1.28725900	0.03759000	-0.58210600
C	0.17566700	0.40134400	-0.67196400
C	1.16880500	-0.35944100	-0.19752100
N	2.49784800	0.10512600	-0.35727900
C	0.95665700	-1.70853500	0.43954800
C	3.60357300	-0.35609000	0.25716600
C	4.90035500	0.35374900	-0.17926800
O	3.70117100	-1.25009300	1.07574400
F	5.69367300	-0.51011400	-0.81722600
F	4.68647400	1.39561800	-0.99614900
F	5.55568100	0.79852800	0.89246900
H	-1.10044700	1.63741900	1.61694200
H	-2.47861100	3.60545800	2.20439700

H	-4.28794000	4.36076100	0.67870200
H	-4.70184000	3.13364500	-1.44032400
H	-3.31935000	1.16353800	-2.02312100
H	-1.61369800	-0.31609600	-1.57049000
H	0.41452400	1.34929800	-1.15162400
H	2.61207600	0.91759700	-0.95349600
H	1.15013300	-1.64345300	1.51548700
H	1.69021000	-2.41535200	0.04195900
C	-4.81056400	-2.85828000	-0.70412500
O	-3.45130200	-1.90158100	1.50753200
C	-3.55171500	-2.02140900	-0.87210200
C	-2.89463900	-1.68042000	0.44986300
C	-1.48765100	-1.10052000	0.43687100
C	-0.46042700	-2.21361800	0.17447700
H	-5.26662900	-3.06670800	-1.67473600
H	-4.58391300	-3.81076600	-0.21792100
H	-5.54088000	-2.33476000	-0.08325800
H	-3.78235300	-1.07068200	-1.37078000
H	-2.81405300	-2.51988800	-1.51306800
H	-1.31648800	-0.70761700	1.44641500
H	-0.66624100	-3.07657500	0.81482400
H	-0.54458900	-2.54639900	-0.86699400

R2ad

C	4.02157300	-0.83377300	0.26244900
C	2.79421400	-0.84715300	-0.25388600
C	1.81996800	0.25522200	-0.09914000
N	0.48692000	-0.21637200	-0.04044500
C	2.16661500	1.54707100	-0.03906400
C	-0.63436300	0.53116000	-0.01312700
C	-1.93989000	-0.28603700	0.02873500
O	-0.72672100	1.74268500	-0.02488600
F	-1.73315700	-1.60889500	0.09437700
F	-2.66234700	0.07101300	1.09050600
F	-2.66304500	-0.03681200	-1.06418200
H	4.37455800	-0.00513100	0.87033200
H	2.45281000	-1.71062200	-0.82396200
H	0.36810400	-1.22222700	-0.01056500
H	1.44636300	2.33929000	0.09892200
H	3.21426900	1.80223000	-0.14717600
H	4.70746100	-1.65711300	0.09253100

COMadI-1

C	-1.97011400	1.77079000	-0.45317300
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C	-3.28786700	1.45118800	-0.87653000
C	-4.03703900	2.45085000	-1.44582100
C	-3.51512000	3.75856000	-1.62571100
C	-2.20109400	4.06370500	-1.17083500
C	-1.43297800	3.03781500	-0.52712400
C	-4.28505800	4.76779600	-2.26334700
C	-3.76802700	6.02157700	-2.46360700
C	-2.45011000	6.31738600	-2.04063000
C	-1.68601300	5.36649000	-1.41151900
C	-0.06885700	3.27274900	0.02013300
C	0.19755800	4.23296900	1.04952000
C	1.53090700	4.36674700	1.53288400
C	2.55303700	3.52485700	1.02668100
C	2.29370700	2.56687400	0.07564200
C	0.96591000	2.47196700	-0.41251900
C	-0.82047300	5.02898900	1.64376200
C	-0.51719800	5.93343200	2.62990500
C	0.81568100	6.09322600	3.08082400
C	1.81407200	5.32138100	2.54733000
O	0.68806100	1.50117200	-1.36943600
O	-1.21070500	0.73750600	0.08619900
P	0.00962200	0.15405200	-0.79474600
O	0.90959000	-0.67434500	0.03475300
O	-0.59567400	-0.49171000	-2.06850600
C	-3.82367400	0.07381800	-0.70610900
C	3.36520100	1.66317800	-0.42892000
C	-4.15245200	-0.65619800	-1.80396000
C	-4.66455900	-1.99291100	-1.69974200
C	-4.84604400	-2.58047900	-0.42416700
C	-4.51944100	-1.80011500	0.76350300
C	-4.01796700	-0.48048300	0.62107800
C	4.00396700	0.71507300	0.46514800
C	5.11251200	-0.04578500	0.00605300
C	5.55001400	0.08203000	-1.37855100
C	4.85401000	0.96861100	-2.23606900
C	3.76992300	1.75507900	-1.72225900
C	-4.68387400	-2.31751900	2.06919000
C	-4.38516000	-1.56240300	3.18265600
C	-3.91698100	-0.24554600	3.03757500
C	-3.73768700	0.28108800	1.77864100
C	-4.95056300	-2.73583500	-2.86621400
C	-5.40511300	-4.03336300	-2.78131000
C	-5.58857000	-4.62256100	-1.51714200
C	-5.31552500	-3.91183000	-0.36607400

C	3.52052900	0.50503400	1.77800900
C	4.13847300	-0.38503300	2.62964700
C	5.26919800	-1.09786400	2.19670800
C	5.73725700	-0.93517500	0.91018300
C	6.62804600	-0.65590700	-1.91765600
C	6.99234700	-0.52156100	-3.24150200
C	6.29550200	0.35908500	-4.08878400
C	5.24331600	1.09291200	-3.58836300
H	-5.05223800	2.24006500	-1.77097000
H	-5.28931100	4.51915600	-2.59483900
H	-4.36058800	6.78643600	-2.95493200
H	-2.03807700	7.30515600	-2.22081100
H	-0.67305800	5.60272500	-1.10380400
H	3.56043800	3.62947300	1.42172000
H	-1.84824200	4.90894400	1.31934500
H	-1.30831300	6.52888200	3.07428400
H	1.03835500	6.81699200	3.85801300
H	2.83875100	5.41547600	2.89568800
H	-0.25305400	-1.45296400	-2.28627800
H	-3.99928500	-0.23999700	-2.79646900
H	3.28121600	2.45515000	-2.39549100
H	-5.05642100	-3.32558200	2.20983200
H	-4.51674900	-1.98576400	4.17342500
H	-3.68956200	0.35169000	3.91467300
H	-3.37882900	1.29970200	1.67074000
H	-4.79708000	-2.26383800	-3.83288300
H	-5.61990200	-4.59956900	-3.68191700
H	-5.94537800	-5.64509500	-1.44434300
H	-5.46242900	-4.39854500	0.59125800
H	2.63734000	1.04201700	2.10785700
H	3.74468600	-0.54244600	3.62910700
H	5.75938200	-1.79735400	2.86653000
H	6.59200700	-1.52020500	0.59074600
H	7.18537000	-1.34413600	-1.29285800
H	7.82319700	-1.10146000	-3.63080200
H	6.58748400	0.45808800	-5.12933500
H	4.69358900	1.78012200	-4.22566400
C	3.61993400	-3.97915800	-0.29348400
C	3.12629600	-3.03646100	0.50856000
C	2.54771600	-3.29622700	1.84654200
N	1.51166700	-2.38399900	2.14262400
C	2.95945400	-4.27151000	2.66694300
C	0.60109400	-2.48308500	3.12882600
C	-0.51315000	-1.42494500	2.97326200

