

Supporting Information

Why Electrostatically Enhanced Thiourea Is Better Than Schreiner's Thiourea in Both Catalytic Activity and Regioselectivity?

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Table of Contents

1. Free energy correction.....	S3
2. Identification of the conformations of active catalysts.....	S4
3. QTAIM analyses of the complexes COM-I~VIII	S6
4. Optimized structures of eleven unfavorable transition states TS1s	S9
5. Evaluation of basis set	S10
6. QTAIM analyses of the intermediates, transition states and products.	S12
7. Cartesian coordinates.....	S24

1. Free energy correction

According to the Supporting Information of Kass' results (Org. Lett. 2016, 18, 188-191), the aminolysis reaction is carried out as follows: "In a 3 dram vial, 0.093 g (1.0 mmol) of aniline, 0.12 g (1.0 mmol) of styrene oxide and 0.1 or 1.0 mol% of the desired catalyst were added under argon at 60 °C". Thereby, the concentrations of two substrates and catalysts: $\rho(\text{aniline}) = 1.022 \text{ g/mL}$ and $\rho(\text{styrene oxide}) = 1.054 \text{ g/mL}$, therefore $V(\text{aniline}) = 0.091 \text{ mL}$ and $V(\text{styrene oxide}) = 0.114 \text{ mL}$, the total volume $V(\text{total})$ is approximately 0.205 mL, $c(\text{aniline}) = c(\text{styrene oxide}) = 4.9 \text{ M}$, $c(\text{Cat-I}) = c(\text{Cat-II}) = 4.9 \text{ M} \times 1\% = 0.049 \text{ M}$, $c(\text{BAr}^{\text{F}_4}) = 2c(\text{Cat-II}) = 0.098 \text{ M}$.

In terms of the ideal gas law $pV = nRT$, when $p = 101.325 \text{ kPa}$, $n = 1 \text{ mol}$, $R = 8.3145 \text{ J/(mol}\cdot\text{K)}$ = $1.986 \times 10^{-3} \text{ kcal/(mol}\cdot\text{K)}$, $T = 333 \text{ K}$, the molar volume of gas is $V_m = (nRT/p) = 0.027 \text{ m}^3/\text{mol} = 27.3 \text{ L/mol}$. That is, in 1 atm gas-phase condition, the molar concentration $c = (1/27.3) \text{ mol/L}$.

At 333.0K, the correction from 1 atm to 4.9 M concentration is

$$RT \ln(4.9 \times 27.3) = 1.986 \times 10^{-3} \text{ kcal/(mol}\cdot\text{K)} \times 333 \text{ K} \times \ln(4.9 \times 27.3) = 3.2 \text{ kcal/mol}$$

while at 333.0K, the correction from 1 atm to 0.098 M concentration is

$$RT \ln(0.098 \times 27.3) = 1.986 \times 10^{-3} \text{ kcal/(mol}\cdot\text{K)} \times 333 \text{ K} \times \ln(0.098 \times 27.3) = 0.7 \text{ kcal/mol}$$

Therefore, the following free energy corrections were applied:

(1) For the **Cat-I**(*syn-anti*) + **R1** → **COM-I** procedure, it is a 2 to 1 component procedure.

The calculated free energy change without correction is 6.6 kcal/mol, while the free energy change after correction is $6.6 + (1-2) \times 3.2 = 3.4 \text{ kcal/mol}$.

(2) For the **Cat-I**(*syn-anti*) + **R1** + **R2** → **TS1(IA)** procedure, it is a 3 to 1 component procedure. The calculated free energy change without correction is 39.9 kcal/mol, while the free energy change after correction is $39.9 + (1-3) \times 3.2 = 33.5 \text{ kcal/mol}$.

(3) For the **Cat-II**(*anti-anti*)-1 + 2**BAr**^{F₄} → **Cat-II**(*anti-anti*)-1•(**BAr**^{F₄})₂ procedure, it is a 3 to 1 component procedure. The calculated free energy change without correction is 16.8 kcal/mol, while the free energy change after correction is $16.8 + (1-3) \times 0.7 = 15.4 \text{ kcal/mol}$.

In this work, a correction of 3.2 kcal/mol was applied to per component change, that is, the Gibbs free energy change of a reaction from n to m components should be added the correction of $(m-n) \times 3.2 \text{ kcal/mol}$.

2. Identification of the conformations of active catalysts

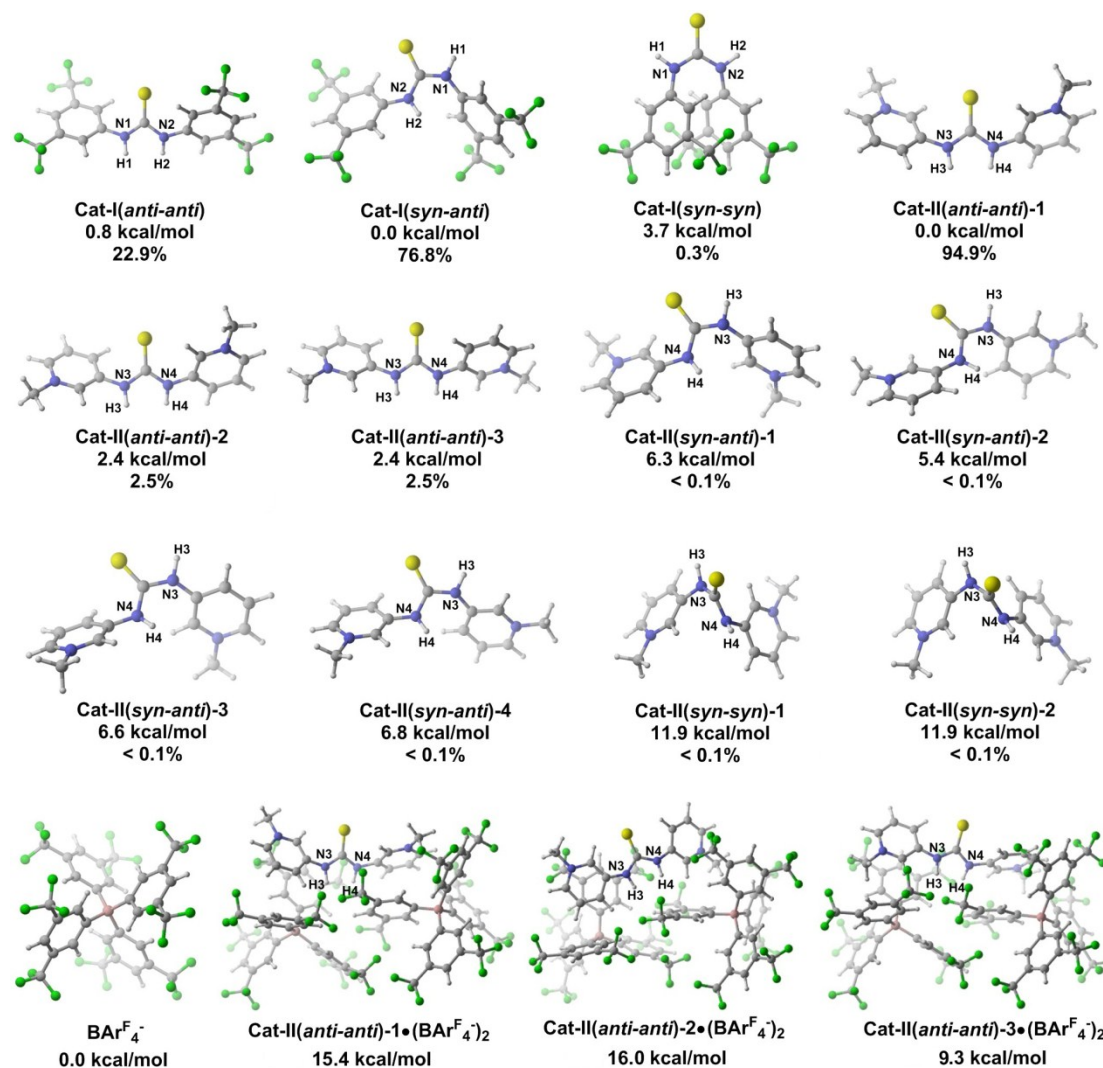


Fig. S1. Optimized structures, relative Gibbs free energies and Boltzmann distribution (%) of all possible catalysts. The Boltzmann distributions of **Cat-II**•($\text{BAr}^{\text{F}_4^-}$)₂ are not displayed because we do not consider their existence in polar solvent.

For **Cat-I**, three possible conformations (i.e., *anti-anti*, *syn-anti*, *syn-syn*) were taken into account. For **Cat-II**, besides all possible conformations, we also consider the combination of two tetrakis(3,5-bis(trifluoromethyl)phenyl) borate (i.e., $\text{BAr}^{\text{F}_4^-}$) anions. The corresponding optimized structures and relative Gibbs free energies are displayed in Fig. 1. For **Cat-I**, the *syn-anti* conformation is of majority in Boltzmann distribution, while for **Cat-II**, the *anti-anti* conformation is overwhelming majority. In practice, the isolated **Cat-II** rather than **Cat-II**•($\text{BAr}^{\text{F}_4^-}$)₂ catalyzes the reaction, the reasons are as follows: (1) The formation of **Cat-II**•($\text{BAr}^{\text{F}_4^-}$)₂ is energetically unfavorable in solvent; (2) The N-H moieties of **Cat-II** are totally blocked when the combination of **Cat-II** with $\text{BAr}^{\text{F}_4^-}$ anion,

HB donor cannot reach the reactants unless removing $\text{BAr}^{\text{F}_4^-}$ anions. (3) In large polar solvent the solvent-separated ion pairs are preferred while in non-polar solvent the tight ion pairs are majority, herein all reactants and products are polar molecules, therefore the formation of tight ion pairs is unlikely (M. Samet, J. Buhle, Y. Zhou and S. R. Kass, *J. Am. Chem. Soc.*, 2015, 137, 4678-4680.). (4) In previous research by Kass and co-workers (M. Samet, J. Buhle, Y. Zhou and S. R. Kass, *J. Am. Chem. Soc.*, 2015, 137, 4678-4680.) using I^- anion to replace $\text{BAr}^{\text{F}_4^-}$ anion lowers the interaction between O-H group of phenol and counterion, indicating that $\text{BAr}^{\text{F}_4^-}$ can hardly combine with HB donor catalyst. Based on the discussions above, we consider three conformations of **Cat-I** and three *anti-anti* conformations of **Cat-II** as active catalysts involved in the whole reactions.

3. QTAIM analyses of the complexes COM-I~VIII

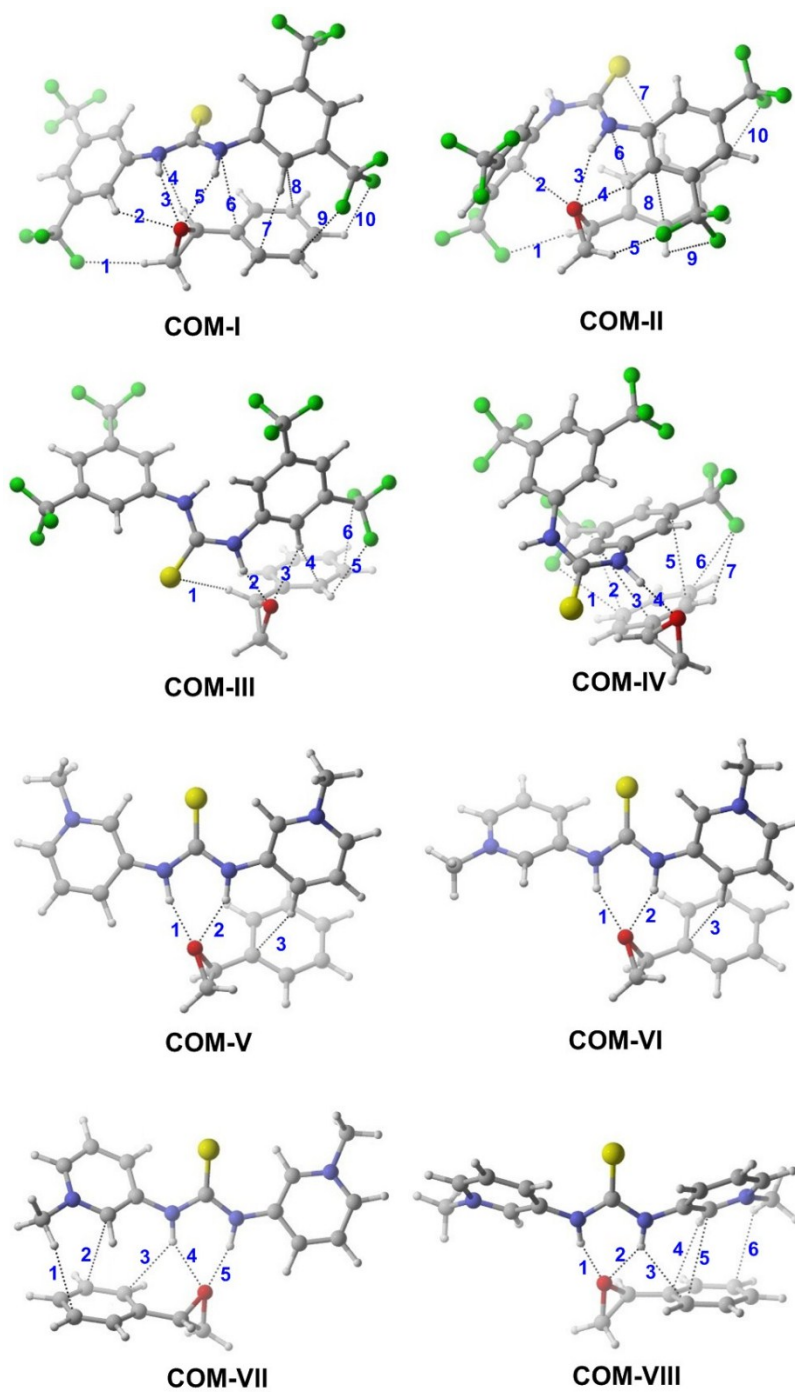


Fig. S2 Intermolecular interactions in COM-I~VIII and numbers of bond critical points (BCPs No.).

Table S1 Numbers of bond critical points (BCPs No.) 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 kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **COM-I~VIII**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
COM-I	1	C-H...F	2.58	0.0056	0.0249	0.0050	-0.0038	0.0012
	2	C-H...O	2.47	0.0109	0.0382	0.0088	-0.0080	0.0008
	3	N-H...O	2.18	0.0178	0.0627	0.0152	-0.0148	0.0004
	4	C-H...N	2.65	0.0097	0.0363	0.0077	-0.0064	0.0013
	5	N-H...O	2.38	0.0098	0.0388	0.0089	-0.0080	0.0009
	6	lp... π	3.34	0.0066	0.0203	0.0044	-0.0038	0.0006
	7	C-H... π	2.65	0.0091	0.0281	0.0060	-0.0050	0.0010
	8	π ... π	3.38	0.0064	0.0200	0.0041	-0.0032	0.0009
	9	lp... π	3.07	0.0068	0.0287	0.0059	-0.0046	0.0013
	10	C-H...F	2.59	0.0072	0.0340	0.0068	-0.0050	0.0018
COM-II	1	C-H...F	2.45	0.0085	0.0361	0.0078	-0.0066	0.0012
	2	lp... π	3.02	0.0101	0.0357	0.0080	-0.0071	0.0009
	3	N-H...O	2.14	0.0168	0.0518	0.0134	-0.0139	-0.0005
	4	C-H...O	2.40	0.0124	0.0399	0.0096	-0.0092	0.0004
	5	C-H...F	2.60	0.0054	0.0248	0.0050	-0.0037	0.0013
	6	lp... π	3.11	0.0095	0.0278	0.0063	-0.0057	0.0006
	7	C-H...S	3.24	0.0052	0.0152	0.0029	-0.0021	0.0008
	8	π ... π	3.16	0.0091	0.0265	0.0056	-0.0046	0.0010
	9	C-H...F	2.65	0.0063	0.0307	0.0060	-0.0043	0.0017
	10	C-H...F	2.95	0.0024	0.0133	0.0024	-0.0014	0.0010
COM-III	1	C-H...S	2.93	0.0080	0.0232	0.0048	-0.0037	0.0011
	2	N-H...O	1.90	0.0279	0.0913	0.0231	-0.0234	-0.0003
	3	C-H...O	2.39	0.0108	0.0388	0.0090	-0.0082	0.0007
	4	C-H... π	2.61	0.0085	0.0269	0.0057	-0.0046	0.0011
	5	C-H...F	2.76	0.0051	0.0249	0.0048	-0.0034	0.0014
	6	lp... π	3.25	0.0043	0.0194	0.0038	-0.0027	0.0011
COM-IV	1	lp... π	3.11	0.0066	0.0279	0.0057	-0.0044	0.0013
	2	lp... π	3.29	0.0046	0.0198	0.0039	-0.0028	0.0011
	3	π ... π	3.30	0.0075	0.0214	0.0045	-0.0036	0.0009
	4	N-H...O	2.06	0.0211	0.0700	0.0178	-0.0181	-0.0003
	5	π ... π	3.32	0.0068	0.0008	0.0041	-0.0033	0.0008
	6	lp... π	3.19	0.0054	0.0268	0.0052	-0.0037	0.0015
	7	C-H...F	2.69	0.0058	0.0286	0.0056	-0.0040	0.0016
COM-V	1	N-H...O	1.86	0.0283	0.0990	0.0242	-0.0236	0.0006
	2	N-H...O	2.02	0.0232	0.0647	0.0176	-0.0190	-0.0014
	3	C-H... π	2.59	0.0104	0.0325	0.0071	-0.0061	0.0010

COM-VI	1	N-H...O	1.93	0.0245	0.0832	0.0207	-0.0207	0.0000
	2	N-H...O	1.94	0.0271	0.0781	0.0208	-0.0221	-0.0013
	3	C-H... π	2.59	0.0104	0.0323	0.0071	-0.0061	0.0010
COM-VII	1	C-H... π	2.79	0.0069	0.0213	0.0042	-0.0031	0.0011
	2	π ... π	3.31	0.0072	0.0222	0.0045	-0.0034	0.0011
	3	N-H... π	2.62	0.0080	0.0271	0.0057	-0.0046	0.0011
	4	N-H...O	2.12	0.0176	0.0541	0.0141	-0.0147	-0.0006
	5	N-H...O	1.87	0.0280	0.0961	0.0235	-0.0231	0.0004
COM-VIII	1	N-H...O	1.90	0.0261	0.0883	0.0218	-0.0215	0.0003
	2	N-H...O	2.09	0.0189	0.0573	0.0151	-0.0158	-0.0007
	3	N-H... π	2.61	0.0082	0.0284	0.0059	-0.0048	0.0011
	4	C-H... π	2.76	0.0077	0.0244	0.0051	-0.0040	0.0011
	5	π ... π	3.33	0.0073	0.0223	0.0045	-0.0035	0.0010
	6	C-H... π	2.81	0.0066	0.0207	0.0041	-0.0030	0.0011

4. Optimized structures of eleven unfavorable transition states TS1s

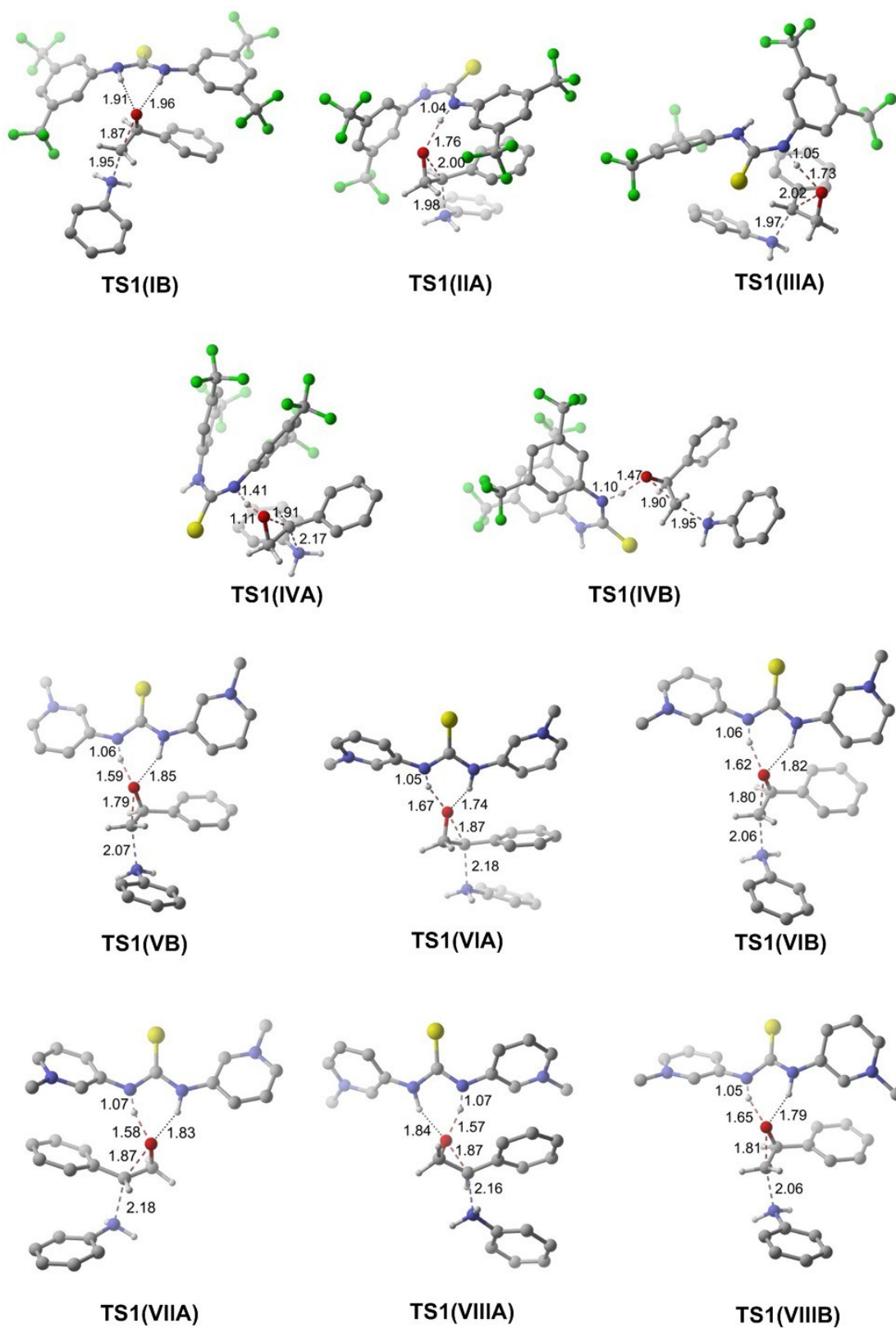


Fig. S3. Optimized structures of eleven unfavorable transition states **TS1s**. Distances are in Å. Some hydrogen atoms and intermolecular interactions are omitted for clarity.

5. Evaluation of basis set

Because there are strong electrostatic interactions in **Cat-II**, we also calculated single-point energies at the M06-2X-D3/6-311++G(2df,2pd)/IEFPCM(aniline) level of theory for **TS1** structures. The solution-phase Gibbs free energy using diffuse function is denoted as $G(\text{diffuse})$, which is the sum of gas-phase thermal correction to Gibbs free energy at M06-2X/6-31G(d,p) (333.0 K) level and solution-phase single-point energy at M06-2X-D3/6-311++G(2df,2pd)/IEFPCM(aniline) level. The calculated results are displayed in **Table S2**. It can be seen that the theoretical regioselectivity significantly deviates from the experimental result after considering the diffuse function.

Table S2 Relative activation Gibbs free energies ($G_{\text{act}}(\text{diffuse})$, in kcal•mol⁻¹), relative reaction rates (k_{rel}) and their summary ($k_{\text{rel}}(\text{sum})$), the calculated and real regioselectivities (dr) of **TS1s** when using $G(\text{diffuse})$. The Gibbs free energies of **R1**, **R2**, **Cat-I** (*syn-anti*) and **Cat-II** (*anti-anti*)-1 are set to 0.0 kcal/mol as reference.

Pathways	TSs	$G_{\text{act}}(\text{diffuse})$	k_{rel}^a	$k_{\text{rel}}(\text{sum})$	$\text{dr}(\mathbf{A}:\mathbf{B})_{\text{Theor}}^b$	$\text{dr}(\mathbf{A}:\mathbf{B})_{\text{Exp}}$
path IA	TS1(IA)	31.0	1.0000	1.0315	5.97:1	1.86:1
path IIA	TS1(IIA)	33.5	0.0241			
path IIIA	TS1(IIIA)	35.1	0.0021			
path IVA	TS1(IVA)	34.5	0.0053			
path IB	TS1(IB)	35.7	0.0008	0.1727		
path IIB	TS1(IIB)	32.2	0.1670			
path IIIB	TS1(IIIB)	34.6	0.0040			
path IVB	TS1(IVB)	35.6	0.0009			
path VA	TS1(VA)	25.1	1.0000	1.1383	379:1	9:1
path VIA	TS1(VIA)	27.6	0.0239			
path VIIA	TS1(VIIA)	26.8	0.0795			
path VIIIA	TS1(VIIIA)	27.3	0.0349			
path VB	TS1(VB)	30.1	0.0006	0.0030		
path VIB	TS1(VIB)	30.6	0.0003			
path VIIB	TS1(VIIB)	29.2	0.0021			
path VIIB	TS1(VIIB)	31.8	0.0000			

^a For paths **IA-IVB**, k_{rel} of **TS1(IA)** is set to 1.0000 as reference, and k_{rel} of other TSs (denoted as **TS1(X)**)

is calculated as: $k_{\text{rel}}(\mathbf{TS1(X)}) : k_{\text{rel}}(\mathbf{TS1(IA)}) = \exp\left(\frac{-G_{\text{act}}(\mathbf{TS1(X)})}{RT}\right) : \exp\left(\frac{-G_{\text{act}}(\mathbf{TS1(IA)})}{RT}\right) = \exp\left(-\frac{G_{\text{act}}(\mathbf{TS1(X)}) - G_{\text{act}}(\mathbf{TS1(IA)})}{RT}\right)$;

For paths **VA-VIIIB**, k_{rel} of **TS1(VA)** is set to 1.0000 as reference, and k_{rel} of other TSs (denoted as **TS1(Y)**) is calculated as: $k_{\text{rel}}(\mathbf{TS1(Y)}) : k_{\text{rel}}(\mathbf{TS1(VA)}) = \exp\left(\frac{-G_{\text{act}}(\mathbf{TS1(Y)})}{RT}\right) :$

$$\exp\left(\frac{-G_{act}(TS1(VA))}{RT}\right) = \exp\left(\frac{G_{act}(TS1(Y)) - G_{act}(TS1(VA))}{RT}\right); \text{ where } R = 1.986 \times 10^{-3} \text{ kcal}\cdot(\text{mol}\cdot\text{K})^{-1} \text{ and } T = 333.0 \text{ K.}$$

^bThe theoretical dr (**A:B**) = $k_{rel}(\text{sum pathA}) : k_{rel}(\text{sum pathB})$.

6. QTAIM analyses of the intermediates, transition states and products.

QTAIM analyses were carried out on some optimized intermediates, transition states and products to figure out the intermolecular interactions. No intramolecular hydrogen bond is found in product **A** or **B**.

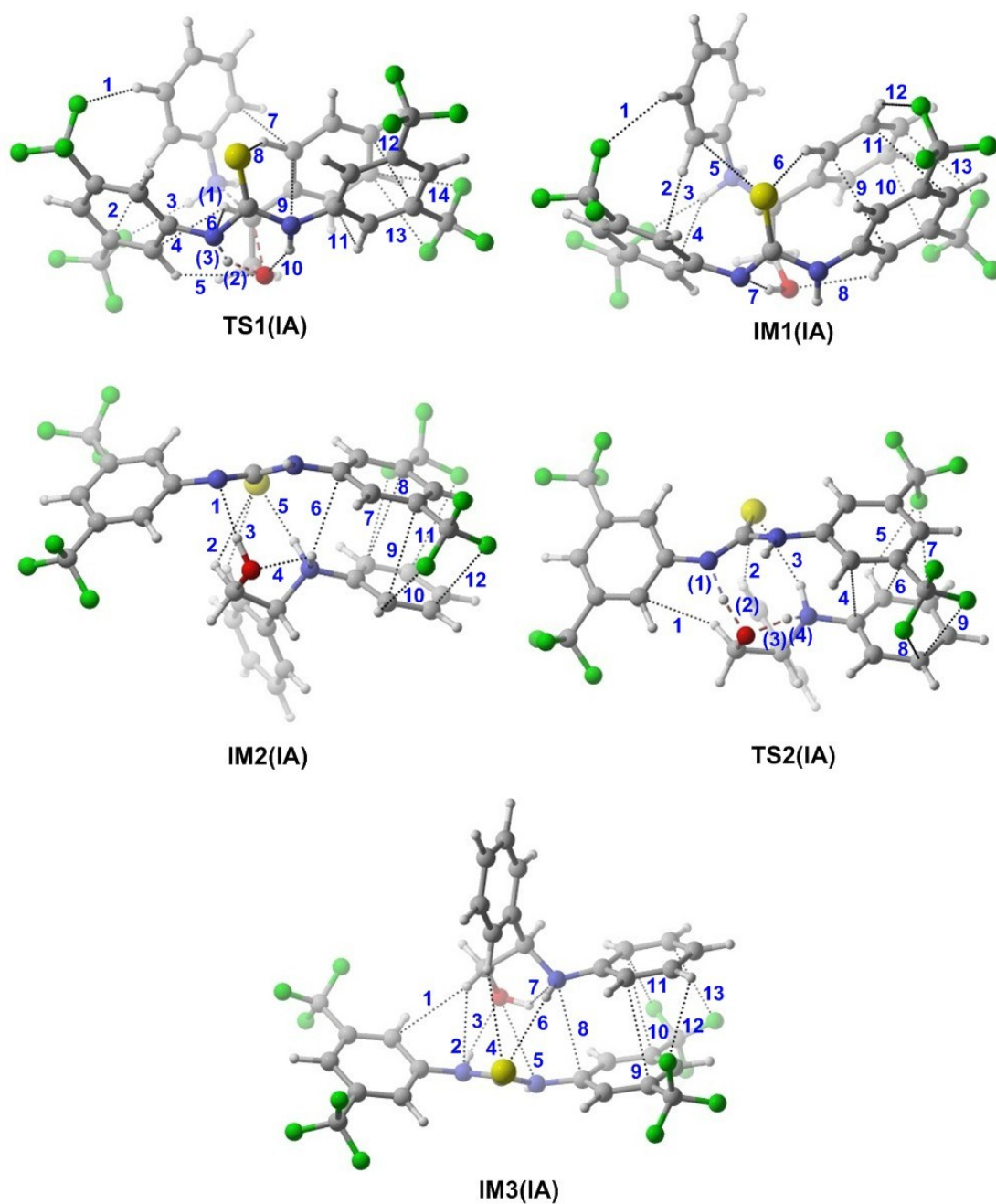


Fig. S4 Intermolecular interactions in **TS1(IA)**, **IM1(IA)**, **IM2(IA)**, **TS2(IA)** and **IM3(IA)**, and numbers of bond critical points (BCPs No.) The BCPs No. of TSs are in parentheses.

