

# Supporting information

## Mechanism and origin of enantioselectivity for organocatalyzed asymmetric heteroannulation of alkynes in construction of axially chiral C2-arylquinoline

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## 1. Mayer bond order

The Mayer bond order are carried out on the optimized complexes, intermediates and transition states of the hydrogen-transfer process (**COM1A** to **IM1A** through **TS1A** and from **COM1B** to **IM1B** through **TS1B**) to verify the transfer process of H3 from O3 to C1 atom.

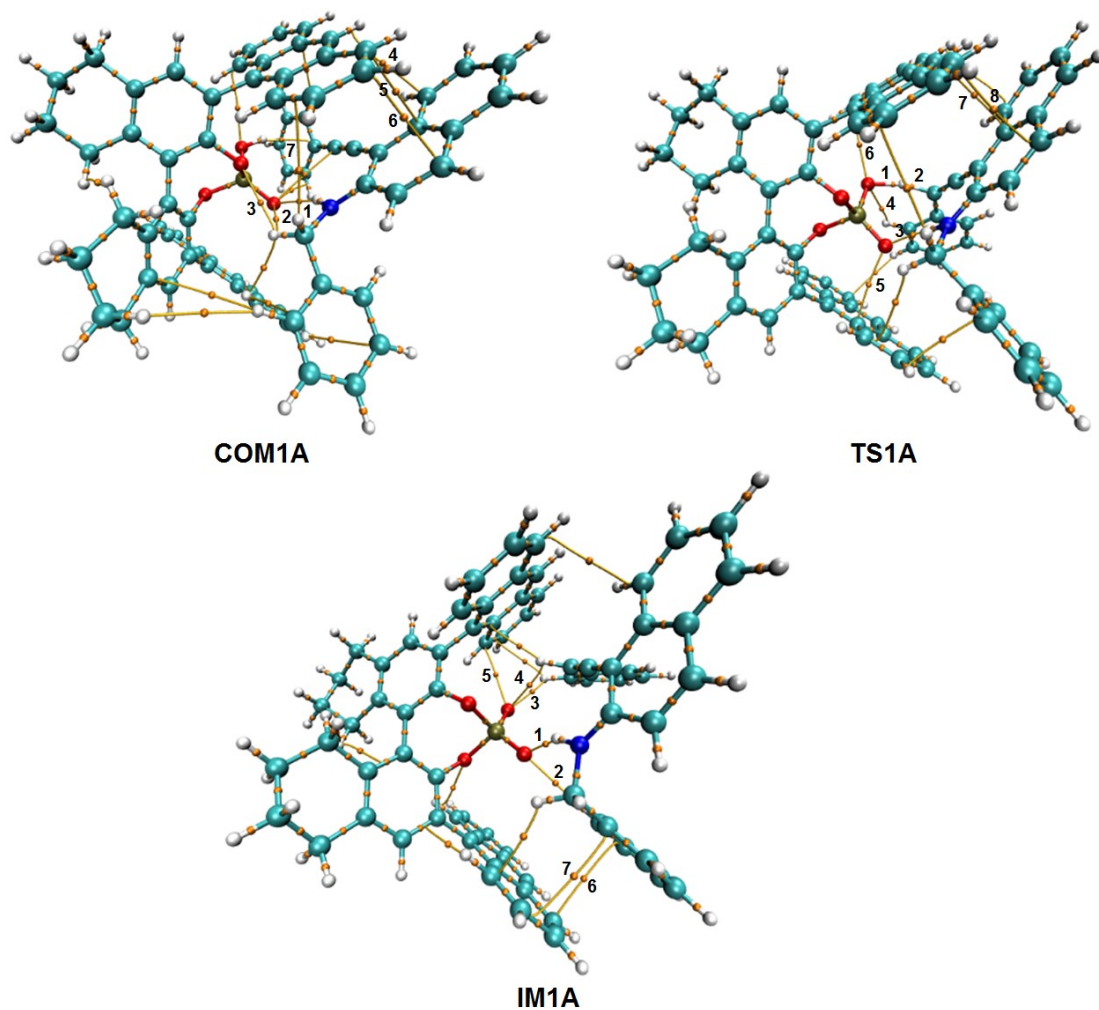
**Table S1** The Mayer bond order for the complexes, transition states and intermediates from the hydrogen-transfer processes.

	<b>COM1A</b>	<b>TS1A</b>	<b>IM1A</b>	<b>COM1B</b>	<b>TS1B</b>	<b>IM1B</b>
<b>O3-H3</b>	0.77	0.31	0.00	0.80	0.35	0.06
<b>C1-H3</b>	0.00	0.48	0.91	0.00	0.42	0.83
<b>C1-C2</b>	2.57	2.28	1.85	2.78	2.32	2.04
<b>C2-C3</b>	1.09	1.36	1.64	1.09	1.43	1.60
<b>C3-C4</b>	1.38	1.18	1.08	1.35	1.15	1.05
<b>C4-N5</b>	1.03	1.33	1.52	1.16	1.33	1.50
<b>N5-H5</b>	0.81	0.83	0.76	0.89	0.83	0.78
<b>O2-H5</b>	0.06	0.09	0.15	0.04	0.12	0.16

## 2. QTAIM Analyses

QTAIM analyses are carried out on the optimized complexes, intermediates and transition states of the hydrogen-transfer process, pathways **I**, **I'**, **II** and **II'** to figure out the intermolecular interactions.

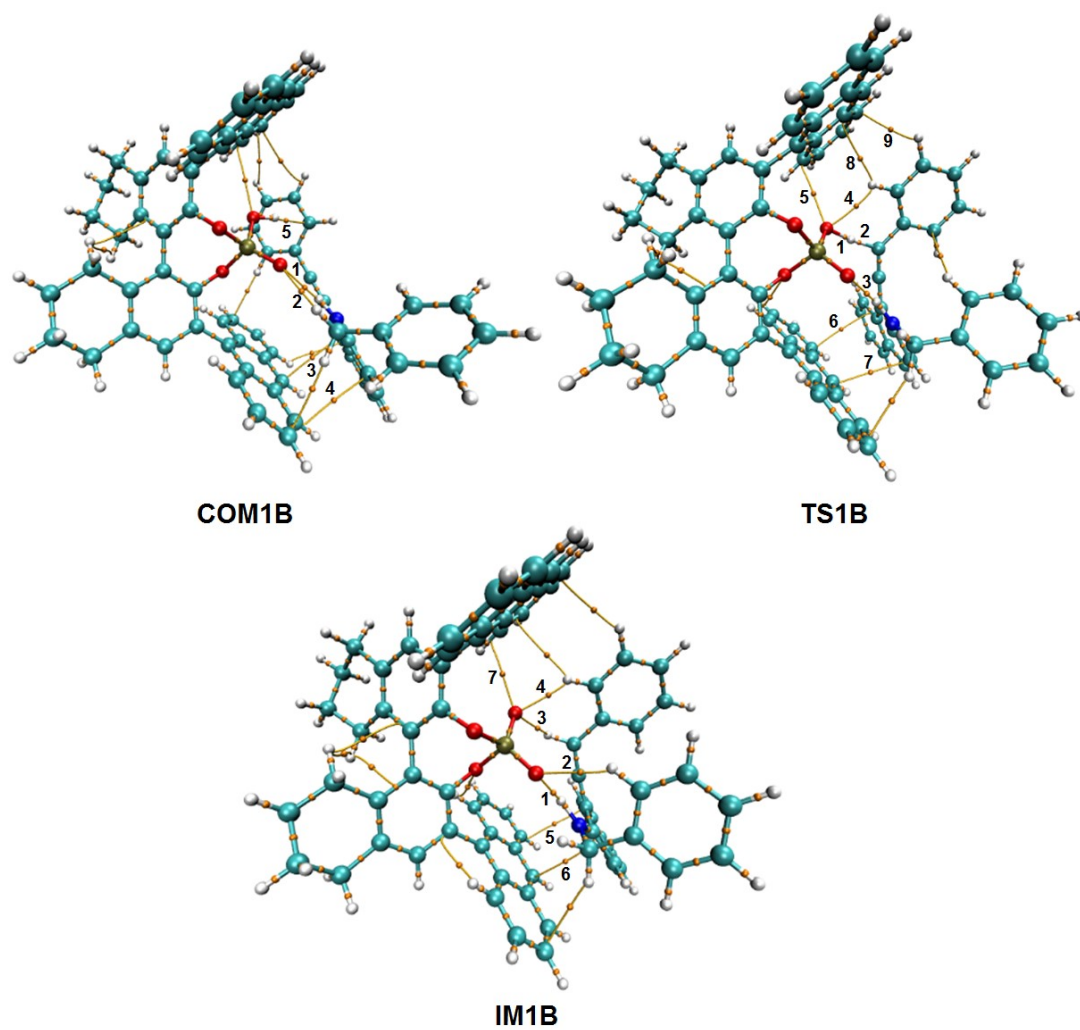
### 2.1 QTAIM analyses of COM1A, TS1A, IM1A, COM1B, TS1B and IM1B



**Figure S1** QTAIM analyses of intermolecular interactions in **COM1A**, **TS1A** and **IM1A** in the hydrogen-transfer process and numbers of bond critical points (BCPs No.).

**Table S2** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **COM1A**, **TS1A** and **IM1A** in hydrogen-transfer processes.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>COM1A</b>	1	N-H...O	2.01	0.0224	0.07	0.0182	-0.0189	-0.0007
	2	C-H...O	2.67	0.0078	0.0296	0.0063	-0.0053	0.0011
	3	C-H...O	2.67	0.0072	0.0272	0.0058	-0.0049	0.001
	4	$\pi$ - $\pi$	3.23	0.0036	0.0109	0.0022	-0.0016	0.0006
	5	$\pi$ - $\pi$	3.15	0.0086	0.0272	0.0056	-0.0044	0.0012
	6	$\pi$ - $\pi$	3.28	0.0073	0.0225	0.0047	-0.0037	0.001
	7	van der Waals	2.24	0.0166	0.0469	0.011	-0.0103	0.0007
<b>TS1A</b>	1	O...H	1.33	0.1223	0.0416	0.0777	-0.1449	-0.0673
	2	H...C	1.29	0.1614	-0.3448	0.0347	-0.1555	-0.1208
	3	N-H...O	1.76	0.0389	0.1352	0.0363	-0.0388	-0.0025
	4	C-H...O	2.52	0.0097	0.037	0.0075	-0.0058	0.0017
	5	p- $\pi$	3.07	0.0078	0.0304	0.0061	-0.0047	0.0015
	6	p- $\pi$	3.09	0.0081	0.0308	0.0062	-0.0048	0.0015
	7	$\pi$ - $\pi$	3.24	0.0074	0.0225	0.0048	-0.0039	0.0009
	8	$\pi$ - $\pi$	3.22	0.0073	0.0212	0.0045	-0.0037	0.0008
<b>IM1A</b>	1	N-H...O	1.57	0.0631	0.1508	0.0545	-0.0712	-0.0168
	2	C-H...O	2.35	0.0112	0.0441	0.009	-0.0069	0.0021
	3	C-H...O	2.24	0.0143	0.0596	0.0124	-0.0099	0.0025
	4	C-H...O	2.40	0.0132	0.0497	0.0104	-0.0083	0.002
	5	p- $\pi$	3.17	0.0066	0.0249	0.005	-0.0038	0.0012
	6	$\pi$ - $\pi$	3.36	0.0066	0.0192	0.004	-0.0032	0.0008
	8	$\pi$ - $\pi$	3.35	0.0066	0.0195	0.004	-0.0032	0.0008

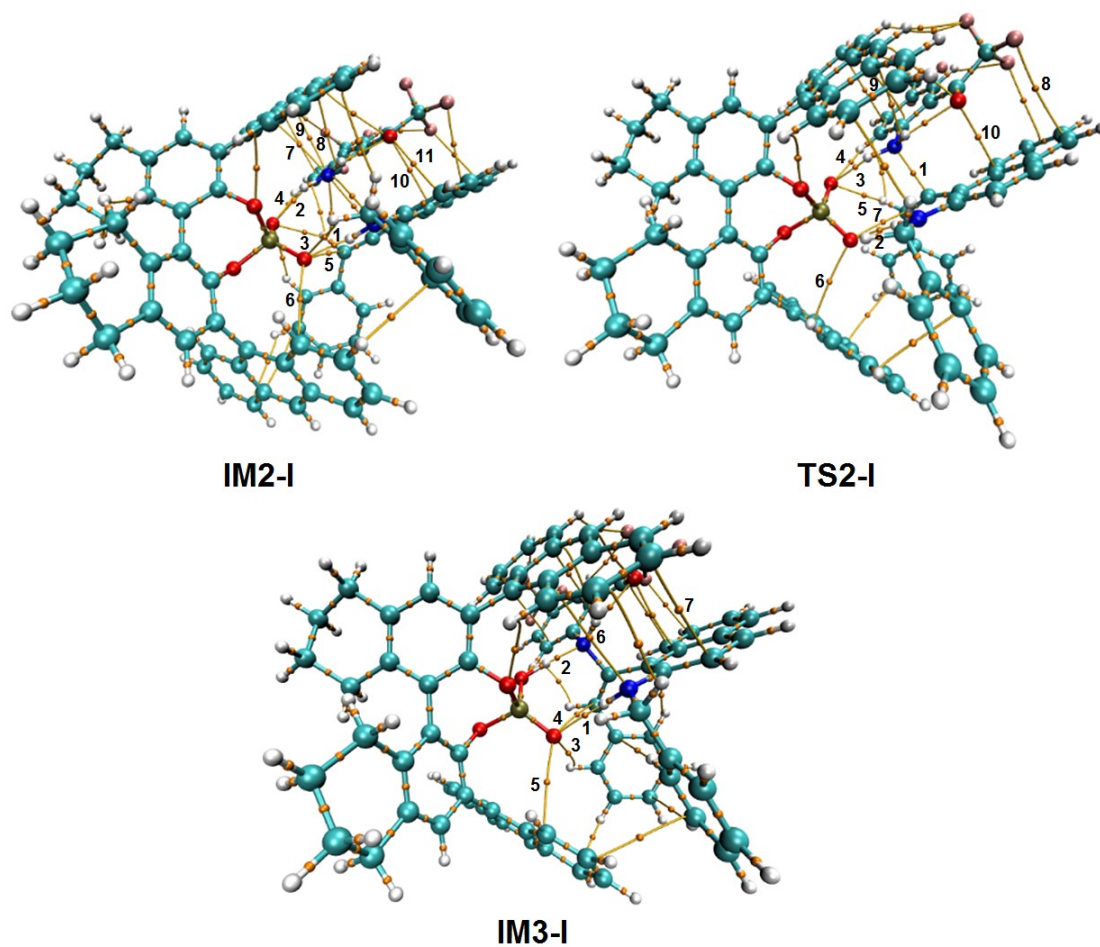


**Figure S2** QTAIM analyses of intermolecular interactions in **COM1B**, **TS1B** and **IM1B** in the hydrogen-transfer process and numbers of bond critical points (BCPs No.).