O	0.54980900	-3.29610600	4.03135900
F	-1.27462400	-1.71582600	1.90892000
F	-1.28622500	-1.40230500	4.05363500
F	-0.00873500	-0.19813700	2.78774300
H	3.61701700	-5.02984800	-0.01440800
H	3.10506200	-1.99727500	0.17965900
H	1.36672800	-1.63508700	1.45796100
H	2.50400800	-4.44749300	3.63058500
H	3.78524500	-4.89879900	2.35159000
C	-1.71810400	-3.44971500	-0.64504900
O	0.27852500	-2.72624200	-2.70843200
C	-0.21281200	-3.74393800	-0.61136500
C	0.37200700	-3.73359300	-1.99548300
C	1.04613900	-4.90369600	-2.58559300
C	1.29987700	-6.04241500	-1.93671700
H	-2.12830600	-3.53143600	0.36313000
H	-1.91601600	-2.43599500	-1.00608300
H	-2.24965200	-4.15481100	-1.29182700
H	-0.01788400	-4.68970900	-0.10599100
H	0.29499900	-2.95175500	-0.05195000
H	1.35412000	-4.76580600	-3.61863300
H	1.81506700	-6.85595000	-2.43811500
H	1.01924900	-6.20825500	-0.90156900
H	4.04809700	-3.71911400	-1.25679900

TSadI-1

C	-1.67386700	2.07119800	-0.36056300
C	-3.02276900	1.95207700	-0.79584200
C	-3.61925600	3.05236200	-1.36061500
C	-2.91694300	4.27470800	-1.52526400
C	-1.57665400	4.38531700	-1.05851700
C	-0.96834600	3.25560500	-0.41839600
C	-3.53121100	5.38895700	-2.15707900
C	-2.84076700	6.55889200	-2.34182100
C	-1.49744100	6.66068300	-1.90733300
C	-0.88110700	5.60500900	-1.28295300
C	0.40617800	3.29501700	0.15008800
C	0.78083500	4.20709400	1.18980000
C	2.11320700	4.16680700	1.69129700
C	3.02374800	3.20449200	1.18774900
C	2.65292600	2.29167100	0.22918500
C	1.32743100	2.36026700	-0.27669400
C	-0.13307500	5.12524100	1.77811600
C	0.27076900	5.97827800	2.77412300

C	1.60718700	5.96357700	3.24229000
C	2.50432200	5.07216000	2.71503600
O	0.94380300	1.44967500	-1.24078300
O	-1.07452200	0.95068000	0.17789900
P	0.05493200	0.17784300	-0.72240800
O	0.84421300	-0.67676900	0.21236700
O	-0.57521600	-0.40774900	-1.96033300
C	-3.75735100	0.66691600	-0.64901900
C	3.61916300	1.27843000	-0.27744300
C	-4.20952000	0.02921200	-1.76060900
C	-4.93694100	-1.20500100	-1.68538800
C	-5.19865000	-1.79298100	-0.42396300
C	-4.72549600	-1.11817300	0.77832200
C	-4.02143000	0.10875800	0.66439000
C	4.18384500	0.28884800	0.62157000
C	5.21423700	-0.57414500	0.16044000
C	5.64635800	-0.50156200	-1.22993400
C	5.01556600	0.42756200	-2.09263500
C	4.01197500	1.31325900	-1.57742600
C	-4.95000700	-1.64739900	2.06964700
C	-4.51475300	-0.98962500	3.19914000
C	-3.84130900	0.23852200	3.08508900
C	-3.60406300	0.77458200	1.83952800
C	-5.37481800	-1.84483600	-2.86642100
C	-6.05688700	-3.03994500	-2.80952600
C	-6.32591100	-3.62626500	-1.55901600
C	-5.90770800	-3.01571300	-0.39403800
C	3.69532900	0.13469600	1.94044500
C	4.23404800	-0.80387900	2.79409000
C	5.29326200	-1.61817200	2.35901600
C	5.76452900	-1.50786500	1.06825200
C	6.65154800	-1.33608900	-1.77035000
C	7.00652500	-1.25419300	-3.10123100
C	6.37401100	-0.33088600	-3.95357900
C	5.39541100	0.49751100	-3.45158200
H	-4.65185800	2.99064100	-1.69390800
H	-4.55810800	5.28837500	-2.49752200
H	-3.31553400	7.40442400	-2.82898600
H	-0.94788500	7.58152300	-2.07510800
H	0.15264200	5.69219000	-0.96584400
H	4.03383100	3.18048800	1.58943900
H	-1.16353700	5.13985300	1.44076500
H	-0.44325400	6.66804800	3.21288900
H	1.91149200	6.64906700	4.02657600

H	3.52850200	5.03212000	3.07553000
H	-0.13018400	-1.72692500	-2.36370500
H	-4.00169500	0.44398300	-2.74368800
H	3.57753400	2.04356100	-2.25537700
H	-5.47457000	-2.58888600	2.18511300
H	-4.69475100	-1.42159400	4.17855600
H	-3.50824700	0.76279900	3.97522800
H	-3.08783900	1.72533300	1.75573300
H	-5.15564100	-1.37615300	-3.82204500
H	-6.38702000	-3.52743500	-3.72123900
H	-6.86673600	-4.56601500	-1.50807900
H	-6.13263300	-3.49354700	0.55263200
H	2.87051500	0.75578700	2.27211800
H	3.83987500	-0.91211000	3.79958300
H	5.72935000	-2.34931300	3.03233700
H	6.56236500	-2.16853900	0.74868200
H	7.16004100	-2.05767300	-1.14105700
H	7.78035800	-1.90766100	-3.49144600
H	6.65795100	-0.27303200	-4.99941600
H	4.89680300	1.21903200	-4.09291600
C	3.68632200	-3.78784500	-0.59382400
C	2.90570000	-3.16663400	0.29813400
C	1.89675200	-3.84622800	1.10005200
N	0.92346000	-2.98442000	1.54262500
C	1.81271800	-5.22470000	1.19132300
C	-0.13356700	-3.28712300	2.35489700
C	-0.99050100	-2.04227900	2.67964200
O	-0.44405000	-4.37112100	2.79243100
F	-1.73565200	-1.70719600	1.62354300
F	-1.79405900	-2.30539200	3.70312400
F	-0.22433900	-0.99488000	2.99506700
H	3.65556000	-4.86121400	-0.75726500
H	2.94493700	-2.08344800	0.39039500
H	0.95815800	-2.01150300	1.16493200
H	1.14326500	-5.68063400	1.90596500
H	2.71157100	-5.77779900	0.94708200
C	-2.45472900	-3.73199000	-1.95260800
O	0.32998300	-2.64652000	-2.53205500
C	-1.34133500	-3.34959300	-0.96401800
C	-0.01704000	-3.54168800	-1.65072900
C	0.77329300	-4.68074500	-1.53044000
C	0.64430900	-5.59546200	-0.47279300
H	-3.43053300	-3.64633600	-1.46965400
H	-2.44132500	-3.07045400	-2.82303600