Table S3 Numbers of Bond Critical Point (BCPs No.) 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 kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TS1(IA)**, **IM1(IA)**, **IM2(IA)**, **TS2(IA)** and **IM3(IA)**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TS1(IA)	1	C-H...F	2.41	0.3085	-0.8242	0.1008	-0.4076	-0.3068
	2	C-H... π	2.64	0.0090	0.0280	0.0060	-0.0050	0.0010
	3	N-H...F	2.25	0.0104	0.0412	0.0097	-0.0092	0.0007
	4	C-H... π	2.56	0.0102	0.0348	0.0074	-0.0061	0.0013
	5	C-H...O	2.61	0.0093	0.0336	0.0074	-0.0064	0.0010
	6	C-H...N	2.53	0.0107	0.0386	0.0085	-0.0074	0.0011
	7	π ... π	3.13	0.0097	0.0288	0.0060	-0.0047	0.0013
	8	C-H...S	2.99	0.0074	0.0224	0.0045	-0.0034	0.0011
	9	lp... π	3.20	0.0081	0.0250	0.0056	-0.0049	0.0007
	10	N-H...O	1.84	0.0319	0.1073	0.0270	-0.0271	-0.0001
	11	C-H... π	2.91	0.0067	0.0215	0.0043	-0.0032	0.0011
	12	π ... π	3.32	0.0071	0.0203	0.0042	-0.0033	0.0009
	13	lp... π	3.14	0.0059	0.0258	0.0052	-0.0039	0.0013
	14	lp... π	3.06	0.0073	0.0335	0.0068	-0.0051	0.0017
	(1)	C...N	2.07	0.0671	0.1035	0.0390	-0.0521	-0.0131
	(2)	O...H	1.84	0.0358	0.1052	0.0280	-0.0296	-0.0016
	(3)	H...N	1.03	0.3253	-1.7473	0.0473	-0.5313	-0.4840
IM1(IA)	1	C-H...F	2.50	0.0065	0.0295	0.0061	-0.0049	0.0012
	2	C-H... π	2.67	0.0087	0.0278	0.0059	-0.0049	0.0010
	3	N-H...F	2.06	0.0169	0.0561	0.0147	-0.0154	-0.0007
	4	N-H... π	2.89	0.0054	0.0185	0.0037	-0.0028	0.0009
	5	lp... π	3.75	0.0052	0.0143	0.0028	-0.0020	0.0008
	6	C-H...S	2.65	0.0130	0.0353	0.0080	-0.0073	0.0007
	7	O-H...N	1.76	0.0479	0.0989	0.0299	-0.0351	-0.0052
	8	C-H...O	2.58	0.0084	0.0293	0.0065	-0.0056	0.0009
	9	π ... π	3.40	0.0067	0.0183	0.0038	-0.0031	0.0007
	10	lp... π	3.16	0.0059	0.0246	0.0050	-0.0038	0.0012
	11	π ... π	3.32	0.0070	0.0197	0.0041	-0.0033	0.0008
	12	C-H...F	2.63	0.0051	0.0243	0.0048	-0.0035	0.0013
13	lp... π	3.07	0.0071	0.0297	0.0061	-0.0047	0.0014	
IM2(IA)	1	O-H...N	1.93	0.0315	0.0798	0.0213	-0.0227	-0.0014
	2	C-H...S	3.03	0.0076	0.0232	0.0048	-0.0038	0.0010
	3	C-H...S	2.82	0.0096	0.0286	0.0060	-0.0049	0.0011
	4	N-H...O	2.07	0.0071	0.0251	0.0052	-0.0041	0.0011
	5	N-H...S	2.12	0.0373	0.0480	0.0178	-0.0237	-0.0059
	6	N-H... π	2.58	0.0100	0.0378	0.0078	-0.0061	0.0017
	7	lp... π	3.10	0.0065	0.0293	0.0059	-0.0045	0.0014

IM2(IA)	8	$\pi \dots \pi$	3.25	0.0077	0.0224	0.0047	-0.0037	0.0010
	9	$\pi \dots \pi$	3.22	0.0082	0.0239	0.0050	-0.0040	0.0010
	10	C-H...F	2.54	0.0075	0.0359	0.0072	-0.0054	0.0018
	11	lp... π	3.24	0.0047	0.0209	0.0041	-0.0029	0.0012
	12	lp... π	3.25	0.0046	0.0208	0.0040	-0.0028	0.0012
TS2(IA)	1	C-H... π	2.73	0.0079	0.0278	0.0056	-0.0043	0.0013
	2	C-H...S	2.85	0.0090	0.0258	0.0054	-0.0044	0.0010
	3	N-H...S	2.66	0.0124	0.0321	0.0075	-0.0069	0.0006
	4	$\pi \dots \pi$	3.32	0.0074	0.0207	0.0044	-0.0035	0.0009
	5	C-H...F	2.69	0.0058	0.0292	0.0057	-0.0041	0.0016
	6	$\pi \dots \pi$	3.46	0.0066	0.0188	0.0039	-0.0031	0.0008
	7	lp... π	3.17	0.0056	0.0278	0.0054	-0.0039	0.0015
	8	lp... π	3.09	0.0069	0.0288	0.0059	-0.0046	0.0013
	9	lp... π	3.10	0.0068	0.0281	0.0058	-0.0045	0.0013
	(1)	N...H	1.25	0.1727	-0.4827	0.0663	-0.2532	-0.1869
	(2)	H...O	1.25	0.1557	-0.2559	0.0876	-0.2391	-0.1515
	(3)	O...H	1.38	0.1148	0.0545	0.0754	-0.1371	-0.0617
	(4)	H...N	1.18	0.2160	-0.8688	0.0610	-0.3391	-0.2781
IM3(IA)	1	C-H... π	2.85	0.0064	0.0223	0.0045	-0.0034	0.0011
	2	C-H...N	2.66	0.0089	0.0335	0.0072	-0.0061	0.0010
	3	N-H...O	2.05	0.0239	0.0709	0.0189	-0.0200	-0.0011
	4	C-H...S	3.07	0.0058	0.0166	0.0033	-0.0024	0.0009
	5	lp...lp	3.12	0.0096	0.0364	0.0080	-0.0068	0.0012
	6	N-H...S	2.71	0.0109	0.0318	0.0070	-0.0061	0.0009
	7	O-H...N	2.03	0.0290	0.0864	0.0228	-0.0239	-0.0011
	8	lp... π	3.15	0.0088	0.0273	0.0061	-0.0053	0.0008
	9	$\pi \dots \pi$	3.34	0.0069	0.0199	0.0041	-0.0033	0.0008
	10	$\pi \dots \pi$	3.36	0.0071	0.0193	0.0040	-0.0033	0.0007
	11	lp... π	3.10	0.0067	0.0285	0.0058	-0.0045	0.0013
	12	C-H...F	2.65	0.0061	0.0301	0.0059	-0.0043	0.0016
	13	lp... π	3.13	0.0061	0.0255	0.0052	-0.0040	0.0012

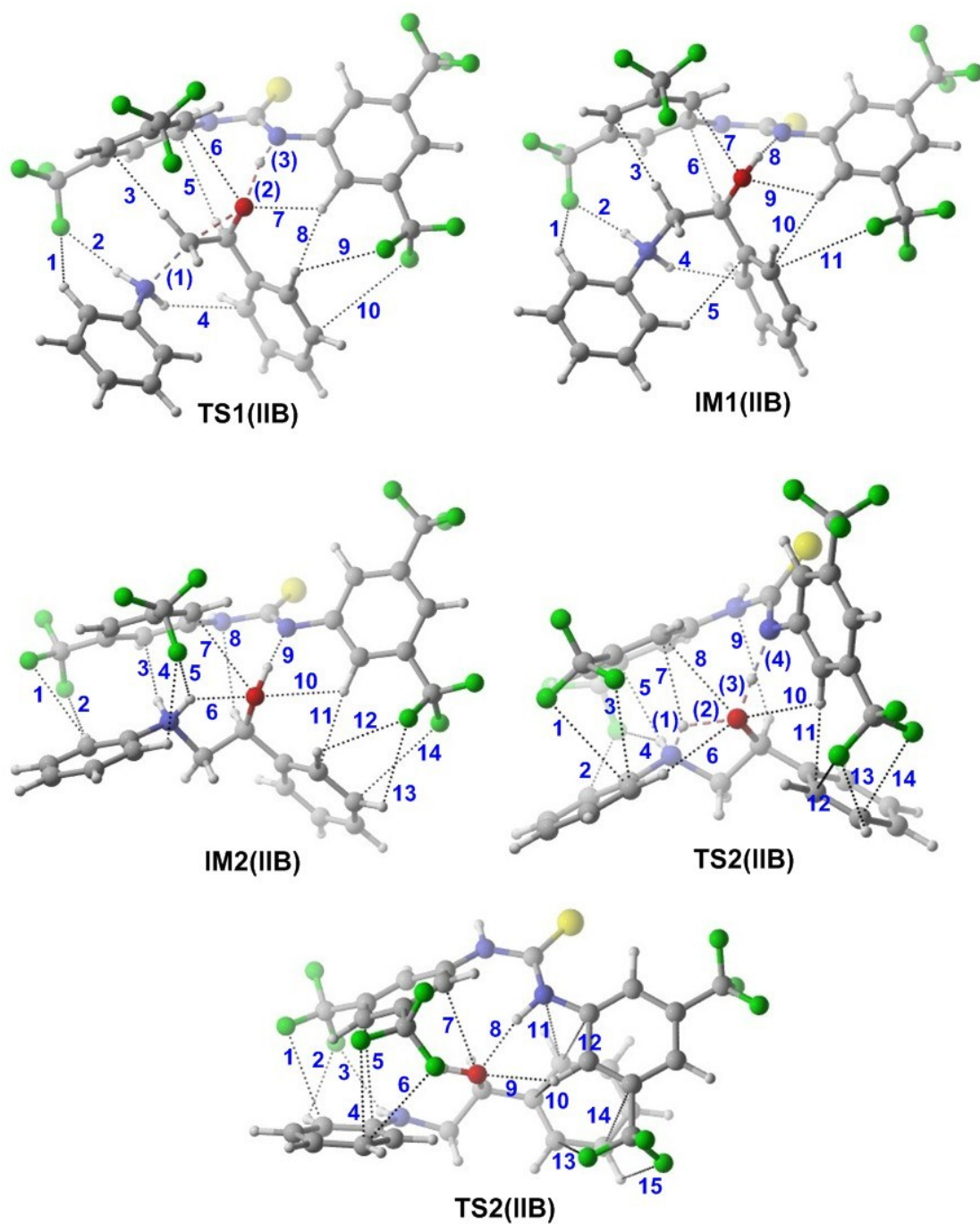


Fig. S5 Intermolecular interactions in TS1(IIB), IM1(IIB), IM2(IIB), TS2(IIB) and IM3(IIB), and numbers of bond critical points (BCPs No.) The BCPs No. of TSs are in parentheses.

Table S4 Numbers of Bond Critical Point (BCPs No.) 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 kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TS1(IIB)**, **IM1(IIB)**, **IM2(IIB)**, **TS2(IIB)** and **IM3(IIB)**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TS1(IIB)	1	C-H...F	2.58	0.0059	0.0265	0.0054	-0.0041	0.0013
	2	N-H...F	2.12	0.0143	0.0523	0.0131	-0.0132	-0.0001
	3	C-H... π	2.56	0.0104	0.0347	0.0075	-0.0063	0.0012
	4	N-H... π	2.61	0.0087	0.0292	0.0061	-0.0048	0.0013
	5	C-H... π	2.95	0.0053	0.0196	0.0039	-0.0029	0.0010
	6	lp... π	2.99	0.0109	0.0352	0.0080	-0.0072	0.0008
	7	C-H...O	2.31	0.0150	0.0480	0.0118	-0.0115	0.0003
	8	C-H... π	2.67	0.0077	0.0271	0.0054	-0.0041	0.0013
	9	C-H...F	2.67	0.0053	0.0266	0.0051	-0.0036	0.0015
	10	lp... π	3.61	0.0020	0.0107	0.0019	-0.0012	0.0007
	(1)	N...C	1.95	0.0843	0.0968	0.0481	-0.0720	-0.0239
	(2)	O...H	1.56	0.0671	0.1562	0.0500	-0.0610	-0.0110
	(3)	H...N	1.07	0.2846	-1.4383	0.0502	-0.4599	-0.4097
IM1(IIB)	1	C-H...F	2.35	0.0099	0.0409	-0.0081	0.0092	0.0011
	2	N-H...F	2.00	0.0192	0.0641	-0.0178	0.0169	-0.0009
	3	C-H... π	2.55	0.0108	0.0335	-0.0063	0.0073	0.0010
	4	N-H... π	2.32	0.0156	0.0479	-0.0098	0.0109	0.0011
	5	C-H... π	2.92	0.0059	0.0187	-0.0029	0.0038	0.0009
	6	C-H... π	2.54	0.0104	0.0370	-0.0063	0.0078	0.0015
	7	lp... π	2.95	0.0113	0.0380	-0.0076	0.0085	0.0009
	8	O-H...N	1.60	0.0688	0.1043	-0.0587	0.0424	-0.0163
	9	C-H...O	2.42	0.0123	0.0445	-0.0089	0.0100	0.0011
	10	C-H... π	2.74	0.0068	0.0217	-0.0034	0.0044	0.0010
IM2(IIB)	11	lp... π	3.48	0.0027	0.0140	-0.0016	0.0026	0.0010
	1	lp... π	2.78	0.0055	0.0262	0.0050	-0.0035	0.0015
	2	lp... π	2.36	0.0101	0.0398	0.0090	-0.0081	0.0009
	3	C-H... π	2.46	0.0126	0.0369	0.0084	-0.0077	0.0007
	4	C-H...F	2.60	0.0073	0.0340	0.0069	-0.0052	0.0017
	5	N-H...F	2.24	0.0119	0.0480	0.0113	-0.0106	0.0007
	6	N-H...O	1.98	0.0296	0.1025	0.0258	-0.0260	-0.0002
	7	lp... π	3.04	0.0098	0.0329	0.0073	-0.0064	0.0009
	8	C-H...N	2.83	0.0065	0.0202	0.0044	-0.0038	0.0006
	9	O-H...N	1.55	0.0775	0.0907	0.0464	-0.0701	-0.0237
	10	C-H...O	2.62	0.0085	0.0346	0.0072	-0.0057	0.0015
	11	C-H... π	2.45	0.0112	0.0358	0.0078	-0.0067	0.0011
	12	C-H...F	2.81	0.0043	0.0219	0.0041	-0.0028	0.0013
13	C-H...F	2.83	0.0040	0.0209	0.0039	-0.0026	0.0013	

TS2(IIb)	14	lp... π	3.37	0.0033	0.0161	0.0030	-0.0020	0.0010
	1	lp... π	3.22	0.0057	0.0246	0.0050	-0.0038	0.0012
	2	C-H...F	2.45	0.0081	0.0352	0.0075	-0.0062	0.0013
	3	lp... π	3.11	0.0062	0.0269	0.0054	-0.0041	0.0013
	4	N-H...F	2.30	0.0099	0.0402	0.0093	-0.0085	0.0008
	5	N-H... π	2.50	0.0110	0.0377	0.0081	-0.0067	0.0014
	6	C-H...O	2.68	0.0075	0.0284	0.0060	-0.0049	0.0011
	7	H... π	2.51	0.0110	0.0359	0.0078	-0.0066	0.0012
	8	lp... π	3.03	0.0107	0.0335	0.0076	-0.0068	0.0008
	9	C-H...N	3.10	0.0039	0.0140	0.0029	-0.0023	0.0006
	10	C-H...O	2.62	0.0086	0.0349	0.0073	-0.0058	0.0015
	11	C-H... π	2.45	0.0113	0.0352	0.0077	-0.0066	0.0011
	12	lp... π	3.30	0.0044	0.0219	0.0042	-0.0029	0.0013
	13	C-H...F	2.73	0.0050	0.0254	0.0049	-0.0034	0.0015
IM3(IIb)	14	lp... π	3.22	0.0047	0.0210	0.0041	-0.0029	0.0012
	(1)	N...H	1.07	0.2908	-1.5124	0.0448	-0.4677	-0.4229
	(2)	H...O	1.65	0.0590	0.1604	0.0462	-0.0523	-0.0061
	(3)	O...H	1.11	0.2234	-0.8305	0.0864	-0.3803	-0.2939
	(4)	H...N	1.40	0.1139	-0.0374	0.0620	-0.1334	-0.0714
	1	lp... π	3.02	0.0081	0.0331	0.0070	-0.0057	0.0013
	2	C-H...F	2.50	0.0090	0.0413	0.0085	-0.0067	0.0018
	3	N-H...F	2.35	0.0104	0.0486	0.0105	-0.0089	0.0016
	4	lp... π	3.24	0.0048	0.0208	0.0041	-0.0030	0.0011
	5	π ... π	3.30	0.0071	0.0209	0.0044	-0.0035	0.0009
	6	lp... π	3.12	0.0063	0.0283	0.0057	-0.0043	0.0014
	7	lp... π	2.99	0.0115	0.0404	0.0088	-0.0075	0.0013
	8	N-H...O	1.93	0.0281	0.0826	0.0218	-0.0229	-0.0011
	9	C-H...F	2.45	0.0103	0.0357	0.0082	-0.0075	0.0007
	10	C-H... π	2.90	0.0076	0.0247	0.0049	-0.0037	0.0012
11	lp... π	3.19	0.0080	0.0244	0.0055	-0.0048	0.0007	
12	π ... π	3.27	0.0072	0.0234	0.0048	-0.0038	0.0010	
13	lp... π	3.16	0.0060	0.0258	0.0052	-0.0039	0.0013	
14	π ... π	3.41	0.0065	0.0185	0.0038	-0.0031	0.0007	
15	C-H...F	2.60	0.0072	0.0340	0.0068	-0.0050	0.0018	

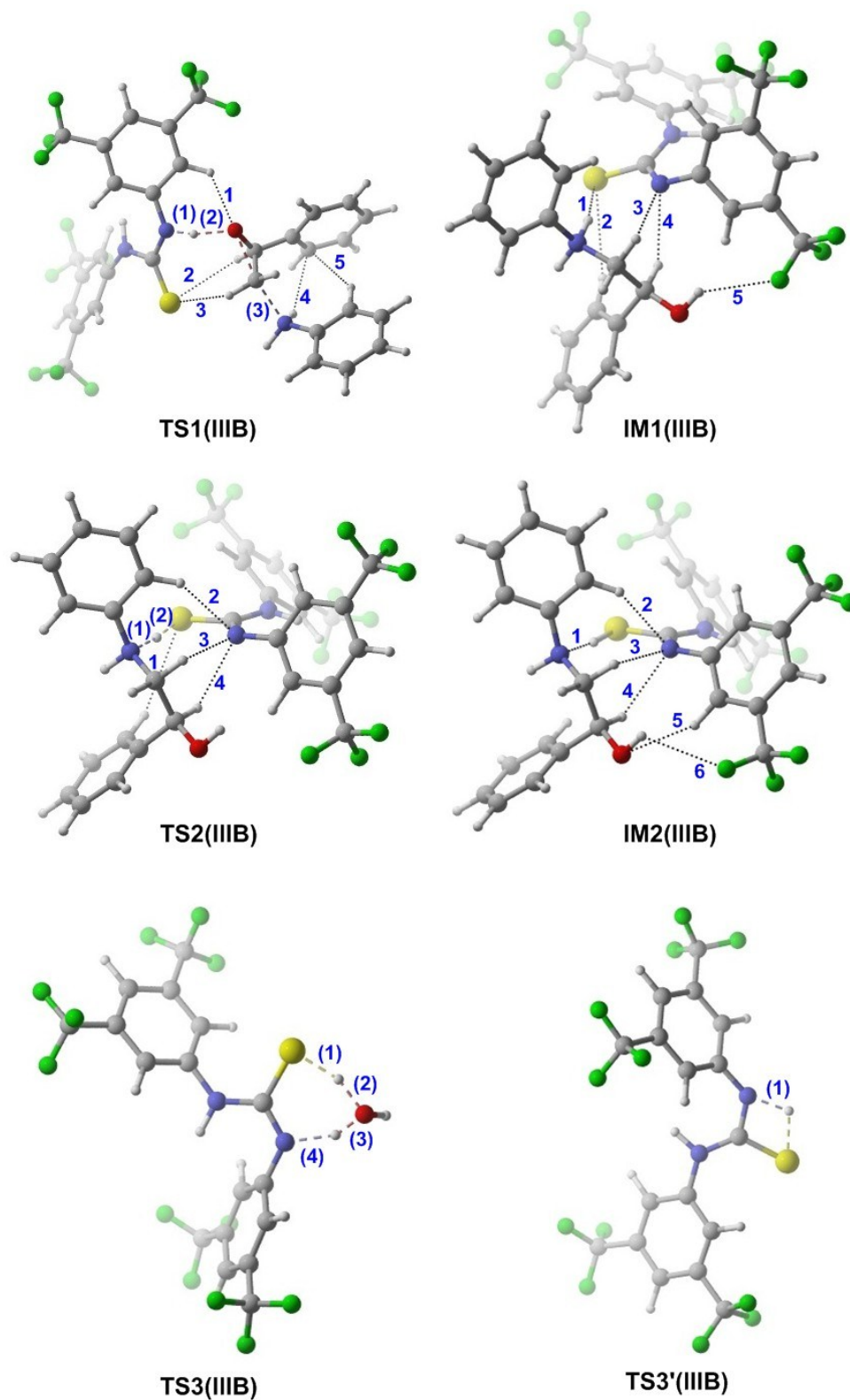


Fig. S6 Intermolecular interactions in **TS1(IIIB)**, **IM1(IIIB)**, **TS2(IIIB)**, **IM2(IIIB)**, **TS3(IIIB)** and **TS3'(IIIB)**, and numbers of bond critical points (BCPs No.) The BCPs No. of TSs are in parentheses.

Table S5 Numbers of Bond Critical Point (BCPs No.) 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 kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TS1(IIIB)**, **IM1(IIIB)**, **TS2(IIIB)**, **IM2(IIIB)**, **TS3(IIIB)** and **TS3'(IIIB)**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TS1(IIIB)	1	C-H...O	2.31	0.0144	0.0460	0.0113	-0.0110	0.0003
	2	C-H...S	2.90	0.0092	0.0278	0.0058	-0.0046	0.0012
	3	C-H...S	2.75	0.0115	0.0346	0.0073	-0.0060	0.0013
	4	N-H... π	2.63	0.0085	0.0294	0.0061	-0.0048	0.0013
	5	C-H... π	2.82	0.0070	0.0225	0.0047	-0.0037	0.0010
	(1)	N...H	1.09	0.2688	-1.3228	0.0511	-0.4328	-0.3817
	(2)	H...O	1.52	0.0766	0.1496	0.0559	-0.0743	-0.0186
	(3)	C...N	1.95	0.0846	0.0962	0.0483	-0.0725	-0.0242
IM1(IIIB)	1	N-H...S	1.98	0.0516	0.0403	0.0219	-0.0336	-0.0117
	2	C-H...S	3.09	0.0061	0.0171	0.0034	-0.0025	0.0009
	3	C-H...N	2.48	0.0138	0.0471	0.0104	-0.0091	0.0013
	4	C-H...N	2.52	0.0123	0.0371	0.0085	-0.0078	0.0007
	5	O-H...F	2.51	0.0094	0.0390	0.0079	-0.0061	0.0018
TS2(IIIB)	1	C-H...S	3.16	0.0050	0.0149	0.0029	-0.0021	0.0008
	2	C-H...N	2.57	0.0098	0.0279	0.0065	-0.0060	0.0005
	3	C-H...N	2.50	0.0129	0.0430	0.0095	-0.0083	0.0012
	4	C-H...N	2.50	0.0125	0.0377	0.0086	-0.0079	0.0007
	(1)	N...H	1.44	0.1113	-0.0228	0.0518	-0.1092	-0.0574
	(2)	H...S	1.55	0.1372	-0.2127	0.0304	-0.1140	-0.0836
IM2(IIIB)	1	S-H...N	1.84	0.0437	0.0803	0.0239	-0.0277	-0.0038
	2	C-H...N	2.61	0.0090	0.0264	0.0060	-0.0054	0.0006
	3	C-H...N	2.59	0.0107	0.0359	0.0078	-0.0067	0.0011
	4	C-H...N	2.51	0.0120	0.0356	0.0082	-0.0075	0.0007
	5	C-H...O	2.47	0.0105	0.0405	0.0087	-0.0073	0.0014
	6	O-H...F	2.75	0.0033	0.0201	0.0037	-0.0023	0.0014
TS3(IIIB)	(1)	S...H	1.60	0.0814	0.0867	0.0492	-0.0768	-0.0276
	(2)	H...O	1.26	0.2656	-1.2614	0.0796	-0.4745	-0.3949
	(3)	O...H	1.05	0.1514	-0.2256	0.0826	-0.2216	-0.1390
	(4)	H...N	1.53	0.1215	-0.1518	0.0312	-0.1004	-0.0692
TS3'(IIIB)	(1)	N...H	1.40	0.1184	-0.0330	0.0606	-0.1294	-0.0688

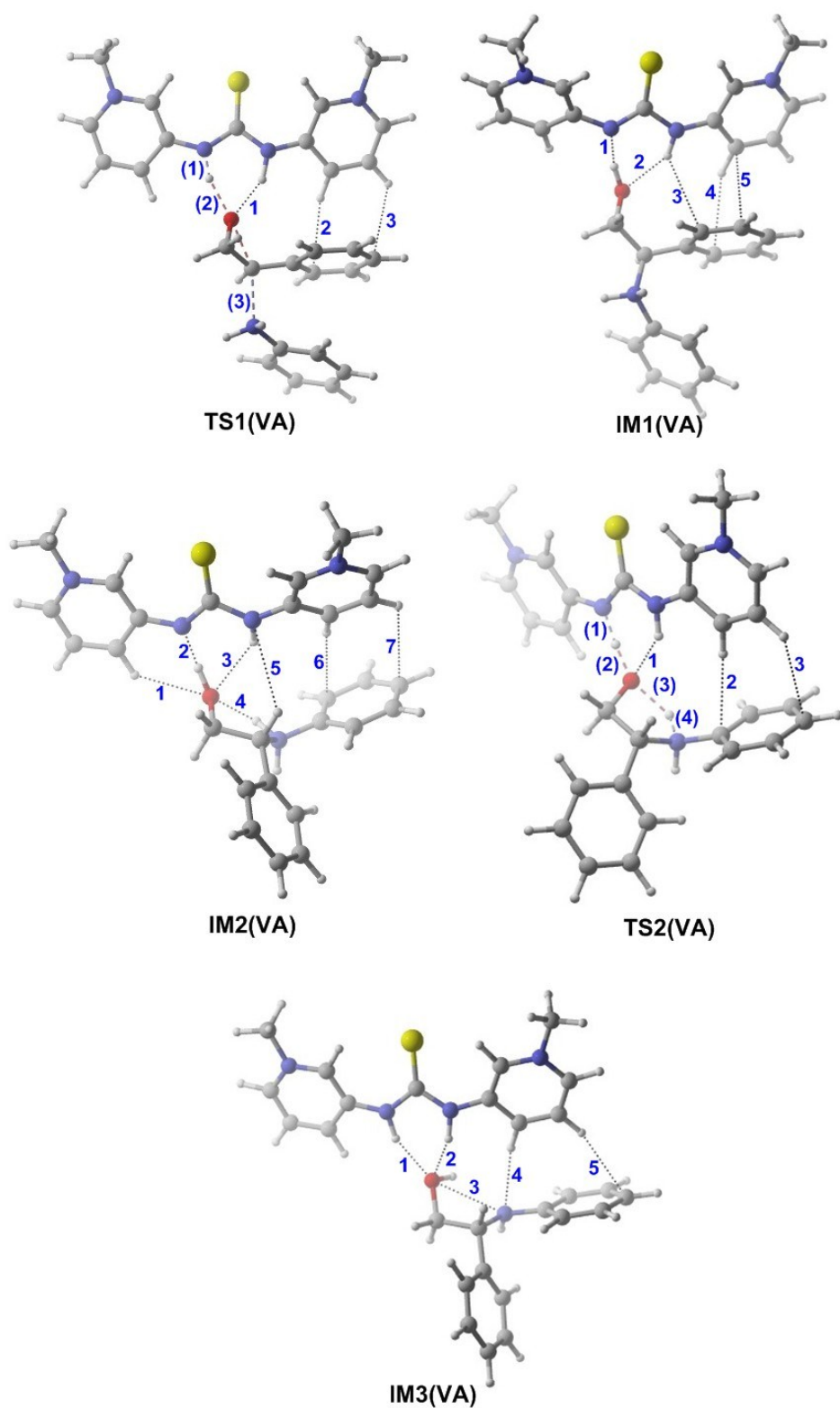


Fig. S7 Intermolecular interactions in TS1(VA), IM1(VA), IM2(VA), TS2(VA) and IM3(VA), and numbers of bond critical points (BCPs No.) The BCPs No. of TSs are in parentheses.

Table S6 Numbers of Bond Critical Point (BCPs No.) 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 kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TS1(VA)**, **IM1(VA)**, **IM2(VA)**, **TS2(VA)** and **IM3(VA)**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TS1(VA)	1	N-H...O	1.77	0.0400	0.1178	0.0308	-0.0322	-0.0014
	2	C-H... π	2.65	0.0088	0.0278	0.0059	-0.0049	0.0010
	3	C-H... π	2.97	0.0050	0.0163	0.0032	-0.0022	0.0010
	(1)	N...H	1.05	0.3030	-1.5854	0.0477	-0.4917	-0.4440
	(2)	H...O	1.63	0.0545	0.1531	0.0424	-0.0465	-0.0041
	(3)	C...N	2.18	0.0540	0.0973	0.0315	-0.0387	-0.0072
IM1(VA)	1	O-H...N	1.61	0.0680	0.1073	0.0423	-0.0578	-0.0155
	2	N-H...O	2.08	0.0207	0.0650	0.0166	-0.0170	-0.0004
	3	N-H... π	3.02	0.0043	0.0146	0.0029	-0.0021	0.0008
	4	C-H... π	2.82	0.0065	0.0212	0.0044	-0.0034	0.0009
	5	π ... π	3.36	0.0066	0.0211	0.0042	-0.0032	0.0010
IM2(VA)	1	C-H...O	2.52	0.0098	0.0408	0.0085	-0.0068	0.0017
	2	O-H...N	1.53	0.0828	0.0841	0.0497	-0.0784	-0.0287
	3	N-H...O	2.31	0.0142	0.0534	0.0124	-0.0114	0.0010
	4	N-H...O	1.78	0.0408	0.1375	0.0352	-0.0359	-0.0007
	5	C-H...N	2.97	0.0049	0.0179	0.0035	-0.0026	0.0009
	6	C-H... π	2.78	0.0070	0.0216	0.0045	-0.0036	0.0009
	7	C-H... π	3.13	0.0037	0.0118	0.0023	-0.0016	0.0007
TS2(VA)	1	N-H...O	2.02	0.0253	0.0722	0.0195	-0.0210	-0.0015
	2	C-H... π	2.71	0.0082	0.0246	0.0053	-0.0044	0.0009
	3	C-H... π	3.09	0.0035	0.0113	0.0021	-0.0015	0.0006
	(1)	N...H	1.23	0.1792	-0.5425	0.0685	-0.2726	-0.2041
	(2)	H...O	1.23	0.1586	-0.2697	0.0929	-0.2532	-0.1603
	(3)	O...H	1.60	0.0636	0.1703	0.0502	-0.0578	-0.0076
	(4)	H...N	1.07	0.2894	-1.4950	0.0462	-0.4663	-0.4201
IM3(VA)	1	N-H...O	1.97	0.0246	0.0756	0.0197	-0.0204	-0.0007
	2	N-H...O	1.89	0.0314	0.0909	0.0241	-0.0254	-0.0013
	3	lp...lp	2.75	0.0188	0.0741	0.0170	-0.0156	0.0014
	4	C-H...N	2.37	0.0142	0.0408	0.0101	-0.0100	0.0001
	5	C-H... π	2.69	0.0082	0.0251	0.0054	-0.0045	0.0009

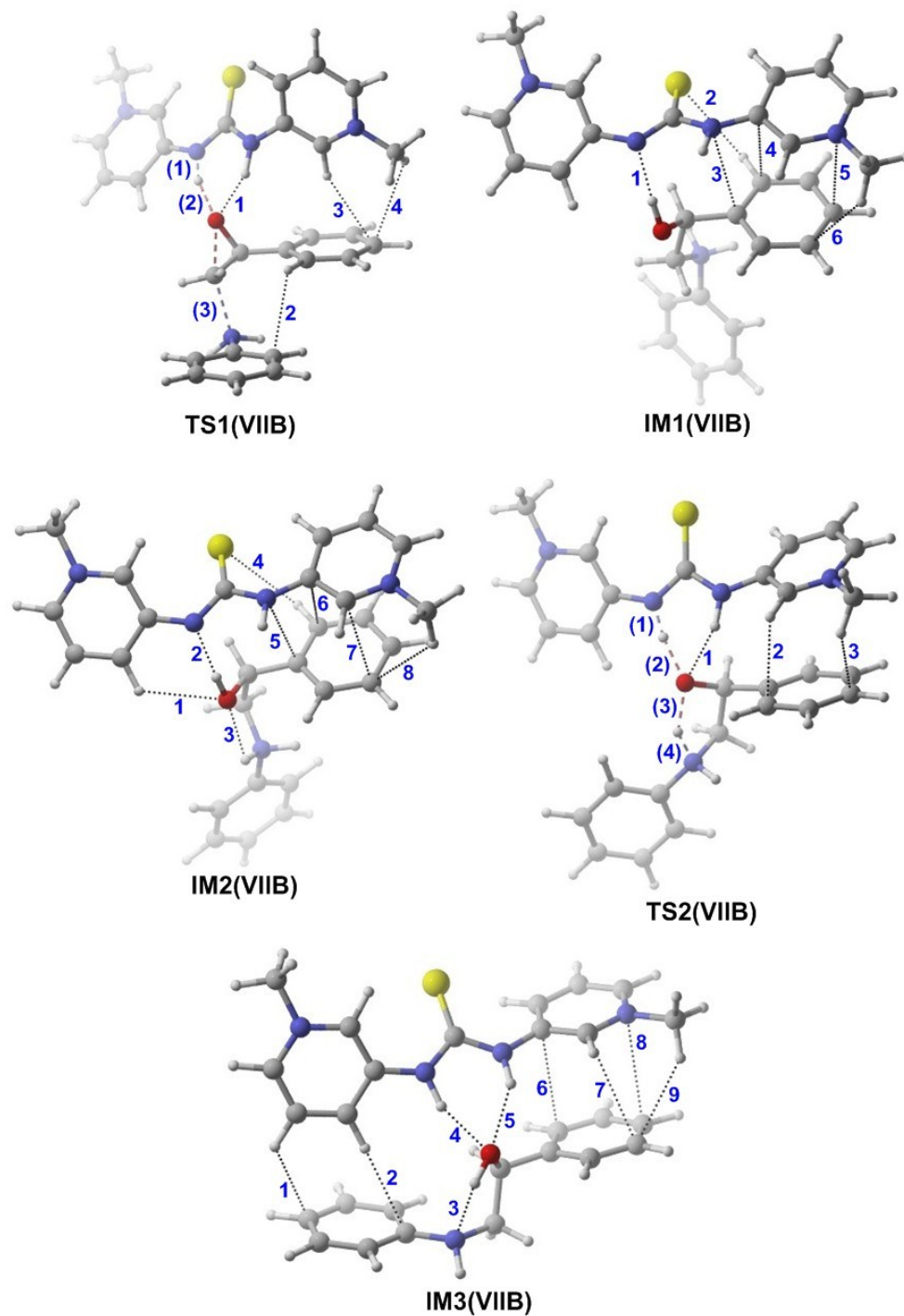


Fig. S8 Intermolecular interactions in **TS1(VIIB)**, **IM1(VIIB)**, **IM2(VIIB)**, **TS2(VIIB)** and **IM3(VIIB)**, and numbers of bond critical points (BCPs No.) The BCPs No. of TSs are in parentheses.