**Table S3** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **COM1B**, **TS1B** and **IM1B** in the hydrogen-transfer processes.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>COM1B</b>	1	N-H...O	2.08	0.0175	0.0791	0.0164	-0.0131	0.0033
	2	C-H...O	2.38	0.0111	0.0455	0.0093	-0.0073	0.002
	3	$\pi$ - $\pi$	3.29	0.008	0.0232	0.005	-0.0042	0.0008
	4	$\pi$ - $\pi$	3.33	0.0064	0.0193	0.0041	-0.0033	0.0008
	5	van der Waals	2.25	0.0157	0.049	0.0106	-0.0091	0.0016
<b>TS1B</b>	1	O...H	1.26	0.1442	-0.0497	0.0857	-0.1838	-0.0981
	2	H...C	1.33	0.1464	-0.264	0.0367	-0.1394	-0.1027
	3	N-H...O	1.74	0.0389	0.1384	0.0367	-0.0389	-0.0021
	4	C-H...O	2.53	0.0087	0.0352	0.0071	-0.0054	0.0017
	5	$\rho$ - $\pi$	3.13	0.0069	0.0268	0.0054	-0.004	0.0013
	6	$\pi$ - $\pi$	3.40	0.0059	0.0179	0.0037	-0.0029	0.0008
	7	$\pi$ - $\pi$	3.35	0.0072	0.0217	0.0045	-0.0037	0.0009
	8	van der Waals	2.85	0.006	0.0194	0.004	-0.0032	0.0008
	9	van der Waals	2.76	0.0069	0.0219	0.0046	-0.0038	0.0009
<b>IM1B</b>	1	N-H...O	1.61	0.0569	0.151	0.0503	-0.0629	-0.0126
	2	C-H...O	2.49	0.0088	0.0328	0.0066	-0.0051	0.0016
	3	C-H...O	2.08	0.0216	0.0845	0.0187	-0.0163	0.0024
	4	C-H...O	2.3	0.0127	0.0504	0.0103	-0.0081	0.0023
	5	$\pi$ - $\pi$	3.32	0.0073	0.0222	0.0047	-0.0038	0.0009
	6	$\pi$ - $\pi$	3.24	0.0075	0.0227	0.0048	-0.004	0.0008
	7	van der Waals	3.02	0.0088	0.0348	0.0071	-0.0055	0.0016

2.2 QTAIM analyses of the intermediates and transition states in pathways I, I', II and II'

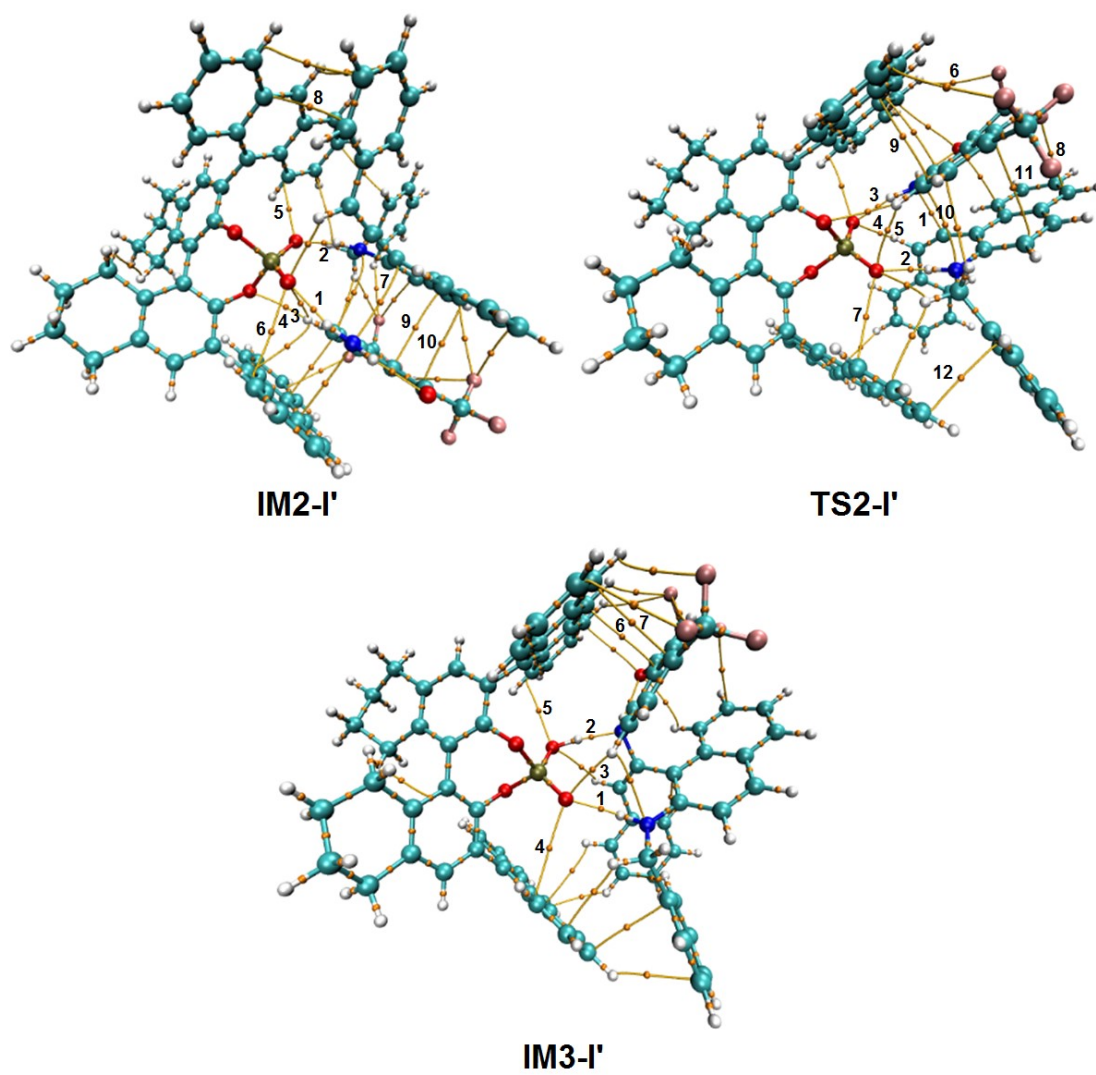


**Figure S3** QTAIM analyses of intermolecular interactions in **IM2-I**, **TS2-I** and **IM3-I** in pathway **I** and numbers of bond critical points (BCPs No.).

**Table S4** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM2-I**, **TS2-I** and **IM3-I** in pathway I.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-I</b>	1	N-H...O	1.70	0.0438	0.1374	0.0349	-0.0355	-0.0006
	2	N-H...O	1.89	0.0314	0.0948	0.0248	-0.0258	-0.0011
	3	C-H...O	2.50	0.0109	0.0430	0.0095	-0.0082	0.0013
	4	C-H...O	2.37	0.0114	0.0404	0.0093	-0.0085	0.0008
	5	p- $\pi$	3.07	0.0091	0.0290	0.0065	-0.0057	0.0008
	6	p- $\pi$	3.31	0.0052	0.0187	0.0039	-0.0031	0.0008
	7	p- $\pi$	3.19	0.0087	0.0272	0.0061	-0.0053	0.0007
	8	p- $\pi$	3.21	0.0088	0.0284	0.0062	-0.0054	0.0009
	9	$\pi$ - $\pi$	3.40	0.0063	0.0180	0.0038	-0.0030	0.0007
	10	$\pi$ - $\pi$	3.26	0.0065	0.0222	0.0044	-0.0033	0.0011
	11	$\pi$ - $\pi$	2.96	0.0105	0.0362	0.0080	-0.0069	0.0011
<b>TS2-I</b>	1	C...N	2.20	0.0516	0.0804	0.0281	-0.0362	-0.0080
	2	N-H...O	1.72	0.0423	0.1377	0.0387	-0.0430	-0.0043
	3	N-H...O	1.76	0.0398	0.1291	0.0357	-0.0391	-0.0034
	4	C-H...O	2.35	0.0114	0.0458	0.0094	-0.0073	0.0021
	5	C-H...O	2.28	0.0148	0.0562	0.0118	-0.0096	0.0022
	6	p- $\pi$	3.34	0.0055	0.0200	0.0039	-0.0028	0.0011
	7	p- $\pi$	1.08	0.2861	-1.0204	0.0364	-0.3280	-0.2915
	8	p- $\pi$	3.67	0.0023	0.0083	0.0015	-0.0010	0.0005
	9	$\pi$ - $\pi$	3.21	0.0077	0.0242	0.0051	-0.0041	0.0010
	10	$\pi$ - $\pi$	2.91	0.0107	0.0433	0.0090	-0.0072	0.0018
<b>IM3-I</b>	1	N-H...O	1.92	0.0270	0.1110	0.0257	-0.0236	0.0021
	2	O-H...N	1.62	0.0669	0.0673	0.0406	-0.0645	-0.0238
	3	C-H...O	2.81	0.0055	0.0211	0.0041	-0.0030	0.0011
	4	p- $\pi$	3.14	0.0082	0.0268	0.0057	-0.0046	0.0010
	5	p- $\pi$	3.22	0.0058	0.0222	0.0044	-0.0032	0.0012
	6	$\pi$ - $\pi$	3.98	0.0023	0.0066	0.0013	-0.0009	0.0004
	7	$\pi$ - $\pi$	4.04	0.0020	0.0058	0.0011	-0.0007	0.0004

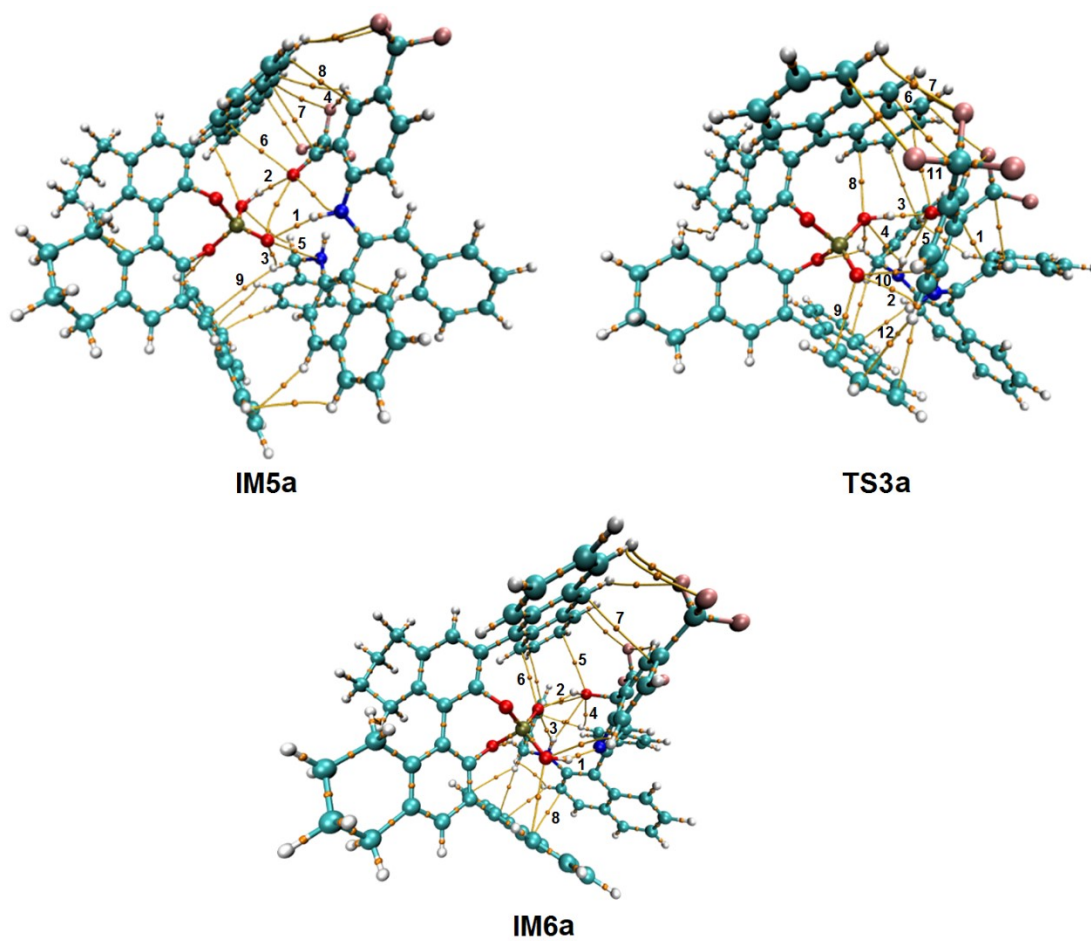




**Figure S4** QTAIM analyses of intermolecular interactions in **IM2-I'**, **TS2-I'** and **IM3-I'** in pathway **I'** and numbers of bond critical points (BCPs No.).