H	-2.32583900	-4.76205700	-2.29748800
H	-1.41688000	-3.95877300	-0.06265700
H	-1.45654500	-2.30281000	-0.67579200
H	1.61349900	-4.75827700	-2.21311200
H	1.12501300	-6.56355600	-0.57797700
H	-0.27366000	-5.61053000	0.10519600
H	4.38724400	-3.21617800	-1.19559700

INTadI-2

C	-2.33076900	1.63614200	-0.25528000
C	-3.57916700	1.16384400	-0.73834900
C	-4.37447300	2.04840300	-1.42319100
C	-3.95906500	3.38514400	-1.66173400
C	-2.70315200	3.83791100	-1.16498700
C	-1.89049200	2.93241600	-0.40574000
C	-4.77514700	4.27554500	-2.40958000
C	-4.35773400	5.55404700	-2.67482900
C	-3.09543200	5.99483900	-2.21043900
C	-2.28857900	5.16136700	-1.47675500
C	-0.56842900	3.31319700	0.16572100
C	-0.41278400	4.36979600	1.12169900
C	0.88877100	4.65598600	1.62470500
C	1.99907200	3.88831900	1.18819700
C	1.85061700	2.84828600	0.30363400
C	0.54291300	2.57387900	-0.17945300
C	-1.51277500	5.11527600	1.62814000
C	-1.31933700	6.11059800	2.55280000
C	-0.02028200	6.41699300	3.02500800
C	1.05707700	5.70046200	2.57338400
O	0.37920000	1.48628200	-1.03125500
O	-1.53257300	0.72693600	0.42393700
P	-0.23243400	0.15006500	-0.34324100
O	0.67223500	-0.17976000	0.87196100
O	-0.47772200	-0.87436100	-1.37710800
C	-3.97518200	-0.25616100	-0.52833300
C	3.01935400	2.07088200	-0.20055100
C	-4.07713200	-1.08260100	-1.60149900
C	-4.45951600	-2.45972400	-1.46566800
C	-4.76151200	-2.98450600	-0.18595000
C	-4.63402500	-2.11563800	0.97790500
C	-4.24984900	-0.76002000	0.80452800
C	3.77797100	1.18381400	0.66281500
C	4.90651900	0.49318500	0.13942900
C	5.29252900	0.68586000	-1.25164200

C	4.50710000	1.53604000	-2.06589300
C	3.37415800	2.21224900	-1.50523200
C	-4.87851800	-2.58146100	2.28948800
C	-4.76350300	-1.74661100	3.38043600
C	-4.40250400	-0.40057400	3.20349100
C	-4.15222700	0.07960000	1.93698400
C	-4.53505900	-3.29188400	-2.60486900
C	-4.91982300	-4.60967800	-2.48997100
C	-5.24686800	-5.12952900	-1.22424500
C	-5.16852100	-4.33490000	-0.09896300
C	3.38937800	0.95159300	2.00147500
C	4.09294300	0.07964300	2.80596700
C	5.20458300	-0.60678600	2.29131500
C	5.59684100	-0.40535600	0.98443900
C	6.38578700	0.01806800	-1.84814600
C	6.67748200	0.18401500	-3.18652000
C	5.89418400	1.03330200	-3.99000400
C	4.82804300	1.70257400	-3.43190300
H	-5.33940100	1.72182000	-1.80159100
H	-5.73395300	3.91591300	-2.77234000
H	-4.98571900	6.22708900	-3.24944300
H	-2.76027300	7.00082000	-2.44198700
H	-1.31838800	5.50788000	-1.13734200
H	2.98686100	4.12887500	1.57340800
H	-2.51552700	4.88314200	1.28628000
H	-2.17190800	6.66545100	2.93121100
H	0.11539000	7.21059300	3.75256000
H	2.05890600	5.91052300	2.93737600
H	-0.85915000	-2.61913600	-2.21707400
H	-3.85017300	-0.70833300	-2.59661500
H	2.79357600	2.86182600	-2.15600300
H	-5.15803400	-3.61583700	2.45297800
H	-4.95378800	-2.13180900	4.37710800
H	-4.31871600	0.25914700	4.06103900
H	-3.87725300	1.12112500	1.80327400
H	-4.28550000	-2.86936300	-3.57440400
H	-4.97463800	-5.24322900	-3.36936500
H	-5.55998500	-6.16452700	-1.12992200
H	-5.42386500	-4.76793500	0.86141700
H	2.51038600	1.45556100	2.38909500
H	3.77640600	-0.08795200	3.82982900
H	5.75183500	-1.30334800	2.91867600
H	6.45252300	-0.95383400	0.60784700
H	7.01223300	-0.64094400	-1.25812900

H	7.52036500	-0.34378400	-3.62135500
H	6.13180400	1.15902200	-5.04140200
H	4.20983400	2.36267000	-4.03425300
C	3.32918800	-1.64417900	-2.61631300
C	2.87609100	-1.46223100	-1.37045700
C	2.95757500	-2.45192200	-0.29860500
N	2.34415300	-2.11648900	0.81030300
C	3.60163300	-3.78883900	-0.53494700
C	2.42895100	-2.85561200	1.98714800
C	1.32981900	-2.45314600	2.99963400
O	3.25075700	-3.67556000	2.31242400
F	0.11461000	-2.53282000	2.45124800
F	1.36737900	-3.25417600	4.05858300
F	1.50499800	-1.19514000	3.41467900
H	3.79473100	-2.56279600	-2.95640600
H	2.43104800	-0.50709300	-1.10279200
H	1.37572700	-0.95580700	0.80139600
H	4.25834200	-4.04010200	0.29713300
H	4.20132400	-3.74642100	-1.44339900
C	-1.67597100	-4.85408000	-0.16265200
O	-0.49595700	-3.47417600	-2.50861800
C	-0.45465100	-3.93027600	-0.13972700
C	0.25879700	-3.94515500	-1.46304200
C	1.48143500	-4.42594200	-1.71693900
C	2.49022900	-4.86529900	-0.69412400
H	-2.23073100	-4.78485100	0.77735000
H	-2.34908300	-4.57984100	-0.97975800
H	-1.37067600	-5.89520300	-0.30750400
H	0.21946000	-4.21960300	0.66841900
H	-0.78072700	-2.90296000	0.06452600
H	1.82550000	-4.35672100	-2.74774000
H	2.98285500	-5.79687300	-0.98973900
H	2.02589100	-5.04444500	0.27876800
H	3.23016900	-0.84692200	-3.34682300