Table S7 Numbers of Bond Critical Point (BCPs No.) 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 kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TS1(VIIB)**, **IM1(VIIB)**, **IM2(VIIB)**, **TS2(VIIB)** and **IM3(VIIB)**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TS1(VIIB)	1	N-H...O	1.78	0.0388	0.1143	0.0300	-0.0314	-0.0014
	2	C-H... π	2.88	0.0058	0.0186	0.0037	-0.0027	0.0010
	3	C-H... π	2.75	0.0076	0.0249	0.0053	-0.0043	0.00010
	4	C-H... π	2.96	0.0054	0.0170	0.0034	-0.0025	0.0009
	(1)	N...H	1.05	0.3055	-1.6088	0.0469	-0.4960	-0.4491
	(2)	H...O	1.65	0.0518	0.1475	0.0402	-0.0434	-0.0032
	(3)	C...N	2.06	0.0681	0.1036	0.0395	-0.0531	-0.0136
IM1(VIIB)	1	O-H...N	1.79	0.0439	0.1004	0.0287	-0.0323	-0.0036
	2	C-H...S	3.08	0.0064	0.0186	0.0037	-0.0027	0.0010
	3	lp... π	3.27	0.0074	0.0213	0.0048	-0.0043	0.0005
	4	π ... π	3.27	0.0069	0.0210	0.0043	-0.0034	0.0009
	5	π ... π	3.34	0.0066	0.0199	0.0042	-0.0035	0.0007
	6	C-H... π	2.88	0.0055	0.0175	0.0035	-0.0025	0.0010
IM2(VIIB)	1	C-H...O	2.63	0.0076	0.0322	0.0065	-0.0049	0.0016
	2	O-H...N	1.80	0.0427	0.0965	0.0275	-0.0309	-0.0034
	3	N-H...O	2.15	0.0195	0.0831	0.0190	-0.0173	0.0017
	4	C-H...S	3.42	0.0041	0.0115	0.0023	-0.0017	0.0006
	5	lp... π	3.20	0.0082	0.0236	0.0054	-0.0048	0.0006
	6	π ... π	3.39	0.0061	0.0168	0.0035	-0.0027	0.0008
	7	π ... π	3.26	0.0076	0.0210	0.0044	-0.0036	0.0008
	8	C-H... π	3.13	0.0035	0.0124	0.0025	-0.0018	0.0007
TS2(VIIB)	1	N-H...O	2.08	0.0224	0.0670	0.0180	-0.0192	-0.0012
	2	C-H... π	2.90	0.0073	0.0232	0.0046	-0.0033	0.0013
	3	C-H... π	2.89	0.0062	0.0196	0.0039	-0.0029	0.0010
	(1)	N...H	1.09	0.2661	-1.2922	0.0532	-0.4294	-0.3762
	(2)	H...O	1.48	0.0820	0.1502	0.0606	-0.0837	-0.0231
	(3)	O...H	1.45	0.0944	0.1334	0.0669	-0.1004	-0.0335
	(4)	H...N	1.13	0.2425	-1.1023	0.0554	-0.3863	-0.3309
	4	C-H... π	3.13	0.0035	0.0124	0.0025	-0.0018	0.0007
IM3(VIIB)	1	C-H... π	2.88	0.0061	0.0194	0.0038	-0.0027	0.0011
	2	C-H... π	2.67	0.0088	0.0269	0.0059	-0.0050	0.0009
	3	O-H...N	1.92	0.0359	0.1005	0.0273	-0.0295	-0.0022
	4	N-H...O	1.86	0.0332	0.0963	0.0254	-0.0266	-0.0012
	5	N-H...O	2.00	0.0229	0.0749	0.0192	-0.0198	-0.0006
	6	π ... π	3.32	0.0069	0.0202	0.0042	-0.0033	0.0009
	7	C-H... π	3.38	0.0065	0.0189	0.0039	-0.0030	0.0009
	8	π ... π	3.33	0.0065	0.0191	0.0042	-0.0036	0.0006
	9	C-H... π	2.79	0.0065	0.0208	0.0041	-0.0031	0.0010

7. Cartesian coordinates

R1

C	2.56026000	-0.00021800	0.74564300
C	1.60079400	0.59131300	-0.20612200
O	2.46398000	-0.46574000	-0.58851300
H	2.17630800	-0.67966900	1.50472300
H	3.47790000	0.52972000	0.99216300
H	1.85137900	1.55971500	-0.63999600
C	0.14691700	0.27651400	-0.12114900
C	-0.28331400	-1.05058000	-0.08857400
C	-0.79086400	1.30644300	-0.05384200
C	-1.63856600	-1.34146500	0.02356400
H	0.45528800	-1.84203100	-0.17358600
C	-2.14663600	1.01394900	0.06080100
H	-0.45730200	2.34042800	-0.09161800
C	-2.57291200	-0.31078500	0.10166700
H	-1.96862400	-2.37534900	0.04328800
H	-2.87044000	1.82104000	0.11389100
H	-3.63042500	-0.53896400	0.18732000

R2

N	2.32895000	-0.00002300	-0.07626000
H	2.76643200	-0.83547200	0.28494500
H	2.76642300	0.83553600	0.28468800
C	0.93515400	-0.00005500	-0.01036000
C	0.22128600	-1.20489600	-0.00614600
C	0.22128700	1.20490700	-0.00618600
C	-1.16804800	-1.19928500	0.00350700
H	0.76521900	-2.14574700	-0.01576500
C	-1.16793200	1.19934400	0.00356400
H	0.76535800	2.14568000	-0.01575900
C	-1.87555100	-0.00000700	0.00914600
H	-1.70175300	-2.14485600	0.00824500
H	-1.70171500	2.14487100	0.00826300
H	-2.95978900	0.00010200	0.01805000

H2O

O	0.00000000	0.00000000	0.11779300
H	0.00000000	0.76021000	-0.47117300
H	0.00000000	-0.76021000	-0.47117300

A

O	-0.58614500	3.63790600	0.21685000
C	-0.61566900	1.21324600	0.27386000
C	-1.34268600	2.50527700	-0.11892100
C	-1.50121400	-0.00236900	0.05283900
C	-2.57776500	-0.21498500	0.91822100
C	-3.44602200	-1.28294000	0.72532200
C	-3.24537100	-2.15863300	-0.33970300
C	-2.17119800	-1.96003900	-1.20084500
C	-1.30332200	-0.88759800	-1.00550500
H	-0.38778900	1.29948600	1.34405400
H	-1.56796400	2.46069600	-1.19963300
H	-2.29814800	2.56821200	0.40899100
H	-2.73168200	0.46457400	1.75392800
H	-4.27633600	-1.43530400	1.40750600
H	-3.91965800	-2.99504700	-0.49261000
H	-2.00192900	-2.64491200	-2.02575500
H	-0.45448800	-0.75327700	-1.66970400
N	0.65184300	1.22051900	-0.43476700
H	0.54151700	1.35432400	-1.43478300
H	0.33126200	3.41677400	0.00300600
C	1.66983300	0.30381700	-0.12370400
C	1.61288500	-0.53756100	0.99231300
C	2.80361700	0.26004800	-0.94750400
C	2.68024500	-1.38504200	1.27952300
H	0.73291900	-0.55177500	1.62539500
C	3.85438700	-0.59736100	-0.65794200
H	2.85518200	0.91872600	-1.81075300
C	3.80433100	-1.42492600	0.46290300
H	2.61959400	-2.03042900	2.15034600
H	4.72313200	-0.61302400	-1.30862700
H	4.62834300	-2.09150400	0.69205900

B

O	0.82257600	-1.78379100	1.14785600
C	0.80080800	-0.51419700	0.54252900
C	0.02732600	-0.60770600	-0.78600500
C	2.20949500	-0.04256400	0.27878300
C	2.46041300	1.31593200	0.08055400
C	3.74077900	1.75933100	-0.23441400
C	4.78460900	0.84428800	-0.34873400
C	4.53980300	-0.51132900	-0.14614800
C	3.25707800	-0.95547200	0.16351000
H	0.29799400	0.21362000	1.20049300
H	0.59780200	-1.27531400	-1.43855200
H	-0.02690800	0.37436300	-1.27557900
H	1.64772500	2.03249200	0.18317900
H	3.92564700	2.81853200	-0.38313500
H	5.78566300	1.18794900	-0.58895900
H	5.35206500	-1.22701500	-0.22752100
H	3.05335400	-2.00677500	0.33490500
N	-1.28809800	-1.19312100	-0.57695800
H	-1.50506000	-1.94647200	-1.21371000
H	-0.08436000	-2.11490200	1.07343100
C	-2.40151100	-0.38714600	-0.30445500
C	-3.68504900	-0.93995200	-0.42823000
C	-2.28210100	0.94311800	0.11496800
C	-4.81211300	-0.18362400	-0.14548500
H	-3.78745500	-1.97365100	-0.74898300
C	-3.42181100	1.69164400	0.39884000
H	-1.30517500	1.40010000	0.22464400
C	-4.69129500	1.14117500	0.27239800
H	-5.79411300	-0.63364100	-0.25360700
H	-3.30659000	2.72116600	0.72356000
H	-5.57308600	1.73073200	0.49702400

Cat-I(anti-anti)

C	-5.18802400	0.08629000	-0.16741400
C	-4.74360000	-0.89350700	0.70592600
C	-3.39416500	-1.22672200	0.78178700
C	-2.47244800	-0.58509400	-0.03978600
C	-2.90716900	0.39316300	-0.93921500
C	-4.25349000	0.72246000	-0.98188200
N	-1.12778300	-1.00622900	0.00993100
C	-0.00049100	-0.21497700	0.00011700
N	1.12546700	-1.00712400	-0.04270200
S	0.00155000	1.43808300	0.03793100
C	2.47054800	-0.58858700	0.02033500
C	2.90952700	0.34489200	0.96418800
C	4.25598000	0.67174400	1.01612300
C	5.18653100	0.07589500	0.16728300
C	4.73794500	-0.85989000	-0.75092400
C	3.38796400	-1.18915300	-0.83619700
C	-4.71658100	1.81535600	-1.90762500
F	-3.90936900	1.93850900	-2.96846600
F	-4.74566400	3.00112400	-1.28695800
F	-5.95539500	1.57523700	-2.35977300
C	-5.70906000	-1.64429400	1.57992700
F	-6.93183100	-1.10501400	1.55510600
F	-5.29358600	-1.66556200	2.85455900
F	-5.82052800	-2.92294300	1.18898700
C	5.69975900	-1.56879400	-1.66323600
F	6.91658200	-1.01650100	-1.63533400
F	5.26734500	-1.55074000	-2.93231500
F	5.83133300	-2.85861100	-1.31816800
C	4.72621200	1.71793800	1.99077700
F	3.91345400	1.80721300	3.05070100
F	4.77635200	2.92832400	1.42095500
F	5.95841000	1.44176400	2.44041600
H	-6.23883600	0.34527000	-0.22088700
H	-3.06443600	-1.98221100	1.48994900
H	-2.20247100	0.88262600	-1.59870800
H	-0.99781100	-1.94928800	0.35299700
H	0.99433000	-1.93336900	-0.42843800
H	2.20783600	0.80160100	1.64986500
H	6.23763600	0.33222000	0.22889700
H	3.05462200	-1.90822800	-1.57965400

Cat-I(syn-anti)

C	4.36449900	0.61464800	0.51438400
C	4.51071600	-0.29808800	-0.52263900
C	3.51002800	-1.21492900	-0.81958400
C	2.34314000	-1.24571100	-0.05290700
C	2.19574900	-0.34953100	1.01226400
C	3.19759300	0.57836600	1.27019900
N	1.37232800	-2.22426800	-0.34306600
C	0.00376800	-2.11789500	-0.38890600
N	-0.45905500	-0.83866800	-0.27077500
S	-0.91675600	-3.48235900	-0.62519900
C	-1.79637000	-0.39170300	-0.27878800
C	-2.82769600	-1.08552000	0.36072900
C	-4.10867300	-0.55215100	0.34834600
C	-4.39020300	0.66815300	-0.25999400
C	-3.35138000	1.35387900	-0.87070200
C	-2.06302400	0.83036500	-0.89198800
C	2.99418400	1.58656500	2.37040900
F	2.25340400	1.08318800	3.36486600
F	2.35786900	2.67382600	1.91286400
F	4.16030200	1.99142600	2.88415100
C	5.77444900	-0.32558000	-1.34123200
F	6.49604300	0.78705900	-1.17408800
F	5.49921100	-0.44895900	-2.64663000
F	6.54688000	-1.36574300	-1.00202700
C	-3.57968800	2.70050000	-1.49932800
F	-4.88082300	2.98266500	-1.61953400
F	-3.02875400	2.76577500	-2.72028800
F	-3.01931100	3.67549000	-0.76854000
C	-5.23151200	-1.33391800	0.97575800
F	-4.79602100	-2.10307100	1.98123000
F	-5.82192800	-2.13923700	0.08364100
F	-6.17994500	-0.52034600	1.46111200
H	5.14410300	1.33535600	0.73144500
H	3.62820800	-1.90129900	-1.65266100
H	1.31874000	-0.39414300	1.64963600
H	1.69852500	-3.14580300	-0.60140700
H	0.22545000	-0.10440500	-0.40575400
H	-2.63149000	-2.02523700	0.85877800
H	-5.39422300	1.07551300	-0.24956700
H	-1.26993800	1.37495700	-1.39732000

Cat-I(syn-syn)

C	1.18433700	-1.10707600	-1.49919600
C	2.29274200	-0.48367600	-0.94482800
C	2.27679200	0.87640500	-0.64638700
C	1.14228600	1.63049500	-0.93441900
C	0.05529600	1.03417300	-1.57818700
C	0.07004800	-0.33120600	-1.81392900
N	1.07484800	2.96942800	-0.48912300
C	0.00065800	3.66833600	-0.00062600
N	-1.07403000	2.97007800	0.48774300
S	0.00124900	5.33368800	-0.00053800
C	-1.14197500	1.63139300	0.93372600
C	-0.05517100	1.03502400	1.57777300
C	-0.07030000	-0.33024900	1.81409200
C	-1.18480600	-1.10592600	1.49968800
C	-2.29301900	-0.48244100	0.94502600
C	-2.27670000	0.87751600	0.64602400
C	-1.15065000	-1.01231200	-2.37195600
F	-2.17235400	-0.16044500	-2.51875200
F	-1.55946600	-1.99771500	-1.55369900
F	-0.90488200	-1.57228100	-3.56123100
C	3.52677100	-1.27866700	-0.61124600
F	3.28522400	-2.59312200	-0.61530200
F	4.00507800	-0.94760200	0.59495600
F	4.50475600	-1.04331900	-1.49802000
C	-3.52717000	-1.27732000	0.61162300
F	-3.28581800	-2.59182000	0.61597700
F	-4.00540600	-0.94646900	-0.59466200
F	-4.50513900	-1.04163800	1.49832400
C	1.15026300	-1.01144700	2.37230900
F	2.17220900	-0.15979100	2.51861000
F	1.55874700	-1.99734500	1.55447000
F	0.90447800	-1.57075900	3.56188700
H	1.18158600	-2.17867100	-1.66561200
H	3.11612800	1.32993100	-0.12724900
H	-0.82069900	1.62291000	-1.82484900
H	1.86905200	3.56728500	-0.67701000
H	-1.86782900	3.56844700	0.67572100
H	0.82101400	1.62359200	1.82416500
H	-1.18235600	-2.17745100	1.66655100
H	-3.11587000	1.33103400	0.12661300

Cat-II(anti-anti)-1

C	5.06921500	0.09984700	-0.38338400
N	4.21213100	0.66014400	0.49147500
C	2.93764700	0.24424000	0.60607100
C	2.45490400	-0.77378000	-0.20964800
C	3.33466500	-1.38045900	-1.11040700
C	4.64975000	-0.94277100	-1.18960600
N	1.13236300	-1.22977000	-0.10547900
C	4.65915900	1.77942700	1.35710500
C	0.00236700	-0.44424300	0.00633200
N	-1.12636000	-1.23147400	0.11708500
S	-0.00101500	1.20659700	0.00597100
C	-2.44895900	-0.77304600	0.22031900
C	-2.93114700	0.23147200	-0.61728000
N	-4.20231900	0.64929100	-0.51066900
C	-5.06057600	0.10596700	0.37876100
C	-4.64292900	-0.91739400	1.20505300
C	-3.32534300	-1.35840400	1.13365900
C	-4.69793100	1.73549600	-1.39203300
H	6.07387200	0.50369500	-0.41243600
H	2.33007200	0.73809200	1.35242100
H	2.98888100	-2.18298500	-1.75570100
H	5.34927000	-1.39147200	-1.88446000
H	0.99585900	-2.18969300	-0.40197600
H	5.73320700	1.90754000	1.24224800
H	4.13896100	2.68740700	1.05063100
H	4.42787200	1.53601500	2.39375300
H	-0.99049200	-2.19100500	0.41517900
H	-2.31840400	0.70383500	-1.37228200
H	-6.06468700	0.51438000	0.39424400
H	-5.34125200	-1.35089100	1.91068700
H	-2.97914200	-2.14652100	1.79616100
H	-3.89248100	2.05406700	-2.04970100
H	-5.53245700	1.35566700	-1.98155600
H	-5.01846700	2.57086000	-0.76928000

Cat-II(anti-anti)-2

C	5.18347500	-0.22381500	-0.09295400
N	4.31759100	0.63804100	0.47222300
C	2.99815000	0.38121000	0.54918000
C	2.47976300	-0.79360200	0.01231100
C	3.36820100	-1.70916800	-0.56240800
C	4.72465800	-1.42299100	-0.60800000
N	1.11716600	-1.11041500	0.08107100
C	4.80776300	1.92991100	1.01321100
C	0.05120400	-0.24862300	-0.09331800
N	-1.14523300	-0.92489800	0.07260000
S	0.16702300	1.35421000	-0.45146000
C	-2.41706300	-0.37880700	-0.16207100
C	-3.42132300	-0.59292600	0.77230300
N	-4.67138200	-0.13796700	0.55909600
C	-4.98205900	0.56281100	-0.54722400
C	-4.01663000	0.81331600	-1.50597000
C	-2.72674900	0.33178500	-1.32845200
C	-5.73665700	-0.39212900	1.56049200
H	6.22522300	0.07176700	-0.11534500
H	2.38735900	1.12586400	1.04039400
H	2.99625900	-2.63976900	-0.98163200
H	5.42913600	-2.11610500	-1.05148400
H	0.91829800	-2.09892600	-0.02369900
H	5.89152200	1.88860000	1.09721800
H	4.51269200	2.72906300	0.33223800
H	4.37068900	2.08624100	1.99867100
H	-1.12345500	-1.78447700	0.60888400
H	-3.25005100	-1.12460100	1.70134400
H	-6.00933300	0.89880800	-0.63453300
H	-4.28723900	1.36759400	-2.39648700
H	-1.96957400	0.49117500	-2.08622600
H	-5.31777900	-0.95598600	2.39104600
H	-6.11646900	0.56471500	1.91852000
H	-6.53303300	-0.96649100	1.08691900

Cat-II(anti-anti)-3

C	-5.06478100	0.46794400	-0.58081700
N	-4.74006800	-0.44706400	0.34669200
C	-3.46097000	-0.83924100	0.52891900
C	-2.44098800	-0.33037400	-0.25882800
C	-2.76440800	0.61298700	-1.24623800
C	-4.08197800	1.01609300	-1.39079800
N	-1.13601600	-0.81165400	-0.07683000
C	-5.78952800	-1.05089600	1.20357100
C	-0.00296900	-0.01674600	-0.00475600
N	1.13336400	-0.80786900	0.04476400
S	-0.00849600	1.62528600	0.01869000
C	2.43741300	-0.33122400	0.24439300
C	3.46155700	-0.83224100	-0.54816100
N	4.73787200	-0.44802700	-0.35313700
C	5.06115900	0.45320300	0.59228100
C	4.07837500	0.99131200	1.40404100
C	2.75795400	0.59356100	1.24634400
C	5.82177100	-1.01286200	-1.19458600
H	-6.11163400	0.73590500	-0.65855000
H	-3.28988700	-1.56492600	1.31684100
H	-1.99194000	1.01025600	-1.89306700
H	-4.36397200	1.74284600	-2.14324500
H	-1.05796500	-1.75401300	0.28779700
H	-6.73466600	-0.54872000	1.00953000
H	-5.87617400	-2.11061500	0.96172800
H	-5.51163000	-0.91586300	2.24878200
H	1.05694900	-1.74227000	-0.34011100
H	3.28619900	-1.54395400	-1.34667700
H	6.11073600	0.71249900	0.67490000
H	4.35746500	1.70540300	2.16959900
H	1.98425000	0.98413200	1.89569300
H	5.38788700	-1.68231400	-1.93400600
H	6.33819100	-0.19491200	-1.69648500
H	6.51042100	-1.56482500	-0.55438200

Cat-II(syn-anti)-1

C	4.69968700	-0.86313000	0.00972500
N	3.53764300	-1.27009200	-0.52315800
C	2.41783800	-0.51431300	-0.46728800
C	2.43089300	0.72105600	0.17211400
C	3.64626600	1.16188100	0.73092700
C	4.77548400	0.37088000	0.64286600
N	1.33166000	1.57662300	0.21491500
C	3.46004000	-2.58118700	-1.21343300
C	-0.02383800	1.33943500	0.05959300
N	-0.40238400	0.04765800	0.42127800
S	-1.02660600	2.53500700	-0.43709000
C	-1.74501700	-0.36680200	0.49210200
C	-2.61505600	-0.15335600	-0.57603800
N	-3.89882600	-0.53719200	-0.49249500
C	-4.38746400	-1.16212100	0.59964100
C	-3.55720000	-1.43365000	1.66829500
C	-2.22773300	-1.02612000	1.62151400
C	-4.82585000	-0.23178200	-1.61055800
H	5.54592300	-1.53277800	-0.08475600
H	1.54181700	-0.91524200	-0.96246200
H	3.68929000	2.12623500	1.22945500
H	5.72004100	0.69389700	1.06460100
H	1.54777900	2.56747500	0.17206900
H	4.46407700	-2.98653300	-1.31624200
H	2.84619100	-3.25817900	-0.61888000
H	3.02502800	-2.43266300	-2.20141300
H	0.19254100	-0.38499100	1.12175700
H	-2.30493800	0.32592600	-1.49418300
H	-5.43901100	-1.42382800	0.57946600
H	-3.95749100	-1.93984700	2.53851900
H	-1.57628200	-1.20624700	2.47207400
H	-4.24476900	0.00500200	-2.49917100
H	-5.44815700	-1.10540100	-1.79978000
H	-5.44128500	0.62333200	-1.32816300

Cat-II(syn-anti)-2

C	-4.41358100	-1.30981300	0.78476400
N	-4.58068600	-0.30245100	-0.08987500
C	-3.55544000	0.48346200	-0.46492500
C	-2.27671900	0.30434000	0.06353200
C	-2.08900500	-0.73577600	0.98884500
C	-3.16159000	-1.54470800	1.33194000
N	-1.29193000	1.21574000	-0.31403100
C	-5.92689500	-0.02139200	-0.65189600
C	0.09075900	1.12992200	-0.23997700
N	0.56784200	-0.17164700	-0.31487500
S	1.00123200	2.48982500	-0.15000300
C	1.93057800	-0.51004800	-0.35921000
C	2.83626000	0.03823400	0.54799200
N	4.13668900	-0.29133200	0.49111000
C	4.61162000	-1.17188900	-0.41492500
C	3.74977500	-1.77180900	-1.31086800
C	2.40035300	-1.43553100	-1.29100600
C	5.09222300	0.35675600	1.42357900
H	-5.28937400	-1.89634400	1.03324500
H	-3.77998500	1.26391400	-1.18467500
H	-1.12074800	-0.88803200	1.45194600
H	-3.04468200	-2.34709400	2.05060700
H	-1.59620100	2.16976700	-0.47751100
H	-6.58218800	-0.86041400	-0.42862800
H	-6.31424800	0.88939700	-0.19365000
H	-5.83933100	0.09915300	-1.73118100
H	-0.03750200	-0.83074800	-0.79382800
H	2.54133500	0.73933500	1.31651300
H	5.67743100	-1.36654700	-0.39056500
H	4.13934400	-2.48197400	-2.03006700
H	1.72000100	-1.88014000	-2.01160900
H	4.54094300	0.76743800	2.26695100
H	5.79956700	-0.39178700	1.77750900
H	5.61249600	1.15422600	0.89161800

Cat-II(syn-anti)-3

C	-4.61702400	-1.07630000	-0.22466800
N	-3.49070600	-1.34636700	0.45344900
C	-2.41395500	-0.53097900	0.41453900
C	-2.43398400	0.62746100	-0.35745000
C	-3.61145500	0.92378800	-1.07048200
C	-4.69892700	0.07468200	-0.99687000
N	-1.38503800	1.54183600	-0.40829700
C	-3.44044800	-2.53850300	1.33515400
C	-0.05519300	1.43444300	-0.03068000
N	0.45562400	0.14095600	-0.17685900
S	0.79311800	2.74320100	0.45536800
C	1.81069100	-0.13849100	0.08978600
C	2.60806200	-0.69705400	-0.89644100
N	3.90311500	-0.99013800	-0.65394000
C	4.46770100	-0.72957700	0.53799500
C	3.71819100	-0.16387600	1.55607400
C	2.37982600	0.12937000	1.34187100
C	4.72263100	-1.62414900	-1.71627200
H	-5.42981100	-1.78596200	-0.12831700
H	-1.56669100	-0.81850500	1.02420000
H	-3.65731400	1.82263800	-1.67869900
H	-5.61285700	0.28664100	-1.53908400
H	-1.66122300	2.51075900	-0.53050400
H	-4.19133500	-3.25287700	1.00362600
H	-2.45255700	-2.99043800	1.26328500
H	-3.64559800	-2.22704700	2.36031300
H	0.04843200	-0.38963300	-0.94152500
H	2.24412500	-0.91091300	-1.89518800
H	5.51519000	-0.98755400	0.64601700
H	4.18899400	0.03527700	2.51127900
H	1.77602600	0.56147500	2.13149900
H	4.26959500	-1.41939200	-2.68428900
H	5.72324900	-1.19535400	-1.68753200
H	4.76423000	-2.69922900	-1.53678100

Cat-II(syn-anti)-4

C	-4.35797900	-1.43174700	0.74946700
N	-4.54040300	-0.52900800	-0.22999700
C	-3.54724900	0.28007100	-0.63831400
C	-2.28647000	0.23873500	-0.04082200
C	-2.08394300	-0.69053900	0.99349100
C	-3.12281900	-1.52744600	1.37118600
N	-1.34527700	1.16718500	-0.47812700
C	-5.87313700	-0.38918300	-0.87056800
C	0.02083100	1.24572000	-0.23377200
N	0.63161300	0.00089900	-0.10944300
S	0.78261500	2.69075200	-0.18308300
C	2.01258900	-0.13106100	0.12562900
C	2.78369900	-0.91338500	-0.71953200
N	4.10427600	-1.07766900	-0.49469100
C	4.71907500	-0.47123500	0.53574000
C	3.99706500	0.32871200	1.40600900
C	2.63453900	0.49805800	1.21266100
C	4.89527600	-1.95584400	-1.39156200
H	-5.20850300	-2.04593400	1.01765500
H	-3.78433300	0.96856600	-1.44275000
H	-1.13174300	-0.73832300	1.50862800
H	-2.99252400	-2.24753200	2.17017300
H	-1.71162600	2.05855100	-0.79565100
H	-6.47748400	-1.25705800	-0.61635100
H	-6.34614400	0.52003600	-0.49746000
H	-5.74147100	-0.33779200	-1.95069600
H	0.19817400	-0.75486900	-0.63027500
H	2.37615100	-1.41409500	-1.59057300
H	5.78352700	-0.64878900	0.63901400
H	4.50803600	0.80634100	2.23321800
H	2.05145100	1.10787600	1.89281000
H	4.38576500	-2.03580500	-2.34982800
H	5.87692900	-1.50896000	-1.54087300
H	4.99163300	-2.93922500	-0.92959400

Cat-II(syn-syn)-1

C	3.59725300	-1.70255200	0.45297400
N	3.15294300	-0.96398100	-0.57668400
C	2.16451000	-0.05556400	-0.43230500
C	1.55661200	0.13736800	0.80360400
C	2.01261400	-0.62633300	1.88978800
C	3.03572400	-1.54101100	1.71143600
N	0.56479900	1.10758800	1.02082300
C	3.79773300	-1.08867100	-1.90767500
C	0.01147200	1.89635300	-0.00302900
N	-0.57425600	1.13044600	-1.02163600
S	0.05001700	3.51509400	-0.00665700
C	-1.56368600	0.15676500	-0.80304300
C	-2.19186100	-0.00931200	0.42994000
N	-3.17769400	-0.91482300	0.57846300
C	-3.60377400	-1.67943300	-0.44420700
C	-3.02588300	-1.54429400	-1.69471500
C	-2.00065500	-0.62819000	-1.87758500
C	-3.85158700	-1.06297500	1.89323000
H	4.39950500	-2.40088400	0.24765700
H	1.89957500	0.51305800	-1.31506100
H	1.56537000	-0.48786000	2.86982400
H	3.40671800	-2.13610700	2.53752500
H	0.73291000	1.66092400	1.85714700
H	4.44053500	-1.96615800	-1.90784000
H	3.02418100	-1.20126900	-2.66617700
H	4.39085300	-0.19279600	-2.09558000
H	-0.74208500	1.68938600	-1.85432600
H	-1.93683400	0.58130900	1.30006000
H	-4.40772200	-2.37434400	-0.22935900
H	-3.38323600	-2.15673300	-2.51412300
H	-1.54136700	-0.50726400	-2.85431400
H	-3.43510700	-0.34069700	2.59149600
H	-4.91690600	-0.87328400	1.76186800
H	-3.68801500	-2.07632300	2.26046800

Cat-II(syn-syn)-2

C	-3.60451300	-1.28039000	1.01580700
N	-3.56416000	-1.04223100	-0.30606300
C	-2.59441300	-0.29151900	-0.85953200
C	-1.59234600	0.29008900	-0.08281500
C	-1.62584900	0.05616300	1.30198000
C	-2.63100000	-0.73448200	1.83706100
N	-0.66041100	1.10038800	-0.74189400
C	-4.60029800	-1.62502700	-1.19579800
C	0.23854800	1.98395800	-0.11164700
N	1.04910200	1.37623100	0.85217600
S	0.31755600	3.55975400	-0.48197600
C	1.83843100	0.23761900	0.63120900
C	2.08241200	-0.26498800	-0.64454500
N	2.89352600	-1.32671900	-0.81675000
C	3.50488100	-1.93154500	0.21873500
C	3.30964900	-1.46298200	1.50706900
C	2.47109900	-0.37936200	1.71921300
C	3.18913200	-1.80730400	-2.18976800
H	-4.41966300	-1.89236300	1.38172600
H	-2.65203600	-0.15255100	-1.93414600
H	-0.88825800	0.50946000	1.95216700
H	-2.68336500	-0.91537700	2.90414500
H	-1.02703300	1.53121200	-1.58554000
H	-5.42300000	-1.98905600	-0.58421200
H	-4.96304600	-0.84909400	-1.86899900
H	-4.15957600	-2.44837700	-1.75886900
H	1.48488300	2.06452500	1.46048100
H	1.66244400	0.17845600	-1.53852800
H	4.14537800	-2.77304800	-0.01896000
H	3.81353400	-1.95273100	2.33188700
H	2.30938300	0.00272000	2.72324300
H	2.45620900	-1.39274600	-2.87821600
H	4.19086300	-1.47714000	-2.46779700
H	3.13159300	-2.89502400	-2.20086200

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C	-0.96845700	1.24031500	-0.47377400
C	-0.77635700	1.99867400	-1.63180800
C	-2.06772200	1.60727600	0.32566400
C	-1.61381900	3.06680100	-1.96558900
H	0.04312800	1.75877000	-2.30513000
C	-2.89916100	2.67206600	-0.00067000
H	-2.27376200	1.04222100	1.23264200
C	-2.68029300	3.42030000	-1.15552100
H	-3.32284600	4.25514100	-1.40993900
C	0.96888700	-0.47330100	-1.24012700
C	2.06772700	0.32675700	-1.60700800
C	0.77765500	-1.63158700	-1.99832500
C	2.89955900	0.00077900	-2.67159900
H	2.27311100	1.23394000	-1.04204000
C	1.61551800	-1.96501200	-3.06624800
H	-0.04144300	-2.30538700	-1.75844400
C	2.68154200	-1.15432400	-3.41969300
H	3.32440500	-1.40847600	-4.25437700
C	-0.96842900	-1.24055100	0.47309400
C	-0.77699300	-1.99874600	1.63134500
C	-2.06697200	-1.60790400	-0.32715400
C	-1.61439400	-3.06709200	1.96457400
H	0.04191200	-1.75853400	2.30526500
C	-2.89834600	-2.67291500	-0.00136900
H	-2.27248000	-1.04298500	-1.23434000
C	-2.68013800	-3.42098300	1.15371200
H	-3.32263600	-4.25599400	1.40771500
C	0.96794700	0.47357200	1.24072500
C	0.77569900	1.63162600	1.99901300
C	2.06688800	-0.32608200	1.60819400
C	1.61272700	1.96524100	3.06753300
H	-0.04355700	2.30509500	1.75873500
C	2.89789400	0.00009000	2.67336800
H	2.27301500	-1.23309800	1.04323000
C	2.67889000	1.15497500	3.42151300
H	3.32110600	1.40927000	4.25665300
B	-0.00001500	0.00000800	-0.00002300
C	4.08684700	0.85693800	-2.99607700
C	-4.08692000	2.99663900	0.85479900
C	-4.08534800	-2.99788400	-0.85773500
C	4.08535400	-0.85557900	2.99850300
C	1.32593100	-3.21928500	-3.83478400
F	2.22822300	-3.44748100	-4.80451900

F	0.11865000	-3.17510000	-4.42318900
F	1.32007000	-4.30208400	-3.03919800
F	4.34491500	0.87073200	-4.31709900
F	5.20615300	0.41228900	-2.39689900
F	3.91905100	2.12901000	-2.60911900
F	5.20492100	-0.41012200	2.40041400
F	3.91854200	-2.12759700	2.61095400
F	4.34234200	-0.86971200	4.31973400
F	-5.20497300	-2.39913100	-0.41331400
F	-3.91747100	-2.61088800	-2.12978700
F	-4.34289400	-4.31900700	-0.87154700
F	-3.92000900	2.60943500	2.12691200
F	-4.34471800	4.31771600	0.86865300
F	-5.20607200	2.39778200	0.40933900
C	1.32209900	3.21927400	3.83606500
C	-1.32332200	3.83544700	-3.21958300
C	-1.32462300	-3.83557000	3.21883900
F	-1.31945500	-3.04007600	4.30171200
F	-0.11698600	-4.42326200	3.17485400
F	-2.22639500	-4.80585300	3.44676100
F	2.22341600	3.44749400	4.80670000
F	0.11427000	3.17465200	4.42331400
F	1.31671600	4.30224500	3.04070600
F	-2.22505400	4.80565400	-3.44798900
F	-1.31736400	3.04007100	-4.30253900
F	-0.11577800	4.42326600	-3.17475200

Cat-II(*syn-anti*)-1•(BAr^F₄)₂

C	-5.30748100	4.99778700	1.64768200
N	-4.76837400	5.49829700	0.51524300
C	-3.72023500	4.91912500	-0.09085100
C	-3.13735600	3.78517100	0.46640900
C	-3.65704100	3.27203100	1.65313300
C	-4.76389500	3.87778700	2.23751500
N	-2.10192000	3.10228600	-0.16970700
C	-5.42268400	6.66194000	-0.11284400
C	-0.98633200	3.63928900	-0.75071800
N	-0.19686000	2.66328700	-1.29580600
S	-0.63436400	5.26525500	-0.78490000
C	1.14881500	2.78972000	-1.66010500
C	2.02181900	3.51429200	-0.85886600
N	3.32175800	3.60369400	-1.17107900
C	3.84174700	2.98391300	-2.24964600
C	3.01673500	2.23300500	-3.06576100
C	1.66306300	2.11681500	-2.76869400
C	4.19756300	4.34496400	-0.24109700
H	-6.17075700	5.52042000	2.04133700
H	-3.37603500	5.35315800	-1.01860600
H	-3.18533100	2.41416200	2.12075800
H	-5.20484800	3.48042700	3.14273600
H	-2.09658300	2.10188600	0.01150800
H	-5.53538600	7.44693500	0.63406200
H	-4.80361000	7.01582900	-0.93383800
H	-6.39242000	6.34269500	-0.49414600
H	-0.60789200	1.75367700	-1.48959500
H	1.70177900	4.01120400	0.04565100
H	4.90765600	3.10115900	-2.41578900
H	3.44142300	1.73116100	-3.92749100
H	1.01318300	1.51413300	-3.39256300
H	3.69380900	5.26713200	0.04657500
H	4.38536500	3.71930800	0.63532400
H	5.13419500	4.56646500	-0.74595900
C	3.35904000	-0.13006000	-0.07518200
C	2.56500000	0.63562200	0.79406400
C	2.65509200	-0.86933200	-1.03773500
C	1.17111200	0.59630000	0.75796900
H	3.03877900	1.24060500	1.56561200
C	1.26282900	-0.88851700	-1.09524600
H	3.20510300	-1.48672500	-1.74435300
C	0.49591200	-0.18369500	-0.17670000
H	-0.58772600	-0.28054000	-0.17342000

C	5.71182200	1.02805300	0.63639300
C	5.56573700	1.54504300	1.93893500
C	6.53148200	1.78027000	-0.21728100
C	6.17350900	2.73166300	2.34282000
H	4.98760000	0.98715800	2.67302100
C	7.15522900	2.96053800	0.19080000
H	6.72538300	1.43111300	-1.22879300
C	6.98388800	3.45875600	1.47376000
H	7.46635200	4.37576600	1.79304900
C	5.69050100	-0.91616600	-1.18330600
C	6.65187200	-1.93291300	-1.23900200
C	5.43395100	-0.26320300	-2.39213000
C	7.31676200	-2.25009000	-2.42482400
H	6.90302800	-2.48710300	-0.33773200
C	6.11177000	-0.55189900	-3.57038700
H	4.68613300	0.52443000	-2.40530700
C	7.06799900	-1.55817900	-3.60574700
H	7.60822800	-1.79214300	-4.51546300
C	5.09165400	-1.49811800	1.36830100
C	4.10481200	-2.46805700	1.59458400
C	6.24693700	-1.59768800	2.15645100
C	4.26367600	-3.47358800	2.54547000
H	3.18072600	-2.45708600	1.02106800
C	6.40553000	-2.59998000	3.11133100
H	7.05367700	-0.87910700	2.02155800
C	5.41454700	-3.55178300	3.31939700
H	5.53961900	-4.33379500	4.05857300
B	4.97035200	-0.37476700	0.18142400
C	5.85631000	3.30493400	3.69360900
C	0.61228400	-1.72840500	-2.15663400
C	5.78051600	0.28095200	-4.76648600
C	7.66200500	-2.61382300	3.93235500
C	7.93905900	3.72756900	-0.83085400
F	8.58077800	4.77761900	-0.31279200
F	7.09841900	4.22186800	-1.78760500
F	8.82621100	2.97133900	-1.47706000
F	6.84517400	4.07828500	4.15921900
F	5.60514500	2.36038000	4.60265200
F	4.75487700	4.08359800	3.61965100
F	7.71605200	-1.56152300	4.76649300
F	8.75650900	-2.54307300	3.15825100
F	7.76779900	-3.71985700	4.68147900
F	4.50914500	0.08772200	-5.17978200
F	5.85330900	1.60429300	-4.46881300