**Table S5** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM2-I'**, **TS2-I'** and **IM3-I'** in pathway **I'**.

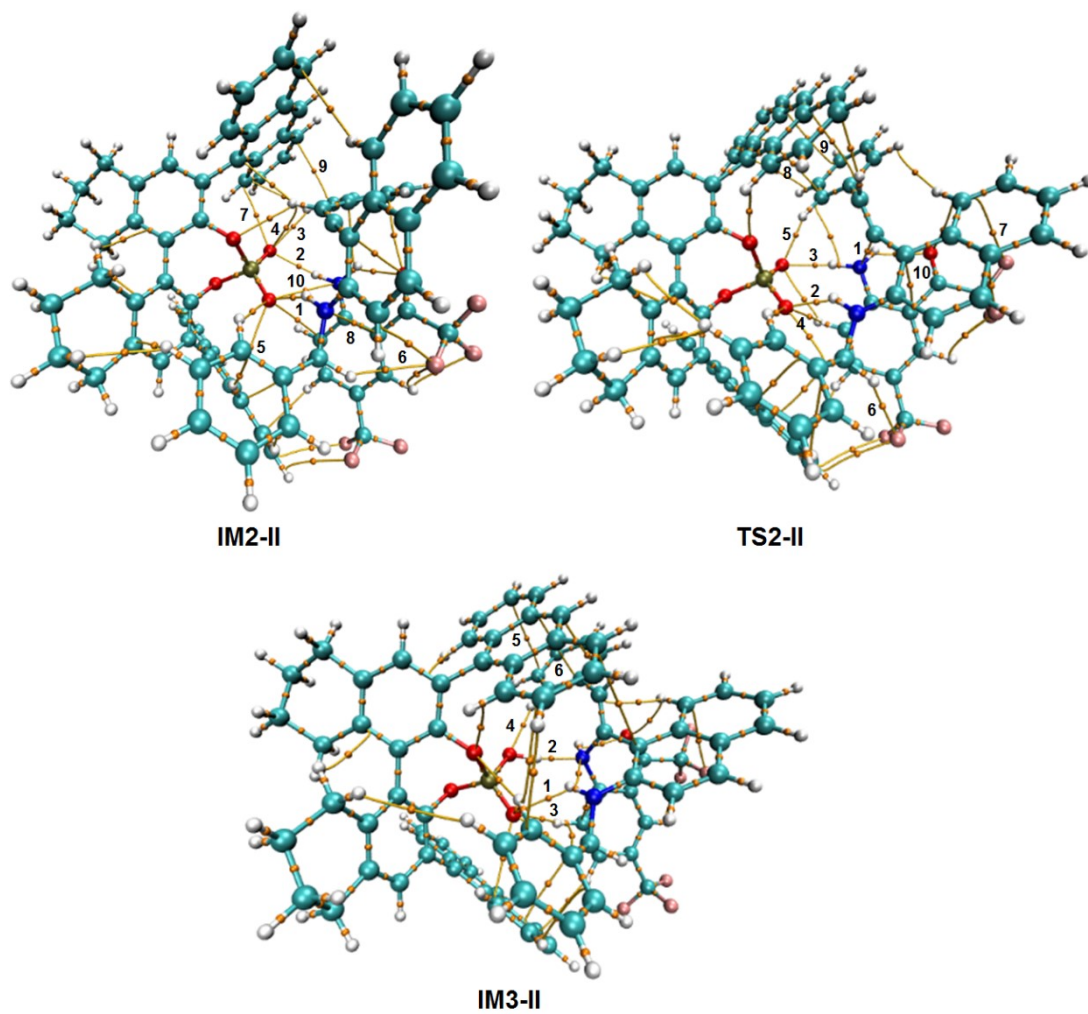
	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-I'</b>	1	N-H...O	1.87	0.0277	0.1132	0.0264	-0.0244	0.002
	2	N-H...O	1.54	0.0677	0.1491	0.0574	-0.0775	-0.0201
	3	C-H...O	2.47	0.0122	0.0437	0.0092	-0.0074	0.0017
	4	C-H...O	2.37	0.0114	0.0451	0.0091	-0.0069	0.0022
	5	p- $\pi$	3.03	0.0084	0.0330	0.0067	-0.0052	0.0015
	6	p- $\pi$	3.43	0.0044	0.0150	0.0030	-0.0022	0.0008
	7	p- $\pi$	3.24	0.0079	0.0273	0.0057	-0.0045	0.0012
	8	$\pi$ - $\pi$	3.41	0.0061	0.0188	0.0038	-0.003	0.0009
	9	$\pi$ - $\pi$	3.42	0.0066	0.0195	0.0040	-0.0032	0.0008
	10	$\pi$ - $\pi$	3.24	0.0072	0.0220	0.0047	-0.0038	0.0008
<b>TS2-I'</b>	1	C...N	2.26	0.0466	0.0770	0.0253	-0.0314	-0.0061
	2	N-H...O	1.85	0.0309	0.1221	0.0295	-0.0285	0.0010
	3	N-H...O	1.74	0.0410	0.1304	0.0367	-0.0407	-0.0041
	4	C-H...O	2.15	0.0181	0.0710	0.0153	-0.0128	0.0025
	5	C-H...O	2.48	0.0109	0.0380	0.0078	-0.0062	0.0017
	6	C-H...F	2.94	0.0029	0.0114	0.0022	-0.0015	0.0007
	7	p- $\pi$	3.37	0.0047	0.0167	0.0033	-0.0024	0.0009
	8	p- $\pi$	3.05	0.0070	0.0286	0.0056	-0.0041	0.0015
	9	$\pi$ - $\pi$	3.30	0.0078	0.0237	0.0050	-0.0040	0.0009
	10	$\pi$ - $\pi$	3.12	0.0091	0.0296	0.0063	-0.0053	0.0011
	11	$\pi$ - $\pi$	3.73	0.0044	0.0128	0.0025	-0.0018	0.0007
	12	$\pi$ - $\pi$	3.32	0.0071	0.0218	0.0046	-0.0037	0.0009
<b>IM3-I'</b>	1	N-H...O	2.00	0.0210	0.0932	0.0201	-0.0168	0.0032
	2	O-H...N	1.68	0.0565	0.0755	0.0357	-0.0526	-0.0168
	3	C-H...O	2.31	0.0128	0.0488	0.0099	-0.0076	0.0023
	4	p- $\pi$	3.58	0.0031	0.0110	0.0021	-0.0014	0.0007
	5	p- $\pi$	3.26	0.0055	0.0212	0.0041	-0.0030	0.0012
	6	$\pi$ - $\pi$	3.30	0.0075	0.0211	0.0045	-0.0037	0.0008
	7	$\pi$ - $\pi$	3.22	0.0080	0.0225	0.0048	-0.0041	0.0008



**Figure S5** QTAIM analyses of intermolecular interactions in **IM5a**, **TS3a** and **IM6a** in annulation processes by **IM4a** and numbers of bond critical points (BCPs No.).

**Table S6** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM5a**, **TS3a** and **IM6a** in annulation processes by **IM4a**.

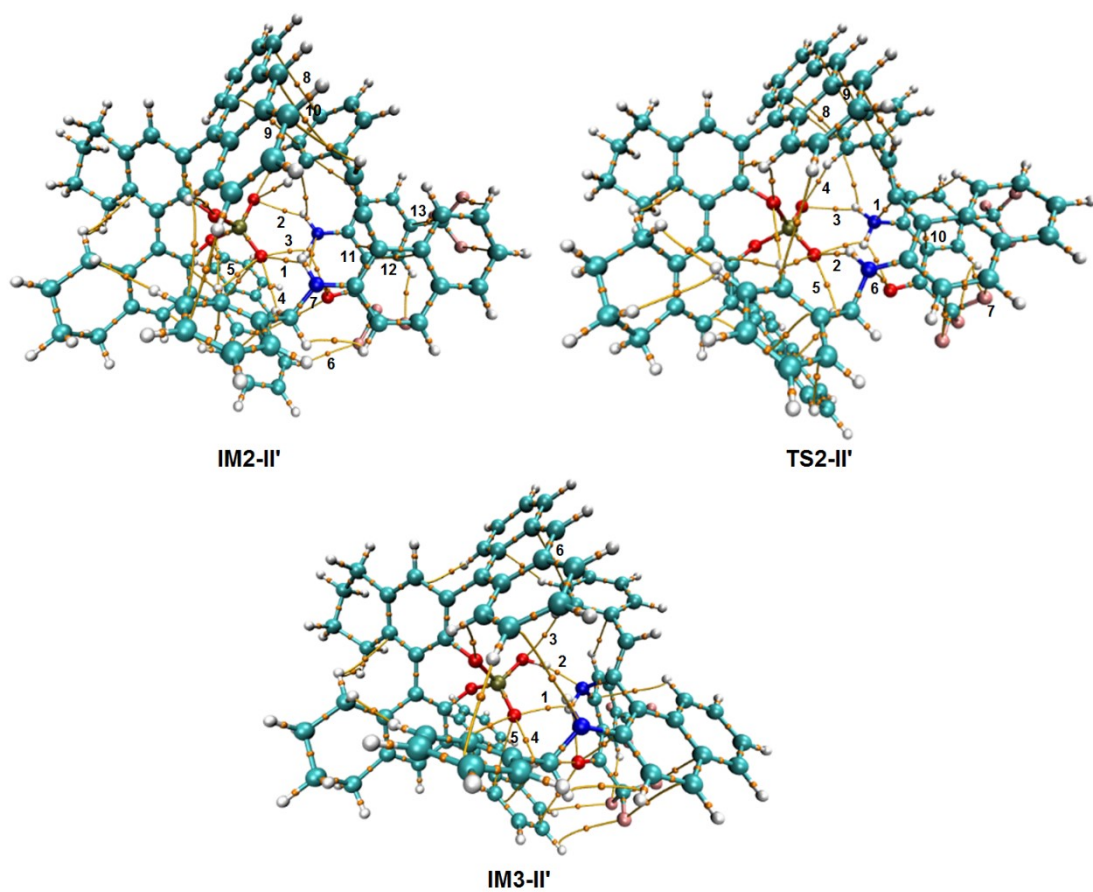
	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM5a</b>	1	N-H...O	2.00	0.0199	0.0849	0.0180	-0.0148	0.0032
	2	O-H...O	1.81	0.0311	0.1285	0.0313	-0.0304	0.0009
	3	C-H...O	2.60	0.0098	0.0372	0.0077	-0.0061	0.0016
	4	C-H...F	2.28	0.0131	0.0615	0.0124	-0.0095	0.0029
	5	p- $\pi$	2.94	0.0112	0.0473	0.0100	-0.0083	0.0018
	6	$\pi$ - $\pi$	3.44	0.0047	0.0163	0.0032	-0.0022	0.0009
	7	$\pi$ - $\pi$	3.36	0.0060	0.0167	0.0035	-0.0029	0.0006
	8	$\pi$ - $\pi$	3.16	0.0083	0.0257	0.0055	-0.0046	0.0009
	9	van der Waals	3.62	0.0016	0.0045	0.0009	-0.0006	0.0003
<b>TS3a</b>	1	C...C	2.22	0.0567	0.0482	0.0220	-0.0320	-0.0100
	2	N-H...O	2.21	0.0167	0.0767	0.0162	-0.0132	0.0030
	3	O-H...O	1.56	0.0631	0.1303	0.0521	-0.0717	-0.0196
	4	N-H...O	2.35	0.0120	0.0528	0.0106	-0.0081	0.0026
	5	N-H...O	2.26	0.0129	0.0516	0.0105	-0.0081	0.0024
	6	C-H...F	2.64	0.0062	0.0272	0.0053	-0.0037	0.0015
	7	C-H...F	2.52	0.0081	0.0355	0.0070	-0.0051	0.0019
	8	p- $\pi$	2.95	0.0095	0.0366	0.0076	-0.0061	0.0015
	9	p- $\pi$	2.90	0.0104	0.0403	0.0084	-0.0068	0.0017
	10	p- $\pi$	2.80	0.0133	0.0550	0.0118	-0.0098	0.0020
	11	$\pi$ - $\pi$	3.60	0.0033	0.0116	0.0022	-0.0015	0.0007
	12	$\pi$ - $\pi$	3.22	0.0084	0.0262	0.0056	-0.0047	0.0009
<b>IM6a</b>	1	N-H...O	1.60	0.0682	0.0815	0.0439	-0.0674	-0.0235
	2	O-H...O	1.98	0.0206	0.0895	0.0195	-0.0166	0.0029
	3	N-H...O	1.98	0.0246	0.1027	0.0233	-0.0208	0.0024
	4	C-H...O	2.46	0.0112	0.0441	0.0092	-0.0073	0.0018
	5	p- $\pi$	3.34	0.0055	0.0185	0.0037	-0.0027	0.0010
	6	p- $\pi$	3.02	0.0085	0.0322	0.0066	-0.0052	0.0014
	7	$\pi$ - $\pi$	3.50	0.0051	0.0143	0.0029	-0.0023	0.0006
	8	$\pi$ - $\pi$	3.23	0.0077	0.0224	0.0048	-0.0040	0.0008



**Figure S6** QTAIM analyses of intermolecular interactions in **IM2-II**, **TS2-II** and **IM3-II** in pathway **II** and numbers of bond critical points (BCPs No.).