TSadI-2

C	-2.75981800	1.08629600	-0.08838300
C	-3.92758500	0.36270400	-0.45861500
C	-4.92507500	1.03776200	-1.11693800
C	-4.79490000	2.41195800	-1.44849300
C	-3.61557200	3.12018100	-1.07881600
C	-2.59346200	2.43282700	-0.34312400
C	-5.81707700	3.08360400	-2.17116000
C	-5.67125400	4.39643000	-2.53798400

C	-4.48464000	5.09208600	-2.20465300
C	-3.48455900	4.47331300	-1.49662200
C	-1.32384700	3.09090400	0.07714700
C	-1.28828000	4.24025700	0.93178700
C	-0.02778900	4.81858600	1.25810000
C	1.16523400	4.23335400	0.76157400
C	1.14028800	3.09795300	-0.01157300
C	-0.12716500	2.53525100	-0.33231300
C	-2.45981200	4.80871600	1.50416800
C	-2.38097400	5.90783900	2.32197700
C	-1.12989100	6.50252500	2.61544300
C	0.01937800	5.96436700	2.09771600
O	-0.15526800	1.39227700	-1.09658200
O	-1.76553800	0.39841500	0.56836300
P	-0.42952100	-0.02308800	-0.29402100
O	0.64142100	-0.25236000	0.72842100
O	-0.74692700	-1.01154600	-1.36787600
C	-4.02644000	-1.09771600	-0.18443100
C	2.38479300	2.47740000	-0.54663800
C	-4.07723800	-1.96203500	-1.23191900
C	-4.15274300	-3.38280600	-1.04400000
C	-4.19430000	-3.91901900	0.26598000
C	-4.16450200	-3.00385100	1.40063700
C	-4.07675200	-1.60509000	1.17386500
C	3.40617000	1.95092500	0.34115100
C	4.60635500	1.41437000	-0.20266400
C	4.76818500	1.33005000	-1.64819200
C	3.72899500	1.81249100	-2.47880300
C	2.55971900	2.39933400	-1.89256600
C	-4.21430800	-3.46537700	2.73576700
C	-4.18446800	-2.58900300	3.79943600
C	-4.10925700	-1.20466000	3.57107400
C	-4.05873600	-0.72639000	2.28060200
C	-4.14507200	-4.24800800	-2.16018900
C	-4.18044400	-5.61477300	-1.99241700
C	-4.22752200	-6.15341500	-0.69392900
C	-4.23451000	-5.32389300	0.40930700
C	3.21598400	1.92230800	1.74136800
C	4.18730600	1.42366600	2.58335000
C	5.38975500	0.92746600	2.05147100
C	5.58771800	0.91954800	0.68631800
C	5.88166600	0.71395300	-2.26260900
C	5.95061700	0.57266500	-3.63356300
C	4.91224800	1.05092900	-4.45431700

C	3.82244300	1.66840300	-3.88110000
H	-5.83091700	0.51126400	-1.40612700
H	-6.71299300	2.52797000	-2.43430600
H	-6.45525800	4.90133100	-3.09305200
H	-4.36201400	6.12415400	-2.51770500
H	-2.57577000	5.01607400	-1.26076500
H	2.11761600	4.69224100	1.01607700
H	-3.42362300	4.35583500	1.29756600
H	-3.28623400	6.32328000	2.75331600
H	-1.08545300	7.37499400	3.25926300
H	0.98931800	6.39731500	2.32646400
H	-0.63819600	-2.66996200	-2.08924100
H	-4.02488800	-1.58123500	-2.24868500
H	1.78756900	2.77361700	-2.55998800
H	-4.27999300	-4.52796200	2.93902800
H	-4.22324600	-2.97103200	4.81460200
H	-4.09166700	-0.51401600	4.40801500
H	-4.00623400	0.34330700	2.10474700
H	-4.10331000	-3.81234700	-3.15483600
H	-4.16978100	-6.27367200	-2.85473900
H	-4.25490900	-7.22970200	-0.55596100
H	-4.26430200	-5.77234700	1.39572900
H	2.28131900	2.28522300	2.15414300
H	4.01593900	1.40494900	3.65462200
H	6.15537600	0.53318300	2.71258000
H	6.51545400	0.51540500	0.29754700
H	6.69508000	0.32803000	-1.65882600
H	6.81233900	0.08722900	-4.08075000
H	4.97243700	0.93321100	-5.53149000
H	3.00907000	2.04275100	-4.49686900
C	2.59928000	-1.55787800	-2.67444900
C	2.71006000	-1.07544700	-1.39699600
C	3.47467900	-1.77227500	-0.45668600
N	3.22138500	-1.45898600	0.85220600
C	4.25702200	-2.95147400	-0.87723600
C	3.88807500	-1.92689500	1.95623200
C	3.17284100	-1.64074700	3.29238600
O	4.91835400	-2.55649900	1.98235900
F	2.67722800	-2.78844300	3.76312100
F	4.04743100	-1.17438200	4.18196600
F	2.16975900	-0.77186700	3.17580800
H	3.36237900	-2.16536500	-3.14329100
H	2.05232400	-0.29001700	-1.04773800
H	2.39919800	-0.84784000	1.00457200

H	4.97181500	-3.26702700	-0.12412400
H	4.79316500	-2.70510200	-1.79529300
C	-0.82979300	-3.74004800	0.23616900
O	-0.09484600	-3.39868800	-2.46719500
C	0.61722500	-3.42681800	-0.15016500
C	0.91099500	-3.61269900	-1.61184200
C	2.14062800	-3.97936300	-2.08863600
C	3.31122700	-4.21273200	-1.19763700
H	-0.93056700	-3.70627100	1.32432800
H	-1.52034300	-3.00318000	-0.17982700
H	-1.13164000	-4.73499700	-0.10556900
H	1.29904400	-4.04577400	0.43735800
H	0.83472500	-2.38478700	0.11309700
H	2.23164700	-4.16637700	-3.15449600
H	3.99451500	-4.93279800	-1.65237300
H	3.01026100	-4.61383700	-0.22865000
H	1.80994600	-1.18511200	-3.32164600