F	6.57948800	0.06098000	-5.80804600
F	0.94277000	-3.01639600	-2.04963800
F	-0.72638400	-1.64232000	-2.11224200
F	0.99414800	-1.31996100	-3.38158100
C	3.14818400	-4.46537900	2.72238200
C	0.41276200	1.41800300	1.75467800
C	8.29971700	-3.38788100	-2.42096600
F	7.67612400	-4.57466400	-2.41882600
F	9.08459100	-3.35749900	-1.33542400
F	9.09821500	-3.36196600	-3.49954500
F	3.48336500	-5.45938000	3.55817500
F	2.79589400	-5.02014300	1.55399000
F	2.04456100	-3.88207300	3.21946900
F	-0.92716100	1.23070400	1.63714100
F	0.60469600	2.74909800	1.57169200
F	0.75160200	1.16044600	3.00944900
C	-6.03720500	-1.58216500	-0.24275700
C	-6.81785200	-1.27461800	-1.35885000
C	-6.54158200	-2.58115900	0.61014400
C	-8.03711600	-1.91225100	-1.60668300
H	-6.48160100	-0.52623900	-2.07334500
C	-7.75217800	-3.21508300	0.36725500
H	-5.97053300	-2.86642100	1.49154500
C	-8.52080100	-2.88470900	-0.74854800
H	-9.47043700	-3.37239300	-0.93558000
C	-4.30054100	0.35191900	-0.91527200
C	-5.19648100	1.43630500	-0.94181000
C	-3.25479200	0.40397800	-1.85192400
C	-5.08192100	2.47489900	-1.86330100
H	-6.02638000	1.45271100	-0.23702400
C	-3.12865000	1.45666000	-2.76319000
H	-2.53984600	-0.41237000	-1.89685700
C	-4.04131800	2.50305400	-2.78792900
H	-3.94586900	3.31173100	-3.50542700
C	-3.46028900	-2.10839900	-0.16814800
C	-2.45218900	-2.56726700	0.68902800
C	-3.51998700	-2.74675800	-1.42374700
C	-1.54422500	-3.56090300	0.30719100
H	-2.35275800	-2.18446100	1.69784500
C	-2.63908300	-3.75242300	-1.79326200
H	-4.28894900	-2.45054000	-2.13435600
C	-1.63223300	-4.17494400	-0.92968300
H	-0.92611300	-4.94368200	-1.22521000
C	-4.62096500	-0.29746200	1.62439600

C	-5.82876900	0.13918900	2.20125600
C	-3.47219200	-0.07066700	2.39353200
C	-5.87748100	0.73344500	3.45956800
H	-6.76224600	-0.00627700	1.66349400
C	-3.52037900	0.48723100	3.67156600
H	-2.49950600	-0.33063000	1.99710600
C	-4.72564800	0.89704900	4.22492800
H	-4.77043100	1.31565600	5.22549500
B	-4.57372500	-0.92327700	0.10466900
C	-6.12105500	3.55481900	-1.90760500
C	-8.22303000	-4.30677800	1.28518600
C	-2.65173000	-4.30427700	-3.18757900
C	-2.24145900	0.74483200	4.41401800
C	-2.02865700	1.44842000	-3.78297600
F	-1.51775400	2.68024600	-3.97222300
F	-2.41685700	0.99473900	-4.97079100
F	-0.99549000	0.66847400	-3.37518900
F	-5.59212800	4.73507400	-2.32061500
F	-6.65262400	3.79667500	-0.68893700
F	-7.13019300	3.27820300	-2.72753100
F	-1.74763100	1.96688600	4.09809500
F	-1.29595600	-0.14714900	4.11238400
F	-2.41845400	0.73798000	5.73951900
F	-2.41818200	-5.62428400	-3.20670200
F	-3.81367100	-4.08550300	-3.81635600
F	-1.68643900	-3.72972900	-3.93094700
F	-7.81368100	-4.10798000	2.54684800
F	-9.56271400	-4.39263100	1.30392300
F	-7.76028800	-5.50817700	0.90850900
C	-7.16837900	1.27953900	3.99564500
C	-8.82902200	-1.48874500	-2.80857200
C	-0.37795800	-3.88184200	1.19963200
F	-0.65298100	-3.66202500	2.49063200
F	0.67742000	-3.09658900	0.88301100
F	0.02702500	-5.14803600	1.07053200
F	-7.28193400	1.10120200	5.31561200
F	-8.24072300	0.75003500	3.40725800
F	-7.23564900	2.62303300	3.78971300
F	-9.90483300	-2.26017100	-3.00973500
F	-8.08764800	-1.52631400	-3.92691400
F	-9.26489700	-0.22146800	-2.68518300

Cat-II(*syn-anti*)-2•(BAR^F₄)₂

C	-5.48872700	3.76141200	2.34231900
N	-4.97339700	4.81786300	1.68946400
C	-3.72259700	4.82505900	1.18665200
C	-2.89166200	3.71888500	1.37072300
C	-3.40994000	2.62466900	2.07602100
C	-4.71153600	2.64133200	2.54898800
N	-1.58257500	3.58581300	0.90697900
C	-5.81537400	6.02182500	1.53689800
C	-0.77241800	4.44151800	0.20479600
N	0.47595500	3.88839900	0.03530400
S	-1.23162100	5.93568800	-0.35387000
C	1.42499000	4.16504400	-0.94981700
C	2.21813100	3.09067200	-1.35652200
N	3.17331000	3.24892400	-2.28546300
C	3.39382100	4.43751700	-2.87421900
C	2.63421300	5.53129800	-2.51350700
C	1.65726600	5.41559500	-1.53375100
C	3.97088200	2.06751200	-2.68492100
H	-6.51561700	3.84328800	2.67682900
H	-3.41514400	5.70677400	0.64793000
H	-2.78606000	1.75840000	2.26206900
H	-5.13068000	1.79014200	3.07194100
H	-1.20729500	2.66017200	1.09255000
H	-5.88446000	6.52390200	2.50247600
H	-5.36342800	6.67887200	0.79834600
H	-6.79894100	5.71204500	1.18808600
H	0.66512900	3.03509000	0.55397700
H	2.09309500	2.08328300	-0.96353400
H	4.18119100	4.47116700	-3.61593800
H	2.83092000	6.48783800	-2.98098100
H	1.08647800	6.27659000	-1.22061400
H	4.32533600	1.57456800	-1.77902500
H	3.33104700	1.39382300	-3.25582600
H	4.81540200	2.39276600	-3.28819200
C	3.36269500	-0.45751100	0.01737200
C	2.53311500	-0.10868300	1.09738100
C	2.72235300	-0.62930100	-1.21585300
C	1.16591500	0.08242400	0.94078100
H	2.97511600	0.01415400	2.08510600
C	1.34612000	-0.44130300	-1.37256500
H	3.30980100	-0.92040300	-2.08557500
C	0.54704200	-0.08916000	-0.29528000
H	-0.52305200	0.02936100	-0.40736900

C	5.60004500	0.88711100	0.59844100
C	4.82328100	2.03619000	0.78879000
C	6.99180200	1.08631600	0.66059400
C	5.38139600	3.29231100	1.02286800
H	3.73994700	1.96530700	0.77063600
C	7.55458400	2.33173500	0.92281200
H	7.65803100	0.24309500	0.48965600
C	6.75646400	3.45785400	1.10372900
H	7.19876100	4.42781800	1.30446600
C	5.66753200	-1.20073100	-1.08959600
C	5.58799500	-2.56571300	-1.41232900
C	6.22400300	-0.37590500	-2.07344500
C	6.01294700	-3.05915600	-2.64219400
H	5.17267000	-3.26488000	-0.69027300
C	6.62819300	-0.86278600	-3.31680700
H	6.36069900	0.68558200	-1.87579800
C	6.52741800	-2.21161000	-3.62033900
H	6.83629800	-2.59567400	-4.58543300
C	5.16469100	-1.62585800	1.54555000
C	4.24614600	-2.67114900	1.72570500
C	6.18800800	-1.54174200	2.49745900
C	4.33387400	-3.56835200	2.78513100
H	3.41645600	-2.78587100	1.03337000
C	6.28600900	-2.44608900	3.55409300
H	6.93386500	-0.75356400	2.43503800
C	5.35889600	-3.46909100	3.71653100
H	5.43300100	-4.16519500	4.54376500
B	4.98161000	-0.60333000	0.27601800
C	4.48199000	4.48614600	1.08395200
C	0.75748700	-0.52917600	-2.75023100
C	7.12203700	0.12551200	-4.32800400
C	7.37758700	-2.25471900	4.56675000
C	9.05034600	2.48715300	0.93326300
F	9.43724400	3.48186800	1.74611700
F	9.51644700	2.78030500	-0.29156900
F	9.66358100	1.36839100	1.33289300
F	4.94228900	5.45129500	1.88049700
F	3.23547000	4.17348700	1.49267700
F	4.32940800	5.04207100	-0.14596900
F	7.08991900	-1.25532400	5.41857800
F	8.54377300	-1.93684500	3.98437100
F	7.57996300	-3.35480100	5.30579400
F	6.13172700	0.98639500	-4.68353200
F	8.11262200	0.88927300	-3.84816900

F	7.55455600	-0.45005900	-5.45214100
F	1.07784100	-1.66576000	-3.37154100
F	-0.57510300	-0.42244000	-2.74624700
F	1.22299800	0.48464900	-3.52220500
C	3.24744200	-4.59505600	2.92855900
C	0.36882200	0.58379300	2.09790100
C	5.95376700	-4.53839900	-2.90512200
F	4.87290800	-5.09837600	-2.34584500
F	7.02688900	-5.16890800	-2.40565600
F	5.91612900	-4.80608600	-4.21971100
F	3.53090700	-5.50499600	3.87073500
F	3.02692700	-5.25038800	1.78019200
F	2.08100500	-4.01798900	3.26962000
F	-0.96450200	0.51383600	1.85858700
F	0.59744800	1.92689600	2.28250800
F	0.62288300	-0.00366800	3.24824500
C	-5.86256500	-1.65660900	-0.76987200
C	-6.47743100	-1.13480600	-1.90938200
C	-6.39626100	-2.86112400	-0.27216800
C	-7.57282200	-1.76071400	-2.51212000
H	-6.10244000	-0.21908200	-2.36096100
C	-7.48485700	-3.48291300	-0.86702100
H	-5.94640100	-3.32176300	0.60468000
C	-8.09241100	-2.93503600	-1.99729700
H	-8.94584600	-3.41720400	-2.46131200
C	-4.27152600	0.51361900	-0.64557900
C	-5.27465400	1.50099900	-0.57660500
C	-3.08633900	0.90023000	-1.28025300
C	-5.10565200	2.76649400	-1.12932400
H	-6.22178700	1.26067900	-0.09453500
C	-2.90604100	2.17776200	-1.82262500
H	-2.29537700	0.16814700	-1.40723600
C	-3.91306900	3.12688000	-1.76165700
H	-3.78326400	4.11205000	-2.19672400
C	-3.24540300	-1.95871000	-0.40885800
C	-2.24028600	-2.38833000	0.47106100
C	-3.03725400	-2.29423600	-1.75824400
C	-1.06461700	-2.99312300	0.02802700
H	-2.33708200	-2.25138800	1.54032900
C	-1.89077700	-2.95181700	-2.19903500
H	-3.78914800	-2.01772200	-2.49656500
C	-0.86876400	-3.27994900	-1.31634400
H	0.05083000	-3.73283900	-1.66920500
C	-4.82517700	-0.79773600	1.56025300

C	-6.10792900	-0.71538100	2.12885600
C	-3.76926200	-0.56945000	2.45040300
C	-6.29763300	-0.46182400	3.48838800
H	-6.98424200	-0.85095800	1.49901400
C	-3.94618100	-0.38351900	3.81837200
H	-2.75867500	-0.53306600	2.07091900
C	-5.22175700	-0.33034400	4.36484100
H	-5.37847900	-0.17279100	5.42632400
B	-4.54748800	-1.00638700	-0.04616400
C	-6.23843200	3.74708500	-1.14027100
C	-8.00966500	-4.78841700	-0.34230000
C	-1.74815400	-3.24461800	-3.66662500
C	-2.71759500	-0.16208600	4.65036400
C	-1.62149700	2.48569200	-2.53536000
F	-0.55166000	2.08037000	-1.79859700
F	-1.44856900	3.80132700	-2.74450100
F	-1.52349200	1.87828100	-3.71467500
F	-5.78322200	5.02423100	-1.12505400
F	-7.03662200	3.62127500	-0.05561800
F	-7.01967800	3.62999200	-2.21067600
F	-2.18584800	1.06363500	4.40069300
F	-1.75727600	-1.04634600	4.36389600
F	-2.96594600	-0.21664000	5.96090800
F	-0.60107300	-3.87800600	-3.94710700
F	-2.75372500	-4.01129000	-4.11182800
F	-1.77140100	-2.11820600	-4.39935700
F	-7.56686700	-5.05412200	0.89375100
F	-9.35257300	-4.79410600	-0.30034400
F	-7.64582000	-5.81522100	-1.12604100
C	-7.67595800	-0.16651400	4.00079700
C	-8.20192700	-1.10458700	-3.70563800
C	0.01776600	-3.29992300	1.02651800
F	0.01253500	-2.40824800	2.04007900
F	1.23524000	-3.23858800	0.45375100
F	-0.10359100	-4.51175500	1.57105200
F	-7.82439600	-0.49797800	5.28852600
F	-8.63156400	-0.77947900	3.30029100
F	-7.91833400	1.16538200	3.91417400
F	-9.11024500	-1.88956100	-4.29976000
F	-7.28550000	-0.77502700	-4.62890700
F	-8.82614000	0.03744800	-3.36498100

Cat-II(*syn-anti*)-3•(BAr^F₄)₂

C	5.49342100	-5.18745700	0.62905000
N	5.15333700	-4.03216600	1.22289900
C	3.92142800	-3.51457000	1.09729500
C	2.94669800	-4.15288900	0.33835500
C	3.27848600	-5.36002900	-0.29275600
C	4.55833300	-5.86865400	-0.13070300
N	1.74759100	-3.47962200	0.18746100
C	6.12910600	-3.27355100	2.03442200
C	0.51012000	-3.97618500	-0.15617800
N	-0.28506700	-2.94798900	-0.58808100
S	0.04175300	-5.55774100	-0.05921600
C	-1.63470000	-3.06323800	-0.94102400
C	-2.02472100	-2.58987900	-2.18164300
N	-3.31972900	-2.63662700	-2.55398200
C	-4.26135000	-3.15804200	-1.74828700
C	-3.91313300	-3.65098300	-0.50191500
C	-2.59780200	-3.58606800	-0.07265900
C	-3.69256400	-2.08046400	-3.87029100
H	6.51460600	-5.51992500	0.75919700
H	3.74426500	-2.57355000	1.60676900
H	2.54977700	-5.86588700	-0.91180500
H	4.85343800	-6.78721300	-0.62216100
H	1.77707700	-2.49170400	0.41757300
H	6.16788900	-2.24929500	1.65646100
H	5.78582100	-3.27289500	3.06916100
H	7.10702800	-3.73977100	1.94663200
H	0.18014800	-2.11124400	-0.92661500
H	-1.32588900	-2.15980000	-2.88978000
H	-5.28270900	-3.16340900	-2.11572500
H	-4.69074400	-4.05028300	0.13634300
H	-2.31936200	-3.91484300	0.92259100
H	-3.66015200	-0.99221000	-3.81547200
H	-2.97830600	-2.43226200	-4.61375600
H	-4.69766100	-2.41024000	-4.12015700
C	-3.36202200	0.30644600	-0.25055200
C	-2.37386700	-0.06872100	0.67965000
C	-2.87921900	0.65273400	-1.52241600
C	-1.01750900	-0.05100000	0.37879100
H	-2.65942900	-0.34022200	1.69080000
C	-1.51571100	0.64149100	-1.83720100
H	-3.57446200	0.98485500	-2.29033600
C	-0.56169600	0.32103400	-0.88302500
H	0.49903800	0.39515400	-1.10554000

C	-5.53285800	-0.97718400	0.78473300
C	-5.02259200	-1.56293000	1.95882400
C	-6.55816800	-1.70210000	0.16202000
C	-5.45497200	-2.79830600	2.43197500
H	-4.28445500	-1.03172900	2.55250900
C	-7.00539200	-2.93512200	0.64032000
H	-7.04442600	-1.30889200	-0.72580900
C	-6.46008200	-3.50818500	1.77984800
H	-6.80082100	-4.46963200	2.14780100
C	-5.85417500	0.97842200	-1.03080900
C	-6.63163100	2.14405000	-1.02976900
C	-5.93823300	0.19799400	-2.19064300
C	-7.44419700	2.48779300	-2.11050700
H	-6.62057300	2.79399700	-0.15887300
C	-6.76414300	0.51974800	-3.26271600
H	-5.36256100	-0.72595800	-2.23835400
C	-7.53064700	1.67776300	-3.23723600
H	-8.18780500	1.93425400	-4.06014000
C	-4.98930100	1.55697700	1.44859700
C	-4.07791700	2.61872000	1.54857100
C	-6.00667400	1.51887800	2.41006500
C	-4.16973600	3.57169700	2.55948900
H	-3.27600300	2.71650200	0.82208500
C	-6.10261300	2.47373500	3.42078600
H	-6.75465600	0.72950300	2.37268300
C	-5.18283500	3.50941600	3.51068500
H	-5.26102600	4.25782300	4.29112800
B	-4.94366100	0.46877100	0.22785000
C	-4.72786800	-3.44180500	3.57512000
C	-1.08186200	0.89560400	-3.25155900
C	-6.80338100	-0.40860500	-4.43445600
C	-7.19385000	2.33522900	4.44237200
C	-7.97703300	-3.70657000	-0.19942500
F	-8.54039200	-4.72167400	0.46141200
F	-7.32827900	-4.24709000	-1.26585100
F	-8.94960500	-2.94103400	-0.69857300
F	-5.47941700	-4.34299600	4.21617900
F	-4.28614400	-2.55480400	4.46951800
F	-3.63840200	-4.10455100	3.11356600
F	-6.92849600	1.34673900	5.31302900
F	-8.37013300	2.03541400	3.87037700
F	-7.36463600	3.45605200	5.15707500
F	-5.68761500	-0.32067200	-5.19089300
F	-6.86105700	-1.70294300	-4.02889300

F	-7.84257500	-0.19644100	-5.23906400
F	-1.70462300	1.92979200	-3.80794300
F	0.23762500	1.07150200	-3.35939700
F	-1.37938500	-0.18861200	-4.02912400
C	-3.13574000	4.65768200	2.65735100
C	-0.03346100	-0.46720700	1.42850300
C	-8.21717100	3.77734700	-2.07499200
F	-7.46805700	4.80836000	-2.49382900
F	-8.63591700	4.07114000	-0.83844700
F	-9.29662200	3.72769000	-2.87102400
F	-3.64412600	5.77506300	3.20126600
F	-2.63923800	4.98087700	1.45618200
F	-2.09972900	4.29021100	3.43082600
F	1.17944200	-0.74738900	0.84111900
F	-0.40628000	-1.59267800	2.05383100
F	0.20959100	0.44448200	2.35933300
C	5.81758200	1.79706800	-0.57900000
C	6.52109300	1.55981400	-1.76077000
C	6.17184700	2.95920400	0.13199200
C	7.53584800	2.41513800	-2.20115900
H	6.28871500	0.68981500	-2.37120800
C	7.18165300	3.80705100	-0.29982400
H	5.64583200	3.20140800	1.05331800
C	7.88264400	3.54189500	-1.47631400
H	8.67962500	4.19643700	-1.81025800
C	4.49599600	-0.53304400	-0.87104000
C	5.61126800	-1.38458000	-0.94743300
C	3.36092200	-0.95307800	-1.58072100
C	5.60228600	-2.56468800	-1.69013600
H	6.52819900	-1.09822800	-0.43194300
C	3.34662200	-2.13229600	-2.32515100
H	2.47779700	-0.32142600	-1.58731500
C	4.46700800	-2.95480000	-2.39325000
H	4.46013700	-3.86822300	-2.97970000
C	3.22148800	1.75533400	-0.17151800
C	2.34865700	2.14535100	0.85466900
C	2.91484000	2.23824700	-1.45611300
C	1.23036300	2.94199400	0.60554500
H	2.53637000	1.84918200	1.88217700
C	1.80892300	3.04515100	-1.70491900
H	3.57453600	1.99576100	-2.28742000
C	0.94571200	3.39976500	-0.67492900
H	0.07919500	4.02679500	-0.86278500
C	4.92372900	0.38914400	1.53224400

C	6.21305500	0.40548500	2.08790300
C	3.93418300	-0.22277600	2.31889200
C	6.48200000	-0.13879300	3.34530400
H	7.03484200	0.84496100	1.52794900
C	4.19636300	-0.75220800	3.57939900
H	2.92259300	-0.28772600	1.93464500
C	5.47746800	-0.70720000	4.11848100
H	5.69132200	-1.12131500	5.09902200
B	4.59560000	0.86977400	-0.00553700
C	6.85712300	-3.38390600	-1.78069400
C	7.50311500	5.05557300	0.47139800
C	1.58391100	3.62391100	-3.07325800
C	3.13074400	-1.53194000	4.28940500
C	2.12777000	-2.54259600	-3.09631700
F	1.72214900	-3.78689400	-2.76123800
F	2.32422500	-2.54674200	-4.41269400
F	1.07184100	-1.72301200	-2.85379000
F	6.60059700	-4.66172100	-2.12114800
F	7.50113600	-3.42519000	-0.59005000
F	7.72220100	-2.90082800	-2.66909200
F	3.26602900	-2.85661600	3.99872700
F	1.89707000	-1.18879000	3.90291000
F	3.20414600	-1.42573100	5.61546200
F	2.12041900	4.84753500	-3.18178600
F	2.12825200	2.86677100	-4.03593900
F	0.27365000	3.74909400	-3.34522600
F	7.14869500	4.95094700	1.75982400
F	8.81663600	5.33241400	0.43337300
F	6.86683000	6.12518900	-0.02844500
C	7.90271600	-0.28653500	3.80509700
C	8.24384800	2.07602300	-3.47993800
C	0.28029100	3.32850900	1.70518000
F	0.72595600	2.98131800	2.91719300
F	-0.91811200	2.72783400	1.52904300
F	0.05528800	4.64640200	1.71250500
F	8.01442200	-0.23960900	5.13720100
F	8.71354700	0.63462000	3.28449700
F	8.37693700	-1.49652800	3.41942700
F	9.23438600	2.93340900	-3.75854600
F	7.40121200	2.08005500	-4.52518200
F	8.78046100	0.84429900	-3.42996600

COM-I

C	-4.94661900	0.99380700	-0.38461200
C	-4.49443700	-0.31901000	-0.40528800
C	-3.14454600	-0.61229000	-0.56249200
C	-2.22731000	0.42611100	-0.71524500
C	-2.66744700	1.75125300	-0.71222900
C	-4.01805800	2.01832100	-0.53594100
N	-0.87716300	0.09909500	-0.95696600
C	0.22828200	0.73081400	-0.44123400
N	1.36781500	0.29550800	-1.06524800
S	0.17584400	1.83682500	0.80133000
C	2.70688200	0.41304900	-0.64927600
C	3.24986600	1.55354200	-0.04981700
C	4.59382200	1.55436400	0.30580700
C	5.42086600	0.45984900	0.07522900
C	4.87250800	-0.65430000	-0.54442800
C	3.53308700	-0.68313900	-0.90960800
O	0.87508900	-2.53268100	-1.01503300
C	0.74174600	-2.40890000	0.41165200
C	1.54895400	-3.48114300	-0.18771400
C	-4.49239100	3.44463300	-0.47925800
F	-3.65337200	4.27381400	-1.11182500
F	-4.60090200	3.87311200	0.78550600
F	-5.70243900	3.57665300	-1.04270200
C	-5.48875400	-1.42709800	-0.20141300
F	-6.62988200	-1.18782200	-0.86184200
F	-5.81493000	-1.56289300	1.09526700
F	-5.01814600	-2.61115300	-0.61710600
C	5.69674400	-1.87899900	-0.82155900
F	6.95817000	-1.74567500	-0.40469000
F	5.72369200	-2.16579100	-2.13022800
F	5.17739700	-2.95930900	-0.20497800
C	5.17361900	2.81077200	0.89974300
F	4.29937900	3.42285800	1.70564800
F	5.50970500	3.68716600	-0.05755700
F	6.28085000	2.55459400	1.60995800
C	-0.62426300	-2.62827100	0.96113000
C	-1.11101900	-1.76456800	1.94198300
C	-2.39339300	-1.94301000	2.45725300
C	-3.19346800	-2.98282200	1.99445800
C	-2.71517100	-3.83904300	1.00185200
C	-1.43825200	-3.65994500	0.48225800
H	-6.00226400	1.21544400	-0.27092700
H	-2.80725700	-1.64488900	-0.56164900

H	-1.96483200	2.56228800	-0.85308900
H	-0.72692000	-0.81156100	-1.38045300
H	1.23363500	-0.48892000	-1.69509100
H	2.63172300	2.41879700	0.14450300
H	6.46268300	0.47684600	0.37106400
H	3.11715100	-1.56280300	-1.39472900
H	1.28112600	-1.55665600	0.82979000
H	2.63398100	-3.39797600	-0.17545000
H	1.14618400	-4.49016400	-0.22751000
H	-0.49382800	-0.93767200	2.28530700
H	-2.77034600	-1.25824600	3.20950600
H	-4.19627900	-3.11374500	2.38530500
H	-3.34758200	-4.63485400	0.62259100
H	-1.07914300	-4.30971600	-0.31126300

COM-II

C	-3.98010500	1.14664600	0.37106300
C	-2.73077700	1.71634900	0.14354600
C	-1.56854500	1.00399800	0.37336000
C	-1.62377700	-0.32323200	0.82142400
C	-2.86780200	-0.90147800	1.07976600
C	-4.02165900	-0.15554300	0.84452600
N	-0.37234000	-0.95204600	0.95379100
C	-0.04877700	-2.26558000	1.09049300
N	1.29976000	-2.51733800	1.00378100
S	-1.08241800	-3.55971300	1.30808000
C	2.34354000	-1.57140300	0.86102700
C	2.51909300	-0.56802500	1.81642400
C	3.51248900	0.38483700	1.63512600
C	4.34358100	0.34949000	0.52129000
C	4.17455300	-0.66864700	-0.40820800
C	3.18635000	-1.63248700	-0.24666700
O	1.45110900	0.75965900	-0.85897600
C	1.13716400	0.34332800	-2.20164000
C	1.38451200	1.75410100	-1.87664400
C	-5.34998700	-0.83942900	1.01079500
F	-5.35024400	-1.68784500	2.04494500
F	-5.66077500	-1.55382200	-0.08529200
F	-6.34340800	0.03983000	1.20060700
C	-2.65699500	3.07638900	-0.48536200
F	-3.05909800	3.03463800	-1.77056000
F	-1.40650800	3.56841700	-0.48843800
F	-3.44278000	3.96232100	0.13546100
C	4.97495900	-0.64187700	-1.67809100
F	6.20354200	-0.15301100	-1.48572300
F	4.37687600	0.14621000	-2.59544900
F	5.08873800	-1.85776500	-2.22378300
C	3.73729600	1.44302600	2.68128900
F	4.72391500	1.09602500	3.51838400
F	2.63956500	1.64915000	3.41794600
F	4.08598500	2.60931200	2.12276900
C	-0.23243500	-0.22003500	-2.38775400
C	-0.43493300	-1.57121600	-2.09049900
C	-1.71545200	-2.11100900	-2.09039000
C	-2.80702300	-1.30261600	-2.41007800
C	-2.60796000	0.02950500	-2.75753400
C	-1.32339800	0.57018000	-2.74738900
H	-4.89208500	1.70197200	0.18203300
H	-0.60405900	1.45735300	0.16813100

H	-2.94285200	-1.91672200	1.44160000
H	0.38040900	-0.35011000	0.62182300
H	1.52414200	-3.50294000	1.00060200
H	1.87396500	-0.53302400	2.68845200
H	5.10823800	1.10562100	0.37941500
H	3.05043900	-2.40995100	-0.99223000
H	1.95782100	-0.20809700	-2.66067100
H	2.34331100	2.19395000	-2.14056400
H	0.54827900	2.44465300	-1.78527400
H	0.41496200	-2.19241900	-1.81199200
H	-1.86455800	-3.14903700	-1.81271900
H	-3.81215100	-1.71070100	-2.37365600
H	-3.45276000	0.66201900	-3.00933900
H	-1.18096400	1.61849300	-2.99312600

COM-III

C	5.19227400	-0.10835800	0.75880200
C	4.16515400	0.34737700	1.57453000
C	2.84977200	0.36273400	1.12680100
C	2.54567400	-0.07516900	-0.16179100
C	3.56998600	-0.51500400	-1.00229900
C	4.87490800	-0.53550200	-0.52560700
N	1.20569100	0.02742100	-0.58823700
C	0.49782800	-0.85214800	-1.35763900
N	-0.79647900	-0.49615600	-1.59744500
S	1.07467100	-2.30355600	-1.95654400
C	-1.51909700	0.62400200	-1.14148300
C	-1.02574200	1.92762400	-1.23322800
C	-1.80830200	2.99033500	-0.78759100
C	-3.08566800	2.78893100	-0.28292500
C	-3.57710700	1.48749500	-0.22809100
C	-2.80874500	0.41079200	-0.64343100
O	-2.71152900	-2.56605700	-1.85739400
C	-2.33380900	-3.29761200	-0.68674500
C	-2.71480200	-3.98669900	-1.93310100
C	5.95909300	-1.05950600	-1.42837300
F	5.76186200	-0.68407000	-2.69903100
F	6.00159700	-2.39784900	-1.41410400
F	7.16781300	-0.61783200	-1.05423500
C	4.45598400	0.77632900	2.98582900
F	3.65768500	1.78580400	3.36367100
F	5.72404200	1.17804600	3.12984300
F	4.25495700	-0.22592100	3.85348400
C	-4.94375300	1.20774200	0.33919600
F	-4.86457000	0.70184500	1.57653900
F	-5.60624700	0.31059100	-0.40701700
F	-5.68999900	2.31697900	0.40284400
C	-1.22797500	4.37587500	-0.87739300
F	-0.78160000	4.63505800	-2.11334800
F	-0.18111500	4.51180500	-0.04919300
F	-2.12339200	5.31497300	-0.55803000
C	-3.25627900	-3.17653200	0.47681600
C	-2.82505500	-3.56342200	1.74590700
C	-3.67367500	-3.43682500	2.84100500
C	-4.95015700	-2.90339200	2.67824500
C	-5.37933400	-2.50529600	1.41452700
C	-4.54026600	-2.65077800	0.31468200
H	6.21801900	-0.11360100	1.10751400
H	2.06229300	0.71920600	1.78476300

H	3.35145000	-0.82953500	-2.01433800
H	0.65923800	0.71282200	-0.08064700
H	-1.35116200	-1.24880000	-2.00717200
H	-0.05488800	2.11816100	-1.68120900
H	-3.68960600	3.62662600	0.04344200
H	-3.20306400	-0.59921100	-0.58819600
H	-1.26600800	-3.24856700	-0.46764900
H	-1.93656200	-4.41036000	-2.56259000
H	-3.70517300	-4.43116700	-1.99992800
H	-1.82198500	-3.96131200	1.87477700
H	-3.33322100	-3.74298500	3.82484000
H	-5.60511300	-2.78984300	3.53586300
H	-6.36363900	-2.06754400	1.28378400
H	-4.86230800	-2.33021300	-0.67229500

COM-IV

C	-3.42770100	0.43214400	-0.33301300
C	-3.37413500	-0.82308400	0.26590000
C	-2.63700800	-1.03270300	1.42244900
C	-1.94923800	0.03346800	2.00484900
C	-2.04531600	1.30844100	1.45242900
C	-2.76114300	1.48828600	0.27434400
N	-1.10683200	-0.22055700	3.11082800
C	0.14156100	0.28284600	3.35968700
N	0.79188100	0.90584100	2.33063500
S	0.83932100	0.13644400	4.86695200
C	0.74565700	0.54440000	0.96229700
C	0.47975300	-0.76318000	0.56269900
C	0.44472900	-1.07566700	-0.78980900
C	0.70758400	-0.11410800	-1.75705700
C	1.00515300	1.17892400	-1.34113000
C	1.01709500	1.51957600	0.00479200
O	3.55506400	1.16286500	1.79566800
C	3.71200000	-0.25368900	1.72061200
C	4.78062400	0.60966000	2.25636600
C	-2.72690000	2.84186100	-0.38082700
F	-1.57895700	3.01930300	-1.05534400
F	-2.80375000	3.82543400	0.52469100
F	-3.73094500	3.00026900	-1.24986800
C	-4.11961900	-1.96275200	-0.37467000
F	-3.96097500	-1.95615400	-1.70361100
F	-5.43601400	-1.87416200	-0.13492900
F	-3.70777800	-3.14977800	0.08531100
C	1.39541600	2.21599800	-2.35530800
F	0.89671100	1.94066900	-3.56626000
F	2.73360500	2.28341700	-2.48688700
F	0.97789400	3.43755000	-2.00288600
C	0.06891900	-2.47426700	-1.18759100
F	-1.26707200	-2.63615700	-1.17549000
F	0.57291900	-3.38283900	-0.33778700
F	0.49640500	-2.78120400	-2.41660200
C	3.77002600	-0.84210400	0.35201900
C	3.50637000	-2.20065600	0.16928700
C	3.51564200	-2.75145200	-1.10789500
C	3.78593600	-1.94559900	-2.21180700
C	4.04985800	-0.58970200	-2.03286400
C	4.04083800	-0.03749600	-0.75491300
H	-3.97311900	0.58189300	-1.25810700
H	-2.55059200	-2.03066200	1.84024600

H	-1.52438200	2.14170100	1.91261100
H	-1.47131400	-0.77890300	3.87108800
H	1.67147100	1.33592800	2.61179800
H	0.31012300	-1.53714000	1.30543700
H	0.69722600	-0.36913900	-2.81014600
H	1.23293100	2.53734400	0.31358100
H	3.10850700	-0.79989000	2.44918100
H	4.93780400	0.66447700	3.33071400
H	5.64040300	0.82133000	1.62413600
H	3.26448900	-2.82237700	1.02794900
H	3.28893000	-3.80392300	-1.24345100
H	3.77812000	-2.37232000	-3.20967900
H	4.23919800	0.04935200	-2.88950900
H	4.20021300	1.02729700	-0.61079100