**Table S7** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM2-II**, **TS2-II** and **IM3-II** in pathway **II**.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-II</b>	1	N-H...O	1.64	0.0519	0.1587	0.0419	-0.0441	-0.0022
	2	N-H...O	2.05	0.0215	0.0610	0.0163	-0.0173	-0.0010
	3	C-H...O	2.33	0.0126	0.0435	0.0102	-0.0095	0.0007
	4	C-H...O	2.60	0.0097	0.0360	0.0076	-0.0061	0.0014
	5	C-H...O	2.41	0.0120	0.0384	0.0092	-0.0088	0.0004
	6	C-H...F	2.45	0.0083	0.0351	0.0077	-0.0065	0.0011
	7	p- $\pi$	3.20	0.0066	0.0230	0.0049	-0.0040	0.0009
	8	p- $\pi$	3.21	0.0084	0.0246	0.0056	-0.0050	0.0006
	9	$\pi$ - $\pi$	3.27	0.0073	0.0224	0.0046	-0.0037	0.0010
	10	van der Waals	3.06	0.0097	0.0334	0.0077	-0.0071	0.0006
<b>TS2-II</b>	1	C...N	2.21	0.0513	0.0748	0.0265	-0.0342	-0.0078
	2	N-H...O	1.76	0.0392	0.1410	0.0374	-0.0395	-0.0021
	3	N-H...O	1.93	0.0259	0.0980	0.0227	-0.0209	0.0018
	4	C-H...O	2.43	0.0134	0.0511	0.0108	-0.0089	0.0019
	5	C-H...O	2.01	0.0230	0.0933	0.0208	-0.0182	0.0026
	6	C-H...F	2.66	0.0051	0.0204	0.0040	-0.0029	0.0011
	7	p- $\pi$	3.20	0.0063	0.0253	0.0049	-0.0035	0.0014
	8	$\pi$ - $\pi$	3.29	0.0072	0.0215	0.0045	-0.0036	0.0009
	9	$\pi$ - $\pi$	3.41	0.0070	0.0204	0.0043	-0.0034	0.0008
	10	$\pi$ - $\pi$	3.20	0.0098	0.027	0.0060	-0.0052	0.0008
<b>IM3-II</b>	1	N-H...O	2.11	0.0197	0.0846	0.0183	-0.0155	0.0028
	2	O-H...N	1.71	0.0528	0.0730	0.0329	-0.0475	-0.0146
	3	C-H...O	2.12	0.0183	0.0730	0.0155	-0.0128	0.0027
	4	C-H...O	2.20	0.0143	0.0612	0.0125	-0.0097	0.0028
	5	$\pi$ - $\pi$	3.39	0.0064	0.0192	0.0040	-0.0031	0.0008
	6	$\pi$ - $\pi$	3.36	0.0066	0.0200	0.0041	-0.0032	0.0009

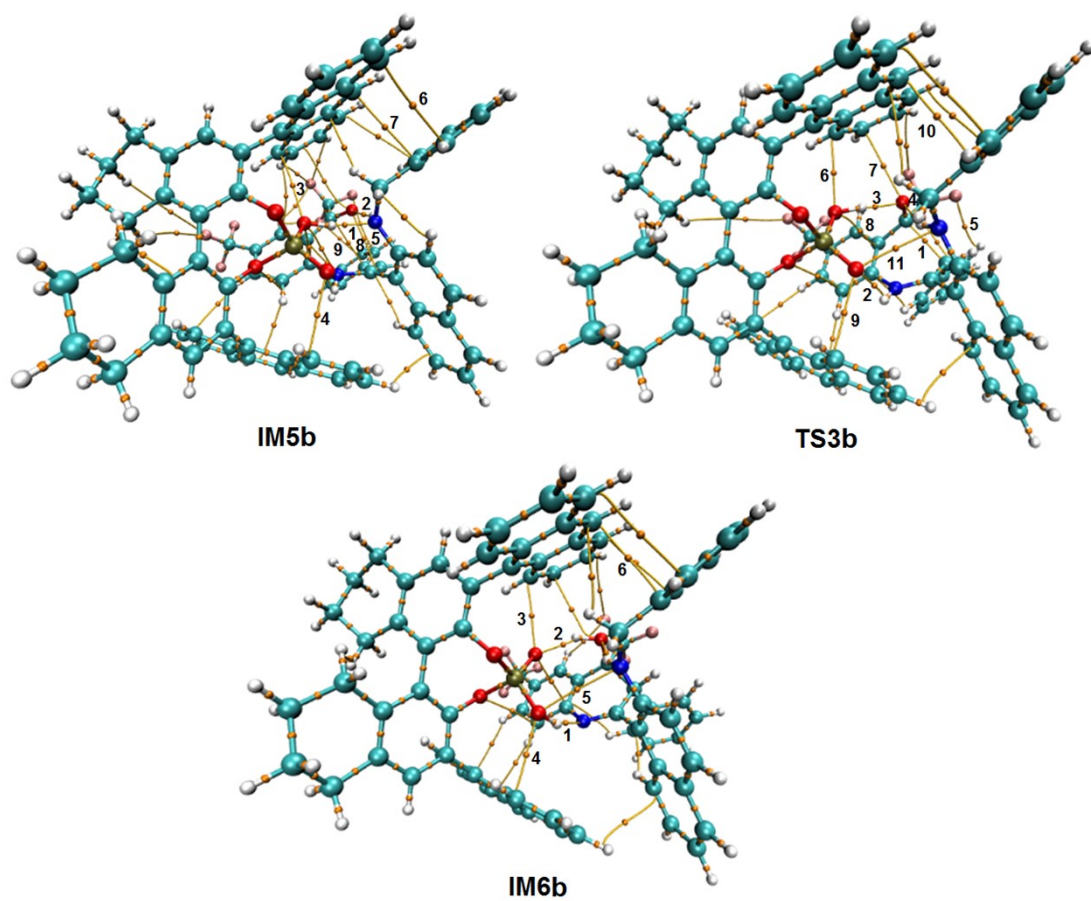


**Figure S7** QTAIM analyses of intermolecular interactions in **IM2-II'**, **TS2-II'** and **IM3-II'** in pathway **II'** and numbers of bond critical points (BCPs No.).

**Table S8** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM2-II'**, **TS2-II'** and **IM3-II'** in pathway **II'**.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-II'</b>	1	N-H...O	2.03	0.0226	0.0965	0.0214	-0.0186	0.0027
	2	N-H...O	2.20	0.0152	0.0623	0.0127	-0.0098	0.0029
	3	N-H...O	2.15	0.0189	0.0832	0.0180	-0.0151	0.0028
	4	C-H...O	2.19	0.0183	0.0780	0.0169	-0.0143	0.0026
	5	C-H...O	2.34	0.0137	0.0528	0.0111	-0.0090	0.0021
	6	C-H...F	2.49	0.0066	0.0305	0.0059	-0.0041	0.0017
	7	p- $\pi$	3.00	0.0092	0.0373	0.0076	-0.0059	0.0017
	8	$\pi$ - $\pi$	3.38	0.0063	0.0185	0.0038	-0.0030	0.0008
	9	$\pi$ - $\pi$	3.26	0.0076	0.0228	0.0048	-0.0039	0.0009
	10	$\pi$ - $\pi$	3.38	0.0067	0.0196	0.0041	-0.0033	0.0008
	11	$\pi$ - $\pi$	3.31	0.0064	0.0201	0.0042	-0.0033	0.0008
	12	$\pi$ - $\pi$	3.39	0.0066	0.0194	0.0040	-0.0032	0.0008
	13	$\pi$ - $\pi$	3.39	0.0071	0.0202	0.0042	-0.0034	0.0008
<b>TS2-II'</b>	1	C...N	2.22	0.0511	0.0751	0.0264	-0.0341	-0.0077
	2	N-H...O	1.74	0.0410	0.1453	0.0392	-0.0420	-0.0028
	3	N-H...O	2.19	0.0157	0.0642	0.0132	-0.0104	0.0028
	4	C-H...O	2.04	0.0225	0.0910	0.0202	-0.0176	0.0026
	5	C-H...O	2.35	0.0134	0.0572	0.0121	-0.0099	0.0022
	6	p- $\pi$	2.79	0.0133	0.0542	0.0117	-0.0099	0.0018
	7	p- $\pi$	2.91	0.0090	0.0394	0.0079	-0.0059	0.0020
	8	$\pi$ - $\pi$	3.18	0.0083	0.0253	0.0054	-0.0044	0.0009
	9	$\pi$ - $\pi$	3.36	0.0067	0.0198	0.0041	-0.0033	0.0008
	10	$\pi$ - $\pi$	3.25	0.0088	0.0262	0.0057	-0.0048	0.0009
<b>IM3-II'</b>	1	N-H...O	2.10	0.0193	0.0828	0.0178	-0.0148	0.0029
	2	O-H...N	1.73	0.0507	0.0796	0.0326	-0.0453	-0.0127
	3	C-H...O	2.41	0.0124	0.0523	0.0107	-0.0084	0.0023
	4	C-H...O	2.22	0.0151	0.0636	0.0133	-0.0108	0.0026
	5	p- $\pi$	3.13	0.0068	0.0265	0.0053	-0.0040	0.0013
	6	$\pi$ - $\pi$	3.27	0.0073	0.0238	0.0050	-0.0040	0.0010





**Figure S8** QTAIM analyses of intermolecular interactions in **IM5b**, **TS3b** and **IM6b** in annulation processes by **IM4b** and numbers of bond critical points (BCPs No.).

**Table S9** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM5b**, **TS3b** and **IM6b** in annulation processes by **IM4b**.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM5b</b>	1	O-H...N	1.61	0.0685	0.0715	0.0426	-0.0672	-0.0247
	2	N-H...O	1.98	0.0217	0.0945	0.0204	-0.0172	0.0032
	3	p- $\pi$	3.13	0.0068	0.0258	0.0052	-0.0039	0.0013
	4	p- $\pi$	2.86	0.0116	0.0464	0.0097	-0.0078	0.0019
	5	p- $\pi$	3.11	0.0064	0.0245	0.0049	-0.0036	0.0013
	6	$\pi$ - $\pi$	3.46	0.0051	0.0157	0.0032	-0.0024	0.0007
	7	$\pi$ - $\pi$	3.26	0.0071	0.0213	0.0046	-0.0038	0.0008
	8	$\pi$ - $\pi$	3.61	0.0042	0.0139	0.0027	-0.0019	0.0008
	9	$\pi$ - $\pi$	2.99	0.0099	0.0336	0.0073	-0.0062	0.0011
<b>TS3b</b>	1	C...C	2.30	0.0499	0.0448	0.0184	-0.0256	-0.0072
	2	N-H...O	2.05	0.0212	0.0907	0.0198	-0.0169	0.0029
	3	O-H...O	1.64	0.0522	0.1204	0.0431	-0.0562	-0.0131
	4	N-H...O	1.86	0.0292	0.1204	0.0284	-0.0268	0.0017
	5	C-H...F	2.61	0.0068	0.0295	0.0058	-0.0042	0.0016
	6	p- $\pi$	2.90	0.0105	0.0422	0.0088	-0.0070	0.0018
	7	p- $\pi$	3.22	0.0063	0.0222	0.0045	-0.0034	0.0011
	8	p- $\pi$	3.06	0.0098	0.0392	0.0081	-0.0064	0.0017
	9	p- $\pi$	2.90	0.0109	0.0424	0.0089	-0.0071	0.0017
	10	$\pi$ - $\pi$	3.19	0.0081	0.0246	0.0053	-0.0044	0.0009
	11	van der Waals	2.95	0.0106	0.0436	0.0091	-0.0072	0.0018
<b>IM6b</b>	1	O-H...N	1.78	0.0427	0.0905	0.0299	-0.0373	-0.0073
	2	O-H...O	1.84	0.0292	0.1204	0.0288	-0.0275	0.0013
	3	p- $\pi$	2.93	0.0101	0.0392	0.0081	-0.0065	0.0016
	4	p- $\pi$	2.84	0.0112	0.0444	0.0093	-0.0075	0.0018
	5	$\pi$ - $\pi$	3.09	0.0084	0.0325	0.0066	-0.0050	0.0016
	6	$\pi$ - $\pi$	3.16	0.0085	0.0258	0.0056	-0.0047	0.0009

### 3. Reaction mechanisms for pathways III, III', IV, IV' and QTAIM Analyses

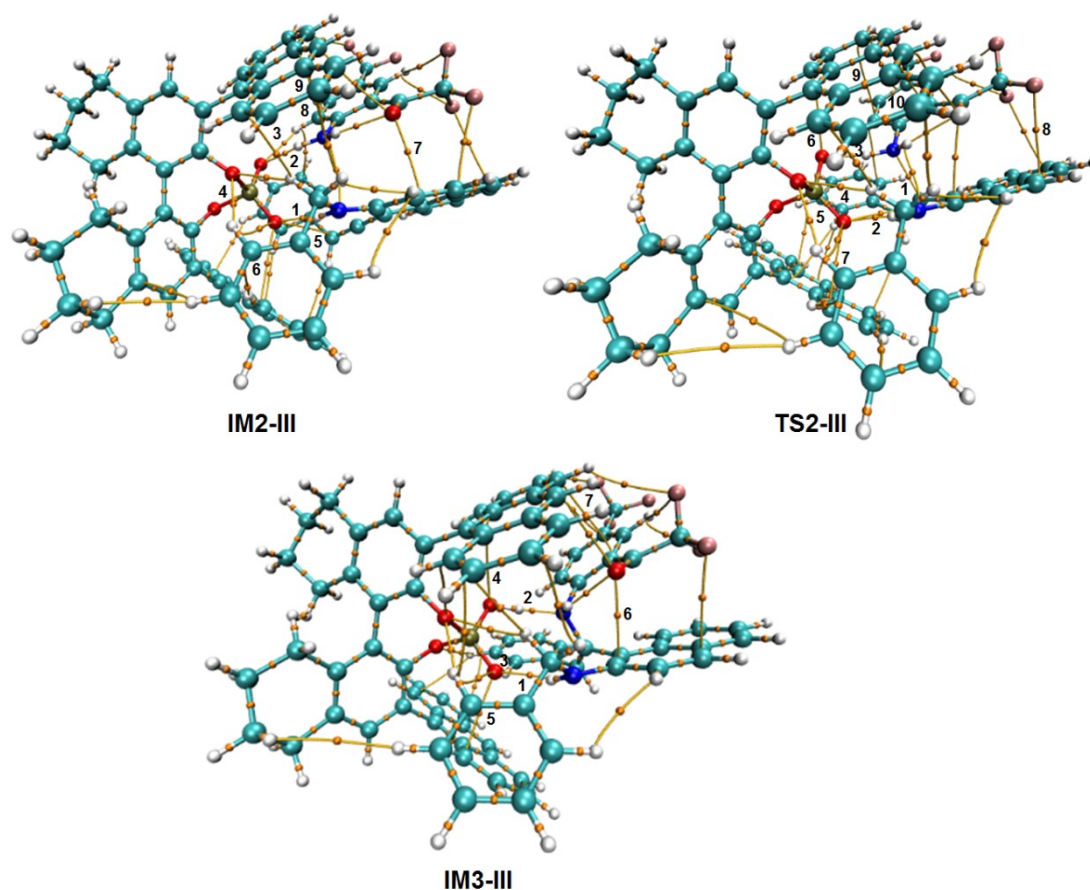
With respect to pathway **III** or **III'** (Figures 4, 9 and 10), it is the reaction process starting from the interaction between **R2** and **IM1B** containing (*S*)-**H-VQM**, leading to the major product **P**. Initially, **R2** interacts with **IM1B** through dual hydrogen bonds (i.e. N5-H5...O2 and N1-H1...O3) and forms the possible intermediate **IM2-III** or **IM2-III'** with an energy release of 0.7 kcal/mol or 1.4 kcal/mol (Figure 9). In **IM2-III** (or **IM2-III'**), the H5...O2 and H1...O3 distances are 1.63 and 1.82 Å (or 1.55 and 1.83 Å), respectively (Figures 10, S9 and S10, Tables S10 and S11). The distance between the reaction sites involving the N1 and C2 atoms in **IM2-III** (or **IM2-III'**) is 3.71 Å (or 3.48 Å) (Figures 10, S9 and S10, Tables S10 and S11). After going through the transition state **TS2-III** (or **TS2-III'**) and overcoming an energy barrier of 16.8 kcal/mol (or 13.6 kcal/mol), the N1-C2 bond forms in the intermediate **IM3-III** (or **IM3-III'**) (Figure 9). In **TS2-III** (or **TS2-III'**), the distance between N1 and C2 atoms is 2.21 Å (or 2.17 Å), and the N5-H5...O2 hydrogen bond retains in which the H5...O2 distances is 1.73 Å (or 1.69 Å). But the N1-H1...O3 hydrogen bond in **TS2-III** (or **TS2-III'**) varies in which the H1 atom transfers towards O3 atom and forms N1...H1...O3 interactions with N1...H1 and H1...O3 distances of 1.05 and 1.64 Å (or 1.04 and 1.74 Å), respectively (Figures 10, S9 and S10, Tables S10 and S11). Then the N1-C2 bond in **IM3-III** (or **IM3-III'**), and also the new O3-H1...N1 hydrogen bond with the H1...N1 distance of 1.58 Å (or 1.76 Å) forms which coexists with the N5-H5...O2 hydrogen bond (Figures 10, S9 and S10, Tables S10 and S11). Then the recovered catalyst **C1** separates from **IM3-III** (or **IM3-III'**) and the same intermediate **IM4c** is produced