PadI

C	-2.02754500	-2.16556200	-0.41709100
C	-0.57659700	-1.82053400	-0.60465400
C	0.06005700	-0.88562200	0.10881900
N	1.43505400	-0.65394000	-0.15717600
C	-0.58842800	-0.10121400	1.22159100
C	2.16832100	0.40887600	0.21914900
C	3.65043500	0.32184700	-0.19365300
O	1.81916000	1.38903900	0.85047400
F	4.01605900	1.44163200	-0.81674900
F	4.41353900	0.19006000	0.89475700
F	3.91587100	-0.71097800	-1.00693400
H	-2.11488000	-3.15169300	0.05682700
H	-0.02656000	-2.36470700	-1.37088900
H	1.88780600	-1.33158800	-0.76055700
H	-0.75468000	0.93267100	0.89470700
H	0.09784100	-0.03759600	2.07047600
C	-4.40807100	2.28387600	-0.57870500
O	-2.90238900	0.18252900	-1.57560200
C	-3.81057200	1.24424300	0.35738800
C	-3.12783200	0.11003700	-0.38402300
C	-2.75987100	-1.12818200	0.43090300
C	-1.90141100	-0.75654600	1.65096400
H	-4.87868600	3.08916900	-0.00987400
H	-3.63524400	2.71702100	-1.21749200
H	-5.16319600	1.83520600	-1.22966100

H	-4.56615700	0.81497000	1.02633700
H	-3.06034800	1.70404700	1.01431200
H	-3.71172000	-1.54328200	0.78745400
H	-1.68559800	-1.67662400	2.20499900
H	-2.44364300	-0.09230800	2.32933200
H	-2.50462000	-2.24398900	-1.39850700

COMadII-1

C	2.79577000	0.52949000	-0.43926500
C	3.16563200	1.82744200	-0.87869300
C	4.34249500	1.95889300	-1.56916000
C	5.15101400	0.82711000	-1.86324000
C	4.76217800	-0.46595000	-1.40711600
C	3.56187900	-0.59959800	-0.63287500
C	6.33987400	0.96675600	-2.62774900
C	7.09996800	-0.12784500	-2.95021200
C	6.69601900	-1.41670400	-2.52792600
C	5.55884400	-1.58316600	-1.77755300
C	3.08116100	-1.89165100	-0.06523100
C	3.85246000	-2.67483600	0.85569000
C	3.28499800	-3.87042000	1.38542000
C	1.95280900	-4.23047700	1.05432200
C	1.18778900	-3.45466200	0.21884000
C	1.79435200	-2.30155400	-0.34417400
C	5.14653600	-2.28762500	1.30112200
C	5.84958700	-3.06974600	2.18249000
C	5.30146000	-4.27928900	2.67303600
C	4.04436500	-4.66445900	2.28699900
O	1.03265500	-1.53808800	-1.22119500
O	1.58156600	0.42714500	0.22620900
P	0.35059000	-0.21527700	-0.60566500
O	-0.78400800	-0.43294000	0.30814700
O	0.10657400	0.63294700	-1.88098900
C	2.25375500	2.96647900	-0.57060900
C	-0.24778300	-3.74648800	-0.06585700
C	1.42500900	3.45023200	-1.53066500
C	0.46603900	4.48197700	-1.25118300
C	0.39689800	5.05199400	0.04247500
C	1.28502100	4.54619600	1.08157100
C	2.19930100	3.50387800	0.77548300
C	-1.25598200	-3.48599500	0.94630200
C	-2.62532400	-3.71028300	0.64595100
C	-3.00365100	-4.20827200	-0.67020600
C	-1.98878300	-4.44973100	-1.62733400

C	-0.61636600	-4.20099800	-1.29084100
C	1.25419200	5.04361800	2.40424200
C	2.08807400	4.53955500	3.38044700
C	2.99348200	3.50979900	3.07283000
C	3.04426600	3.00353000	1.79197700
C	-0.44065300	4.89489900	-2.25358800
C	-1.38714800	5.86203100	-1.99254200
C	-1.44447800	6.44960600	-0.71542800
C	-0.57086500	6.05396400	0.27783000
C	-0.90633700	-2.96674100	2.21468600
C	-1.86752500	-2.68759000	3.16158400
C	-3.22334100	-2.91452300	2.86863600
C	-3.58993800	-3.41201000	1.63647500
C	-4.34442700	-4.44883600	-1.04681100
C	-4.65812400	-4.90880900	-2.30899800
C	-3.64476300	-5.14911400	-3.25480900
C	-2.33018600	-4.92188400	-2.91416800
H	4.66228800	2.93849800	-1.91402400
H	6.62668200	1.96101500	-2.95861500
H	8.00465600	-0.01231100	-3.53818700
H	7.28840100	-2.28265600	-2.80562500
H	5.25245300	-2.57762200	-1.47067300
H	1.52359200	-5.12226500	1.50393300
H	5.57583300	-1.35750200	0.94596300
H	6.83442400	-2.75472200	2.51237400
H	5.87335700	-4.88902900	3.36487000
H	3.59832800	-5.57734500	2.67155000
H	-0.81656300	1.11347300	-1.92848300
H	1.44465400	3.02324000	-2.52956800
H	0.13755000	-4.37488900	-2.05472800
H	0.56675800	5.83922600	2.66780900
H	2.04368800	4.94095900	4.38791800
H	3.65106300	3.11447300	3.84042400
H	3.74735600	2.21152800	1.55345200
H	-0.37765200	4.43074500	-3.23441400
H	-2.08123400	6.17299000	-2.76728100
H	-2.18243700	7.21789800	-0.50681800
H	-0.64975100	6.51966800	1.25364200
H	0.13805000	-2.77239100	2.43570400
H	-1.57840000	-2.28313600	4.12676600
H	-3.98493900	-2.68678300	3.60796700
H	-4.64249200	-3.56728900	1.43100600
H	-5.14922200	-4.27351200	-0.34275200
H	-5.69610500	-5.08494300	-2.57300700

H	-3.90030600	-5.50933500	-4.24616100
H	-1.53270900	-5.09771000	-3.63097500
C	-0.60409700	1.96643500	3.48548800
C	-1.29355800	0.94151800	2.98350000
C	-2.76047100	0.95207800	2.77652000
N	-3.13955500	0.24536500	1.61370300
C	-3.61321900	1.58370100	3.59594900
C	-4.35300600	0.27288200	1.03873000
C	-4.44699300	-0.49351500	-0.29594500
O	-5.36380500	0.83026200	1.43074300
F	-3.29072700	-1.01469300	-0.70377800
F	-5.33862200	-1.48455900	-0.19114600
F	-4.88157400	0.33876500	-1.25291600
H	-1.08580600	2.89671100	3.77713200
H	-0.77186800	0.04402800	2.65779200
H	-2.37729300	-0.20121300	1.09542300
H	-4.67775900	1.61318000	3.41976800
H	-3.21172500	2.06797300	4.47873300
C	-4.37941000	2.84713100	-3.17101200
O	-2.09970600	1.74984800	-2.14997500
C	-3.96487400	3.15759800	-1.74178200
C	-2.66708800	2.50122100	-1.34898800
C	-2.08051400	2.75624900	-0.02339300
C	-2.62145800	3.59549100	0.86395200
H	-5.32724400	3.33806400	-3.40180300
H	-3.62557900	3.20105600	-3.87921400
H	-4.49941200	1.77191100	-3.31749500
H	-4.72508000	2.83037600	-1.02217900
H	-3.84523300	4.23625800	-1.58757100
H	-1.15584800	2.23032300	0.20695700
H	-2.13958900	3.76578600	1.82197700
H	-3.54521900	4.13471000	0.67399200
H	0.47127200	1.89926000	3.61936000