COM-V

C	5.81351700	-0.61694200	0.03669700
N	5.23431500	0.51024400	0.47357100
C	3.90664300	0.73959000	0.36920200
C	3.07571600	-0.21395000	-0.21691300
C	3.67256700	-1.40554900	-0.67268000
C	5.03316000	-1.60412900	-0.54671900
C	6.05628600	1.56553700	1.11363400
C	0.82523800	0.92308600	-0.15429800
S	1.22966600	2.39696000	0.48895500
C	-1.64007300	1.26327200	-0.44956500
C	-1.72540300	2.65282000	-0.50792000
N	-2.92744700	3.26352500	-0.46132700
C	-4.08105300	2.58000600	-0.37479000
C	-4.05465200	1.19645400	-0.34621200
C	-2.83918900	0.53514000	-0.38325600
C	-2.94932700	4.74359800	-0.54034300
O	0.08328700	-2.29974200	-1.21926500
C	-0.66256600	-3.33133100	-0.53314300
C	-0.68403400	-3.23193100	-1.99780500
C	-1.79434700	-2.83420000	0.30333300
C	-1.51054000	-2.08324500	1.45005000
C	-2.54518100	-1.59502100	2.24157800
C	-3.87089000	-1.86477800	1.89685800
C	-4.15822800	-2.61850000	0.76061600
C	-3.12130900	-3.10148300	-0.03853300
H	6.88523800	-0.70435300	0.16449500
H	3.54345900	1.67960000	0.75603800
H	3.04867600	-2.17027900	-1.12852900
H	5.50188900	-2.51509300	-0.89831200
H	1.29383600	-0.94634900	-0.81037300
H	7.10488400	1.28278500	1.05451700
H	5.89571100	2.50414700	0.58393100
H	5.75470100	1.66001400	2.15705400
H	-0.57387300	-0.44470900	-0.74736400
H	-0.86197100	3.29546900	-0.59290800
H	-4.99428900	3.16055800	-0.33646800
H	-4.98420400	0.64391900	-0.28231700
H	-2.81233300	-0.55092000	-0.35490100
H	-2.67897300	5.04648900	-1.55243400
H	-3.95093400	5.09512900	-0.30264600
H	-2.23846200	5.14462100	0.18101600
H	-0.01632100	-4.08611600	-0.08843700
H	-0.09075000	-3.91685700	-2.59497800

H	-1.55374100	-2.79855300	-2.48442100
H	-0.47581800	-1.89000000	1.72523900
H	-2.32036100	-1.02270800	3.13537600
H	-4.67777700	-1.50480800	2.52695100
H	-5.18726300	-2.84873300	0.50464200
H	-3.34567300	-3.70315600	-0.91467800
N	1.70152500	-0.10976700	-0.39107700
N	-0.44905300	0.54254400	-0.51093900

COM-VI

C	5.73351100	0.32167300	0.83049200
N	5.33816400	-0.14475100	-0.36627500
C	4.03029200	-0.21892100	-0.69304300
C	3.04588500	0.15856100	0.20711300
C	3.44143200	0.62554400	1.47056600
C	4.79277400	0.71602900	1.76756900
C	6.33917300	-0.57989100	-1.36853900
C	0.73161900	0.98016800	-0.00354400
S	1.01635300	2.46135000	0.68619500
C	-1.70633300	1.18955000	-0.47640200
C	-1.84862000	2.57281400	-0.55594700
N	-3.07571700	3.13190300	-0.55403000
C	-4.20087100	2.39786300	-0.49650100
C	-4.11553100	1.01743800	-0.45655100
C	-2.87139800	0.40831900	-0.44711300
C	-3.15616700	4.61080800	-0.60535800
O	0.21637200	-2.17481900	-1.27228200
C	-0.45220900	-3.28273500	-0.62686300
C	-0.46961600	-3.13738900	-2.08747600
C	-1.62659900	-2.89903900	0.21135400
C	-1.41001000	-2.16150400	1.38052200
C	-2.48562900	-1.76392300	2.16839200
C	-3.78522000	-2.11358900	1.79728800
C	-4.00528900	-2.85784600	0.64032400
C	-2.92737500	-3.24876000	-0.15539800
H	6.80070900	0.35921900	1.01227800
H	3.80076300	-0.58144800	-1.68929600
H	2.69372200	0.89979300	2.20387000
H	5.12972400	1.07428100	2.73260400
H	1.46832800	-0.80733900	-0.72429200
H	6.18296500	-0.01908500	-2.29002100
H	7.33583100	-0.37845300	-0.98208300
H	6.22075100	-1.64916900	-1.54557800
H	-0.51590900	-0.45165900	-0.75241200
H	-1.00810400	3.24816600	-0.62041400
H	-5.13919600	2.93830300	-0.48844000
H	-5.02233100	0.42605000	-0.42116800
H	-2.79628700	-0.67501400	-0.40828400
H	-4.19595600	4.90450100	-0.73095000
H	-2.76236000	5.01732700	0.32643800
H	-2.57015600	4.96474300	-1.45308100
H	0.24665900	-3.99945000	-0.19956100
H	0.17885900	-3.75625000	-2.69916600

H	-1.36736400	-2.75836900	-2.56875300
H	-0.39415000	-1.90453600	1.67317500
H	-2.31259800	-1.19982400	3.07885500
H	-4.62348300	-1.82291300	2.42200400
H	-5.01284500	-3.15013800	0.36336000
H	-3.09832700	-3.84037000	-1.05037800
N	1.70514100	0.01612800	-0.17035000
N	-0.47541500	0.53494400	-0.48004400

COM-VII

C	5.97112600	0.82442700	-0.41778200
N	5.50513000	-0.39406400	-0.09842600
C	4.19736700	-0.63449200	0.12817000
C	3.26510300	0.39542600	0.01570900
C	3.74188500	1.67894800	-0.29538800
C	5.09243600	1.89125900	-0.50940900
C	6.43880900	-1.54110700	0.00683600
C	1.10669200	-0.86072200	0.11273200
S	1.62733900	-2.37193100	-0.32733200
C	-1.26170000	-1.48375500	0.29186800
C	-2.38860600	-1.17976800	-0.46254600
N	-3.40889600	-2.05511500	-0.54759200
C	-3.37502400	-3.24217500	0.09008100
C	-2.28658300	-3.58450700	0.86748100
C	-1.21989600	-2.70041900	0.97891400
C	-4.59181200	-1.73963500	-1.38011900
O	0.10467500	2.46925100	0.45971900
C	-0.98910600	3.06352100	-0.26059400
C	-0.33853300	3.77391200	0.85297300
C	-2.31075900	2.39683700	-0.08708100
C	-3.24352300	2.43060100	-1.12597300
C	-4.50553900	1.86446700	-0.95041000
C	-4.83365300	1.24688900	0.25636300
C	-3.89652900	1.19053400	1.28796500
C	-2.63939400	1.76522500	1.11783100
H	7.03626200	0.91524900	-0.59011700
H	3.92673500	-1.64681800	0.38974000
H	3.03698300	2.50187000	-0.37552900
H	5.47405900	2.87378400	-0.75862500
H	1.41288700	1.13964400	0.37915800
H	6.20414900	-2.25746100	-0.78080600
H	7.45790800	-1.17938100	-0.10938400
H	6.32037200	-2.00058200	0.98775600
H	-0.47203300	0.42548800	0.49267000
H	-2.49543600	-0.24366400	-1.00321500
H	-4.23697300	-3.88605000	-0.04447200
H	-2.28243200	-4.53524000	1.38638300
H	-0.36310800	-2.94328200	1.59524300
H	-5.47210500	-1.69475100	-0.73828800
H	-4.43897400	-0.77525600	-1.85879500
H	-4.70746400	-2.52001900	-2.13227900
H	-0.73640700	3.36978700	-1.27371800
H	0.36429500	4.57402800	0.64063300

H	-0.84493700	3.81472200	1.81368100
H	-2.99665400	2.92792800	-2.05994500
H	-5.23960000	1.93014000	-1.74768700
H	-5.82811700	0.83670100	0.40325700
H	-4.15383700	0.72558100	2.23429300
H	-1.91846800	1.74153000	1.93262300
N	1.90005200	0.25322200	0.24104400
N	-0.21321400	-0.55116500	0.35801000

COM-VIII

C	-6.08417700	-0.28755400	0.01870400
N	-5.38359100	0.72622000	0.55301300
C	-4.03689400	0.77088500	0.46800400
C	-3.32719400	-0.21788700	-0.19694100
C	-4.04733800	-1.27206600	-0.78360100
C	-5.42709100	-1.30296500	-0.65782900
C	-6.07856500	1.81986800	1.27053500
C	-1.03045500	-1.10730200	-0.13347400
S	-1.43030100	-2.65745600	0.28949000
C	1.39941900	-1.46256200	-0.17301300
C	2.45947200	-0.98666100	0.58976700
N	3.56998000	-1.72899200	0.75786500
C	3.69434300	-2.94864700	0.19698800
C	2.67874800	-3.46038900	-0.58524600
C	1.52192700	-2.71518900	-0.78325900
C	4.68111300	-1.22409400	1.59546900
O	-0.32847100	2.29473500	-0.44660500
C	0.74332200	3.04588400	0.14980400
C	-0.03714900	3.59595500	-0.97038700
C	2.11015700	2.48897600	-0.05594800
C	3.08914500	2.67507200	0.92304300
C	4.38328500	2.19958400	0.71608200
C	4.69968400	1.52027900	-0.46012400
C	3.71927100	1.31443400	-1.43108900
C	2.42987700	1.79984100	-1.23121700
H	-7.16013200	-0.25577200	0.13858300
H	-3.54979000	1.61286900	0.94759700
H	-3.52502200	-2.04322500	-1.33436100
H	-6.00819400	-2.10338800	-1.09949100
H	-1.57531200	0.86657700	-0.32940700
H	-5.70399900	1.86552500	2.29321300
H	-5.89136600	2.75965400	0.75076900
H	-7.14622300	1.61235800	1.28122300
H	0.40732800	0.33676000	-0.47889700
H	2.44208100	-0.01367400	1.07174100
H	4.61915200	-3.47854400	0.39481400
H	2.80065700	-4.43507600	-1.04157500
H	0.72212000	-3.09259300	-1.40775700
H	4.38505200	-0.27649200	2.03943100
H	4.88925700	-1.95658900	2.37534800
H	5.55902300	-1.07543000	0.96578800
H	0.52191600	3.41324000	1.14996300
H	-0.79931600	4.34448300	-0.77547800

H	0.40621000	3.60259900	-1.96270600
H	2.84896500	3.21896200	1.83249700
H	5.14888000	2.38011200	1.46441300
H	5.71560700	1.17881700	-0.63387200
H	3.96585600	0.80085400	-2.35475000
H	1.67376300	1.65894500	-2.00086500
N	-1.94055800	-0.08547900	-0.29663900
N	0.25712100	-0.65922300	-0.32035800

TS1(IA)Value of imaginary frequency = -479.6 cm⁻¹

C	-5.15910300	0.57468900	-0.40787600
C	-4.55069800	-0.60732700	-0.82782500
C	-3.24653000	-0.61700600	-1.28383700
C	-2.50116600	0.57314400	-1.31517100
C	-3.10586100	1.77049000	-0.93280600
C	-4.42379300	1.74678000	-0.47778300
N	-1.17694400	0.42672400	-1.74413600
C	-0.06381900	1.16902500	-1.46577100
N	1.04273300	0.52950700	-1.98409300
S	-0.02297600	2.59003200	-0.59261900
C	2.37363800	0.60634500	-1.56761600
C	3.02675500	1.73740400	-1.06297900
C	4.34599200	1.62211400	-0.62851800
C	5.04640700	0.42210900	-0.67482400
C	4.39513100	-0.68419000	-1.21109100
C	3.09092600	-0.59587200	-1.66927700
O	0.06591500	-2.06670900	-1.98923500
C	0.49829900	-2.05199400	-0.04443400
C	0.64230200	-3.00548200	-1.15986700
C	-5.02221000	3.03450300	0.01605400
F	-4.67334700	4.07113200	-0.75632000
F	-4.60692100	3.31558400	1.26167600
F	-6.36138300	2.98223100	0.04948200
C	-5.33703300	-1.88262900	-0.73374100
F	-6.43804300	-1.84287700	-1.49627700
F	-5.75477000	-2.10122000	0.52857400
F	-4.62452800	-2.95411500	-1.10602600
C	5.02235900	-2.04396000	-1.15683500
F	6.34746500	-1.99655000	-1.02188100
F	4.73266500	-2.78245700	-2.23207500
F	4.54549000	-2.73579100	-0.08554200
C	5.00294700	2.83954200	-0.03557400
F	4.61953200	3.02732600	1.24149000
F	4.68246600	3.95124700	-0.70417800
F	6.33750100	2.73103700	-0.02989700
C	-0.76486700	-1.83896300	0.67850600
C	-0.99166700	-0.59545700	1.28133400
C	-2.17530100	-0.35317700	1.97256400
C	-3.13043500	-1.35923500	2.08251400
C	-2.90327300	-2.60961800	1.50303300
C	-1.72797100	-2.84989200	0.80401300
H	-6.18063700	0.57877800	-0.04443600

H	-2.77365600	-1.55001500	-1.57930600
H	-2.56101000	2.70264800	-0.97237600
H	-0.96611600	-0.54362400	-2.00422000
H	0.82381100	-0.42157200	-2.31805100
H	2.51353500	2.68716200	-1.00876700
H	6.06569300	0.35364500	-0.31457700
H	2.59961800	-1.46894000	-2.09261800
H	1.13882700	-1.17880800	-0.11969900
H	1.69436600	-3.26298000	-1.38041800
H	0.07812200	-3.94389800	-1.05154500
H	-0.24810000	0.19417600	1.18703600
H	-2.35278100	0.62686200	2.40382400
H	-4.06630400	-1.16940900	2.59861000
H	-3.66135400	-3.38233200	1.57199100
H	-1.56935800	-3.81534100	0.33290900
N	1.72739600	-2.64703500	1.51148800
H	1.34625100	-3.48329400	1.94402300
H	2.60672700	-2.85897500	1.04299900
C	1.83031700	-1.54572400	2.40503200
C	1.00856300	-1.47313500	3.52758200
C	2.64872600	-0.47046800	2.05623900
C	1.01511300	-0.31979200	4.30579300
H	0.34763500	-2.30098100	3.77120900
C	2.64140400	0.68129800	2.83506800
H	3.28544400	-0.53916600	1.17788400
C	1.82401400	0.75977800	3.96106200
H	0.37202200	-0.26325500	5.17775300
H	3.27011500	1.51727400	2.54788900
H	1.81500300	1.66110400	4.56380000

TS1(IB)Value of imaginary frequency = -603.5 cm⁻¹

C	5.43141300	-0.06853100	-0.19810300
C	4.56081400	0.86946400	-0.74701200
C	3.26851100	0.52235100	-1.09629600
C	2.80403000	-0.78338600	-0.88507800
C	3.67024500	-1.74118300	-0.35494000
C	4.96891000	-1.36369600	-0.01836100
N	1.47749800	-1.01103400	-1.27595300
C	0.56761400	-1.93984900	-0.85419500
N	-0.63985100	-1.71283900	-1.48365000
S	0.83523100	-3.13148100	0.27932700
C	-1.91117600	-2.07232200	-1.01333700
C	-2.26599400	-3.32363300	-0.49689200
C	-3.55823800	-3.51101900	-0.01739400
C	-4.50841600	-2.49304100	-0.01858000
C	-4.14964400	-1.26986200	-0.56925100
C	-2.88018400	-1.06859600	-1.08988400
O	-0.44008200	1.07903800	-1.58994400
C	-0.60836600	1.11355800	-0.20380200
C	-1.59765800	2.13395300	-0.55942600
C	5.88293100	-2.38195400	0.60602700
F	5.57553700	-3.62786700	0.22645300
F	5.81448900	-2.34722200	1.94604500
F	7.16412400	-2.15921200	0.27572700
C	5.05349100	2.27394400	-0.94567000
F	4.14084900	3.05582100	-1.53905300
F	6.16154000	2.30269900	-1.69988200
F	5.37522700	2.85459100	0.22520900
C	-5.06613700	-0.08859200	-0.48900000
F	-6.34824600	-0.42764700	-0.36998400
F	-4.94158900	0.72904000	-1.54495900
F	-4.76641800	0.68096100	0.59796400
C	-3.97514100	-4.86463400	0.49173200
F	-2.92724000	-5.64812900	0.76019400
F	-4.73765500	-5.50405600	-0.40801800
F	-4.70636700	-4.75665900	1.61196300
C	0.59031700	1.52517400	0.61489900
C	1.09355500	0.65788700	1.58504200
C	2.26207200	0.97153000	2.27675100
C	2.92849300	2.16319900	2.00948700
C	2.42595700	3.04154600	1.04905600
C	1.26677500	2.72093200	0.35118600
H	6.44823800	0.20068700	0.06643700

H	2.59533000	1.26744900	-1.50904100
H	3.34359800	-2.75973000	-0.20471100
H	1.05164300	-0.18648900	-1.71211300
H	-0.67306200	-0.79004000	-1.93529300
H	-1.54421800	-4.12699400	-0.45559900
H	-5.49656100	-2.65426000	0.39761700
H	-2.60528200	-0.12061300	-1.54308000
H	-1.04910500	0.20096200	0.23561100
H	-2.53543200	1.81802300	-1.00140200
H	-1.22701100	3.10668500	-0.86191400
H	0.59583700	-0.29381600	1.76263800
H	2.66016300	0.27350500	3.00609600
H	3.85102300	2.40119300	2.52854000
H	2.96419400	3.95503100	0.81838500
H	0.91553300	3.37757000	-0.44147000
N	-2.47053700	2.79311500	1.05813700
H	-3.12794800	2.05709100	1.30907400
H	-1.72587500	2.84154400	1.75089800
C	-3.10817000	4.04771100	0.82848100
C	-4.40023600	4.07238500	0.30650500
C	-2.39718600	5.22956000	1.02848200
C	-4.98823900	5.29573600	0.00469000
H	-4.93138100	3.13951100	0.14128000
C	-2.99724100	6.44647600	0.72292300
H	-1.38378700	5.19206200	1.42045800
C	-4.29225200	6.48405600	0.21280400
H	-5.99636200	5.31803300	-0.39536600
H	-2.44886800	7.36821600	0.88597900
H	-4.75683700	7.43522900	-0.02241100

TS1(IIA)Value of imaginary frequency = -497.0 cm⁻¹

C	4.38699100	-0.96576200	-0.72500300
C	3.18709100	-1.36434600	-1.30773100
C	2.00189300	-1.36551600	-0.59361900
C	1.98337100	-0.94016400	0.74568000
C	3.18234600	-0.55701400	1.35166000
C	4.35888300	-0.57440900	0.60411000
N	0.70531700	-0.91185100	1.33609300
C	0.31958000	-0.51719100	2.57127600
N	-1.04062000	-0.56056200	2.78196500
S	1.26850600	0.04512600	3.83731500
C	-2.03348700	-1.06475200	1.90954100
C	-2.00040200	-2.39255800	1.48349700
C	-2.93619000	-2.83828900	0.56165000
C	-3.91106700	-1.98624400	0.05666500
C	-3.95360000	-0.67618400	0.51625300
C	-3.03471100	-0.21326700	1.45122000
O	-0.99755800	-0.98451800	-0.86628100
C	-1.16874500	0.99054900	-1.13815300
C	-1.35178400	-0.23031200	-1.95218700
C	5.60680000	-0.04065800	1.24638500
F	5.70639000	-0.39662900	2.53186100
F	5.62820200	1.30737900	1.21487400
F	6.71458300	-0.45980000	0.61836500
C	3.15241400	-1.66362400	-2.77617600
F	4.27925700	-2.25269200	-3.19767400
F	3.02356300	-0.52541800	-3.49569600
F	2.12455800	-2.44905400	-3.11677300
C	-4.90932600	0.29697200	-0.10212300
F	-6.01432600	-0.28449600	-0.56711600
F	-4.33452200	0.93118400	-1.16395300
F	-5.27141800	1.26919300	0.74645000
C	-2.92568700	-4.27488400	0.11706300
F	-3.78210100	-5.01127400	0.84302100
F	-1.71573300	-4.82758200	0.24716500
F	-3.30038000	-4.39159800	-1.16365800
C	0.17741800	1.50432600	-0.81391500
C	0.41555400	2.04572500	0.45373000
C	1.68192100	2.50196400	0.79988500
C	2.71664900	2.44734300	-0.13324400
C	2.47946200	1.94310300	-1.41049200
C	1.21552700	1.47038800	-1.74962500
H	5.31218000	-0.96456300	-1.28993300

H	1.06272700	-1.64622100	-1.06513100
H	3.20094400	-0.23211900	2.38178400
H	-0.03321600	-0.97841900	0.60977800
H	-1.31892900	-0.15246800	3.66336100
H	-1.22475800	-3.05784900	1.84803300
H	-4.62052600	-2.33861800	-0.68398500
H	-3.05952700	0.81983300	1.78810800
H	-1.90948100	1.08676600	-0.35142100
H	-2.39375900	-0.36408400	-2.29830600
H	-0.68354100	-0.29859300	-2.82992500
H	-0.39186800	2.07570500	1.18341300
H	1.86449900	2.87284700	1.80282000
H	3.71564800	2.76525900	0.14645800
H	3.28679200	1.87637500	-2.13263100
H	1.05604600	1.03056600	-2.73023100
N	-1.93581700	2.55600800	-2.07901100
H	-1.39362600	2.68083700	-2.92969100
H	-2.87722400	2.24337000	-2.30529500
C	-1.91792400	3.70344500	-1.23459900
C	-0.83944200	4.58442100	-1.28954700
C	-2.91778300	3.86177100	-0.27481200
C	-0.77198700	5.63987300	-0.38780300
H	-0.04635900	4.42583500	-2.01550900
C	-2.83794200	4.92286700	0.62187400
H	-3.74855700	3.16288900	-0.23408400
C	-1.76895800	5.81357800	0.56893600
H	0.06951100	6.32301700	-0.42942100
H	-3.61769200	5.05196300	1.36511200
H	-1.71092800	6.63679700	1.27239100

TS1(IIb)Value of imaginary frequency = -620.6 cm⁻¹

C	-5.24683900	0.70689400	0.59548000
C	-4.04410100	1.38636300	0.46269000
C	-2.89238100	0.72968000	0.04949100
C	-2.92752300	-0.63489900	-0.23697100
C	-4.12669000	-1.33756300	-0.09577800
C	-5.26750600	-0.65642000	0.31190300
N	-1.70309200	-1.24176900	-0.58636300
C	-1.52276500	-2.14188200	-1.57170900
N	-0.20383300	-2.53932800	-1.75707100
S	-2.67012700	-2.74857800	-2.62385500
C	0.88953300	-2.53422700	-0.88793500
C	0.76660200	-2.54351100	0.50932400
C	1.90581400	-2.60064900	1.29746500
C	3.18295800	-2.66369400	0.74483900
C	3.29505400	-2.64902600	-0.63946900
C	2.16972900	-2.57679500	-1.45416500
O	0.16188700	0.37954000	0.26804600
C	0.81085900	0.91189600	-0.83543700
C	1.99228600	0.69341900	0.01201900
C	-6.56669500	-1.40663700	0.41056400
F	-6.37695500	-2.68351800	0.77031000
F	-7.21977500	-1.41984300	-0.76005500
F	-7.38912500	-0.84868300	1.31244100
C	-3.95218100	2.86243200	0.72513100
F	-2.89332000	3.16035700	1.50135100
F	-5.04492100	3.33541700	1.33787400
F	-3.79479200	3.55879200	-0.41025500
C	4.65712200	-2.59139000	-1.26324700
F	5.07601300	-1.29816100	-1.38432100
F	4.67993000	-3.10585200	-2.49411100
F	5.57918500	-3.21201200	-0.52756200
C	1.77799600	-2.49740900	2.79283900
F	0.56770800	-2.86639800	3.22137400
F	1.98451800	-1.23560700	3.19609300
F	2.68791100	-3.26246000	3.41267800
C	0.51553100	2.35536800	-1.16014200
C	0.88281100	2.90650400	-2.38938100
C	0.67215600	4.26030800	-2.64474900
C	0.06924300	5.06328600	-1.67953300
C	-0.31763300	4.51172000	-0.45909700
C	-0.08125300	3.16620500	-0.19360100
H	-6.14328600	1.21866000	0.92471100

H	-1.95289300	1.26431000	-0.03950500
H	-4.16670300	-2.40054500	-0.29661700
H	-0.86181900	-0.68837600	-0.22736200
H	-0.09369100	-3.06278100	-2.61523600
H	-0.20995700	-2.50319600	0.97603500
H	4.06116400	-2.71753300	1.37815100
H	2.28182900	-2.56191100	-2.53415900
H	0.78220300	0.28547800	-1.74574100
H	2.35141300	-0.31967300	0.13526900
H	2.10117400	1.37545300	0.84820100
H	1.30520300	2.26672700	-3.16363400
H	0.95694800	4.68188000	-3.60358600
H	-0.11456400	6.11275300	-1.88517400
H	-0.81324600	5.12610000	0.28584600
H	-0.37339100	2.71699800	0.75122500
N	3.58719200	1.36219200	-0.89599800
H	4.07519700	0.57413000	-1.31639700
H	3.18421700	1.95250600	-1.62278300
C	4.41372200	2.11392900	-0.00683300
C	5.55050400	1.53542500	0.55117300
C	4.00707000	3.39631700	0.36153200
C	6.29742000	2.25939700	1.47530600
H	5.84382000	0.53144300	0.25779400
C	4.76421500	4.10905100	1.28418100
H	3.10211500	3.82088900	-0.06970500
C	5.90922400	3.54489300	1.84267700
H	7.18721300	1.81453800	1.90807000
H	4.45430700	5.10841200	1.57058900
H	6.49471700	4.10480100	2.56357400

TS1(III A)Value of imaginary frequency = -490.1 cm⁻¹

C	4.25875300	1.37398000	0.65224300
C	3.10781900	1.25951800	1.41894200
C	1.85868800	1.16905100	0.81892400
C	1.73969700	1.18356600	-0.57092200
C	2.88631700	1.32594100	-1.35723000
C	4.12502500	1.40727100	-0.73283100
N	0.44173900	1.07341500	-1.10194800
C	0.03365300	0.21710500	-2.10082200
N	-1.30539700	0.01939100	-2.18675100
S	1.08078000	-0.60175100	-3.12677900
C	-2.31035400	0.63009400	-1.41164600
C	-2.32307700	1.99950100	-1.14453000
C	-3.33095900	2.53974400	-0.34389500
C	-4.34173700	1.74856300	0.17192600
C	-4.34608400	0.38954500	-0.15074300
C	-3.36136000	-0.17524000	-0.94042600
O	-2.21912600	-2.49841100	-2.39637000
C	-0.72809100	-3.01494500	-1.14250800
C	-1.58899100	-3.68567600	-2.14198700
C	5.36222700	1.42675600	-1.58598000
F	5.16304900	2.06552700	-2.74272900
F	5.75140500	0.17362100	-1.88611100
F	6.39006600	2.01446900	-0.95983900
C	3.18811900	1.20188600	2.91757200
F	2.90332100	2.37980500	3.48438100
F	4.41158300	0.84071400	3.33330000
F	2.31450400	0.30757500	3.41468400
C	-5.44567300	-0.46553800	0.41418400
F	-5.39894000	-0.48391600	1.75996700
F	-5.37557600	-1.73433300	-0.00458200
F	-6.65514300	0.00731800	0.08212900
C	-3.27863000	4.01383900	-0.05759900
F	-3.31521400	4.73345000	-1.18731700
F	-2.13656500	4.34087800	0.57100000
F	-4.29392600	4.41493500	0.71527700
C	-1.27595600	-2.49915300	0.13249600
C	-0.55141000	-1.53442700	0.84304600
C	-1.04542000	-1.02017500	2.03979600
C	-2.27785200	-1.45043600	2.52402700
C	-3.00334500	-2.41288900	1.82241700
C	-2.50267100	-2.94114600	0.63885600
H	5.23630200	1.42701700	1.11736900

H	0.96991700	1.05378000	1.43331800
H	2.80856700	1.35802600	-2.43528400
H	-0.27959200	1.28091600	-0.41865200
H	-1.56868500	-0.91179300	-2.58870300
H	-1.56464400	2.65239000	-1.56631400
H	-5.11599400	2.17733300	0.79824800
H	-3.37120700	-1.22776300	-1.21369700
H	0.03549600	-2.39223200	-1.60275400
H	-1.00256900	-4.11254400	-2.97633700
H	-2.22857500	-4.48758100	-1.72935900
H	0.41075500	-1.19922900	0.45769600
H	-0.46025800	-0.29864000	2.60328700
H	-2.67749200	-1.03638700	3.44403600
H	-3.97489000	-2.73070800	2.18470700
H	-3.09792300	-3.64679500	0.06734800
N	0.64110000	-4.27691700	-0.48529200
H	0.16421300	-4.95326600	0.10567400
H	0.95374000	-4.73369100	-1.33930300
C	1.69959600	-3.59849100	0.19484700
C	1.72495000	-3.56699900	1.58683000
C	2.60906000	-2.85005000	-0.55206600
C	2.67129300	-2.77943500	2.23474100
H	0.98805800	-4.12676600	2.15674600
C	3.55374900	-2.06895800	0.10480700
H	2.55544200	-2.84776000	-1.63722400
C	3.58577800	-2.03142300	1.49827600
H	2.68388900	-2.73908800	3.31864800
H	4.25343900	-1.47812500	-0.47852400
H	4.31467200	-1.41167300	2.01053900

TS1(IIIB)Value of imaginary frequency = -598.7 cm⁻¹

C	5.02118900	-2.85154500	0.66148500
C	4.76690600	-1.71692200	1.41734600
C	3.71665400	-0.86466700	1.09638600
C	2.90311600	-1.13500500	-0.00371500
C	3.16145600	-2.26283800	-0.78906700
C	4.20631800	-3.10706700	-0.43785300
N	1.90396700	-0.19335200	-0.31221300
C	0.61785400	-0.40806500	-0.74136200
N	-0.13935200	0.69934900	-0.88753100
S	-0.01835100	-1.94498700	-1.01874800
C	0.25660600	2.04421700	-0.80240600
C	1.46314000	2.53402600	-1.30984200
C	1.75379200	3.89463000	-1.21165700
C	0.85640500	4.78710700	-0.65008600
C	-0.36404100	4.29351300	-0.18650400
C	-0.67100500	2.94633000	-0.25171300
O	-2.70679700	0.64818300	-0.62628300
C	-2.93248100	-0.36077500	0.29996400
C	-3.42721300	-1.08899400	-0.88036600
C	4.44060500	-4.35220000	-1.24895900
F	4.07947600	-4.18749800	-2.52783800
F	3.73631900	-5.38722900	-0.76937400
F	5.73155800	-4.71340200	-1.23123800
C	5.59347800	-1.41053700	2.63458700
F	5.87390300	-0.10142200	2.71767300
F	6.75297700	-2.07848500	2.62955100
F	4.94644600	-1.73991200	3.76266300
C	-1.33515900	5.26162200	0.43191500
F	-0.91661700	5.66043300	1.64339500
F	-2.55182900	4.72852600	0.58272500
F	-1.46106500	6.36637200	-0.31746400
C	3.08957900	4.36915300	-1.71289300
F	3.36166800	3.87568000	-2.92893600
F	4.07982800	3.96512800	-0.90079000
F	3.15193600	5.70297000	-1.78852000
C	-3.97669400	-0.11197900	1.35566700
C	-4.01428500	-0.90227300	2.50628800
C	-5.06291300	-0.77624800	3.41608700
C	-6.07257600	0.15438400	3.18331900
C	-6.02256200	0.96515700	2.04867200
C	-4.97975700	0.83280400	1.13691500
H	5.84455300	-3.51088800	0.90894600

H	3.53320500	0.01489000	1.70759400
H	2.55632200	-2.47225600	-1.66071700
H	2.07628100	0.72533700	0.07891100
H	-1.21837700	0.57699400	-0.90844700
H	2.16237300	1.87205600	-1.81063400
H	1.08845800	5.84430900	-0.59152900
H	-1.63113600	2.56674000	0.08645800
H	-2.02160000	-0.80085500	0.73778900
H	-2.67284900	-1.45800500	-1.56554900
H	-4.38251400	-0.75372100	-1.26879700
H	-3.20793700	-1.60885800	2.69930200
H	-5.08489100	-1.39341600	4.30871800
H	-6.88749500	0.25971700	3.89217900
H	-6.79978600	1.70353500	1.87796000
H	-4.91724600	1.45200200	0.24671300
N	-4.10883600	-2.82929200	-0.32822000
H	-3.49954800	-3.54941200	-0.70889100
H	-3.98831000	-2.79112600	0.68270000
C	-5.48178900	-3.01050300	-0.68397900
C	-5.81513400	-3.69620100	-1.84939400
C	-6.46925400	-2.41184000	0.09903800
C	-7.15098300	-3.80074800	-2.22338000
H	-5.03520500	-4.14698600	-2.45713300
C	-7.80047000	-2.52616300	-0.28588500
H	-6.19553500	-1.86294500	0.99760400
C	-8.14653800	-3.21863300	-1.44404000
H	-7.41125300	-4.34121000	-3.12724900
H	-8.56990700	-2.06526000	0.32464800
H	-9.18690200	-3.30215000	-1.73864300

TS1(IVA)Value of imaginary frequency = -591.9 cm⁻¹

C	-3.81435400	0.49108000	0.28458100
C	-3.66827400	-0.87045300	0.03313200
C	-2.77206600	-1.63815500	0.76165900
C	-1.99778700	-1.04431400	1.75982300
C	-2.18107700	0.30442000	2.06528500
C	-3.07015800	1.06232400	1.31017400
N	-0.98665100	-1.80712400	2.37303500
C	0.31636900	-1.43666300	2.65976100
N	0.86913100	-0.35285900	2.11592100
S	1.16424600	-2.43818600	3.74519400
C	0.46597100	0.27154100	0.93578000
C	-0.01440500	-0.42173700	-0.18928000
C	-0.41262700	0.28054000	-1.32058500
C	-0.27480300	1.66319200	-1.40505300
C	0.28902700	2.33111800	-0.32452000
C	0.65825700	1.65657700	0.83067300
O	3.25127300	0.34410700	2.33375000
C	3.57511100	-0.61378200	0.71057100
C	4.01778500	-0.82118800	2.09418300
C	-3.17101700	2.54099900	1.57170500
F	-2.22402100	3.22615600	0.90907500
F	-3.01924900	2.82115200	2.87191200
F	-4.35464400	3.03094700	1.18044900
C	-4.44798500	-1.48132200	-1.09778100
F	-4.28979000	-0.77407200	-2.22506600
F	-5.76281600	-1.50560100	-0.83473600
F	-4.06522600	-2.74070700	-1.34889100
C	0.51093600	3.81364800	-0.42367400
F	-0.44404900	4.40541100	-1.15451200
F	1.68469200	4.08935800	-1.02040500
F	0.52994100	4.39975700	0.77767700
C	-0.95526800	-0.46466800	-2.50557800
F	-1.58947100	-1.59418800	-2.14893900
F	0.03047900	-0.82385700	-3.35402500
F	-1.81841200	0.27659700	-3.20827300
C	4.14060400	0.36362200	-0.22495100
C	3.33715500	0.77588200	-1.29564600
C	3.81002600	1.72052400	-2.19860800
C	5.08985400	2.24751500	-2.04204200
C	5.89740000	1.83194000	-0.98335800
C	5.42593800	0.89351300	-0.07439100
H	-4.49119100	1.09561400	-0.30929800

H	-2.60752500	-2.67954800	0.50461000
H	-1.59083600	0.76495900	2.85119500
H	-1.23774800	-2.70534300	2.76268400
H	2.19088000	0.03562000	2.42633000
H	-0.11590200	-1.50284600	-0.15128400
H	-0.61084400	2.20574500	-2.28109100
H	1.06515800	2.19763400	1.67895900
H	2.54586300	-0.90116300	0.53778700
H	3.61631900	-1.71250500	2.58658700
H	5.07514200	-0.66267100	2.31203300
H	2.33649600	0.36168500	-1.40543300
H	3.17458000	2.05491200	-3.01166800
H	5.45876400	2.99016900	-2.74198500
H	6.89087200	2.25035300	-0.86213100
H	6.04709400	0.58892600	0.76197000
N	3.97640000	-2.45902400	-0.35974700
H	4.48087100	-2.24614000	-1.21508700
H	4.55419800	-3.03390400	0.24653900
C	2.69217600	-3.02993200	-0.59063800
C	2.07435600	-2.91415100	-1.83651300
C	2.00616300	-3.59686000	0.48409700
C	0.78826500	-3.41574700	-2.01395600
H	2.59606400	-2.43958500	-2.66375700
C	0.71520700	-4.08239700	0.29906900
H	2.45558000	-3.63541600	1.47318100
C	0.10470100	-4.00361800	-0.95138700
H	0.31161600	-3.32214500	-2.98273500
H	0.19673000	-4.51188000	1.15095300
H	-0.90226000	-4.38055400	-1.09951800