(Figure 9). Due to the proton-donating and accepting characters of the recovered catalyst **C1**, it reconnects with **IM4c** by forming the new dual hydrogen bonding mode (i.e., N1-H1'...O2 and O3-H1...O5 hydrogen bonds) to generate **IM5c**. Afterwards, the hydrogen transfers (i.e., the transfer of H1' atom to O2 atom and the transfer of H1 atom to O5 atom) together with the C1-C4 annulation reaction take place in the transition state **TS3c** (Figures 10 and S11, Table S12). In **TS3c**, the distance between reaction sites of C1 and C4 atoms is 2.28 Å, and the O2...H1', H1'...N1, O3...H1 and H1...O5 distances are 2.12 Å, 1.02 Å, 1.00 Å and 1.65 Å, respectively (Figures 10 and S11, Table S12). The energy barrier for the process from **IM5c** to **TS3c** is 10.0 kcal/mol. After the completion of the hydrogen transfers and C1-C4 annulation reaction, **IM6c** is generated, and the process from **TS3c** to **IM6c** releases an energy of 37.6 kcal/mol (Figure 9). In **IM6c**, two new hydrogen bonds (i.e., O2-H1'...N1 and O5-H1...O3 hydrogen bonds) form and the catalyst **C1** recovers. Subsequently, the O2-H1'...N1 and O5-H1...O3 hydrogen bonds break and give out **IM7c** which needs an energy of 3.3 kcal/mol. After going through an intramolecular dehydration elimination reaction of **IM7c**, the major product **P** is yielded with an energy release of 16.5 kcal/mol (Figure 9). The enantioselectivity-determining step in pathway **III** (or **III'**) is the N1-C2 bonding process from **IM2-III** to **TS2-III** (or from **IM2-III'** to **TS2-III'**) with energy barrier of 16.8 kcal/mol (or 13.6 kcal/mol).

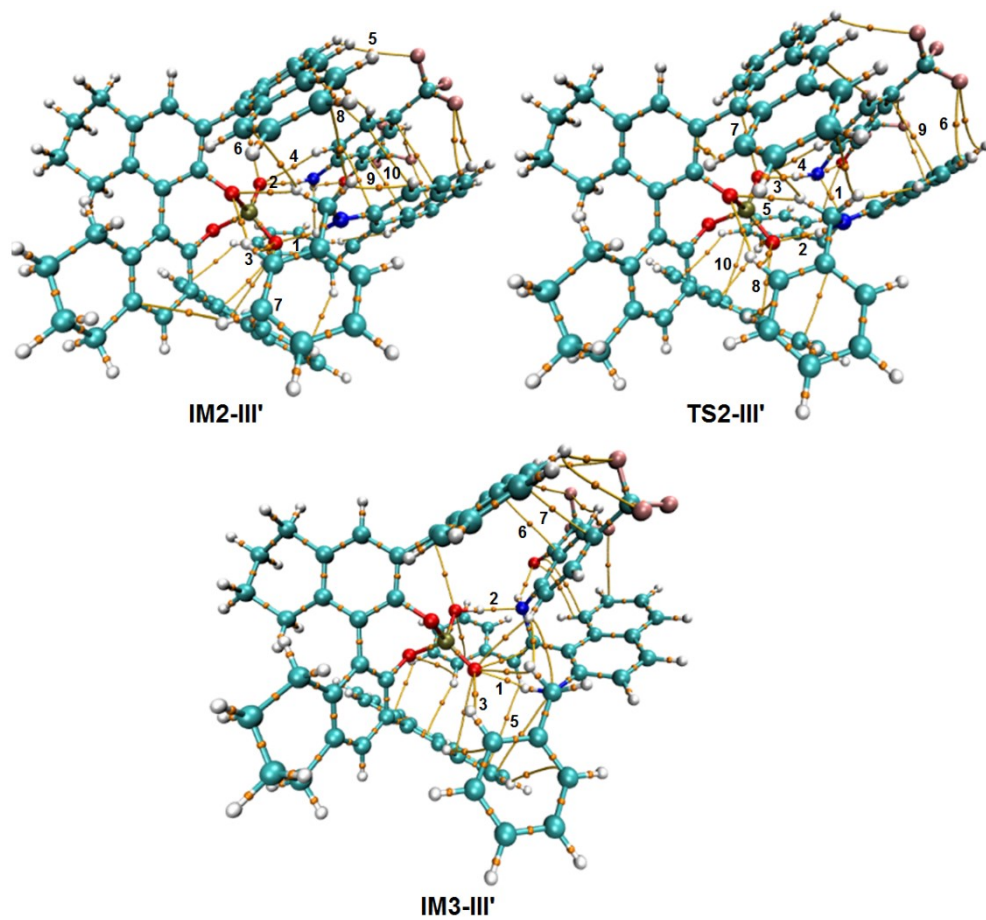
For pathways **IV** and **IV'**, their Gibbs free energy profiles are shown in Figure 11, and the optimized geometries of the intermediates, transition states and the product involving in these two pathways are displayed in Figure 12. The reaction process starts

from the dual hydrogen bonding interaction (i.e., N5-H5 $\cdots$ O2 and N1-H1 $\cdots$ O3 hydrogen bonds) of **R2** with **IM1B**, and two possible complexes **IM2-IV** and **IM2-IV'** form which release an energy of 0.3 and 0.9 kcal/mol, respectively (Figure 11). The H5 $\cdots$ O2 and H1 $\cdots$ O3 distances are 1.66 and 1.90 Å in **IM2-IV** (or 1.69 and 1.87 Å in **IM2-IV'**), and the C2 $\cdots$ N1 distance is 3.65 Å in **IM2-IV** (or 4.00 Å in **IM2-IV'**) (Figures 12, S12, S13, Tables S13 and S14). The C2-N1 bonding process goes through the transition state **TS2-IV** (or **TS2-IV'**) which needs to overcome an energy barrier of 11.2 kcal/mol (or 13.3 kcal/mol), and the C2-N1 bond forms in **IM3-IV** (or **IM3-IV'**) which is accompanied by the transfer of H1 atom to O3 atom (Figure 11). In **TS2-IV** (or **TS2-IV'**), the C2 $\cdots$ N1 distance is shortened to 2.23 Å (or 2.25 Å), while the H1 $\cdots$ O3 and H1 $\cdots$ N1 distances 1.72 are 1.03 Å (or 1.62 and 1.05 Å), respectively (Figures 12, S12, S13, Tables S13 and S14). A new hydrogen bond (i.e., O3-H1 $\cdots$ N1 hydrogen bond) forms in **IM3-IV** (or **IM3-IV'**) which coexists with the N5-H5 $\cdots$ O2 hydrogen bond, so the catalyst recovers. Then the recovered catalyst **C1** breaks away from **IM3-IV** (or **IM3-IV'**) by disconnecting the dual hydrogen bonding interaction (i.e., the N5-H5 $\cdots$ O2 and O3-H1 $\cdots$ N1 hydrogen bonds), leading to the intermediate **IM4d**. Subsequently, the resultant **IM4d** reconnects with the catalyst **C1** via two new hydrogen bonds (i.e., N1-H1' $\cdots$ O2 and O3-H1 $\cdots$ O5 hydrogen bonds) and forms the intermediate **IM5d** in which the H1' $\cdots$ O2 and H1 $\cdots$ O5 distances are 2.19 and 1.81 Å, respectively (Figures 12 and S14, Table S15). The annulation reaction between C1 and C4 atoms occurs in **TS3d** which is accompanied by the double proton transfer (i.e., the transfer of H1 atom to O5 atom and the transfer of H1' atom to O2 atom). After

overcoming an energy barrier of 7.2 kcal/mol, the intermediate **IM6d** is generated (Figure 11). In **TS3d**, the C1...C4 distance is shortened to 2.19 Å, while the C1-C4 bond forms in **IM6d** (Figures 12 and S14, Table S15). The double proton transfer leads to the formations of two new hydrogen bonds (i.e., O2-H1'...N1 and O5-H1...O3 hydrogen bonds) in **IM6d** which makes the catalyst **C1** recover. After the broken of O2-H1'...N1 and O5-H1...O3 hydrogen bonds, **IM7d** breaks away from **IM6d** and then undergoes an intramolecular dehydration reaction which gives out the minor product **mP** (Figure 11). The enantioselectivity of pathway **IV** (or **IV'**) is determined by the step involving the N1-C2 bonding process with an energy barrier of 11.2 kcal/mol (or 13.3 kcal/mol).



**Figure S9** QTAIM analyses of intermolecular interactions in **IM2-III**, **TS2-III** and **IM3-III** in pathway **III** and numbers of bond critical points (BCPs No.).



**Figure S10** QTAIM analyses of intermolecular interactions in **IM2-III'**, **TS2-III'** and **IM3-III'** in pathway **III'** and numbers of bond critical points (BCPs No.).

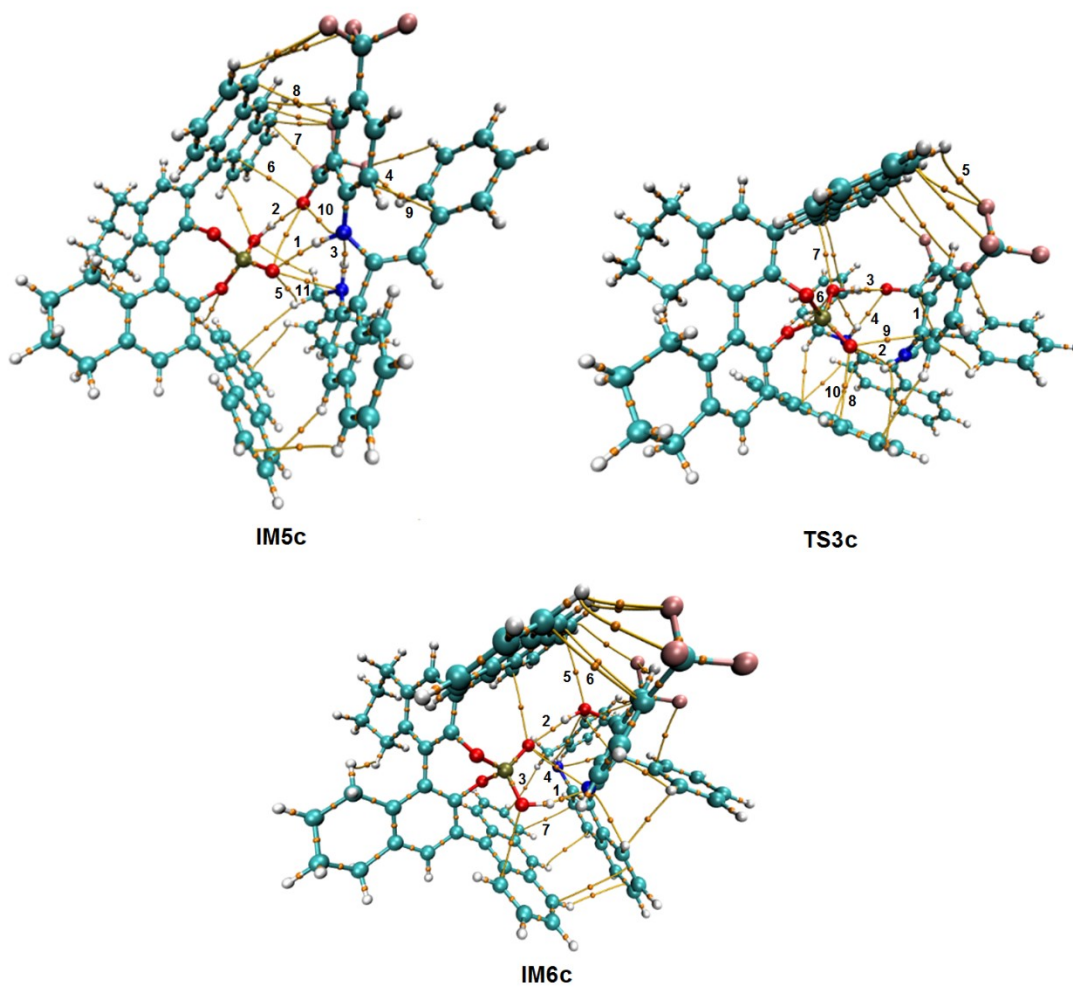
**Table S10** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , in a.u.) and its Laplacian value ( $\nabla^2\rho$ , in a.u.), the electronic kinetic energy density ( $G$ , 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 **IM2-III**, **TS2-III** and **IM3-III** in pathway **III**.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-III</b>	1	N-H...O	1.63	0.0528	0.1448	0.0467	-0.0571	-0.0105
	2	N-H...O	1.82	0.0347	0.1218	0.0315	-0.0325	-0.0010
	3	C-H...O	2.38	0.0105	0.0421	0.0085	-0.0065	0.0020
	4	C-H...O	2.33	0.0120	0.0465	0.0094	-0.0073	0.0022
	5	p- $\pi$	2.98	0.0099	0.0363	0.0076	-0.0061	0.0015
	6	p- $\pi$	3.04	0.0081	0.0315	0.0064	-0.0049	0.0015
	7	p- $\pi$	2.89	0.0114	0.0424	0.0089	-0.0073	0.0017
	8	p- $\pi$	3.27	0.0080	0.0277	0.0057	-0.0046	0.0012
	9	$\pi$ - $\pi$	3.43	0.0071	0.0212	0.0044	-0.0035	0.0009
<b>TS2-III</b>	1	C...N	2.21	0.0517	0.0788	0.0274	-0.0352	-0.0077
	2	N-H...O	1.73	0.0409	0.1388	0.038	-0.0414	-0.0034
	3	N-H...O	1.64	0.0535	0.1408	0.0466	-0.0580	-0.0114
	4	C-H...O	2.41	0.0100	0.0380	0.0077	-0.0059	0.0018
	5	C-H...O	2.44	0.0092	0.0347	0.0070	-0.0052	0.0017
	6	p- $\pi$	3.10	0.0073	0.0278	0.0056	-0.0043	0.0013
	7	p- $\pi$	2.99	0.0090	0.0340	0.0070	-0.0055	0.0015
	8	p- $\pi$	3.18	0.0064	0.0252	0.0049	-0.0035	0.0014
	9	$\pi$ - $\pi$	3.43	0.0064	0.0193	0.0040	-0.0031	0.0009
	10	$\pi$ - $\pi$	3.3	0.0074	0.0211	0.0045	-0.0037	0.0008
<b>IM3-III</b>	1	N-H...O	1.94	0.0247	0.1076	0.0241	-0.0213	0.0028
	2	O-H...N	1.58	0.2851	-1.0126	0.0369	-0.3270	-0.2901
	3	C-H...O	2.37	0.0128	0.0475	0.0098	-0.0076	0.0021
	4	p- $\pi$	3.35	0.0056	0.0203	0.0040	-0.0029	0.0011
	5	p- $\pi$	2.94	0.0097	0.0374	0.0078	-0.0062	0.0016
	6	p- $\pi$	2.89	0.0119	0.0442	0.0096	-0.0082	0.0014
	7	$\pi$ - $\pi$	3.32	0.0071	0.0208	0.0044	-0.0035	0.0008