TSadII-1

C	2.44361900	1.36237000	-0.39956100
C	2.35168600	2.69499900	-0.88533900
C	3.38493900	3.17844000	-1.64607100
C	4.50585900	2.36442300	-1.96426300
C	4.57819100	1.02830400	-1.47292500
C	3.52433800	0.53640500	-0.63319500
C	5.54873100	2.86022700	-2.79154000
C	6.60821600	2.06323500	-3.14111700
C	6.66355100	0.72495600	-2.68438900

C	5.67697900	0.22023500	-1.87434400
C	3.50181900	-0.83936000	-0.05687800
C	4.52202000	-1.34334100	0.81489600
C	4.38920700	-2.66109800	1.34233300
C	3.23285400	-3.43001200	1.04617300
C	2.22621000	-2.93191800	0.25690500
C	2.39703700	-1.63254000	-0.29521700
C	5.64464300	-0.56712100	1.21558700
C	6.59841600	-1.08842800	2.05332700
C	6.48542600	-2.41224800	2.54211100
C	5.40069700	-3.17594100	2.19764500
O	1.39334000	-1.13855100	-1.10323500
O	1.38545800	0.90090000	0.35131800
P	0.33699500	-0.12795400	-0.37644400
O	-0.38506400	-0.79755600	0.74311800
O	-0.38441100	0.55297900	-1.50510200
C	1.12239200	3.48176500	-0.58275600
C	0.96694300	-3.68136800	-0.02696300
C	0.21481300	3.70981800	-1.56672200
C	-1.02870200	4.37940400	-1.31013800
C	-1.31467300	4.86667300	-0.01264700
C	-0.34269200	4.64578800	1.05001100
C	0.85897400	3.94468600	0.76641400
C	-0.05094500	-3.83376300	0.99664500
C	-1.28292500	-4.46106700	0.67325000
C	-1.49417600	-4.99183600	-0.66729800
C	-0.46953400	-4.83631200	-1.63151000
C	0.74511100	-4.16030600	-1.27823100
C	-0.56835800	5.08315300	2.37573700
C	0.34710100	4.83842100	3.37798400
C	1.53493300	4.14299900	3.09336900
C	1.78268400	3.70837300	1.80970700
C	-1.99608800	4.49241600	-2.33381800
C	-3.21908600	5.07753800	-2.08635800
C	-3.49915300	5.58574700	-0.80409500
C	-2.56530500	5.48691200	0.20731500
C	0.13705200	-3.31836600	2.29998100
C	-0.85225700	-3.41007900	3.25355000
C	-2.07901900	-4.01746500	2.93177600
C	-2.28469100	-4.53140500	1.66984200
C	-2.68079700	-5.65271300	-1.05855300
C	-2.83919900	-6.13342700	-2.34167900
C	-1.81750800	-5.97400000	-3.29584900
C	-0.65126600	-5.33398000	-2.94130000

H	3.34683700	4.19472300	-2.02928600
H	5.48113700	3.88431400	-3.14834100
H	7.39847100	2.44959000	-3.77665200
H	7.49167600	0.08990900	-2.98276500
H	5.72483700	-0.81116300	-1.54170400
H	3.13835600	-4.42219300	1.48057100
H	5.73840900	0.45286500	0.85914200
H	7.44577300	-0.47797400	2.34907500
H	7.25120600	-2.81211800	3.19888000
H	5.28676800	-4.18646900	2.58034800
H	-1.74708700	0.86338700	-1.76254500
H	0.39633900	3.33063200	-2.56869200
H	1.49686900	-4.02328900	-2.05177200
H	-1.47317400	5.62920500	2.61862100
H	0.14950800	5.18666500	4.38697800
H	2.25634900	3.95137200	3.88124900
H	2.70332000	3.17726900	1.58850800
H	-1.76165200	4.09295800	-3.31695100
H	-3.96072500	5.15370700	-2.87554700
H	-4.45713100	6.05729100	-0.60744300
H	-2.81662900	5.87832100	1.18680200
H	1.07089500	-2.82099700	2.53820100
H	-0.68944900	-3.00306100	4.24680600
H	-2.86646000	-4.08213100	3.67619200
H	-3.24070000	-4.98902300	1.44409700
H	-3.48709800	-5.79291000	-0.34805900
H	-3.76028100	-6.63809600	-2.61583000
H	-1.95070900	-6.35296200	-4.30409300
H	0.14906400	-5.19841000	-3.66364100
C	-1.20543700	1.55963500	3.85133900
C	-1.58720400	0.47031700	3.17808800
C	-2.90097500	0.31787200	2.53731800
N	-2.90409500	-0.58409800	1.50150300
C	-3.95525300	1.17802000	2.77105900
C	-3.99558900	-0.90848000	0.74824400
C	-3.70559400	-1.75534100	-0.50830800
O	-5.15775400	-0.63649000	0.96930500
F	-2.42057600	-1.77319800	-0.85462700
F	-4.10804400	-3.01323200	-0.30588500
F	-4.41045200	-1.25988500	-1.52799200
H	-1.85347400	2.41851600	4.00280000
H	-0.88736900	-0.34448400	3.01834200
H	-1.95274900	-0.86704800	1.15209600
H	-4.94269700	0.95027300	2.40262800

H	-3.89241500	1.81976900	3.64192300
C	-5.24562300	1.70389000	-2.76860100
O	-2.74107500	1.07705400	-2.00811100
C	-4.86998700	1.83182900	-1.29742200
C	-3.40364000	1.62205200	-1.03489200
C	-2.77118900	1.98411000	0.15477200
C	-3.41780800	2.54392200	1.25956500
H	-6.31437200	1.89024500	-2.89517100
H	-4.69432500	2.42665800	-3.37622100
H	-5.01980800	0.70511000	-3.14591100
H	-5.42009100	1.09398800	-0.69669200
H	-5.15192200	2.81575800	-0.91097100
H	-1.69711900	1.82521200	0.21287400
H	-2.79575400	3.08791300	1.96628600
H	-4.44246200	2.89405300	1.17003700
H	-0.20733800	1.61866100	4.27239100