TS1(IVB)Value of imaginary frequency = -602.7 cm⁻¹

C	-4.25683200	0.15356600	-1.47144500
C	-4.44934700	-1.20283800	-1.25573600
C	-3.36796600	-2.07367200	-1.14964900
C	-2.07147900	-1.58545400	-1.29125100
C	-1.86949300	-0.23556600	-1.59551600
C	-2.95548500	0.62363100	-1.64000500
N	-0.98162600	-2.44500400	-1.03885100
C	0.23675800	-2.14336700	-0.46774900
N	0.35282400	-1.09103600	0.36096700
S	1.54023500	-3.15664500	-0.84776100
C	-0.68491900	-0.37028900	0.97762000
C	-1.84273900	-0.99312200	1.45323800
C	-2.90809000	-0.21823800	1.88188700
C	-2.82058600	1.17231700	1.92146900
C	-1.62622100	1.77105400	1.54474800
C	-0.55618700	1.01569800	1.07348300
O	2.53736400	0.18467700	0.74618100
C	3.30229800	-0.05871600	-0.38882700
C	3.96284700	-1.03763800	0.49047200
C	-2.74371800	2.10349700	-1.81472500
F	-1.44804200	2.41728500	-1.91232500
F	-3.24986600	2.78361000	-0.77197100
F	-3.36123300	2.56383600	-2.91114600
C	-5.83895900	-1.75444800	-1.08709400
F	-6.24645200	-2.38635100	-2.19910900
F	-6.72809300	-0.79097300	-0.82555600
F	-5.89183500	-2.64763400	-0.09069900
C	-1.47861000	3.26667400	1.60085700
F	-2.66075800	3.87962000	1.74214700
F	-0.90092000	3.74171700	0.48928000
F	-0.70702600	3.64340200	2.63183300
C	-4.20641600	-0.87344200	2.26179900
F	-4.17924000	-2.19699000	2.05429400
F	-5.22516200	-0.37474100	1.53902400
F	-4.51367900	-0.67001000	3.54929500
C	4.20345200	1.04851000	-0.86512300
C	4.68527300	1.04978700	-2.17500200
C	5.64021800	1.98359200	-2.57508600
C	6.10879800	2.92779100	-1.66480600
C	5.60804000	2.94583600	-0.36227000
C	4.65830100	2.01149100	0.03656700
H	-5.10013000	0.83499600	-1.48416800

H	-3.53234800	-3.11404500	-0.88474200
H	-0.86329600	0.14823000	-1.71971200
H	-0.98351400	-3.34842700	-1.49328100
H	1.34383100	-0.65926100	0.55678000
H	-1.93188000	-2.07253100	1.41531100
H	-3.66888700	1.77547900	2.22475000
H	0.36433100	1.48486200	0.73533900
H	2.75448300	-0.51765300	-1.22800900
H	3.41032800	-1.94625600	0.70014100
H	4.61550700	-0.62009500	1.24937300
H	4.29979200	0.32407100	-2.88971000
H	6.00986900	1.97960800	-3.59565700
H	6.85030300	3.65779800	-1.97346300
H	5.96119000	3.69278000	0.34188100
H	4.24880500	2.00676900	1.04266200
N	5.41473600	-1.90816800	-0.48103300
H	5.17023400	-2.89066100	-0.58048400
H	5.36583100	-1.45955800	-1.39398200
C	6.68312200	-1.69908900	0.14304400
C	7.19230200	-2.64947600	1.02509200
C	7.35101800	-0.49251400	-0.06733000
C	8.39026900	-2.39693400	1.68626900
H	6.65613800	-3.57980100	1.19187700
C	8.54810000	-0.25443900	0.59849900
H	6.93589700	0.25054700	-0.74452600
C	9.07224900	-1.20211800	1.47468100
H	8.78932400	-3.13921500	2.36945100
H	9.06897900	0.68250400	0.43122500
H	10.00574100	-1.00922900	1.99182900

TS1(VA)Value of imaginary frequency = -529.7 cm⁻¹

C	-5.57160100	-3.77164700	-0.31189800
N	-5.94358100	-2.50162700	-0.08847800
C	-5.05509800	-1.49522700	0.05113900
C	-3.68589800	-1.74714500	-0.04653900
C	-3.28411400	-3.07837800	-0.26654500
C	-4.22370100	-4.08360000	-0.39681400
C	-7.38119600	-2.15624000	0.00242300
C	-2.71655900	0.55396200	-0.03439800
S	-4.06996000	1.45797900	-0.38537100
C	-1.01490700	2.36601300	-0.06415700
C	-1.79138100	3.49081700	0.21463400
N	-1.30197300	4.72827100	0.00097400
C	-0.05486000	4.93994900	-0.45605900
C	0.77337400	3.86043400	-0.70457400
C	0.29855400	2.57280800	-0.51409300
C	-2.19431500	5.87545600	0.28417400
O	-0.09315900	-1.32037900	0.24390200
C	1.74399000	-1.61336500	0.37979900
C	0.63132900	-1.92280100	1.28048700
C	2.36819900	-0.28200200	0.30041900
C	3.02149600	0.08771200	-0.88038700
C	3.69663600	1.30423000	-0.96034800
C	3.73171600	2.15209500	0.14497600
C	3.07954600	1.79091800	1.32560300
C	2.40089500	0.57968100	1.40462600
H	-6.36017500	-4.50540500	-0.41901300
H	-5.46015300	-0.51026900	0.23084600
H	-2.22227800	-3.29624000	-0.34515900
H	-3.92778600	-5.10995100	-0.57547000
H	-1.71446600	-1.21303800	0.17710600
H	-7.56228900	-1.65612200	0.95353200
H	-7.63741700	-1.49851500	-0.82828600
H	-7.96956100	-3.06947800	-0.05052300
H	-0.69687800	0.34565900	0.21112800
H	-2.79858300	3.42788000	0.59955800
H	0.24279700	5.96932400	-0.61058500
H	1.78052000	4.02931300	-1.06528000
H	0.93391400	1.71761000	-0.73293100
H	-3.07425400	5.80216500	-0.35497300
H	-2.48428500	5.84652500	1.33448000
H	-1.66077300	6.79989000	0.07492300
H	1.84515500	-2.26176100	-0.48291700

H	0.43143000	-2.99043400	1.42503100
H	0.61116000	-1.40190700	2.24411800
H	3.02322300	-0.59056000	-1.72872400
H	4.21878100	1.57150900	-1.87298600
H	4.28425000	3.08553000	0.09612700
H	3.11573300	2.44607200	2.18978900
H	1.91513500	0.29980300	2.33495000
N	-2.68106100	-0.80958600	0.09500400
N	-1.44658400	1.06047800	0.12132100
N	3.50016700	-2.60138900	1.20618100
H	3.58889000	-2.31165600	2.17718200
H	3.31023300	-3.60079200	1.18449600
C	4.65880400	-2.26159800	0.44586200
C	5.48755700	-1.22291700	0.86584500
C	4.89026200	-2.90268700	-0.77103600
C	6.55392300	-0.82934600	0.06425500
H	5.29705100	-0.72369700	1.81257400
C	5.96233000	-2.50437900	-1.56367400
H	4.24577600	-3.71874600	-1.08927400
C	6.79361700	-1.46530900	-1.15149800
H	7.20466800	-0.02778900	0.39728700
H	6.15197100	-3.01396600	-2.50227900
H	7.63248300	-1.16321200	-1.76834100

TS1(VB)Value of imaginary frequency = -580.7 cm⁻¹

C	4.04009400	-4.81363000	-0.00236200
N	4.74205800	-3.68698000	0.18882300
C	4.17781000	-2.45983700	0.16404700
C	2.81089300	-2.31954400	-0.08342700
C	2.06206700	-3.49909500	-0.26709700
C	2.67376700	-4.73654000	-0.22677100
C	6.20049100	-3.75641900	0.43963500
C	2.54425900	0.15464000	-0.31052600
S	4.13616300	0.64221900	-0.30092400
C	1.40329900	2.36534400	-0.62451100
C	2.46395600	3.18002000	-1.02016500
N	2.29222700	4.51404800	-1.13827500
C	1.11626300	5.11653500	-0.90171000
C	0.02183700	4.35166000	-0.53384600
C	0.15988900	2.98284900	-0.39610800
C	3.46836200	5.31592000	-1.54694500
O	-0.51453000	-0.98550700	-0.19654500
C	-1.27505400	-0.91462300	0.99570400
C	-2.19549600	-1.55895600	0.06290900
C	-1.55225700	0.47582700	1.49738600
C	-0.63007700	1.05795600	2.37309200
C	-0.80136300	2.36545900	2.81761100
C	-1.90714800	3.10406900	2.39614300
C	-2.83181900	2.53302000	1.52370400
C	-2.65227800	1.22539300	1.07014500
H	4.58709500	-5.74731000	0.02924400
H	4.83250800	-1.61927300	0.34034800
H	0.99532700	-3.41178000	-0.45549500
H	2.10998200	-5.64861800	-0.37867300
H	1.05484000	-1.25227500	-0.15341000
H	6.41309000	-3.29120500	1.40204800
H	6.50843800	-4.79937600	0.45754600
H	6.71964400	-3.22901100	-0.36045200
H	0.54167700	0.51931400	-0.44103700
H	3.44769800	2.79628400	-1.24536500
H	1.08195200	6.19243900	-1.01680200
H	-0.93027900	4.83345200	-0.34815100
H	-0.69346500	2.37685700	-0.10329200
H	3.17373000	6.35931000	-1.63420700
H	4.24540300	5.21068800	-0.78989200
H	3.82535700	4.95117000	-2.50987700
H	-0.89409500	-1.55775500	1.79915000

H	-2.07172500	-2.61519400	-0.13213400
H	-2.69113700	-0.95895800	-0.68928800
H	0.22337600	0.47618900	2.71460900
H	-0.08616200	2.80110100	3.50747600
H	-2.05707000	4.11437600	2.76289400
H	-3.70121600	3.09930800	1.20488200
H	-3.38186000	0.79604300	0.38747100
N	2.10615100	-1.13264700	-0.14268400
N	1.46151700	0.98769100	-0.47730100
N	-4.02556700	-1.88818600	0.97788900
H	-4.03774900	-2.83092200	1.36219400
H	-4.11139000	-1.23368900	1.75351900
C	-5.07100900	-1.70041900	0.01331200
C	-5.24394600	-2.65667500	-0.98660900
C	-5.84877100	-0.54450200	0.02967300
C	-6.21188300	-2.45808900	-1.96487800
H	-4.63660600	-3.55821500	-0.98952000
C	-6.81119300	-0.35216600	-0.95901300
H	-5.72505300	0.18589700	0.82590500
C	-6.99458900	-1.30520600	-1.95624200
H	-6.35700200	-3.20893200	-2.73386100
H	-7.42802500	0.53965500	-0.93839400
H	-7.75097500	-1.15644700	-2.71836500

TS1(VIA)Value of imaginary frequency = -532.1 cm⁻¹

C	-6.09449300	-3.16887400	0.03183900
N	-4.91887000	-3.49051200	-0.53460900
C	-3.86473200	-2.65008600	-0.49344200
C	-3.94602600	-1.42331300	0.15506400
C	-5.16167900	-1.08491600	0.77504800
C	-6.23243500	-1.96142000	0.69621400
C	-4.75590800	-4.79172400	-1.22008400
C	-2.75581600	0.72873000	0.04517300
S	-4.08421400	1.68233000	-0.26272700
C	-0.96623600	2.43380600	-0.13094400
C	-1.67434600	3.60610700	0.13576200
N	-1.14024500	4.80826400	-0.15660800
C	0.09022000	4.94004500	-0.68414300
C	0.85444000	3.81243900	-0.92228100
C	0.33159200	2.55834000	-0.64996500
C	-1.96568000	6.00730700	0.11373600
O	-0.20943000	-1.25316000	0.15387300
C	1.61940000	-1.60086100	0.34716700
C	0.46789100	-1.88013900	1.20726100
C	2.28372100	-0.28859400	0.29136700
C	3.00630200	0.05309700	-0.85742500
C	3.71427400	1.25202600	-0.91315300
C	3.71187000	2.11056500	0.18422800
C	2.99073100	1.77757600	1.33266600
C	2.27987600	0.58376400	1.38775100
H	-6.89375100	-3.89420000	-0.05532800
H	-2.95897700	-2.97662800	-0.99322500
H	-5.25037700	-0.15151900	1.31456400
H	-7.18055200	-1.72402800	1.16313100
H	-1.87606400	-1.12167000	0.15868000
H	-4.30411600	-4.62280400	-2.19695600
H	-4.12134100	-5.43669600	-0.61163900
H	-5.73473900	-5.24875600	-1.34773100
H	-0.74401800	0.39881800	0.18746700
H	-2.66350300	3.60683000	0.57000800
H	0.42624800	5.94636500	-0.89965100
H	1.84906500	3.91812900	-1.33746400
H	0.91695800	1.66537900	-0.85639100
H	-2.86481300	5.96070300	-0.50087100
H	-2.22977900	6.02280300	1.17101900
H	-1.39163600	6.89686800	-0.13536200
H	1.73003900	-2.24950500	-0.51436100

H	0.23457800	-2.94270700	1.33989800
H	0.43381000	-1.36496200	2.17405700
H	3.03497300	-0.63364400	-1.69847600
H	4.28894700	1.49778700	-1.79993700
H	4.28643200	3.03127000	0.15482700
H	2.99738500	2.44145600	2.19082400
H	1.73683400	0.32710000	2.29268900
N	-2.80262300	-0.63747600	0.19477000
N	-1.45470300	1.16106700	0.12637800
N	3.31365400	-2.64060900	1.23515800
H	3.37444500	-2.34787500	2.20742700
H	3.09253900	-3.63347700	1.21108600
C	4.51025600	-2.34241000	0.51744300
C	5.35489600	-1.32695300	0.96170000
C	4.76643300	-2.99919300	-0.68609100
C	6.46250700	-0.97294400	0.19811600
H	5.14451300	-0.81388400	1.89676900
C	5.87871200	-2.63971200	-1.44102100
H	4.10838700	-3.79657500	-1.02333500
C	6.72636400	-1.62410100	-1.00435500
H	7.12539300	-0.18982800	0.55043700
H	6.08678900	-3.16142700	-2.36898700
H	7.59589400	-1.35183600	-1.59191700

TS1(VIB)Value of imaginary frequency = -582.3 cm⁻¹

C	-4.44409200	4.60154500	0.39522800
N	-3.31986900	4.55812600	-0.34441300
C	-2.60437600	3.42292300	-0.46533700
C	-2.98795700	2.25450400	0.18455700
C	-4.14291900	2.29291400	0.98285100
C	-4.87081800	3.47225000	1.06960500
C	-2.85137100	5.78619100	-1.02428700
C	-2.61961200	-0.14132300	-0.21095200
S	-4.22498900	-0.58070700	-0.24114700
C	-1.51126000	-2.34203700	-0.65648600
C	-2.59825000	-3.12990500	-1.03591700
N	-2.44403700	-4.45688200	-1.23125300
C	-1.26269900	-5.07783100	-1.08822600
C	-0.14492800	-4.33975100	-0.73587000
C	-0.26378600	-2.97908700	-0.52075200
C	-3.64518000	-5.22764600	-1.62636700
O	0.44481000	0.93453100	-0.14878300
C	1.21303300	0.80597100	1.03246500
C	2.14002700	1.48079000	0.12783900
C	1.48142400	-0.60730100	1.47317000
C	0.55733500	-1.22112400	2.32464800
C	0.71861800	-2.54922900	2.70755700
C	1.81608400	-3.27720800	2.24796000
C	2.74304300	-2.67434700	1.40002400
C	2.57339200	-1.34574100	1.00812600
H	-4.96604000	5.55021900	0.43213100
H	-1.72462600	3.46074300	-1.09777900
H	-4.45157700	1.41230900	1.52983600
H	-5.76822700	3.52692800	1.67370800
H	-1.13231400	1.28883400	-0.04365800
H	-2.29365000	5.50648000	-1.91607300
H	-3.71666800	6.38028200	-1.31256600
H	-2.21671500	6.35272700	-0.34161400
H	-0.62541800	-0.51292800	-0.38940800
H	-3.58883200	-2.72690500	-1.18529800
H	-1.24340000	-6.14615400	-1.26215100
H	0.81060600	-4.83656000	-0.62131900
H	0.60792000	-2.39556800	-0.23610600
H	-3.37758900	-6.27758200	-1.72223700
H	-4.40805000	-5.10790800	-0.85741800
H	-4.00812500	-4.84886600	-2.58179200
H	0.84383500	1.41640600	1.86650000

H	2.02014800	2.54467100	-0.02305200
H	2.62101500	0.90885600	-0.65506000
H	-0.29056000	-0.64854700	2.69462700
H	0.00137400	-3.01041600	3.37851800
H	1.95753900	-4.30533500	2.56524800
H	3.60604100	-3.23295800	1.05144100
H	3.30338000	-0.89233000	0.34163900
N	-2.17462900	1.13672600	0.02965900
N	-1.55052900	-0.97501900	-0.43026400
N	3.96943200	1.74609800	1.04509500
H	4.00191600	2.67907300	1.45160900
H	4.03482400	1.07167100	1.80560700
C	5.01727700	1.55551100	0.08289500
C	5.20309800	2.51876300	-0.90794000
C	5.78515600	0.39297600	0.09330500
C	6.17400500	2.32034400	-1.88329800
H	4.60269100	3.42491400	-0.90598000
C	6.75049900	0.20079100	-0.89261000
H	5.65065400	-0.34361500	0.88199300
C	6.94672200	1.16071000	-1.88076500
H	6.32904500	3.07607600	-2.64553900
H	7.35954300	-0.69646000	-0.87675000
H	7.70523800	1.01175200	-2.64074600

TS1(VIIA)Value of imaginary frequency = -524.7 cm⁻¹

C	6.45314100	-2.71950500	0.49719000
N	6.46127400	-1.50573800	-0.07631100
C	5.34337400	-0.76763100	-0.23591400
C	4.11281500	-1.24718900	0.21598500
C	4.08948800	-2.52599800	0.80110800
C	5.25486000	-3.25724500	0.93866100
C	7.73613300	-0.92122700	-0.55391000
C	2.64887500	0.76917200	-0.04842600
S	3.79377300	1.96549900	-0.18692900
C	0.67270400	2.21603300	0.04838100
C	-0.36359700	2.36075200	0.96817700
N	-1.04484600	3.51385300	1.06884300
C	-0.75325300	4.57330100	0.28773600
C	0.26187800	4.48487500	-0.64461100
C	0.98198700	3.30298100	-0.77848700
C	-2.10108300	3.65775600	2.09263000
O	0.26594800	-1.38788200	0.44351800
C	-1.49284900	-1.67340900	-0.11899600
C	-0.20785500	-2.09654800	-0.67254800
C	-2.07662000	-0.33931700	-0.35472100
C	-3.06239600	0.12857000	0.52242500
C	-3.69185900	1.34948500	0.28752300
C	-3.33706300	2.11488600	-0.82169500
C	-2.35404900	1.65573200	-1.70047000
C	-1.73296500	0.43206800	-1.47368400
H	7.40449900	-3.22780700	0.58909700
H	5.45716100	0.19565300	-0.71113400
H	3.14515000	-2.92776400	1.15847600
H	5.25018400	-4.23852300	1.39705200
H	2.07547300	-1.14178500	0.32969500
H	7.63300900	-0.66910200	-1.60907400
H	7.95376200	-0.02726000	0.03073400
H	8.53068700	-1.65285400	-0.42614600
H	0.70389400	0.10774900	0.17891400
H	-0.65479400	1.55174400	1.62891900
H	-1.34541900	5.46730700	0.44478100
H	0.48002100	5.34204000	-1.26996100
H	1.76725000	3.21272700	-1.51744700
H	-2.33323300	2.67610500	2.50002100
H	-1.73954000	4.31904400	2.88105000
H	-2.99122300	4.07603500	1.62298500
H	-1.82783700	-2.21438700	0.75897900

H	-0.01541600	-3.17392000	-0.64222100
H	0.07188700	-1.68727300	-1.65081200
H	-3.36627000	-0.48699800	1.36546100
H	-4.48394000	1.68121200	0.95206300
H	-3.84480000	3.05423700	-1.02111000
H	-2.09047900	2.24021600	-2.57606700
H	-0.98374100	0.07862200	-2.17618200
N	2.90764200	-0.57897400	0.09866800
N	1.29561900	0.97439600	-0.01189400
N	-3.03138900	-2.76471000	-1.20793000
H	-3.03800400	-2.45082300	-2.17543700
H	-2.75197200	-3.74299800	-1.18598900
C	-4.28950500	-2.55515400	-0.57068200
C	-5.16660100	-1.58752500	-1.05748800
C	-4.58329500	-3.24798700	0.60452900
C	-6.34701400	-1.32255700	-0.36996400
H	-4.92391600	-1.04307400	-1.96699500
C	-5.76588300	-2.97524000	1.28479400
H	-3.90000800	-4.00857700	0.97485200
C	-6.64876200	-2.01098700	0.80216000
H	-7.03613200	-0.58031400	-0.75854700
H	-6.00211100	-3.52605800	2.18879400
H	-7.57381200	-1.80845200	1.33011300

TS1(VIIB)Value of imaginary frequency = -580.6 cm⁻¹

C	5.27172100	-3.78553800	0.23943900
N	5.67465400	-2.50823200	0.17716600
C	4.81732900	-1.47587700	0.02832500
C	3.44405800	-1.70954800	-0.07452000
C	3.01080500	-3.04891700	-0.00747200
C	3.91895000	-4.07765200	0.14890100
C	7.11811400	-2.18371100	0.25455500
C	2.55656300	0.60271200	-0.43217100
S	3.94981100	1.51261400	-0.42159300
C	1.03906900	2.48037600	-0.87753500
C	0.00977600	3.10158200	-0.18418300
N	-0.31226400	4.38820900	-0.44008700
C	0.35915800	5.11583400	-1.35011900
C	1.39531000	4.54499600	-2.06761600
C	1.73621300	3.21938700	-1.84601700
C	-1.42218800	4.99615900	0.32357800
O	-0.17006500	-1.13894200	-0.21945600
C	-0.94797300	-1.20088500	0.95530700
C	-1.71854900	-2.02466700	0.02410200
C	-1.51899300	0.09930700	1.45966900
C	-0.93563300	0.70728900	2.57502300
C	-1.44348600	1.90158100	3.08453200
C	-2.55335600	2.49478800	2.48460000
C	-3.13212400	1.90572600	1.35948000
C	-2.61123400	0.72063400	0.84265600
H	6.03802300	-4.54068700	0.35829100
H	5.24402300	-0.48420700	-0.00996900
H	1.94775300	-3.25806400	-0.09111100
H	3.59531100	-5.10997300	0.19686700
H	1.48264800	-1.11981900	-0.22197600
H	7.26674800	-1.42882600	1.02582500
H	7.67166100	-3.08462800	0.50941500
H	7.44560400	-1.80528700	-0.71400500
H	0.49908600	0.48818600	-0.51474700
H	-0.56442300	2.59667500	0.58812900
H	0.04097800	6.14217800	-1.48543900
H	1.91575500	5.13976200	-2.80812700
H	2.52464700	2.74717400	-2.41803700
H	-1.50252500	6.04721600	0.05477700
H	-2.34624900	4.47209700	0.07873000
H	-1.21001600	4.89809700	1.38829800
H	-0.46871800	-1.75172300	1.77468600

H	-1.39080400	-3.04149400	-0.14496400
H	-2.29036300	-1.54410900	-0.75795300
H	-0.09041800	0.22984500	3.06425900
H	-0.99389300	2.34910700	3.96481500
H	-2.98072200	3.39960800	2.90641300
H	-4.00800400	2.35348800	0.89892600
H	-3.09102600	0.26854500	-0.02140800
N	2.46380700	-0.75133500	-0.23471400
N	1.30236800	1.13610700	-0.61235600
N	-3.47984400	-2.62891400	0.90134500
H	-3.38744100	-3.59199400	1.21873300
H	-3.62471900	-2.04131800	1.72071000
C	-4.55652900	-2.48742500	-0.03701100
C	-4.66437300	-3.40069000	-1.08455600
C	-5.43510000	-1.41023000	0.05734700
C	-5.66992200	-3.24070200	-2.03193400
H	-3.97725400	-4.24052100	-1.14903000
C	-6.43485700	-1.25614700	-0.90003400
H	-5.35529800	-0.71257700	0.88781300
C	-6.55480000	-2.16823600	-1.94434900
H	-5.76442000	-3.96014600	-2.83792300
H	-7.13125300	-0.42863600	-0.81786600
H	-7.33988100	-2.04998000	-2.68245200

TS1(VIIIA)Value of imaginary frequency = -527.3 cm⁻¹

C	6.69941000	-2.18782400	0.04236000
N	5.65861500	-2.61475800	0.77774200
C	4.45511600	-2.00963400	0.70972800
C	4.23577000	-0.93355100	-0.14179300
C	5.30765900	-0.49327600	-0.93803900
C	6.53878700	-1.12139800	-0.82623400
C	5.81509000	-3.77867500	1.67835600
C	2.65469800	0.96140300	-0.22681300
S	3.78322700	2.17836300	-0.27550800
C	0.66923900	2.36194800	0.00000500
C	-0.32947800	2.45737200	0.96582600
N	-0.99265600	3.60915100	1.16504500
C	-0.72213700	4.71143400	0.43734800
C	0.25085300	4.67137800	-0.54182700
C	0.95430200	3.49445600	-0.77311300
C	-2.00569500	3.70259100	2.23741200
O	0.35142600	-1.27536700	0.17078400
C	-1.40937500	-1.59676300	-0.35542600
C	-0.13003300	-1.84706800	-1.01849700
C	-2.07639800	-0.27980700	-0.36152400
C	-2.97496300	0.01939400	0.66837800
C	-3.69033400	1.21484900	0.65313200
C	-3.51737700	2.11611800	-0.39569900
C	-2.62091000	1.82580700	-1.42609700
C	-1.90502800	0.63294000	-1.41105900
H	7.63490900	-2.71998600	0.16268700
H	3.67796500	-2.40267800	1.35606700
H	5.16391900	0.32079900	-1.63535200
H	7.38244000	-0.80037000	-1.42486700
H	2.17042200	-1.00290900	0.06270100
H	5.34987200	-3.54966900	2.63637000
H	5.34071100	-4.64805800	1.22174200
H	6.87578300	-3.96890300	1.82785600
H	0.73216100	0.23904600	0.00360300
H	-0.60704500	1.61163000	1.58495000
H	-1.29725900	5.59895900	0.67347800
H	0.45174100	5.56274400	-1.12361900
H	1.71041300	3.44217200	-1.54586300
H	-2.17598300	2.71108500	2.65107800
H	-1.63550600	4.37543200	3.01168600
H	-2.93431900	4.08407100	1.81320600
H	-1.66119000	-2.27571400	0.45174000

H	0.13050400	-2.90127800	-1.15774700
H	0.07759200	-1.27837100	-1.93348200
H	-3.14132000	-0.70570000	1.46086200
H	-4.41144800	1.41936200	1.43869200
H	-4.10242300	3.03081200	-0.42969000
H	-2.49771500	2.51941200	-2.25171200
H	-1.22412200	0.40892000	-2.22760500
N	2.95862100	-0.38828600	-0.18675700
N	1.29830000	1.13156200	-0.15761000
N	-2.94788800	-2.59398500	-1.49440700
H	-3.07553200	-2.10784300	-2.37877100
H	-2.60369600	-3.53235100	-1.68600900
C	-4.14518400	-2.61376700	-0.71840200
C	-5.12747800	-1.64635300	-0.92441200
C	-4.27211300	-3.54067600	0.31667600
C	-6.24559300	-1.61711700	-0.09661000
H	-5.01394700	-0.91877200	-1.72469300
C	-5.39405400	-3.50289800	1.13855900
H	-3.50757600	-4.29937700	0.46611100
C	-6.38167100	-2.54100900	0.93637000
H	-7.01612800	-0.87260200	-0.26614200
H	-5.50084300	-4.23469100	1.93190600
H	-7.25899800	-2.52108500	1.57296300

TS1(VIIIB)Value of imaginary frequency = -583.7 cm⁻¹

C	5.47364400	-3.46352900	0.48030700
N	4.49890200	-3.63605700	-0.43190800
C	3.54195900	-2.70520800	-0.61932400
C	3.51017900	-1.53939400	0.13765200
C	4.50440600	-1.35958600	1.11356600
C	5.49102000	-2.32479900	1.26544500
C	4.51641000	-4.83331900	-1.30187800
C	2.61261400	0.71839800	-0.22863400
S	4.01930200	1.55199700	0.06608700
C	1.15801100	2.62017800	-0.87687400
C	-0.14378100	3.06197800	-0.64050100
N	-0.50296400	4.33081100	-0.90692600
C	0.37857400	5.23299400	-1.38137400
C	1.67936600	4.84827700	-1.63751200
C	2.07812200	3.53734000	-1.40782700
C	-1.88709200	4.76541000	-0.62389800
O	-0.12627200	-0.98918800	-0.46963600
C	-0.78276000	-1.04191500	0.77986000
C	-1.62337200	-1.91002400	-0.04199100
C	-1.32336000	0.26641200	1.29482200
C	-0.52189800	1.03765800	2.14258200
C	-0.96476900	2.27252500	2.61191500
C	-2.22692700	2.74164300	2.24852100
C	-3.03224400	1.98174100	1.40032000
C	-2.57765100	0.75505400	0.91537200
H	6.21229600	-4.25197100	0.55941900
H	2.81069700	-2.90399600	-1.39485700
H	4.48927000	-0.48040800	1.74299400
H	6.26989600	-2.20980700	2.00923700
H	1.52065100	-1.03165500	-0.32832700
H	5.05623300	-4.59783400	-2.22001700
H	5.01213400	-5.64560700	-0.77379600
H	3.49134400	-5.12043300	-1.52969300
H	0.61924500	0.62675800	-0.67957100
H	-0.91554800	2.40821400	-0.24482500
H	0.00403900	6.23495900	-1.55218200
H	2.37455800	5.57273500	-2.04365100
H	3.08408800	3.22249300	-1.64586100
H	-2.19472600	5.47648500	-1.38920700
H	-2.53875300	3.89432800	-0.64133200
H	-1.91779200	5.23135900	0.36220600
H	-0.20391600	-1.55473400	1.56001600

H	-1.27808800	-2.91761400	-0.22860800
H	-2.28777000	-1.46174000	-0.76892800
H	0.45300300	0.66195900	2.44570300
H	-0.33851300	2.85467400	3.27984100
H	-2.59226000	3.68341300	2.64638500
H	-4.02376300	2.33310300	1.12962800
H	-3.22195600	0.17438800	0.25998800
N	2.47079800	-0.64464800	-0.09986200
N	1.42204900	1.27853800	-0.62739200
N	-3.24844100	-2.56770100	1.03140800
H	-3.05945400	-3.51220000	1.36192800
H	-3.34712400	-1.96666500	1.84805300
C	-4.42523000	-2.52745200	0.20919900
C	-4.55959800	-3.45783900	-0.82018000
C	-5.38105600	-1.53009600	0.39204500
C	-5.66533200	-3.39465000	-1.66095200
H	-3.81179100	-4.23541200	-0.95304100
C	-6.48090200	-1.47112400	-0.46056500
H	-5.28164400	-0.82239400	1.21192000
C	-6.62559900	-2.40005600	-1.48654100
H	-5.77883600	-4.12798900	-2.45176600
H	-7.23430700	-0.70568500	-0.30943300
H	-7.48867200	-2.35749800	-2.14109700

IM1(IA)

C	-4.83097600	0.55229500	-0.47743300
C	-4.26723900	-0.60501600	-1.00294600
C	-3.02747700	-0.57594000	-1.62707100
C	-2.33199800	0.63316400	-1.75152700
C	-2.89375200	1.80571900	-1.24196200
C	-4.12544200	1.74354400	-0.59743500
N	-1.08465600	0.60764600	-2.40407200
C	0.14119500	0.96131100	-1.83210600
N	1.10869200	0.15888600	-2.27713000
S	0.22794500	2.17785800	-0.64111100
C	2.40251900	0.24295700	-1.80232200
C	3.11343700	1.42125100	-1.48102900
C	4.36076000	1.34241500	-0.87597600
C	4.96467900	0.12317200	-0.56301400
C	4.30123300	-1.03208200	-0.95109700
C	3.06799800	-0.97643100	-1.59384600
O	-0.10180900	-2.27763200	-1.95801400
C	0.24023900	-1.67541300	0.35880600
C	0.35529500	-2.75492500	-0.73427700
C	-4.67285000	2.97916300	0.05563100
F	-4.28254900	4.09715400	-0.56499400
F	-4.25920600	3.07629500	1.33524300
F	-6.01410600	2.97396400	0.08668600
C	-5.02434000	-1.89748200	-0.90132300
F	-5.92488700	-2.02704900	-1.88722100
F	-5.70577500	-1.98268000	0.25589800
F	-4.21422100	-2.96469800	-0.96871900
C	4.82597300	-2.38785900	-0.60196900
F	6.02508700	-2.35888600	-0.02490900
F	4.88138100	-3.21201200	-1.64937000
F	3.98053700	-2.99745100	0.29558300
C	5.02714000	2.61373400	-0.43158300
F	4.61147100	2.97053700	0.80170100
F	4.75737900	3.63755000	-1.24537500
F	6.35928100	2.48119600	-0.36265700
C	-1.09584100	-1.53252500	1.04280600
C	-1.53244600	-0.25453400	1.40893100
C	-2.76018800	-0.08615000	2.04009900
C	-3.56050600	-1.19298900	2.31168900
C	-3.12796300	-2.46857400	1.96004100
C	-1.89920400	-2.63952700	1.32874200
H	-5.79065100	0.52353300	0.02683100
H	-2.56361400	-1.49482100	-1.97596200

H	-2.36602400	2.74484500	-1.34027700
H	-0.97936400	-0.19402300	-3.01544600
H	0.42333800	-1.46130000	-2.19820000
H	2.66881400	2.38706500	-1.67992500
H	5.91937900	0.08283900	-0.05292600
H	2.59255700	-1.88955600	-1.94045600
H	0.54582600	-0.71244300	-0.06061300
H	1.40621300	-3.09204500	-0.78266700
H	-0.23860300	-3.63642700	-0.47705700
H	-0.92278300	0.61144100	1.16056300
H	-3.10531100	0.91475100	2.27891100
H	-4.53312900	-1.06231900	2.77526600
H	-3.76133400	-3.32899600	2.14839000
H	-1.59621200	-3.64204000	1.04020900
N	1.33244200	-1.94942600	1.41077500
H	1.09470900	-2.80685800	1.91878800
H	2.21935000	-2.12803800	0.91529900
C	1.53018500	-0.84652900	2.36404100
C	0.97891500	-0.93558800	3.63324200
C	2.20995600	0.27624700	1.91656400
C	1.13981900	0.14324300	4.49675700
H	0.41728000	-1.81530400	3.93563100
C	2.35849600	1.34878200	2.78990800
H	2.59224100	0.33361800	0.90105100
C	1.82847500	1.27911200	4.07580500
H	0.71713000	0.09691900	5.49413500
H	2.88265400	2.23341200	2.44703400
H	1.94347000	2.11876900	4.75263900