**Table S11** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM2-III'**, **TS2-III'** and **IM3-III'** in pathway **III'**.

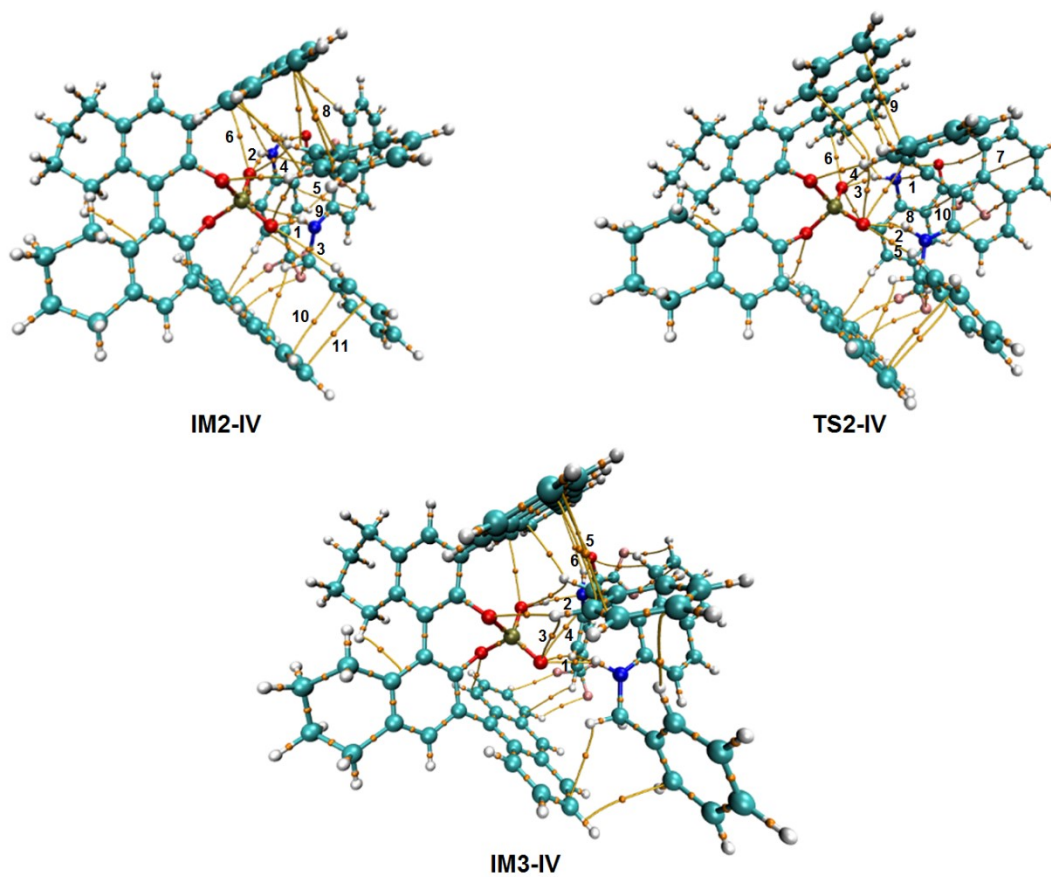
	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-III'</b>	1	N-H...O	1.55	0.0668	0.1469	0.0565	-0.0764	-0.0198
	2	N-H...O	1.83	0.0306	0.1192	0.0288	-0.0279	0.0010
	3	C-H...O	2.89	0.0062	0.0225	0.0045	-0.0034	0.0011
	4	C-H...O	2.51	0.0091	0.0330	0.0067	-0.0051	0.0016
	5	C-H...F	2.91	0.0029	0.0116	0.0022	-0.0015	0.0007
	6	p- $\pi$	3.30	0.0052	0.0195	0.0038	-0.0028	0.0011
	7	p- $\pi$	2.97	0.0090	0.0352	0.0072	-0.0057	0.0016
	8	$\pi$ - $\pi$	3.27	0.0073	0.0234	0.0049	-0.0040	0.0009
	9	$\pi$ - $\pi$	3.23	0.0073	0.0219	0.0047	-0.0038	0.0008
	10	$\pi$ - $\pi$	3.37	0.0066	0.0192	0.0040	-0.0032	0.0008
<b>TS2-III'</b>	1	C...N	2.17	0.0563	0.0761	0.0287	-0.0383	-0.0097
	2	N-H...O	1.69	0.0466	0.1459	0.0429	-0.0492	-0.0064
	3	N-H...O	1.74	0.0389	0.1290	0.0351	-0.038	-0.0029
	4	C-H...O	2.60	0.0080	0.0287	0.0058	-0.0044	0.0014
	5	C-H...O	2.38	0.0108	0.0417	0.0085	-0.0065	0.0019
	6	C-H...F	2.70	0.0059	0.0258	0.0050	-0.0035	0.0015
	7	p- $\pi$	3.48	0.0038	0.0137	0.0026	-0.0018	0.0008
	8	p- $\pi$	2.84	0.0113	0.0459	0.0096	-0.0077	0.0019
	9	$\pi$ - $\pi$	3.45	0.0060	0.0177	0.0036	-0.0028	0.0008
	10	$\pi$ - $\pi$	3.27	0.0073	0.0243	0.0051	-0.0041	0.0010
<b>IM3-III'</b>	1	N-H...O	1.96	0.2622	-0.6891	0.0655	-0.3033	-0.2378
	2	O-H...N	1.76	0.0456	0.0794	0.0300	-0.0401	-0.0101
	3	C-H...O	2.73	0.0063	0.0234	0.0047	-0.0035	0.0012
	4	p- $\pi$	3.29	0.0073	0.0237	0.0048	-0.0038	0.0011
	5	p- $\pi$	3.69	0.0033	0.0102	0.0020	-0.0014	0.0006
	6	$\pi$ - $\pi$	3.33	0.0067	0.0194	0.0041	-0.0033	0.0008
	7	$\pi$ - $\pi$	3.25	0.0079	0.0236	0.0050	-0.0042	0.0008



**Figure S11** QTAIM analyses of intermolecular interactions in **IM5c**, **TS3c** and **IM6c** in annulation processes by **IM4c** and numbers of bond critical points (BCPs No.).

**Table S12** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM5c**, **TS3c** and **IM6c** in annulation processes by **IM4c**.

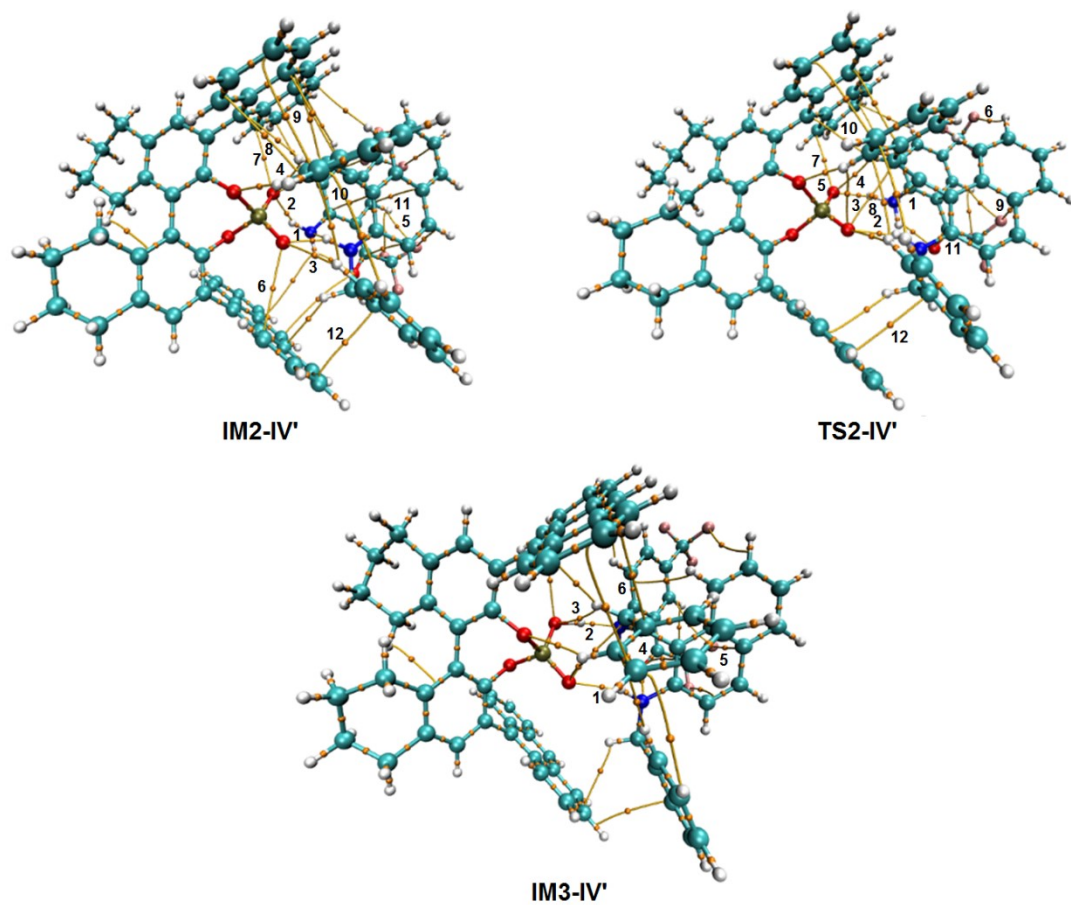
	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM5c</b>	1	N-H...O	1.97	0.0227	0.0711	0.018	-0.0183	-0.0003
	2	O-H...O	1.81	0.0298	0.1139	0.0265	-0.0246	0.0019
	3	N-H...N	2.32	0.0146	0.0533	0.0120	-0.0108	0.0013
	4	C-H...F	2.43	0.0090	0.0392	0.0085	-0.0071	0.0013
	5	C-H...O	2.60	0.0098	0.0373	0.0080	-0.0067	0.0013
	6	p- $\pi$	3.63	0.0031	0.0117	0.0023	-0.0017	0.0006
	7	p- $\pi$	3.00	0.0086	0.0342	0.0073	-0.0061	0.0012
	8	$\pi$ - $\pi$	3.18	0.0078	0.0250	0.0051	-0.0039	0.0011
	9	$\pi$ - $\pi$	2.98	0.0115	0.0398	0.0082	-0.0064	0.0017
	10	van der Waals	2.74	0.0162	0.0659	0.0144	-0.0124	0.0021
	11	van der Waals	2.97	0.0109	0.0373	0.0089	-0.0085	0.0004
<b>TS3c</b>	1	C...C	2.28	0.0523	0.0448	0.0192	-0.0273	-0.0080
	2	N-H...O	2.12	0.0189	0.0864	0.0185	-0.0153	0.0031
	3	O-H...O	1.65	0.0497	0.1251	0.0422	-0.0530	-0.0109
	4	N-H...O	2.08	0.0190	0.0794	0.0170	-0.0142	0.0028
	5	C-H...F	2.51	0.0082	0.0357	0.0070	-0.0052	0.0019
	6	C-H...O	2.41	0.0101	0.0404	0.0083	-0.0064	0.0019
	7	p- $\pi$	2.97	0.0091	0.0349	0.0072	-0.0057	0.0015
	8	p- $\pi$	2.88	0.0108	0.0422	0.0089	-0.0072	0.0017
	9	p- $\pi$	2.77	0.0143	0.0577	0.0125	-0.0106	0.0019
	10	$\pi$ - $\pi$	3.24	0.0083	0.0255	0.0055	-0.0046	0.0009
<b>IM6c</b>	1	O-H...N	1.56	0.0748	0.0745	0.0469	-0.0752	-0.0283
	2	O-H...O	1.81	0.0301	0.1199	0.0293	-0.0286	0.0007
	3	N-H...O	1.91	0.0260	0.1052	0.0241	-0.0220	0.0022
	4	p-p	2.99	0.0109	0.0438	0.0092	-0.0075	0.0017
	5	p- $\pi$	3.20	0.0072	0.0264	0.0053	-0.0041	0.0013
	6	$\pi$ - $\pi$	3.50	0.0050	0.0150	0.0031	-0.0024	0.0007
	7	$\pi$ - $\pi$	3.40	0.0056	0.0169	0.0035	-0.0027	0.0007



**Figure S12** QTAIM analyses of intermolecular interactions in **IM2-IV**, **TS2-IV** and **IM3-IV** in pathway **IV** and numbers of bond critical points (BCPs No.).