INTadII-2

C	-2.25529900	1.62446800	-0.31534300
C	-3.54089700	1.14039600	-0.68722100
C	-4.41547100	2.02370800	-1.27290500
C	-4.05664200	3.37429700	-1.51999400
C	-2.77763500	3.84864400	-1.11323200
C	-1.88200100	2.94752800	-0.45125800
C	-4.95425600	4.26077300	-2.17355700
C	-4.59338000	5.55731500	-2.43493600
C	-3.31007900	6.02214200	-2.05886400
C	-2.42588000	5.19269500	-1.41546700
C	-0.55594100	3.36348900	0.08311900
C	-0.41987600	4.37447500	1.08981400
C	0.87819500	4.66542900	1.59923100
C	1.99192900	3.91097700	1.15295300
C	1.85832400	2.90250200	0.22881300
C	0.56700600	2.66468200	-0.31400100
C	-1.53043800	5.07232000	1.64244000
C	-1.34950900	6.03255300	2.60582800
C	-0.05266400	6.35029500	3.07760400
C	1.03415000	5.67459500	2.58818300
O	0.41972200	1.67644400	-1.26685500
O	-1.36480000	0.72733600	0.23560900
P	-0.11659900	0.23147800	-0.71428600
O	0.89596300	-0.31375500	0.25217100
O	-0.59796000	-0.55384300	-1.88704900
C	-3.92251300	-0.28200800	-0.46820200

C	3.03290200	2.07237100	-0.16281900
C	-4.28082000	-1.04067600	-1.53739600
C	-4.68827000	-2.40957300	-1.40069300
C	-4.72207100	-3.00984900	-0.11965700
C	-4.35471400	-2.20732900	1.04067500
C	-3.96949100	-0.85172500	0.86720300
C	3.64012400	1.17344200	0.80303200
C	4.81504400	0.45736200	0.45552100
C	5.40973200	0.64345000	-0.86215600
C	4.75105400	1.48042400	-1.79462800
C	3.55709900	2.17785100	-1.41071000
C	-4.37635100	-2.73651800	2.35073700
C	-4.05061500	-1.96283000	3.44567300
C	-3.70470600	-0.61220100	3.27337200
C	-3.66678700	-0.07243200	2.00594300
C	-5.03181500	-3.16353900	-2.54296800
C	-5.40211300	-4.48604900	-2.42965000
C	-5.43552600	-5.08893100	-1.16031700
C	-5.10261900	-4.36606800	-0.03177800
C	3.05227000	0.95666900	2.07146800
C	3.59750700	0.06521100	2.96949600
C	4.75898200	-0.64866900	2.62654200
C	5.35115200	-0.45304500	1.39665000
C	6.60713000	0.01076200	-1.26508700
C	7.11749200	0.19270300	-2.53373900
C	6.45179000	1.01618100	-3.45996100
C	5.28706900	1.65096100	-3.09051800
H	-5.40704000	1.68387000	-1.56028100
H	-5.92981800	3.88401100	-2.46832400
H	-5.28310100	6.22725200	-2.93809100
H	-3.02164200	7.04336600	-2.28693200
H	-1.44078400	5.55642500	-1.14232800
H	2.96928400	4.11856800	1.58202600
H	-2.53207700	4.83327900	1.30329100
H	-2.21076800	6.55048200	3.01585900
H	0.07313300	7.11710900	3.83515400
H	2.03480200	5.88823500	2.95374800
H	-1.47652600	-1.97695800	-1.22471900
H	-4.24332900	-0.61497500	-2.53727400
H	3.08855500	2.83216100	-2.14165300
H	-4.65962000	-3.77037200	2.51184800
H	-4.07805600	-2.39568900	4.44105400
H	-3.47103600	0.00630700	4.13454300
H	-3.40510700	0.97294800	1.87934600

H	-4.99250100	-2.68034200	-3.51554700
H	-5.66279800	-5.06067600	-3.31272200
H	-5.72238400	-6.13147500	-1.06453000
H	-5.13416300	-4.86482800	0.93012400
H	2.14231600	1.48966200	2.32537000
H	3.12391900	-0.09266300	3.93379500
H	5.19017500	-1.35766100	3.32647200
H	6.23741600	-1.02580800	1.15030900
H	7.14628900	-0.62795000	-0.57478200
H	8.03961600	-0.30446400	-2.81776200
H	6.85740300	1.15155500	-4.45745600
H	4.76152500	2.29615200	-3.78913400
C	-0.40948500	-2.01747900	3.69324100
C	0.53197300	-1.76815600	2.76865000
C	1.31228600	-2.80231400	2.11886900
C	1.20800900	-4.24266100	2.49954700
C	3.03763000	-3.14221000	0.44817300
C	3.59466400	-2.53695100	-0.86304700
O	3.49462500	-4.18948600	0.81860900
F	3.07251000	-1.34937300	-1.15171500
F	4.91650200	-2.42713300	-0.76016100
F	3.33739500	-3.37244200	-1.87162200
H	-0.68871600	-3.01228400	4.02369300
H	0.72611900	-0.74926400	2.45328700
H	2.19836300	-4.67104500	2.65787400
H	0.65110700	-4.32246800	3.43039900
C	-0.16764800	-3.76013900	-2.78734800
O	-1.75069100	-2.69719500	-0.61663000
C	0.39200800	-3.49909200	-1.38693700
C	-0.68169100	-3.48239300	-0.33044300
C	-0.68662200	-4.18346000	0.81580000
C	0.45824000	-4.99811800	1.35543400
H	0.65026200	-3.81864100	-3.51026400
H	-0.72443400	-4.70124200	-2.81739400
H	-0.83465100	-2.95332000	-3.10003700
H	0.88309200	-2.51778200	-1.39588600
H	1.14112100	-4.25738200	-1.15030400
H	-1.54548400	-4.03531300	1.46926700
H	0.11255800	-5.94403700	1.78269000
H	1.17602300	-5.24996100	0.57272300
N	2.05581300	-2.38419000	1.09786500
H	1.73457900	-1.42331900	0.67235000
H	-0.94748200	-1.18729900	4.13899700