IM2(IA)

C	-4.53170500	-1.35402600	0.45494100
C	-4.01774000	-1.01159700	1.69812700
C	-2.67238100	-1.19623100	1.99543400
C	-1.80405200	-1.74753000	1.04259600
C	-2.32564400	-2.14728900	-0.19416400
C	-3.66908000	-1.92389100	-0.47333200
N	-0.44920800	-1.84935100	1.37491500
C	0.69081800	-1.50090300	0.64005000
N	1.71457600	-1.30817900	1.43060000
S	0.57752800	-1.22668600	-1.07026900
C	3.00565200	-1.07438500	0.95957400
C	3.61013800	-1.79355500	-0.08398400
C	4.92201500	-1.52251000	-0.44640400
C	5.67388400	-0.54361300	0.20044200
C	5.07854400	0.15487700	1.24093000
C	3.77022000	-0.11134300	1.62840000
O	0.59245200	1.18944200	2.19098300
C	-0.22223800	2.35811400	0.28196100
C	1.02349800	1.87607500	1.03133800
C	-4.17406800	-2.29296000	-1.84152700
F	-4.23177700	-3.61875700	-2.01014500
F	-3.36723400	-1.81180100	-2.80270400
F	-5.40084400	-1.80073800	-2.06957700
C	-4.89867600	-0.36825800	2.73124700
F	-5.17773300	-1.20022300	3.74103200
F	-6.06188900	0.04337600	2.21064100
F	-4.30078700	0.71089600	3.27440900
C	5.84572500	1.19539900	2.00394900
F	6.98821300	1.53157500	1.39122400
F	6.16304100	0.77306600	3.23740900
F	5.12302400	2.31833900	2.15794700
C	5.52628700	-2.26483500	-1.60524000
F	5.25759000	-1.65962300	-2.77296800
F	5.05536100	-3.51620700	-1.69543400
F	6.86181000	-2.34013100	-1.50331100
C	0.02055800	2.98769200	-1.06287700
C	-0.59371500	4.20298600	-1.36760400
C	-0.40149100	4.79783400	-2.61050700
C	0.40275700	4.17388900	-3.55960100
C	1.01206200	2.95681100	-3.26402900
C	0.82577200	2.36140700	-2.01979500
H	-5.56712500	-1.15832500	0.20685700
H	-2.28097400	-0.86732300	2.95571800

H	-1.67236400	-2.58827300	-0.93576500
H	-0.24217300	-1.88006100	2.36697100
H	1.04709400	0.32061600	2.21013100
H	3.05147900	-2.56473600	-0.60084300
H	6.69661200	-0.34025900	-0.09295900
H	3.32656400	0.43451900	2.45721000
H	-0.77767500	3.04869400	0.92576800
H	1.61982100	1.22238600	0.38277900
H	1.63199900	2.74999400	1.29061800
H	-1.22813200	4.68312400	-0.62705500
H	-0.88119600	5.74430500	-2.83658500
H	0.55381200	4.63441200	-4.53056000
H	1.63721500	2.46664100	-4.00290900
H	1.29384100	1.40326600	-1.80522200
N	-1.11344000	1.14099400	0.16227300
H	-0.62083400	0.40223300	-0.43165800
H	-1.11998700	0.74160900	1.11314500
C	-2.46972700	1.36640900	-0.31971600
C	-2.79101900	0.99336000	-1.61724000
C	-3.40522200	1.92816000	0.54063400
C	-4.10143300	1.16827200	-2.05439800
H	-2.03824000	0.53834900	-2.25501800
C	-4.70939300	2.10379000	0.09046200
H	-3.13178900	2.18278600	1.56099500
C	-5.05587100	1.72249200	-1.20499400
H	-4.37550400	0.85252800	-3.05491400
H	-5.45522800	2.51679000	0.76083600
H	-6.07660100	1.84812500	-1.55033300

TS2(IA)Value of imaginary frequency = -1167.8 cm⁻¹

C	4.61911600	-1.48466200	-0.35634600
C	4.10170000	-1.05950400	-1.57367200
C	2.73963000	-1.11910500	-1.82866200
C	1.85596300	-1.61120100	-0.85981100
C	2.36831700	-2.07991100	0.35519800
C	3.73694400	-1.99246100	0.58889900
N	0.49260400	-1.58160700	-1.19026000
C	-0.63061200	-1.35233400	-0.42074100
N	-1.60760200	-0.85531900	-1.21351200
S	-0.64482600	-1.50331300	1.26120900
C	-2.96150600	-0.80620900	-0.87805000
C	-3.60811600	-1.74481400	-0.06197300
C	-4.97333100	-1.63575000	0.16582400
C	-5.73522300	-0.61991600	-0.40292900
C	-5.09274100	0.29182900	-1.23041300
C	-3.72869900	0.20285300	-1.47497900
O	-0.51097600	1.26219100	-1.83286600
C	0.18177000	2.57160200	0.03010000
C	-1.02331100	2.12415300	-0.84324200
C	4.25631000	-2.34997500	1.95304600
F	3.54990800	-3.33153700	2.52004200
F	4.18891700	-1.28749800	2.78194600
F	5.53940800	-2.72989700	1.91368800
C	5.02303500	-0.52729800	-2.63574600
F	5.40569200	-1.48809200	-3.48658900
F	6.13585300	0.00001800	-2.10667000
F	4.42839800	0.42987700	-3.36813200
C	-5.88722600	1.35783200	-1.92938700
F	-7.00778000	1.66215200	-1.26061300
F	-6.25501300	0.97276800	-3.16113700
F	-5.17827600	2.48877200	-2.07206600
C	-5.63459200	-2.61113000	1.09973200
F	-5.56841300	-2.19362500	2.37293700
F	-5.05559500	-3.81838500	1.05214900
F	-6.93366300	-2.77030400	0.80630400
C	-0.13344200	3.00254700	1.43468400
C	0.32458800	4.23327300	1.90600500
C	0.04161000	4.63925400	3.20701800
C	-0.69385000	3.81047100	4.04887300
C	-1.14492200	2.57541700	3.58776300
C	-0.87084700	2.17179400	2.28565900
H	5.67939200	-1.40839900	-0.14555400

H	2.35283800	-0.73411700	-2.76882400
H	1.70621500	-2.49067600	1.10433400
H	0.30317700	-1.46331900	-2.17931000
H	-1.12871800	0.18346300	-1.71080600
H	-3.04989600	-2.55443200	0.39110600
H	-6.79925500	-0.54760500	-0.21278700
H	-3.24799600	0.91579000	-2.13920200
H	0.73308100	3.35819300	-0.49339900
H	-1.75503800	1.60610600	-0.20477800
H	-1.50760900	3.00616400	-1.27505600
H	0.90537700	4.87646100	1.25016800
H	0.39882500	5.60003300	3.56263700
H	-0.91500300	4.12448100	5.06380700
H	-1.71722800	1.92455000	4.24041400
H	-1.22719300	1.20273100	1.94017500
N	1.07400500	1.36275900	-0.03942700
H	0.77396600	0.66820700	0.66081500
H	0.61735600	1.03183100	-1.07090900
C	2.49670300	1.60268600	0.04861100
C	3.18534600	1.25314300	1.20224800
C	3.15009800	2.16703800	-1.04455700
C	4.56109200	1.47031300	1.25981500
H	2.66106100	0.79057100	2.03425700
C	4.52030600	2.38501700	-0.97362500
H	2.59205100	2.40026300	-1.94791400
C	5.22645100	2.03605000	0.17730600
H	5.10766800	1.17764100	2.14962800
H	5.04163900	2.79997000	-1.82947900
H	6.29900000	2.19251300	0.22003000

IM3(IA)

C	4.59452300	-1.46050600	-0.43232200
C	4.09862900	-0.83489900	-1.56900700
C	2.74365700	-0.86834900	-1.86655200
C	1.85524900	-1.53673700	-1.02217200
C	2.34157000	-2.20321300	0.10274600
C	3.70250300	-2.14169000	0.38543900
N	0.49114300	-1.51527400	-1.38914500
C	-0.62339700	-1.38152200	-0.61140800
N	-1.69842300	-1.01833400	-1.39339500
S	-0.67359300	-1.57341500	1.04499900
C	-3.03694300	-0.90915400	-0.97498300
C	-3.65747700	-1.88564100	-0.19134800
C	-4.99545700	-1.73509200	0.14252200
C	-5.74249700	-0.64648700	-0.30109900
C	-5.11743100	0.30315000	-1.09560500
C	-3.77310000	0.18293200	-1.43106100
O	-0.35743200	1.40501200	-2.07189200
C	0.36495400	2.52279200	-0.05536100
C	-0.82622200	2.07232300	-0.90859600
C	4.19207800	-2.76406000	1.66321500
F	3.54110900	-3.90060600	1.94049100
F	4.00138300	-1.93974600	2.70765700
F	5.50100900	-3.04067200	1.61249800
C	5.03480500	-0.14391300	-2.52093700
F	5.35112100	-0.94386000	-3.55157100
F	6.17939100	0.21026700	-1.92792500
F	4.48151100	0.96051200	-3.04645800
C	-5.89779500	1.46252800	-1.64941600
F	-6.98609100	1.72360300	-0.91638600
F	-6.30835700	1.22133100	-2.90285100
F	-5.15143500	2.57619000	-1.69113900
C	-5.65059700	-2.74804800	1.04171400
F	-5.59945400	-2.36600200	2.32461800
F	-5.05607400	-3.94485900	0.95874600
F	-6.94419800	-2.90950600	0.72981400
C	-0.07477700	3.14166100	1.25394500
C	0.19668200	4.48053600	1.53263300
C	-0.21458500	5.05167200	2.73428400
C	-0.90059900	4.28420700	3.66997100
C	-1.17272700	2.94421700	3.40121800
C	-0.76322600	2.37576100	2.20017200
H	5.64793200	-1.40619200	-0.18515000
H	2.37556500	-0.33966800	-2.74284500

H	1.67270900	-2.75392400	0.74951200
H	0.33081000	-1.41670300	-2.38474700
H	-1.44166000	-0.33733000	-2.10975800
H	-3.10241700	-2.74998800	0.15048200
H	-6.78855700	-0.54673300	-0.03566500
H	-3.29502700	0.94425100	-2.04250400
H	0.93324900	3.26168900	-0.63017200
H	-1.45981800	1.40199100	-0.30479100
H	-1.43005500	2.93203400	-1.21256800
H	0.73899500	5.07818000	0.80446000
H	0.00534800	6.09431600	2.94013300
H	-1.22140800	4.72625100	4.60777400
H	-1.70703300	2.34083200	4.12794200
H	-0.98337100	1.32741500	2.00171000
N	1.22611400	1.33846500	0.09421500
H	0.79885200	0.67701500	0.74280600
H	0.48925000	1.02473300	-1.76646700
C	2.59051800	1.53423900	0.42213200
C	3.13893200	0.93140800	1.55508700
C	3.42248200	2.25878400	-0.43869900
C	4.50189500	1.04231800	1.81829200
H	2.49749400	0.35594200	2.21849400
C	4.77861700	2.37810100	-0.16248300
H	3.01105500	2.68708300	-1.34861900
C	5.32721700	1.76737900	0.96465800
H	4.91434500	0.55189300	2.69411600
H	5.41560000	2.92671900	-0.84921700
H	6.38912800	1.85268600	1.16918400

IM1(IIb)

C	-5.34392700	0.63924900	0.48408000
C	-4.14671700	1.33501700	0.58105200
C	-2.93914600	0.73728500	0.24215900
C	-2.89512200	-0.58248300	-0.21703800
C	-4.10069200	-1.29137600	-0.31307200
C	-5.29742800	-0.67906900	0.03689600
N	-1.63662000	-1.14880900	-0.47274200
C	-1.41450600	-1.79368900	-1.60056500
N	-0.11162600	-2.32428300	-1.75622400
S	-2.40230600	-2.00727400	-2.96593000
C	0.93181800	-2.46262200	-0.86997800
C	0.76912100	-2.58764300	0.52385000
C	1.88161500	-2.72971500	1.33762500
C	3.18108800	-2.76622600	0.83120800
C	3.33438900	-2.64040600	-0.54404000
C	2.23964500	-2.48556800	-1.38689500
O	0.09234500	0.25462000	0.89748500
C	0.86826900	0.72573800	-0.14879200
C	2.30071000	0.70805300	0.40208600
C	-6.57481600	-1.45541500	-0.11006100
F	-6.41490000	-2.74372800	0.22857600
F	-7.02844100	-1.43820500	-1.37168500
F	-7.55401100	-0.95652400	0.66333000
C	-4.12752900	2.77223200	1.00840900
F	-3.08043900	3.04047100	1.81263000
F	-5.24045900	3.12041200	1.67002500
F	-4.01589400	3.60652700	-0.03953700
C	4.70239600	-2.52000500	-1.13562500
F	5.02542000	-1.18635900	-1.30041400
F	4.79948200	-3.05845500	-2.34892500
F	5.65836600	-3.02844900	-0.36341500
C	1.70544800	-2.70264800	2.83058100
F	0.49160800	-3.10353100	3.21032500
F	1.88401500	-1.45271300	3.29271600
F	2.61063500	-3.47811300	3.44642000
C	0.51430500	2.13434800	-0.59303800
C	0.68269600	2.53311700	-1.92128200
C	0.46341200	3.86061600	-2.29476700
C	0.04863500	4.78549300	-1.34300900
C	-0.16122000	4.38192700	-0.02251100
C	0.08004700	3.06571800	0.35438600
H	-6.28374900	1.10039000	0.76226600
H	-2.01601000	1.29679000	0.34072200

H	-4.09259400	-2.31859500	-0.65841300
H	-0.59477300	-0.36399200	0.45787200
H	0.05002000	-2.61389800	-2.71133100
H	-0.22572200	-2.56002200	0.94969000
H	4.03383000	-2.88283000	1.48972900
H	2.39237900	-2.38573500	-2.45835200
H	0.81253500	0.06451500	-1.03078100
H	2.58562800	-0.29165800	0.73067100
H	2.37756700	1.40640700	1.23713700
H	0.92627400	1.79136000	-2.68263400
H	0.58613500	4.15970400	-3.33055900
H	-0.14348600	5.81330100	-1.63271200
H	-0.52832200	5.09316700	0.71028600
H	-0.10120300	2.72865400	1.37134400
N	3.29348000	1.15850800	-0.65773900
H	3.74153200	0.32971000	-1.06872200
H	2.75271900	1.62713400	-1.39976100
C	4.31317100	2.10693300	-0.18386800
C	5.58322500	1.64595200	0.12382700
C	3.93415900	3.43549500	-0.03147800
C	6.51759700	2.56358300	0.59895900
H	5.83858600	0.59977500	-0.01041600
C	4.88138000	4.33585100	0.44373000
H	2.92157700	3.75491800	-0.27390600
C	6.16791900	3.90111500	0.75821200
H	7.51885800	2.22740600	0.84407000
H	4.61150400	5.37852300	0.56878800
H	6.90011400	4.60934000	1.13026000

IM2(IIb)

C	-5.26540800	-0.35860400	0.77266100
C	-4.40027800	0.70791100	0.58313200
C	-3.12348200	0.51219500	0.06797100
C	-2.67873900	-0.76379900	-0.27621200
C	-3.54945500	-1.84774400	-0.09259400
C	-4.81885500	-1.63372800	0.42552400
N	-1.34598500	-0.90040200	-0.69448700
C	-1.04345900	-1.59652700	-1.77292600
N	0.35004000	-1.69715700	-2.03634800
S	-2.03092700	-2.30616400	-2.94649300
C	1.41361900	-1.73635400	-1.17093300
C	1.29301300	-1.79495200	0.23412300
C	2.43296500	-1.83214900	1.02391000
C	3.72226100	-1.83976300	0.49178400
C	3.83739400	-1.79250600	-0.89297000
C	2.71563600	-1.72245100	-1.71490500
O	0.10390200	1.00610200	0.30002000
C	0.52596900	1.74698500	-0.80961600
C	1.90570800	2.29644100	-0.42755100
C	-5.75908300	-2.79482200	0.58338100
F	-5.10271000	-3.95223000	0.74780000
F	-6.55566000	-2.94047000	-0.48516000
F	-6.56529500	-2.63396200	1.64663000
C	-4.81292900	2.11283900	0.90838800
F	-3.87917400	2.74376500	1.65064100
F	-5.96346100	2.16058500	1.59284500
F	-4.97334400	2.85760300	-0.19645600
C	5.19277500	-1.79416900	-1.54458400
F	5.27694200	-0.81506000	-2.47235100
F	5.44800100	-2.94296800	-2.17244900
F	6.17492700	-1.57970000	-0.66025300
C	2.26292300	-1.67913600	2.50805700
F	1.15943700	-2.26215900	2.96810600
F	2.16142100	-0.35496100	2.80890800
F	3.30718100	-2.14758600	3.19430700
C	-0.38615800	2.90643200	-1.16302600
C	-0.39119200	3.43229200	-2.45388000
C	-1.22068800	4.50447800	-2.76922300
C	-2.05959100	5.04448200	-1.79753800
C	-2.05998600	4.51846100	-0.50787800
C	-1.21181000	3.46326100	-0.18584900
H	-6.25424400	-0.21075600	1.19016200
H	-2.46389400	1.35886400	-0.07884000

H	-3.22581800	-2.84813900	-0.35411200
H	-0.46805000	0.21414300	-0.05902700
H	0.51685800	-2.03852800	-2.97444100
H	0.30953400	-1.79249300	0.68694300
H	4.59655000	-1.85477300	1.13042000
H	2.84225100	-1.66519400	-2.79279300
H	0.63158500	1.09316900	-1.69415800
H	1.80857300	3.06674900	0.34145200
H	2.47916900	2.68542200	-1.27084700
H	0.23623900	2.98595400	-3.22253700
H	-1.22905000	4.90273300	-3.77859800
H	-2.72377000	5.86446000	-2.05012000
H	-2.73434400	4.91224000	0.24507600
H	-1.21683300	3.02992400	0.81008800
N	2.66310200	1.16127800	0.19987000
H	1.98169600	0.75179300	0.86916000
H	2.80802400	0.42186500	-0.50323300
C	3.93802000	1.51031400	0.82263200
C	3.93928000	2.00790100	2.11839500
C	5.10389800	1.35073800	0.08661100
C	5.15843600	2.35332700	2.69280100
H	3.01000200	2.10314500	2.67187700
C	6.31620500	1.69280600	0.67717000
H	5.07030900	0.95308200	-0.92405600
C	6.34227500	2.19558100	1.97541300
H	5.18178700	2.73726600	3.70654200
H	7.23763800	1.55908400	0.12143800
H	7.28932700	2.45961200	2.43335500

TS2(IIb)Value of imaginary frequency = -96.6 cm⁻¹

C	-4.98539700	-0.47338500	0.82852000
C	-4.16059700	0.61441700	0.58464100
C	-2.93329600	0.45699500	-0.04843100
C	-2.49307500	-0.80479700	-0.45121100
C	-3.32064700	-1.91095000	-0.20890300
C	-4.54533800	-1.73157900	0.41966400
N	-1.19844700	-0.89566900	-0.97970200
C	-0.89816200	-1.66705800	-2.01472800
N	0.48539100	-1.69848700	-2.31038900
S	-1.89287100	-2.51358800	-3.07664500
C	1.55961200	-1.68924300	-1.44442300
C	1.44916200	-1.83288000	-0.04586300
C	2.59031100	-1.81520400	0.74593700
C	3.86742900	-1.67216600	0.20687400
C	3.96764500	-1.52698900	-1.17190500
C	2.84475400	-1.52854900	-1.99131900
O	0.28619900	0.96177300	-0.18059000
C	0.62499300	1.88748000	-1.17386300
C	1.98681100	2.45913600	-0.70656900
C	-5.44239300	-2.91889500	0.62887400
F	-4.74255600	-4.04971700	0.79817900
F	-6.25979500	-3.11416500	-0.41566600
F	-6.22432800	-2.76230500	1.70996000
C	-4.56022300	2.00196100	0.99138300
F	-3.60482400	2.58887300	1.74312400
F	-5.69240500	2.01888200	1.70614400
F	-4.74208900	2.80359100	-0.06930900
C	5.28371500	-1.12650900	-1.76623000
F	5.36068600	0.23840500	-1.79147200
F	5.43690000	-1.53307400	-3.02569500
F	6.32571300	-1.54952500	-1.05196600
C	2.43558500	-1.94822300	2.23868400
F	2.29131400	-3.22306000	2.61367300
F	1.35819400	-1.28003600	2.67556700
F	3.50453300	-1.45614400	2.88340100
C	-0.36291700	3.02419300	-1.33112800
C	-0.51869400	3.66206500	-2.56025300
C	-1.41291400	4.72140300	-2.69159300
C	-2.16565600	5.13746500	-1.59708700
C	-2.01557000	4.49996500	-0.36727400
C	-1.10551700	3.45682500	-0.23089800
H	-5.93795900	-0.35278400	1.32996800

H	-2.30873400	1.32138100	-0.24098400
H	-3.00083200	-2.90141600	-0.50889600
H	-0.35659000	0.14014200	-0.55985600
H	0.65893600	-2.07058400	-3.23529800
H	0.46977000	-1.92618500	0.40812100
H	4.74298200	-1.63491400	0.84350000
H	2.95747800	-1.38946700	-3.06266700
H	0.75728600	1.38551200	-2.14841600
H	1.82373900	3.16496100	0.10977200
H	2.56859200	2.93415900	-1.49709600
H	0.04513900	3.31669100	-3.42389900
H	-1.53696600	5.20646500	-3.65436100
H	-2.88057700	5.94626700	-1.70587100
H	-2.62106500	4.79603400	0.48244500
H	-0.99912100	2.93887700	0.71825500
N	2.72897300	1.28376900	-0.13259400
H	1.88794900	0.63329100	0.00693900
H	3.37968600	0.87042000	-0.80648600
C	3.37643500	1.46795700	1.16461100
C	2.55226200	1.56016400	2.27946300
C	4.76017800	1.49477000	1.25518900
C	3.14512600	1.69143500	3.53053200
H	1.47339000	1.50075100	2.15802100
C	5.33703800	1.62694500	2.51571000
H	5.37263700	1.39422700	0.36375400
C	4.53274000	1.72718600	3.64792000
H	2.52006600	1.75111500	4.41458800
H	6.41722300	1.64672900	2.61013300
H	4.98942000	1.82513900	4.62676200

IM3(IIb)

C	4.75768100	-0.88749300	0.62825300
C	3.49505300	-1.46492200	0.51266600
C	2.35243000	-0.68831600	0.46250400
C	2.45150700	0.71022700	0.50951100
C	3.70383800	1.30409800	0.66111800
C	4.83663100	0.49271400	0.71138100
N	1.22862000	1.40234600	0.42484600
C	0.98076000	2.69954600	0.11139900
N	-0.35607700	3.04173900	0.12554600
S	2.07972800	3.87236000	-0.34324600
C	-1.48301900	2.29128400	0.50219500
C	-1.48917200	1.45754800	1.62614100
C	-2.60750700	0.67603400	1.89344500
C	-3.76283500	0.75799800	1.11938700
C	-3.77288100	1.65796400	0.05898600
C	-2.64380500	2.40272600	-0.26574300
O	-0.78369100	-0.45072300	-0.56698700
C	-0.73177000	-0.35676000	-1.99422700
C	-1.75888600	-1.32373100	-2.58748900
C	6.18046700	1.16257300	0.79140700
F	6.15587100	2.22174800	1.61074900
F	6.57496000	1.60631800	-0.41201900
F	7.12885100	0.32503300	1.23406500
C	3.40006500	-2.96227800	0.45267100
F	2.16181500	-3.38443100	0.16218400
F	3.75172000	-3.52520100	1.61723300
F	4.22748800	-3.46357200	-0.48123900
C	-5.00267400	1.85557600	-0.78604400
F	-4.83220500	1.37985500	-2.03729000
F	-5.28184000	3.15994800	-0.91854600
F	-6.07763400	1.25793200	-0.27064300
C	-2.50909800	-0.33645600	3.00291600
F	-1.90458600	0.17907600	4.08144100
F	-1.77530300	-1.39229600	2.61263300
F	-3.70719400	-0.79214800	3.37761600
C	0.70087500	-0.58826400	-2.40492200
C	1.52986400	0.51284200	-2.62473800
C	2.89035300	0.34128400	-2.86462100
C	3.42741700	-0.94240100	-2.91338600
C	2.60263300	-2.04907500	-2.72193400
C	1.24846800	-1.87265200	-2.45515700
H	5.65140400	-1.50052300	0.65897100
H	1.37961700	-1.15762500	0.35139400

H	3.80562200	2.37749700	0.72771600
H	0.43523000	0.76752200	0.29815000
H	-0.51750300	3.95837700	-0.26985300
H	-0.61566300	1.39333600	2.26644200
H	-4.62229200	0.13038100	1.33422900
H	-2.66079200	3.06668300	-1.12550600
H	-1.02548000	0.66317200	-2.29155700
H	-1.52503300	-2.35170200	-2.29005100
H	-1.70667200	-1.27815500	-3.67991300
H	1.11704400	1.51860200	-2.57149500
H	3.52694200	1.21025600	-2.99737500
H	4.48890900	-1.08204500	-3.09188700
H	3.02020800	-3.04986800	-2.74726600
H	0.62918200	-2.74178100	-2.25312200
N	-3.09709000	-0.97537100	-2.14673800
H	-1.70790900	-0.31217900	-0.30157300
H	-3.67709000	-0.51309400	-2.82910400
C	-3.80413800	-1.63872000	-1.14756700
C	-3.16884700	-2.36242700	-0.12515700
C	-5.20154700	-1.50569800	-1.10387000
C	-3.91700900	-2.89763800	0.91994100
H	-2.09005000	-2.47453000	-0.12003400
C	-5.93238700	-2.03906500	-0.05157000
H	-5.70805500	-0.95649500	-1.89177800
C	-5.29776500	-2.73497100	0.97646300
H	-3.39921700	-3.42820300	1.71254200
H	-7.00996600	-1.90674400	-0.03787800
H	-5.86841400	-3.14552000	1.80179900

IM1(IIIB)

C	-5.49489600	-0.91268000	-0.49698900
C	-4.95029000	0.12971300	-1.23268700
C	-3.61669200	0.49362800	-1.08353600
C	-2.79988300	-0.18028900	-0.17468800
C	-3.34445200	-1.21663200	0.59180100
C	-4.67328500	-1.57467100	0.41059500
N	-1.48135100	0.27116100	-0.00932300
C	-0.31430000	-0.45571100	0.16515700
N	0.83097700	0.16802900	0.25707400
S	-0.34408400	-2.18644800	0.19495900
C	0.95450100	1.55312500	0.26196500
C	0.44352500	2.37623900	1.27945300
C	0.74856100	3.73333100	1.30655700
C	1.56635400	4.31759800	0.34452400
C	2.05811200	3.50625100	-0.67152300
C	1.74676500	2.15496300	-0.72769900
O	4.21077000	-0.04465400	-1.90177900
C	3.31999100	-1.03306900	-1.43093900
C	3.53636500	-1.18748400	0.07990300
C	-5.22338000	-2.72564900	1.20721300
F	-4.69847200	-2.76726100	2.43996000
F	-4.95290000	-3.90211300	0.62512300
F	-6.55573700	-2.64508000	1.33499800
C	-5.77643600	0.86064300	-2.25290900
F	-5.60683600	2.18866700	-2.15909700
F	-7.08331500	0.60558100	-2.11688200
F	-5.42772600	0.51456800	-3.50120700
C	2.95085300	4.05983800	-1.74509900
F	2.33224300	4.11026100	-2.93090300
F	4.03516500	3.27412100	-1.91059000
F	3.38535200	5.29054000	-1.45916900
C	0.16931200	4.56571300	2.41773000
F	0.41530300	4.01585300	3.61638900
F	-1.16263600	4.66771100	2.30413300
F	0.67007800	5.80693900	2.42995200
C	3.61408800	-2.33315400	-2.14310400
C	2.58569000	-3.25175300	-2.37160200
C	2.86803700	-4.48586100	-2.95530200
C	4.17318300	-4.80181800	-3.32114500
C	5.19821800	-3.88286100	-3.10121800
C	4.92281100	-2.65459000	-2.50956400
H	-6.53490500	-1.19172300	-0.61403400
H	-3.21066700	1.30535800	-1.68098400

H	-2.73407000	-1.73103600	1.32275700
H	-1.33571800	1.24192800	-0.25789900
H	4.01182500	0.80218700	-1.48209500
H	-0.16947600	1.93821800	2.06268800
H	1.82013600	5.36907200	0.39256300
H	2.11107300	1.54201800	-1.54839500
H	2.26758300	-0.75818800	-1.59160100
H	3.24487700	-0.27588000	0.60454200
H	4.58476400	-1.42831000	0.28161000
H	1.56199900	-2.99379700	-2.10066600
H	2.06419000	-5.19248400	-3.13425300
H	4.39070400	-5.75894100	-3.78410300
H	6.21494700	-4.12372300	-3.39516100
H	5.70930400	-1.92440200	-2.34829700
N	2.69396100	-2.28451200	0.64145400
H	1.62073600	-2.14035400	0.42301800
H	2.93449200	-3.15603000	0.15597700
C	2.84637600	-2.45065300	2.08324300
C	2.12577100	-1.60398500	2.91682400
C	3.70544900	-3.42158200	2.57896000
C	2.27935300	-1.74247900	4.29235300
H	1.45999200	-0.86504500	2.47770400
C	3.84650700	-3.55032400	3.95771400
H	4.25649900	-4.06815500	1.90091900
C	3.13562700	-2.71161100	4.81149700
H	1.72108800	-1.09542500	4.96012100
H	4.51209700	-4.30547300	4.36120200
H	3.24692900	-2.81534600	5.88558400

TS2(IIIB)Value of imaginary frequency = -677.5 cm⁻¹

C	-5.39186000	-0.81070100	-0.59920400
C	-4.80879100	0.13610600	-1.42822500
C	-3.48142100	0.51780900	-1.26040300
C	-2.72005800	-0.03769200	-0.23370500
C	-3.30514900	-0.97209300	0.62735200
C	-4.62182500	-1.35873600	0.42306800
N	-1.40398800	0.42161600	-0.04147600
C	-0.25817500	-0.31194300	0.19256900
N	0.89418300	0.25063600	0.35502200
S	-0.36621500	-2.06173200	0.18740900
C	1.05539700	1.63777300	0.35520300
C	0.52529700	2.46665600	1.35427900
C	0.83534400	3.82294600	1.37500900
C	1.67434900	4.39124800	0.42287900
C	2.19169900	3.56721400	-0.57046400
C	1.88357900	2.21412100	-0.61763300
O	4.17570900	-0.15675400	-1.67717600
C	3.27302000	-1.17530300	-1.29002300
C	3.46177900	-1.46365000	0.20306000
C	-5.22530900	-2.40979800	1.31463300
F	-4.68241000	-2.39219400	2.53896600
F	-5.03904500	-3.63936800	0.81608100
F	-6.54719200	-2.23548600	1.45012800
C	-5.58807000	0.75433300	-2.55595200
F	-5.46530800	2.09020900	-2.55344000
F	-6.89154500	0.46357600	-2.48078300
F	-5.14591700	0.32732400	-3.74747100
C	3.10642900	4.11606200	-1.62994000
F	2.50105000	4.17159800	-2.82316700
F	4.18732900	3.33100200	-1.77829100
F	3.53503900	5.34803400	-1.33485600
C	0.23108500	4.67006200	2.46149100
F	0.44398200	4.13362700	3.67173300
F	-1.09774000	4.77319000	2.31145900
F	0.73427000	5.90975500	2.47066300
C	3.55573700	-2.40712100	-2.11740800
C	2.51653000	-3.27633700	-2.45654900
C	2.78345200	-4.45282900	-3.15418900
C	4.08895700	-4.76124200	-3.52486600
C	5.12689900	-3.89127300	-3.19540300
C	4.86398900	-2.72111100	-2.49107600
H	-6.42671200	-1.10247200	-0.73198100

H	-3.03964500	1.24949000	-1.93095600
H	-2.73912100	-1.38052500	1.45589400
H	-1.24011500	1.39238400	-0.27866500
H	4.08024100	0.59413700	-1.07815000
H	-0.10749100	2.03768600	2.12647500
H	1.92817100	5.44319500	0.46192000
H	2.28782400	1.58499600	-1.40725200
H	2.22793400	-0.86806600	-1.44162200
H	3.22390800	-0.56320000	0.77452900
H	4.50421600	-1.75320900	0.38874700
H	1.49360600	-3.02143000	-2.18340100
H	1.96859300	-5.11923100	-3.41822000
H	4.29760800	-5.67290800	-4.07536200
H	6.14475800	-4.12493600	-3.49149000
H	5.66234000	-2.02934900	-2.24246300
N	2.54366200	-2.52700600	0.66213400
H	1.16246600	-2.24800500	0.37708400
H	2.75666700	-3.38272200	0.14584300
C	2.59391500	-2.77984400	2.07821500
C	2.08030000	-1.81277100	2.94199400
C	3.10657900	-3.97477000	2.57338800
C	2.09859300	-2.04614900	4.31209200
H	1.66221900	-0.89975400	2.52419900
C	3.11058400	-4.20338700	3.94677600
H	3.50224300	-4.72027700	1.88858100
C	2.61185100	-3.23932000	4.81743200
H	1.69963900	-1.29762000	4.98861900
H	3.50828700	-5.13559400	4.33393100
H	2.61828400	-3.41854200	5.88721700

IM2(IIIB)

C	-5.42781900	-0.77175300	-0.67525400
C	-4.83002800	0.14097000	-1.53200400
C	-3.50529800	0.52865400	-1.35768200
C	-2.76539700	0.01455900	-0.29493500
C	-3.36555300	-0.88279400	0.59436300
C	-4.67809700	-1.27941000	0.38206700
N	-1.44718900	0.47035000	-0.09486900
C	-0.31581300	-0.27549800	0.15177200
N	0.84821300	0.23577900	0.33638700
S	-0.48111300	-2.03486700	0.12348700
C	1.05760500	1.61887600	0.36117600
C	0.47063800	2.46251800	1.31359000
C	0.81330700	3.81094600	1.35586600
C	1.74327800	4.35110500	0.47541500
C	2.32340400	3.50762000	-0.46634600
C	1.98533800	2.16314600	-0.53710300
O	4.27846000	-0.11892500	-1.53884600
C	3.38506900	-1.16252000	-1.19044600
C	3.53212200	-1.48526000	0.30020600
C	-5.30376500	-2.29231100	1.30293300
F	-4.75120400	-2.26178000	2.52196800
F	-5.15635600	-3.53662300	0.82944800
F	-6.61857300	-2.07574900	1.44145700
C	-5.59084900	0.71564700	-2.69579300
F	-5.47600200	2.05104500	-2.73383600
F	-6.89296600	0.41763400	-2.63562900
F	-5.12068000	0.25174900	-3.86182200
C	3.33750300	4.02942300	-1.44687200
F	2.83102000	4.10366700	-2.68419100
F	4.40365800	3.21396200	-1.50880600
F	3.77563900	5.24875900	-1.11437500
C	0.12992300	4.68111400	2.37505400
F	0.21596700	4.15446800	3.60454900
F	-1.17741300	4.80613300	2.09825700
F	0.65306700	5.91117600	2.41833600
C	3.69902400	-2.36756800	-2.04543700
C	2.67588700	-3.23446400	-2.43398800
C	2.96659500	-4.38933100	-3.15674800
C	4.28293900	-4.67934600	-3.50411000
C	5.30587400	-3.81163800	-3.12672000
C	5.01737500	-2.66236200	-2.39758800
H	-6.46071000	-1.06788000	-0.81458700
H	-3.04982500	1.23176300	-2.04914600