**Table S13** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM2-IV**, **TS2-IV** and **IM3-IV** in pathway **IV**.

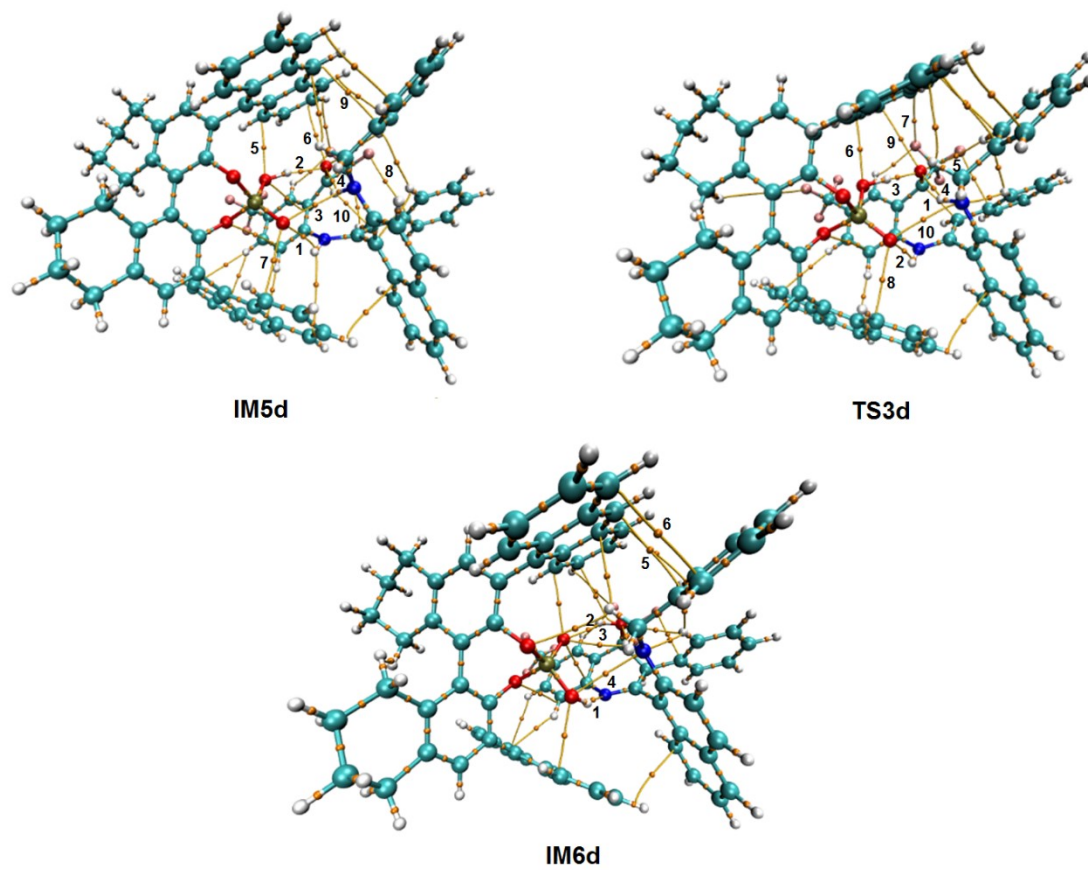
	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-IV</b>	1	N-H...O	1.66	0.0513	0.1387	0.0447	-0.0547	-0.0100
	2	N-H...O	1.90	0.0250	0.1094	0.0245	-0.0216	0.0029
	3	C-H...O	2.76	0.0049	0.0188	0.0037	-0.0027	0.0010
	4	C-H...O	2.27	0.0155	0.0604	0.0128	-0.0105	0.0023
	5	C-H...F	2.25	0.0145	0.0689	0.0141	-0.0110	0.0031
	6	p- $\pi$	3.14	0.0072	0.0263	0.0054	-0.0041	0.0012
	7	p- $\pi$	3.30	0.0069	0.0219	0.0045	-0.0035	0.0010
	8	$\pi$ - $\pi$	3.39	0.0061	0.0185	0.0038	-0.0029	0.0008
	9	$\pi$ - $\pi$	3.53	0.0067	0.0193	0.0040	-0.0032	0.0008
	10	$\pi$ - $\pi$	3.37	0.0068	0.0206	0.0043	-0.0034	0.0008
<b>TS2-IV</b>	11	$\pi$ - $\pi$	3.36	0.0067	0.0198	0.0041	-0.0033	0.0008
	1	C...N	2.23	0.0492	0.0743	0.0257	-0.0328	-0.0071
	2	N-H...O	1.83	0.0324	0.1220	0.0303	-0.0300	0.0002
	3	N-H...O	1.72	0.0419	0.1447	0.0397	-0.0431	-0.0035
	4	N-H...O	2.41	0.0126	0.0461	0.0097	-0.0078	0.0019
	5	C-H...O	2.50	0.0079	0.0305	0.0061	-0.0046	0.0015
	6	C-H...O	3.09	0.0090	0.0305	0.0064	-0.0052	0.0012
	7	p- $\pi$	3.39	0.0039	0.0159	0.0030	-0.0020	0.0010
	8	p- $\pi$	3.17	0.0090	0.0290	0.0062	-0.0052	0.0010
	9	p- $\pi$	3.40	0.0063	0.0188	0.0039	-0.0030	0.0009
	10	$\pi$ - $\pi$	3.14	0.0107	0.0305	0.0068	-0.0061	0.0008
	11	$\pi$ - $\pi$	3.37	0.0065	0.0196	0.0041	-0.0032	0.0009
12	$\pi$ - $\pi$	2.23	0.0492	0.0743	0.0257	-0.0328	-0.0071	
<b>IM3-IV</b>	1	N-H...O	1.96	0.0230	0.1004	0.0221	-0.0191	0.0030
	2	O-H...N	1.63	0.0652	0.0742	0.0411	-0.0636	-0.0225
	3	C-H...O	2.94	0.0048	0.0170	0.0034	-0.0025	0.0009
	4	p- $\pi$	3.16	0.0091	0.0290	0.0062	-0.0052	0.0010
	5	$\pi$ - $\pi$	3.41	0.0063	0.0184	0.0038	-0.0029	0.0008
	6	$\pi$ - $\pi$	3.43	0.0060	0.0182	0.0037	-0.0029	0.0008



**Figure S13** QTAIM analyses of intermolecular interactions in **IM2-IV'**, **TS2-IV'** and **IM3-IV'** in pathway **IV'** and numbers of bond critical points (BCPs No.).

**Table S14** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM2-IV'**, **TS2-IV'** and **IM3-IV'** in pathway **IV'**.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM2-IV'</b>	1	N-H...O	1.69	0.0465	0.1377	0.0413	-0.0482	-0.0069
	2	N-H...O	1.87	0.0309	0.1153	0.0283	-0.0278	0.0005
	3	C-H...O	2.58	0.0071	0.0266	0.0053	-0.0040	0.0013
	4	C-H...O	2.39	0.0105	0.0425	0.0087	-0.0067	0.0020
	5	C-H...F	2.29	0.0136	0.0642	0.0131	-0.0102	0.0029
	6	p- $\pi$	3.39	0.0046	0.0163	0.0032	-0.0023	0.0009
	7	p- $\pi$	3.08	0.0075	0.0285	0.0058	-0.0044	0.0013
	8	$\pi$ - $\pi$	3.42	0.0063	0.0194	0.0040	-0.0031	0.0009
	9	$\pi$ - $\pi$	3.41	0.0065	0.0198	0.0041	-0.0032	0.0009
	10	$\pi$ - $\pi$	3.32	0.0062	0.0197	0.0041	-0.0032	0.0009
	11	$\pi$ - $\pi$	3.40	0.0060	0.0178	0.0037	-0.0029	0.0008
	12	$\pi$ - $\pi$	3.32	0.0068	0.0208	0.0044	-0.0035	0.0008
<b>TS2-IV'</b>	1	C...N	2.25	0.0471	0.0787	0.0259	-0.0322	-0.0063
	2	N-H...O	1.80	0.0335	0.1268	0.0316	-0.0315	0.0001
	3	N-H...O	1.62	0.0559	0.1445	0.0488	-0.0615	-0.0127
	4	C-H...O	2.41	0.0123	0.0447	0.0093	-0.0073	0.0019
	5	C-H...O	2.34	0.0108	0.0428	0.0086	-0.0065	0.0021
	6	C-H...F	2.68	0.0048	0.0204	0.0039	-0.0027	0.0012
	7	p- $\pi$	3.16	0.0066	0.0259	0.0052	-0.0038	0.0013
	8	p- $\pi$	3.10	0.0092	0.0313	0.0066	-0.0054	0.0012
	9	p- $\pi$	2.98	0.0085	0.036	0.0072	-0.0054	0.0018
	10	$\pi$ - $\pi$	3.31	0.0075	0.0228	0.0048	-0.0039	0.0009
	11	$\pi$ - $\pi$	2.97	0.0085	0.0349	0.0072	-0.0056	0.0016
	12	$\pi$ - $\pi$	3.20	0.0078	0.0240	0.0051	-0.0042	0.0009
<b>IM3-IV'</b>	1	N-H...O	1.94	0.0232	0.1015	0.0223	-0.0192	0.0031
	2	O-H...N	1.57	0.0746	0.0654	0.0452	-0.0739	-0.0288
	3	C-H...O	2.57	0.0100	0.0387	0.0079	-0.0062	0.0017
	4	p- $\pi$	3.11	0.0079	0.0247	0.0053	-0.0043	0.0009
	5	p- $\pi$	2.98	0.0081	0.0342	0.0068	-0.0050	0.0018
	6	$\pi$ - $\pi$	3.36	0.0065	0.0194	0.0040	-0.0031	0.0009



**Figure S14** QTAIM analyses of intermolecular interactions in **IM5d**, **TS3d** and **IM6d** in annulation processes by **IM4d** and numbers of bond critical points (BCPs No.).



**Table S15** Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms ( $d$ , in Å), classifications of the intermolecular interactions, electron density ( $\rho$ , 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 **IM5d**, **TS3d** and **IM6d** in annulation processes by **IM4d**.

	BCPs No.	Classification	$d$	$\rho$	$\nabla^2\rho$	$G$	$V$	$H$
<b>IM5d</b>	1	N-H...O	2.19	0.0169	0.0738	0.0156	-0.0128	0.0028
	2	O-H...O	1.81	0.0321	0.1117	0.0290	-0.0301	-0.0011
	3	N-H...O	2.42	0.0121	0.0495	0.0103	-0.0081	0.0021
	4	N-H...O	2.12	0.0178	0.0805	0.0171	-0.0140	0.0031
	5	p- $\pi$	2.89	0.0106	0.0428	0.0089	-0.0071	0.0018
	6	p- $\pi$	3.21	0.0066	0.0247	0.0049	-0.0036	0.0013
	7	p- $\pi$	2.93	0.0100	0.0384	0.0080	-0.0063	0.0016
	8	p- $\pi$	3.39	0.0041	0.0162	0.0031	-0.0021	0.0010
	9	$\pi$ - $\pi$	3.20	0.0081	0.0247	0.0053	-0.0044	0.0009
	10	$\pi$ - $\pi$	2.89	0.0133	0.0405	0.0092	-0.0083	0.0009
<b>TS3d</b>	1	C...C	2.19	0.0597	0.0468	0.0228	-0.0340	-0.0111
	2	N-H...O	2.08	0.0204	0.0884	0.0192	-0.0163	0.0029
	3	O-H...O	1.56	0.0652	0.1212	0.0521	-0.0739	-0.0218
	4	N-H...O	1.93	0.0254	0.1070	0.0244	-0.0220	0.0024
	5	C-H...O	2.89	0.0041	0.0138	0.0028	-0.0021	0.0007
	6	p- $\pi$	1.10	0.2751	-0.9289	0.0418	-0.3158	-0.2740
	7	p- $\pi$	3.17	0.0056	0.0248	0.0048	-0.0033	0.0014
	8	p- $\pi$	2.91	0.0105	0.0409	0.0085	-0.0068	0.0017
	9	$\pi$ - $\pi$	3.25	0.0063	0.0223	0.0045	-0.0033	0.0011
	10	van der Waals	2.94	0.0111	0.0462	0.0095	-0.0076	0.0020
<b>IM6d</b>	1	O-H...N	1.80	0.0417	0.0894	0.0290	-0.0357	-0.0067
	2	O-H...O	1.94	0.0227	0.0973	0.0217	-0.0190	0.0026
	3	N-H...O	2.47	0.0095	0.0358	0.0073	-0.0056	0.0017
	4	p-p	2.98	0.0105	0.0422	0.0088	-0.0070	0.0018
	5	$\pi$ - $\pi$	3.35	0.0082	0.0245	0.0053	-0.0045	0.0008
	6	$\pi$ - $\pi$	3.20	0.0060	0.0178	0.0037	-0.0030	0.0008