TSadII-2

C	-2.32378000	1.57191500	-0.25048100
C	-3.59816800	1.04588100	-0.60531400
C	-4.52002500	1.90221100	-1.15872100
C	-4.22202900	3.26782600	-1.39804200
C	-2.95218900	3.78452100	-1.01783200
C	-2.00838000	2.91073000	-0.38740800
C	-5.16815400	4.12517000	-2.02138000
C	-4.86140500	5.43587500	-2.28037300
C	-3.58652600	5.94414000	-1.93211900
C	-2.65695200	5.14291900	-1.31775600
C	-0.68322200	3.37388600	0.10444300
C	-0.55322600	4.38265300	1.11291900
C	0.74906500	4.72287800	1.57742500
C	1.87135600	4.00722400	1.09322500
C	1.74528500	2.99663900	0.16916100
C	0.44891300	2.72040600	-0.34227500
C	-1.67041500	5.03415700	1.70764600
C	-1.49302300	5.99849800	2.66736100
C	-0.19342600	6.36653500	3.09369400
C	0.90103000	5.73532600	2.56388800
O	0.29940300	1.74740700	-1.31044400
O	-1.37756900	0.70669000	0.26292600
P	-0.15893200	0.26764800	-0.76736400
O	0.93174100	-0.31395800	0.06901300
O	-0.74019200	-0.48035300	-1.93169400
C	-3.93812800	-0.39017900	-0.41162200
C	2.94222100	2.19995400	-0.22249100
C	-4.29001700	-1.13377000	-1.49314300
C	-4.68071900	-2.50945100	-1.38101500
C	-4.71296300	-3.13162600	-0.11063600
C	-4.37356000	-2.34017700	1.06633800
C	-3.98985700	-0.98028900	0.91440800
C	3.58315400	1.34719800	0.76421300
C	4.80827900	0.70463300	0.45069800
C	5.39544100	0.88073700	-0.87171600
C	4.69672600	1.65451900	-1.83028200
C	3.47095300	2.30834400	-1.46774600
C	-4.44471400	-2.87606700	2.37285400
C	-4.16620700	-2.10619100	3.48375300
C	-3.79977700	-0.75834600	3.33122100
C	-3.71324000	-0.21121900	2.06823500
C	-5.00926700	-3.24899400	-2.53698000
C	-5.36060300	-4.57836800	-2.44713200

C	-5.39060900	-5.20358100	-1.18841500
C	-5.07516000	-4.49471900	-0.04615200
C	2.98182300	1.10682700	2.02275100
C	3.57201100	0.27651800	2.95012500
C	4.79772600	-0.34368500	2.65091400
C	5.39879200	-0.13154500	1.42788300
C	6.62051100	0.29114100	-1.25578900
C	7.12224200	0.45618500	-2.53045300
C	6.41977000	1.21884700	-3.48090700
C	5.22622800	1.80993200	-3.13053600
H	-5.50285800	1.52560500	-1.42960300
H	-6.13607200	3.71461900	-2.29551900
H	-5.58707900	6.08411400	-2.76089400
H	-3.34095800	6.97679400	-2.15892400
H	-1.67927500	5.54054100	-1.06657500
H	2.85331200	4.24185200	1.49709600
H	-2.67327400	4.75634700	1.40340500
H	-2.35871300	6.48110100	3.10994700
H	-0.07119100	7.13620300	3.84893700
H	1.90491500	5.98697800	2.89472500
H	-1.43941900	-1.90582500	-1.40855200
H	-4.26008200	-0.68929800	-2.48497600
H	2.98205900	2.93101800	-2.21283400
H	-4.73733600	-3.90974800	2.51811900
H	-4.23623100	-2.54244200	4.47515400
H	-3.58707200	-0.14800700	4.20300400
H	-3.43955000	0.83282900	1.95606300
H	-4.97291600	-2.74908700	-3.50108200
H	-5.60939500	-5.14175000	-3.34077000
H	-5.66306000	-6.25148200	-1.11158700
H	-5.10741500	-5.00838300	0.90797700
H	2.02738500	1.57115800	2.24519100
H	3.08633500	0.09479200	3.90392700
H	5.26937400	-0.99833700	3.37728500
H	6.33591400	-0.63271200	1.21670000
H	7.18646000	-0.30271300	-0.54731200
H	8.06577200	-0.00768500	-2.80013400
H	6.81905300	1.34170500	-4.48258700
H	4.67180000	2.40736300	-3.84906300
C	-0.90094500	-2.66966600	2.40519900
C	0.34424600	-2.09507700	2.28239400
C	1.42473300	-2.94734800	2.06072800
C	1.27011100	-4.40167300	2.26321700
C	3.54834100	-3.07621800	0.84063900

C	4.07186500	-2.58306600	-0.52648300
O	4.09288700	-4.01799800	1.36308000
F	3.47730600	-1.46334800	-0.93549800
F	5.38757400	-2.39538400	-0.48830600
F	3.82116000	-3.53710900	-1.43265800
H	-1.06950300	-3.62585200	2.88435400
H	0.42283900	-1.06303100	1.96341400
H	2.22090200	-4.92576300	2.29162400
H	0.74927300	-4.56985900	3.20623900
C	0.29710000	-3.44465000	-2.80915600
O	-1.71783800	-2.69692100	-0.86077300
C	0.58260000	-3.21491800	-1.31994500
C	-0.66004900	-3.40082000	-0.49178800
C	-0.77184500	-4.26897400	0.57175500
C	0.38438900	-5.05964300	1.08406100
H	1.23403000	-3.38234800	-3.36828800
H	-0.14127800	-4.43192000	-2.98076800
H	-0.38062500	-2.68408400	-3.20228800
H	0.95691900	-2.19742600	-1.17908300
H	1.35988200	-3.90123500	-0.98681300
H	-1.77743000	-4.47236500	0.93037100
H	0.04075400	-6.00460200	1.50951500
H	1.08840600	-5.30043900	0.28669900
N	2.42183500	-2.42082900	1.27944400
H	2.18970000	-1.51857800	0.83455600
H	-1.78302100	-2.06711400	2.20660100

PadII

C	2.12989100	-1.35679100	-1.30225000
C	0.69548000	-0.91852200	-1.37329800
C	-0.07841300	-0.73398100	-0.29822200
C	0.38287700	-0.95358800	1.11626100
C	-2.32241200	0.06858300	0.40658800
C	-3.70015800	0.42762400	-0.18591400
O	-2.19554300	0.16838000	1.61242900
F	-3.75711000	0.31191100	-1.52101800
F	-4.63489800	-0.37086700	0.33355300
F	-4.01418500	1.68489900	0.13031800
H	2.20737600	-2.41811400	-1.57162500
H	0.27347600	-0.75343500	-2.36313000
H	0.41571000	0.00791300	1.63207400
H	-0.35622600	-1.56448300	1.64277400
C	4.75932600	2.17339200	-0.28849200
O	2.46152900	1.10735300	0.85335000

C	4.51326600	0.67316600	-0.28374200
C	3.15893400	0.29206600	0.28169600
C	2.73801700	-1.15967600	0.10127400
C	1.75052200	-1.64382400	1.16710300
H	5.75424100	2.40088100	-0.67842500
H	4.02090500	2.68734100	-0.90971100
H	4.68223800	2.58064500	0.72215000
H	5.26007700	0.15268100	0.33147100
H	4.61131000	0.24140300	-1.28674800
H	3.65216300	-1.76216500	0.15445000
H	1.61244100	-2.72067400	1.01680900
H	2.17999800	-1.51169300	2.16451700
N	-1.42060500	-0.32605100	-0.51082100
H	-1.71736500	-0.29294000	-1.48005000
H	2.71175900	-0.81503600	-2.05674900