H	-2.81669000	-1.25199100	1.45320600
H	-1.26863300	1.43983900	-0.32759900
H	4.26507100	0.55182900	-0.84525900
H	-0.23423200	2.05524500	2.03323000
H	2.01732000	5.39738500	0.52904600
H	2.44425800	1.51791100	-1.28240700
H	2.33936200	-0.86489400	-1.36017100
H	3.24058400	-0.60044600	0.87449100
H	4.58700700	-1.71543000	0.51230100
H	1.64598600	-2.99506300	-2.17561100
H	2.16336400	-5.05433600	-3.45772300
H	4.51145000	-5.57449600	-4.07356100
H	6.33235800	-4.03062900	-3.40383200
H	5.80412200	-1.97228100	-2.11041900
N	2.64651100	-2.58651500	0.69064400
H	0.88483400	-2.23583200	0.29643400
H	2.92518200	-3.43021700	0.19340800
C	2.54936700	-2.84458000	2.08758400
C	2.03770700	-1.85734800	2.93552000
C	2.89852900	-4.08983600	2.60981800
C	1.90093400	-2.11682300	4.29385800
H	1.72970700	-0.90386900	2.51309900
C	2.74325100	-4.34621700	3.96896800
H	3.29585500	-4.85616400	1.94913700
C	2.25148300	-3.35968400	4.81760000
H	1.50423900	-1.34623900	4.94724000
H	3.01754200	-5.31918400	4.36398300
H	2.13663100	-3.55800700	5.87778900

Cat-I'(syn-anti)

C	-4.39032000	0.61434700	0.37894900
C	-3.40606900	1.59287600	0.38938700
C	-2.09355100	1.29562900	0.03969600
C	-1.74422800	-0.01026800	-0.30196300
C	-2.71812600	-1.01279600	-0.27947100
C	-4.03031200	-0.68467800	0.03477500
N	-0.39815000	-0.30340900	-0.59915500
C	0.10173700	-0.98876000	-1.68520700
N	1.34068000	-1.18876700	-1.92342000
S	-1.09613000	-1.56743000	-2.87159500
C	2.32647400	-0.78354000	-1.01215400
C	2.36413000	-1.24066600	0.31128400
C	3.40837000	-0.86277900	1.15025600
C	4.42835100	-0.03236600	0.70494900
C	4.39059200	0.40973600	-0.61417100
C	3.36281000	0.03853000	-1.47037800
C	-5.08583400	-1.75621800	-0.02728800
F	-4.58609500	-2.95681500	0.29145700
F	-5.60044800	-1.85457500	-1.26009400
F	-6.09902800	-1.49639300	0.80824800
C	-3.73504600	3.01455700	0.75738600
F	-2.95633200	3.44360600	1.76050500
F	-5.00882800	3.14992500	1.13915500
F	-3.52827200	3.84175300	-0.27630100
C	5.45712600	1.33537700	-1.13283100
F	5.00110900	2.59331200	-1.23147300
F	5.86699800	0.97285200	-2.35584300
F	6.52903800	1.35974200	-0.33136100
C	3.39058100	-1.36060000	2.56925800
F	3.21377000	-2.68821100	2.61824400
F	2.37960000	-0.81033100	3.26032700
F	4.52501700	-1.07356400	3.21719700
H	-5.41230900	0.85406800	0.64685100
H	-1.34223300	2.08036600	0.02940300
H	-2.45122300	-2.04293700	-0.48798700
H	0.29916600	0.22447600	-0.08751000
H	1.58942800	-1.91063300	0.67360500
H	5.24098800	0.25118000	1.36204100
H	3.35359600	0.36844100	-2.50397900
H	-0.12591400	-2.04284400	-3.66428600

TS3(IIIB)Value of imaginary frequency = -889.1 cm⁻¹

C	4.40682500	-0.80477900	-0.04870100
C	3.44078700	-1.57029500	-0.68261400
C	2.13034200	-1.11480400	-0.80226400
C	1.77402800	0.11922200	-0.26685200
C	2.73268800	0.89203900	0.39523800
C	4.03658900	0.42888900	0.48231000
N	0.42227400	0.52247600	-0.33551200
C	-0.08098100	1.72637200	-0.75332400
N	-1.37435000	1.94457100	-0.77503500
S	1.03103600	2.95074100	-1.32119600
C	-2.30473000	1.02511200	-0.26109600
C	-2.23490800	0.54336300	1.05192400
C	-3.21993200	-0.31167200	1.53609500
C	-4.29290000	-0.69793900	0.74389000
C	-4.36667000	-0.20307500	-0.55492700
C	-3.39221900	0.64824900	-1.05870900
C	5.08757600	1.27700400	1.14573500
F	4.54780700	2.18110500	1.97258000
F	5.81587300	1.94470800	0.24145200
F	5.93934900	0.52586900	1.85757700
C	3.79324000	-2.89864800	-1.29382000
F	2.91299100	-3.84517600	-0.93686300
F	5.01078000	-3.30993100	-0.92283300
F	3.77597000	-2.83768500	-2.63242200
C	-5.49102600	-0.63359400	-1.45749700
F	-5.10924100	-1.63390800	-2.26466800
F	-5.89954900	0.37116800	-2.24375700
F	-6.54792400	-1.06572800	-0.75946000
C	-3.08264800	-0.81821700	2.94584300
F	-2.89253500	0.19125200	3.80724800
F	-2.02292800	-1.63249300	3.06309800
F	-4.16236500	-1.49906500	3.34352700
H	5.42423100	-1.16582800	0.04680800
H	1.38877100	-1.72118500	-1.31440200
H	2.45670800	1.83885900	0.84332200
H	-0.25856500	-0.22249500	-0.24926200
H	-1.41973900	0.85470300	1.69890300
H	-5.06081800	-1.35603100	1.13169000
H	-3.46641300	1.03498800	-2.07010200
H	-0.21032900	3.89117700	-1.68349200
O	-1.41507900	4.24494500	-1.80136200
H	-1.60855700	4.93304500	-1.15037600

H	-1.68711500	3.31758400	-1.38591800
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TS3'(III B)

Value of imaginary frequency = -1596.5 cm⁻¹

C	-4.53645200	0.60384100	-0.21043700
C	-3.53924200	1.40045600	-0.75326000
C	-2.20951500	0.99371100	-0.73984000
C	-1.86514800	-0.22676400	-0.16474700
C	-2.85236700	-1.03103300	0.40849000
C	-4.17477400	-0.61094600	0.36473900
N	-0.50001400	-0.58466500	-0.13249700
C	0.03632300	-1.81463300	-0.29043000
N	1.33111300	-2.07005300	-0.31932300
S	-0.77592100	-3.32278400	-0.56279600
C	2.36791400	-1.16447300	-0.05999100
C	2.32438000	-0.26599300	1.01183300
C	3.39545100	0.59336300	1.24314300
C	4.52688100	0.56606700	0.44180300
C	4.57388600	-0.35069100	-0.60734900
C	3.51528500	-1.20835300	-0.86326500
C	-5.24767300	-1.50832100	0.92285200
F	-4.78079100	-2.27757900	1.91364200
F	-5.73437300	-2.32283000	-0.02171300
F	-6.27580300	-0.79688100	1.40260600
C	-3.86827300	2.71422400	-1.40855300
F	-3.11347500	3.70404800	-0.91090700
F	-5.15055900	3.05065000	-1.24017700
F	-3.62717600	2.66691200	-2.72613800
C	5.77160600	-0.37314000	-1.51900600
F	5.58989200	0.42662200	-2.57922400
F	6.00709000	-1.60465100	-1.98805900
F	6.87574100	0.04700200	-0.88948800
C	3.29273800	1.54664200	2.40219700
F	3.10942000	0.88944900	3.55532700
F	2.24142500	2.36841000	2.25320600
F	4.38592000	2.30423400	2.52994900
H	-5.57075100	0.92622800	-0.22102600
H	-1.44603100	1.62650300	-1.18411100
H	-2.59329200	-1.96343500	0.89641200
H	0.15998700	0.18448700	-0.17309300
H	1.47220000	-0.26033400	1.68596700
H	5.36001300	1.23027400	0.63781300
H	3.56409200	-1.92156200	-1.67905800
H	0.83890000	-3.35682000	-0.55573500

IM1(VA)

C	-4.99456000	-4.19628900	-0.31022100
N	-5.22345100	-3.14743000	0.49931000
C	-4.39707000	-2.08403800	0.56270900
C	-3.24611100	-2.01235600	-0.23781700
C	-2.98742700	-3.13156400	-1.05645300
C	-3.85483800	-4.20887200	-1.09656500
C	-6.43016100	-3.12398300	1.35356900
C	-2.62963200	0.29595800	-0.03048400
S	-4.11099700	0.98203500	0.39178400
C	-1.29385600	2.43392900	-0.34795100
C	-2.22816500	3.42482600	-0.02304200
N	-1.93448800	4.72837500	-0.20683400
C	-0.75414800	5.15226700	-0.68501000
C	0.21896100	4.21805200	-1.00057100
C	-0.04466900	2.87228800	-0.83498800
C	-2.99393100	5.71021000	0.11643600
O	0.09236700	-1.28747700	-1.19930600
C	2.25518300	-1.37002000	-0.31342900
C	0.84076400	-1.94688200	-0.23233800
C	2.39452800	0.08158400	0.06471700
C	3.22654500	0.91131800	-0.69043000
C	3.46235900	2.22482800	-0.28929500
C	2.87065300	2.71393000	0.87329000
C	2.02446600	1.89688800	1.62274500
C	1.78370800	0.58595700	1.21908800
H	-5.72835500	-4.99181800	-0.30510800
H	-4.67524500	-1.29968100	1.25106900
H	-2.10010000	-3.11477900	-1.68250100
H	-3.66885800	-5.05650000	-1.74455100
H	-0.88427600	-1.28494700	-0.90877500
H	-6.12398500	-3.08286700	2.39883800
H	-7.02269300	-2.24546000	1.09891300
H	-7.01039000	-4.02649700	1.17424800
H	-0.67465000	0.53224800	-0.53478900
H	-3.20886200	3.18727400	0.36474000
H	-0.62277800	6.21990500	-0.80392100
H	1.17479900	4.55454400	-1.38303900
H	0.71389600	2.13443800	-1.08919000
H	-3.35596600	5.51786800	1.12576500
H	-2.57795400	6.71360600	0.05791500
H	-3.80584800	5.59960900	-0.60264400
H	2.63804800	-1.53798200	-1.32402100
H	0.89330800	-3.03391900	-0.42292700

H	0.42544300	-1.81739800	0.78118200
H	3.70659400	0.52168500	-1.58415100
H	4.12210600	2.85591700	-0.87560100
H	3.06908600	3.73029400	1.19816000
H	1.55703700	2.27750000	2.52479700
H	1.11776500	-0.03486400	1.81448600
N	-2.33490500	-0.98561900	-0.26888100
N	-1.47736200	1.07770000	-0.22504000
N	3.17775500	-2.19416800	0.59642200
H	2.94645700	-1.97659100	1.57237800
H	2.97179600	-3.19125600	0.46319800
C	4.62366100	-1.97119400	0.38101200
C	5.28519300	-1.03962200	1.16761100
C	5.25111700	-2.68728100	-0.62890200
C	6.64174100	-0.83030600	0.93453600
H	4.75994000	-0.48421000	1.94039000
C	6.60718800	-2.46457700	-0.84870300
H	4.70512300	-3.41176400	-1.22822400
C	7.29851000	-1.54014600	-0.06813300
H	7.18428000	-0.11440100	1.54148200
H	7.12200500	-3.01882600	-1.62518600
H	8.35636800	-1.37531500	-0.24014700

IM2(VA)

C	-5.99055300	-2.35520700	-0.79225500
N	-5.97274600	-1.14952100	-0.20474700
C	-4.84050000	-0.43201000	-0.03703500
C	-3.60285000	-0.92356400	-0.48005600
C	-3.62578100	-2.19525200	-1.09869300
C	-4.80272000	-2.90164400	-1.25217400
C	-7.23462200	-0.54698300	0.27886500
C	-2.10488800	0.88969100	0.10852800
S	-3.12119700	2.02341500	0.82017600
C	-0.01628100	2.31225100	0.23475200
C	-0.31254400	3.12636400	1.33493100
N	0.39836300	4.24339300	1.57296200
C	1.44231300	4.61458700	0.80889200
C	1.82306300	3.81181300	-0.25065200
C	1.09876400	2.66654100	-0.54267700
C	-0.02108800	5.08928100	2.71347000
O	-0.35614300	-1.70734700	-1.18669900
C	1.66991700	-1.68105900	0.08002400
C	0.24714000	-2.27381800	-0.05031400
C	2.60079100	-2.48044900	0.96246600
C	2.14110100	-2.85569400	2.22934800
C	2.94337400	-3.61509800	3.07262200
C	4.21428900	-4.01306900	2.66210200
C	4.68242500	-3.63727900	1.40898200
C	3.88182400	-2.87050900	0.56403400
H	-6.95051200	-2.84716100	-0.88188700
H	-4.94686300	0.52807000	0.44565000
H	-2.68930900	-2.60687400	-1.46318900
H	-4.81721400	-3.87383100	-1.72924600
H	-1.19675600	-1.16127800	-0.90655100
H	-7.44225200	0.35184100	-0.30196000
H	-8.04222400	-1.26485400	0.15378800
H	-7.12315900	-0.29685900	1.33355300
H	-0.28438200	0.56515800	-0.75530100
H	-1.11706800	2.90532200	2.02021100
H	1.93998300	5.53965900	1.06954600
H	2.67185500	4.09921700	-0.85867600
H	1.38306200	2.05472700	-1.39613300
H	0.71135100	5.88060900	2.85613100
H	-0.99849100	5.51818200	2.49063500
H	-0.07454800	4.47138500	3.60930000
H	1.58323100	-0.64116800	0.41767400
H	0.31613100	-3.36416700	-0.15026900

H	-0.31510000	-2.04574700	0.86247300
H	1.15343400	-2.55358300	2.56586300
H	2.57358800	-3.90134300	4.05118400
H	4.83678600	-4.61083500	3.31857400
H	5.67284300	-3.93524500	1.08314700
H	4.30054500	-2.56972400	-0.39504600
N	-2.36891400	-0.31779800	-0.38982700
N	-0.72423900	1.16742000	-0.06694800
N	2.16619400	-1.57392300	-1.34738000
H	2.69977300	-2.41997500	-1.58236600
H	1.27575100	-1.58677500	-1.89189700
C	2.91060700	-0.35525200	-1.71502800
C	3.78786500	0.23117400	-0.81060500
C	2.68617200	0.17504500	-2.98108500
C	4.46577400	1.38458800	-1.19938300
H	3.95220900	-0.20385100	0.17061300
C	3.36980600	1.33023100	-3.35415200
H	1.99801400	-0.30493200	-3.67224300
C	4.25958400	1.93164400	-2.46490200
H	5.16817400	1.84445400	-0.51259400
H	3.21443700	1.74994700	-4.34193100
H	4.80652200	2.81884600	-2.76673900

TS2(VA)Value of imaginary frequency = -527.1 cm⁻¹

C	5.30420400	-3.35609200	0.93706700
N	5.57504400	-2.25114700	0.22543400
C	4.65094600	-1.29886400	-0.02572500
C	3.34597400	-1.42557800	0.46383500
C	3.05300100	-2.59496100	1.19876900
C	4.02422700	-3.54917500	1.43314600
C	6.93602100	-2.03520400	-0.31512300
C	2.35431600	0.74396800	-0.11992600
S	3.70464000	1.64205800	-0.52271700
C	0.58199700	2.53705800	-0.37306700
C	1.29004700	3.55218200	-1.02515400
N	0.72213400	4.75786900	-1.23343800
C	-0.53176900	5.04907800	-0.85467400
C	-1.29059700	4.07490100	-0.22618400
C	-0.74076100	2.83067000	0.01616200
C	1.54275200	5.78048100	-1.92330300
O	0.02390800	-1.27247100	0.87069400
C	-2.06561600	-1.49526200	-0.23208200
C	-0.60739600	-2.01987400	-0.13064700
C	-3.06543700	-2.45515600	-0.82961900
C	-2.68753900	-3.20590800	-1.94767300
C	-3.58054400	-4.09778800	-2.52992100
C	-4.86003700	-4.25620700	-2.00096700
C	-5.24465900	-3.51226000	-0.89152000
C	-4.35372700	-2.61176100	-0.31125900
H	6.11564800	-4.05558500	1.09127900
H	4.97665700	-0.45197900	-0.61111700
H	2.04653000	-2.72028700	1.58808200
H	3.80696700	-4.44276600	2.00502900
H	1.18945200	-0.97264000	0.60263500
H	7.34262200	-1.11875500	0.11239400
H	7.56398400	-2.88125400	-0.04529600
H	6.87437400	-1.95149000	-1.40005500
H	0.36384400	0.62425800	0.26589200
H	2.30357800	3.42161500	-1.37442600
H	-0.89241100	6.04810600	-1.06308000
H	-2.30475700	4.29958200	0.08068700
H	-1.33319200	2.07451700	0.52685000
H	0.99633500	6.72070000	-1.94153900
H	2.47774100	5.90560700	-1.37783900
H	1.74004500	5.44448600	-2.94146500
H	-2.04596200	-0.54379100	-0.77613600

H	-0.62699500	-3.09328800	0.10876600
H	-0.12403100	-1.90082200	-1.11001000
H	-1.69362100	-3.09568900	-2.37197200
H	-3.27587700	-4.67442600	-3.39648300
H	-5.55357900	-4.95668500	-2.45285600
H	-6.23900700	-3.62690900	-0.47416300
H	-4.69571900	-2.02835700	0.54185800
N	2.30126500	-0.54548500	0.27738700
N	1.05937700	1.27088000	-0.11037600
N	-2.39687500	-1.11462100	1.19204300
H	-2.91606100	-1.87886200	1.63864000
H	-1.39758900	-1.07469600	1.58126200
C	-3.04831800	0.18230900	1.41962100
C	-3.95173500	0.69445700	0.49450900
C	-2.70324000	0.87950900	2.57337700
C	-4.52206900	1.94208700	0.73954200
H	-4.21843200	0.13129200	-0.39500700
C	-3.28220600	2.12438000	2.80679000
H	-1.99560700	0.45791500	3.28218000
C	-4.19029400	2.65441700	1.89092000
H	-5.23981000	2.34648300	0.03409200
H	-3.02929000	2.67293800	3.70733500
H	-4.65318100	3.61671000	2.08367700

IM3(VA)

C	-6.47980700	-2.55736400	-0.66007400
N	-6.46533900	-1.38211700	-0.01282500
C	-5.33587800	-0.66760600	0.17691400
C	-4.11873400	-1.13582300	-0.31682000
C	-4.11920400	-2.37353700	-0.98503400
C	-5.29484800	-3.08031600	-1.15385600
C	-7.72884700	-0.81227200	0.51352800
C	-2.59277400	0.81062300	0.14411800
S	-3.69808900	2.01473000	0.41375600
C	-0.45826200	2.12766500	0.23803100
C	-0.84216800	3.31385800	0.85764700
N	0.00804500	4.36187900	0.88500100
C	1.24047800	4.30926000	0.34887100
C	1.68143200	3.14534600	-0.25862900
C	0.82665500	2.05863500	-0.32137700
C	-0.46617300	5.62119300	1.50499700
O	-0.23502700	-1.47918000	-0.94228900
C	2.02813000	-1.57577800	-0.02705500
C	0.75950100	-2.35412700	-0.38508900
C	3.06759800	-2.52018800	0.55383000
C	2.89328400	-2.99858600	1.85518200
C	3.79617800	-3.90473500	2.40119500
C	4.88602500	-4.33796800	1.64922900
C	5.06998900	-3.85842900	0.35621400
C	4.16397800	-2.95286400	-0.19067800
H	-7.43824300	-3.04924900	-0.76845300
H	-5.43586900	0.26449600	0.71295100
H	-3.18500500	-2.76869300	-1.37533600
H	-5.30815100	-4.03122400	-1.67220600
H	-2.09976500	-1.07052600	-0.46635500
H	-7.96584200	0.09261900	-0.04645100
H	-8.52379500	-1.54472600	0.39308200
H	-7.59634400	-0.58321600	1.57051200
H	-0.68455900	0.13635000	-0.07276900
H	-1.80593300	3.45155500	1.32500400
H	1.84146600	5.20743600	0.42020600
H	2.67975200	3.09120800	-0.68354500
H	1.14874300	1.14353700	-0.81566800
H	-1.10612100	6.14533000	0.79411400
H	-1.02279100	5.38033200	2.40930200
H	0.39473000	6.23539500	1.76013800
H	1.74899500	-0.83661900	0.73969000
H	0.99222700	-3.15053400	-1.10278100

H	0.32773000	-2.81145300	0.50639900
H	2.05008500	-2.65335300	2.45112800
H	3.65418600	-4.26796000	3.41340600
H	5.59429400	-5.04114600	2.07362300
H	5.92428300	-4.18253600	-0.22827000
H	4.33854200	-2.57230200	-1.19317300
N	-2.89366700	-0.49920500	-0.17061400
N	-1.23067600	0.97002400	0.16383200
N	2.41524100	-0.81504400	-1.21073000
H	2.65051100	-1.43026100	-1.98736300
H	0.20352500	-1.04484900	-1.69257000
C	3.40338900	0.20515100	-1.07645900
C	3.97004300	0.55576000	0.15210600
C	3.75737700	0.92356000	-2.22612800
C	4.88342500	1.60869400	0.21848900
H	3.74650400	-0.01047600	1.04946200
C	4.68135400	1.95913300	-2.15209300
H	3.31023700	0.65634500	-3.18017600
C	5.24623500	2.31296000	-0.92521500
H	5.33292400	1.85661700	1.17462800
H	4.96212700	2.49008500	-3.05577100
H	5.97570800	3.11335500	-0.86825200

IM1(VIIB)

C	3.52579000	-4.91493200	-0.47493100
N	4.12917600	-3.93049000	0.22010200
C	3.74934900	-2.64486800	0.11987600
C	2.69835600	-2.25901200	-0.72522100
C	2.07469800	-3.28373000	-1.46201000
C	2.48749200	-4.60082400	-1.33340400
C	5.26863100	-4.24778500	1.10755200
C	2.35619800	-0.02669600	0.01000100
S	2.42709900	-0.23317300	1.68999500
C	2.01446300	2.48783800	-0.04902700
C	1.41761500	3.44639900	-0.87053300
N	1.24400400	4.71528400	-0.46373600
C	1.60899800	5.11912600	0.76562500
C	2.21269300	4.21602700	1.62361000
C	2.43692500	2.90604800	1.22892600
C	0.63674200	5.67228600	-1.41065000
O	-0.24942100	-0.83300000	-1.83911800
C	-0.79668500	-0.58720800	-0.57496200
C	-2.12738900	-1.35374500	-0.59610300
C	-1.06622600	0.88747000	-0.31504100
C	-0.91093000	1.43718600	0.96201100
C	-1.28043100	2.76203100	1.20810500
C	-1.81116700	3.53930400	0.18151000
C	-1.95046600	2.99893500	-1.10013000
C	-1.57623000	1.68046900	-1.34911800
H	3.89987200	-5.91945600	-0.32740500
H	4.30304300	-1.92919100	0.71299200
H	1.26134200	-3.01790500	-2.13064300
H	2.01239400	-5.39502300	-1.89626300
H	0.73495800	-0.82090400	-1.73595700
H	5.09935100	-3.78227500	2.07790300
H	5.33810600	-5.32705700	1.22510500
H	6.18542000	-3.86420400	0.65882000
H	2.07699400	1.15550500	-1.59097100
H	1.05799400	3.21040300	-1.86615300
H	1.42880500	6.15676300	1.01562500
H	2.53094600	4.55491100	2.60211100
H	2.93076300	2.20341300	1.88565000
H	0.39711200	6.59190000	-0.88083900
H	1.34651700	5.88040400	-2.21197000
H	-0.27507600	5.23046100	-1.81344200
H	-0.15460000	-0.98006200	0.23159500
H	-1.97596400	-2.43121200	-0.67640200

H	-2.73413100	-1.01343000	-1.43830800
H	-0.46265300	0.84023000	1.75553900
H	-1.15943900	3.17925400	2.20294800
H	-2.12640100	4.55978000	0.37938200
H	-2.37649200	3.59801100	-1.90029500
H	-1.67575500	1.25133800	-2.34283800
N	2.32744000	-0.95653700	-0.94090100
N	2.17192000	1.22910000	-0.58353300
N	-2.93920800	-1.09762300	0.64912900
H	-2.48616500	-1.54442800	1.45364500
H	-2.91017000	-0.08479100	0.84019600
C	-4.34437700	-1.54680100	0.55609200
C	-4.67146900	-2.82827100	0.97160300
C	-5.27236800	-0.66709800	0.01711300
C	-5.99597300	-3.23944200	0.84646500
H	-3.92199500	-3.49510800	1.38976500
C	-6.59131100	-1.09390800	-0.09996000
H	-4.97676600	0.32951300	-0.30232500
C	-6.94995300	-2.37562000	0.31357300
H	-6.28033800	-4.23425100	1.16989200
H	-7.33717200	-0.42282200	-0.51038600
H	-7.97988600	-2.70223100	0.22280600

IM2(VIIB)

C	-0.84511600	5.87882700	-0.29213400
N	-1.96789400	5.26408600	0.13020200
C	-2.16621000	3.94528900	-0.03044900
C	-1.20510400	3.12863500	-0.64652600
C	-0.04223600	3.77260300	-1.10674600
C	0.13293700	5.13667500	-0.92785600
C	-3.03511300	6.04629800	0.79090000
C	-2.05482100	1.00205100	-0.04665600
S	-2.38532000	1.27366800	1.58841600
C	-2.91405200	-1.38532700	-0.25505700
C	-2.90164900	-2.44638600	-1.16521100
N	-3.43028800	-3.64460800	-0.86675100
C	-3.98695900	-3.89374400	0.33180100
C	-4.04059200	-2.88059500	1.27211700
C	-3.51860100	-1.62637300	0.99643100
C	-3.33449100	-4.71691700	-1.87713300
O	1.06329000	0.61212300	-1.12891200
C	1.03368000	0.10247600	0.18536200
C	2.48594200	0.14925200	0.66342700
C	0.49311800	-1.31871900	0.24980300
C	-0.01646400	-1.81779900	1.45166900
C	-0.42672900	-3.14588000	1.54201000
C	-0.32298600	-3.99061200	0.43680800
C	0.16410400	-3.49229100	-0.77065600
C	0.55984600	-2.15664200	-0.86781800
H	-0.77021300	6.94308100	-0.11266700
H	-3.10661000	3.55330300	0.33272000
H	0.72064200	3.17844300	-1.59934600
H	1.02764800	5.63763000	-1.27678000
H	0.16420600	0.99302800	-1.30892100
H	-3.24019200	5.60536700	1.76628400
H	-2.69875800	7.07337900	0.91392900
H	-3.92964300	6.02286500	0.16835700
H	-2.08413200	-0.17640800	-1.66643200
H	-2.46338600	-2.35343700	-2.15276900
H	-4.38786800	-4.88637900	0.49130500
H	-4.51141000	-3.07595800	2.22812900
H	-3.57480400	-0.82839000	1.72411800
H	-3.95018400	-5.55737500	-1.56428000
H	-3.69334300	-4.33950300	-2.83412700
H	-2.29123000	-5.02752200	-1.95707400
H	0.44650300	0.74359800	0.85844000
H	2.64608000	-0.35950700	1.61537100

H	2.85335400	1.17550200	0.71925200
H	-0.10130500	-1.16109300	2.31470300
H	-0.81570300	-3.52550400	2.48152200
H	-0.60916300	-5.03486800	0.52190900
H	0.25680500	-4.14466500	-1.63485300
H	0.90761500	-1.75304900	-1.81596600
N	-1.39315100	1.79156300	-0.89749800
N	-2.35771200	-0.20434200	-0.69006300
N	3.32832400	-0.54137000	-0.37697400
H	3.00388900	-1.51435900	-0.45837800
H	3.08994500	-0.09048000	-1.27222600
C	4.77906300	-0.50569900	-0.12069000
C	5.32984200	-1.48962900	0.68791600
C	5.52892800	0.52591800	-0.66585500
C	6.69518000	-1.43772600	0.95179000
H	4.71446600	-2.28484900	1.10093800
C	6.89338100	0.56354900	-0.39186900
H	5.06804800	1.28113000	-1.29712300
C	7.47242700	-0.41426000	0.41383900
H	7.14985600	-2.19939900	1.57503500
H	7.50257900	1.35525800	-0.81307400
H	8.53622200	-0.38065400	0.62091400

TS2(VIIB)Value of imaginary frequency = -194.9 cm⁻¹

C	-3.71522200	4.38604200	0.00027500
N	-2.48932300	4.92108000	0.10855400
C	-1.36867700	4.17123800	0.17406300
C	-1.44853000	2.77729500	0.12576600
C	-2.73293400	2.20615300	0.02812500
C	-3.85668500	3.00727200	-0.03565700
C	-2.32464700	6.39228300	0.15842300
C	0.94813600	2.14277500	0.05472200
S	1.68038200	3.57504800	-0.36219300
C	2.99299600	0.72308100	0.07216900
C	3.65129200	-0.13891200	0.94356100
N	4.93157400	-0.49415000	0.73702700
C	5.63424100	-0.01973200	-0.30767100
C	5.03337300	0.84643100	-1.20257100
C	3.70710000	1.21731300	-1.02976500
C	5.59343700	-1.37638500	1.72154800
O	-0.76140300	-0.62915700	0.40819400
C	-0.25778900	-1.25735000	-0.73136800
C	-1.37856900	-2.24117400	-1.19311000
C	1.03597100	-2.01206700	-0.44301700
C	1.98795700	-2.21624000	-1.44601300
C	3.14501100	-2.94636000	-1.18619600
C	3.35801200	-3.49155900	0.08080800
C	2.42097200	-3.28110200	1.09105700
C	1.27156900	-2.53216800	0.83284000
H	-4.55016400	5.07278100	-0.05402500
H	-0.43189900	4.70222600	0.26069300
H	-2.81524800	1.12293100	-0.00038800
H	-4.84795200	2.57956500	-0.12028500
H	-0.65417200	0.84788400	0.31161200
H	-1.71649700	6.70592300	-0.68987600
H	-3.30458700	6.86137500	0.10604800
H	-1.83567000	6.65919000	1.09523000
H	1.11071000	0.22010900	0.74081500
H	3.16470500	-0.55990000	1.81511700
H	6.66281800	-0.34807800	-0.39301400
H	5.60563800	1.21262300	-2.04625600
H	3.22345000	1.87441700	-1.74053300
H	6.38927300	-1.92592700	1.22181700
H	6.00598100	-0.76531300	2.52557600
H	4.85651900	-2.07690700	2.11127300
H	-0.07772300	-0.55019700	-1.55760500

H	-1.02276600	-3.08886000	-1.77947000
H	-2.15875900	-1.70838800	-1.73949800
H	1.81960900	-1.80532400	-2.43922100
H	3.87067900	-3.10859400	-1.97697000
H	4.24139200	-4.09328000	0.27327800
H	2.57382300	-3.71379500	2.07597800
H	0.55433000	-2.33664900	1.62639900
N	-0.38653600	1.90125400	0.19992800
N	1.64913100	0.97696100	0.31511600
N	-1.98684700	-2.67693900	0.10032000
H	-1.47936500	-3.48103600	0.47730800
H	-1.66043400	-1.74174200	0.65413800
C	-3.42762500	-2.92304700	0.10914300
C	-3.95170300	-3.97120800	-0.63802300
C	-4.23506700	-2.09080000	0.87293000
C	-5.32570800	-4.18809800	-0.61442900
H	-3.30084700	-4.61218200	-1.22599600
C	-5.60916700	-2.31793500	0.88885500
H	-3.79305400	-1.29328800	1.46430400
C	-6.15214700	-3.36287500	0.14644500
H	-5.75021600	-5.00495800	-1.18744600
H	-6.25238600	-1.68601600	1.49127200
H	-7.22164800	-3.54079300	0.16517500

IM3(VIIB)

C	5.06534800	2.22935600	-0.31375900
N	4.10826100	3.16545100	-0.44934400
C	2.80016700	2.85003700	-0.51136100
C	2.38961300	1.52288500	-0.40926200
C	3.37474300	0.53233900	-0.28771600
C	4.71278300	0.89370700	-0.24536900
C	4.47446900	4.59830400	-0.53785500
C	-0.05316500	1.82160900	-0.03920600
S	-0.03638400	3.28218300	0.74429400
C	-2.49970100	1.41327300	0.05717400
C	-3.52732500	1.11630700	-0.82862400
N	-4.81492800	1.31953000	-0.49245400
C	-5.15734700	1.82791900	0.70360900
C	-4.17449800	2.14179500	1.62571600
C	-2.83949000	1.92359100	1.31913800
C	-5.85570000	0.99147900	-1.48990100
O	-0.05646200	-1.36117400	-1.27381400
C	-0.48472100	-2.03308100	-0.08563400
C	0.02644100	-3.49233700	-0.15484100
C	-1.98935700	-1.96494700	0.03217500
C	-2.59366400	-1.68260700	1.25731700
C	-3.98304100	-1.65993300	1.37041300
C	-4.77638800	-1.92120300	0.25511000
C	-4.17715100	-2.19826300	-0.97505200
C	-2.78865300	-2.21151600	-1.08809900
H	6.08888300	2.57905600	-0.26442200
H	2.10896800	3.67093100	-0.63855100
H	3.09376800	-0.51681200	-0.21196800
H	5.48049700	0.13755500	-0.13861700
H	0.88438500	0.17014600	-0.78812400
H	4.00562300	5.13142500	0.28918600
H	5.55616300	4.69219100	-0.47409100
H	4.12509300	4.99278900	-1.49199000
H	-1.09535000	0.32494300	-0.98008600
H	-3.34445600	0.70907900	-1.81668100
H	-6.21465300	1.96967100	0.89049600
H	-4.46518200	2.53801700	2.59104400
H	-2.06661300	2.13271700	2.04654100
H	-6.83209700	1.04142600	-1.01238500
H	-5.80476900	1.71147400	-2.30738600
H	-5.67367600	-0.01966300	-1.85415900
H	-0.03713800	-1.52208800	0.77875800
H	-0.64949800	-4.06672300	-0.79367100

H	0.00144300	-3.94430000	0.84464600
H	-1.97595100	-1.48505900	2.13058400
H	-4.44400600	-1.46011400	2.33262400
H	-5.85834200	-1.93746300	0.34964300
H	-4.78993300	-2.43764600	-1.83972700
H	-2.31749400	-2.42702600	-2.04354900
N	1.05291800	1.13542000	-0.47839800
N	-1.19707400	1.11322800	-0.34057300
N	1.33573400	-3.50741000	-0.78665100
H	1.49983000	-4.33255600	-1.35079200
H	0.61845400	-1.96013100	-1.66490200
C	2.48610200	-3.11103100	-0.06198600
C	3.72067900	-3.12842900	-0.72745800
C	2.43433300	-2.66894500	1.26405500
C	4.87982900	-2.73832100	-0.06941700
H	3.76491100	-3.47111600	-1.75767300
C	3.60211500	-2.25943900	1.90996000
H	1.50381100	-2.68050000	1.81983000
C	4.82726900	-2.29369000	1.25403400
H	5.83093800	-2.79590600	-0.58991300
H	3.54879000	-1.93923600	2.94538800
H	5.73494000	-2.00731500	1.77472900