#### 4. Calculation of ee Value

To compare the calculated results with the experimental results, the ee values of pathways **I'** and **IV** are calculated using the Gibbs free energy as follows:

$$\Delta G_{act}(TSII - I') = G(TSII - I') - (G(R1) + G(R2) + G(C1)) \quad \text{formula (1)}$$

$$\Delta G_{act}(TSII - IV) = G(TSII - IV) - (G(R1) + G(R2) + G(C1)) \quad \text{formula (2)}$$

$$\begin{aligned} P(TSII - I') : mP(TSII - IV) \\ = \exp\left(-\frac{\Delta G_{act}(TSII - I')}{RT}\right) : \exp\left(-\frac{\Delta G_{act}(TSII - IV)}{RT}\right) \\ = 2.3 \times 10^3 : 1 \end{aligned}$$

In the above formula,  $R = 1.987 \times 10^{-3} \text{ kcal} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ ,  $T = 298.15 \text{ K}$ .

$$e.e. = \frac{[P] - [mP]}{[P] + [mP]} \times 100\% = 99\% \quad \text{formula (3)}$$

## 5. Cartesian Coordinates

### R1

C	0.36728500	5.25794800	0.38336400
C	-0.81164000	4.62919700	0.07575400
C	-0.85468200	3.22877400	-0.13631200
C	0.34020500	2.46803400	-0.02668000
C	1.54581100	3.14353500	0.29297500
C	1.55656100	4.50103800	0.49189300
H	-2.97821700	3.13676900	-0.53270000
H	0.39209100	6.33053500	0.54383100
H	-1.73512000	5.19554600	-0.01130100
C	-2.06325300	2.55583200	-0.45486200
C	0.29358200	1.05515800	-0.24403900
H	2.46001900	2.56464800	0.37768300
H	2.48861200	5.00096100	0.73619300
C	-0.91611300	0.42310400	-0.55968100
C	-2.10235900	1.20504000	-0.65869200
H	-3.04477000	0.71720200	-0.87986000
C	1.47367100	0.26320100	-0.15061100
C	2.45203800	-0.45398300	-0.08335300
C	3.62296700	-1.27042400	0.00556300
C	4.87985400	-0.68338400	0.21649000
C	3.53284500	-2.66502200	-0.11585800
C	6.01601200	-1.47651700	0.30358900
H	4.94988100	0.39520900	0.30973800
C	4.67432800	-3.45073100	-0.02879600
H	2.56175100	-3.12201200	-0.27604600
C	5.91829700	-2.86063800	0.18103300
H	6.98305100	-1.01223800	0.46728400
H	4.59260000	-4.52853100	-0.12429800
H	6.80841900	-3.47719700	0.24895500
N	-0.95366800	-0.93594000	-0.75345600
H	-0.05151900	-1.38469100	-0.80884900
C	-2.08025300	-1.62011900	-1.34363500
H	-2.43748100	-1.09041000	-2.23918400
H	-1.71789000	-2.59435300	-1.68712100
C	-3.24837500	-1.83701500	-0.39575400
C	-3.06953000	-1.83654500	0.98645600
C	-4.52364200	-2.06135900	-0.91700500
C	-4.14962800	-2.06696300	1.83406500
H	-2.07994500	-1.64437700	1.38938600
C	-5.60256600	-2.29568700	-0.07102300
H	-4.67237700	-2.05024400	-1.99445400

C	-5.41730400	-2.29922300	1.30902200
H	-4.00016800	-2.06088100	2.90916100
H	-6.58932300	-2.46803600	-0.48891300
H	-6.25861200	-2.47581900	1.97126800
<b>C1</b>			
P	0.00381100	-1.45560600	0.02320700
O	0.98786700	-0.43959300	0.81027700
O	-0.97186100	-0.45926600	-0.78406300
O	-0.57601900	-2.44846700	0.92725100
C	1.52073900	0.60938200	0.07126700
C	0.69501200	1.68482900	-0.25270900
C	2.85480700	0.53345600	-0.32636800
C	3.34293800	1.58515200	-1.09600200
C	2.53303800	2.64615200	-1.50756800
H	4.38309100	1.55726900	-1.41263100
C	-1.51802400	0.58723600	-0.04595400
C	-0.70427500	1.67664700	0.26677500
C	-2.85303800	0.50341500	0.34383600
C	-3.35080700	1.55715300	1.10542900
C	-2.55284800	2.62833000	1.51204800
H	-4.39161600	1.52120700	1.41873000
C	-1.20947400	2.68555700	1.11086300
C	-0.28463200	3.75108700	1.67256500
C	-1.02848600	4.97464500	2.20068300
H	-1.45159100	5.54198900	1.36088400
C	-2.15287400	4.54171700	3.13631800
H	-2.64058200	5.40798600	3.59285000
C	-3.17818100	3.71446500	2.36623500
H	-3.90277600	3.26219900	3.05096800
H	0.27862200	3.29114500	2.49721900
C	1.18926000	2.69190700	-1.10593800
C	0.25242700	3.74187600	-1.67671200
C	0.98198000	4.96969700	-2.21465900
H	1.39795300	5.54896200	-1.37946200
C	2.11177000	4.54248000	-3.14639400
H	2.58981600	5.41069800	-3.60936700
C	3.14622800	3.73324000	-2.36941600
H	3.71286900	4.41202300	-1.71760800
H	-0.30488300	3.26809000	-2.49753500
H	-3.75344200	4.38149100	1.70985000
H	-1.73066100	3.94246700	3.95271100
H	-0.32577900	5.63854800	2.71273100
H	0.46718900	4.04721500	0.93822900

H	-0.50315500	4.03450000	-0.94489100
H	0.27172200	5.62095500	-2.73242300
H	1.69699600	3.93209900	-3.95833600
H	3.87684300	3.28482900	-3.05033500
O	0.82811400	-1.98184200	-1.23500900
H	1.36397100	-2.76087700	-1.03289500
C	4.17062800	-0.02158100	3.70798900
C	3.74647300	0.14610600	2.42380600
C	4.13048100	-0.77175300	1.39337500
C	4.98268000	-1.86992700	1.75260400
C	5.40622000	-2.00834800	3.11200800
C	5.01292100	-1.11573800	4.06162600
C	3.70992000	-0.62634800	0.05601100
C	5.38405200	-2.77776500	0.77304200
C	4.96627000	-2.65146200	-0.55077100
C	4.10822400	-1.55944100	-0.92212700
C	3.66643100	-1.48532400	-2.28574400
H	2.98762600	-0.68945300	-2.57096400
C	4.06315500	-2.41207400	-3.20380900
C	4.93411900	-3.47999100	-2.83593800
C	5.36703700	-3.59440300	-1.55037500
H	3.86598300	0.68439700	4.47365700
H	3.10880200	0.98514400	2.16753300
H	6.04989000	-2.84560000	3.36671600
H	5.33860100	-1.23030700	5.09028000
H	6.03331700	-3.60553600	1.04890700
H	3.70978100	-2.34166100	-4.22734500
H	5.24144100	-4.20266400	-3.58464400
H	6.02273600	-4.40833000	-1.25404500
C	-4.08382000	-2.40832000	3.23421100
C	-3.65967400	-1.50709000	2.30474600
C	-4.11442500	-1.57770900	0.94740100
C	-5.00226900	-2.64817000	0.58771100
C	-5.42811700	-3.56819700	1.59734800
C	-4.99012600	-3.45053500	2.88065900
C	-3.70906300	-0.65575700	-0.03611300
C	-5.42852000	-2.77288000	-0.73326700
C	-5.00909900	-1.88237900	-1.72116100
C	-4.13519000	-0.79857600	-1.37125400
C	-3.73998400	0.10736300	-2.40813400
H	-3.08714700	0.93717500	-2.15903600
C	-4.17042300	-0.05945200	-3.69054200
C	-5.03304500	-1.14043600	-4.03534600
C	-5.43926400	-2.01982500	-3.07853100

H	-3.71923100	-2.34331300	4.25409800
H	-2.95132500	-0.73354000	2.57914800
H	-6.10735200	-4.36641400	1.31107500
H	-5.31749700	-4.15524500	3.63822400
H	-6.09974100	-3.58591400	-1.00084500
H	-3.85566800	0.63712700	-4.46087600
H	-5.36428900	-1.25523700	-5.06230200
H	-6.09942300	-2.84645000	-3.32637100

**COM1A**

P	-0.61443000	-0.57774200	1.00693200
O	0.03340400	-0.73489800	-0.46728500
O	-2.12131000	-1.10076200	0.79756700
O	-0.42981500	0.80032400	1.48519900
C	-0.18416700	-1.95551800	-1.09915700
C	-1.44676600	-2.21537100	-1.62932900
C	0.86927300	-2.86442300	-1.16179200
C	0.59667500	-4.09772000	-1.74615100
C	-0.67606500	-4.43756100	-2.21212800
H	1.40119700	-4.82594600	-1.81956300
C	-2.78610700	-0.59676800	-0.31651000
C	-2.46717000	-1.12709400	-1.56687000
C	-3.72555500	0.41680800	-0.13498800
C	-4.34894600	0.89954800	-1.28350000
C	-4.01432600	0.44982900	-2.56244900
H	-5.09232200	1.68601600	-1.17580700
C	-3.04512100	-0.55435500	-2.71659600
C	-2.54167300	-0.93108300	-4.09855200
C	-3.52202200	-0.57288700	-5.21194100
H	-4.39832000	-1.23263900	-5.15927700
C	-3.97184500	0.87766700	-5.06913100
H	-4.60789200	1.17694300	-5.90725500
C	-4.72528700	1.06191600	-3.75454300
H	-4.90775200	2.12373400	-3.55900000
H	-1.59951000	-0.38739800	-4.26187700
C	-1.71643000	-3.49840800	-2.14515100
C	-3.13523000	-3.89145500	-2.51492900
C	-3.19989400	-5.11259900	-3.42804600
H	-2.82833400	-4.84853600	-4.42720200
C	-2.34906000	-6.24104700	-2.85357900
H	-2.45380200	-7.15422300	-3.44668600
C	-0.88387700	-5.81619500	-2.80964300
H	-0.48286800	-5.81306100	-3.83232800
H	-3.66698400	-4.11525700	-1.57913300

H	-5.71484100	0.59362600	-3.84358600
H	-3.08937800	1.52997800	-5.08827500
H	-3.05161000	-0.74325600	-6.18471700
H	-2.27696300	-1.98932200	-4.14581000
H	-3.67152000	-3.04981000	-2.95871300
H	-4.24065000	-5.42781600	-3.54702200
H	-2.69825800	-6.47375400	-1.83980600
H	-0.28731500	-6.54484600	-2.25134500
O	-0.08615500	-1.78162600	1.88068200
H	0.69463100	-1.57395100	2.42565100
C	3.24419600	-0.03600700	-3.29304600
C	2.47358900	-0.90762700	-2.58295600
C	2.98971600	-1.57174500	-1.42213200
C	4.33870800	-1.28126900	-1.02514800
C	5.11494100	-0.36426900	-1.80233400
C	4.58838200	0.23503900	-2.90462300
C	2.23305100	-2.50164800	-0.68160200
C	4.87833200	-1.91270300	0.09482900
C	4.13774100	-2.83343000	0.83650900
C	2.78236200	-3.12474000	0.45603700
C	2.03705300	-4.04295500	1.26697700
H	0.99878600	-4.23310400	1.01695400
C	2.60926700	-4.65478900	2.34404200
C	3.96874700	-4.39935000	2.69155200
C	4.70324100	-3.51031600	1.96404300
H	2.83354300	0.45856700	-4.16809900
H	1.45680300	-1.11217900	-2.89991500
H	6.12979700	-0.14301800	-1.47959700
H	5.18283300	0.93731100	-3.47971800
H	5.90226500	-1.68821900	0.38560800
H	2.02518100	-5.34370900	2.94594600
H	4.41035900	-4.90901200	3.54213600
H	5.73573900	-3.29533100	2.22604400
C	-2.67330500	4.44912100	0.84546100
C	-2.99206500	3.15874500	0.54477500
C	-3.64866500	2.31240800	1.49706000
C	-3.92748000	2.85764300	2.79687600
C	-3.57518400	4.21645800	3.07400500
C	-2.97396700	4.99059500	2.12952800
C	-4.00452500	0.97786200	1.21632200
C	-4.52791900	2.05482100	3.76475100
C	-4.87000300	0.72883900	3.50224900
C	-4.61027400	0.17512900	2.20344600
C	-4.99454200	-1.18427900	1.96606100

H	-4.81930100	-1.61605300	0.98649900
C	-5.57515500	-1.93410300	2.94489500
C	-5.82095900	-1.38374800	4.23651800
C	-5.48086800	-0.09249800	4.50168400
H	-2.17857000	5.06665900	0.10246500
H	-2.74336200	2.76290100	-0.43352200
H	-3.79887600	4.61264700	4.06077900
H	-2.71083500	6.02010200	2.35011400
H	-4.73218700	2.47130000	4.74872600
H	-5.85556900	-2.96263200	2.74203600
H	-6.28269400	-1.99841100	5.00234300
H	-5.66706000	0.34274000	5.47972200
C	7.79002800	2.29234200	-0.33351100
C	6.87902400	2.88692500	-1.17162800
C	5.48853900	2.78164900	-0.92767200
C	5.03102800	2.05741100	0.20605300
C	5.99228700	1.46620200	1.06617500
C	7.33489300	1.57615600	0.79779500
H	4.87224100	3.88526100	-2.68385800
H	8.85345800	2.37158500	-0.53289600
H	7.21254400	3.44075800	-2.04578400
C	4.52452300	3.32750200	-1.81777400
C	3.62897000	1.90048100	0.42052600
H	5.64201400	0.91218500	1.93190900
H	8.05637700	1.11003200	1.46205100
C	2.69844300	2.42976200	-0.48744500
C	3.18481300	3.14999400	-1.62197000
H	2.47142300	3.57949200	-2.31725900
C	3.13450800	1.17567800	1.54128100
C	2.63018700	0.58801300	2.47642800
C	2.00100500	-0.13147300	3.54209200
C	2.47031500	-1.40444900	3.90795200
C	0.85536500	0.38748800	4.17186600
C	1.80167500	-2.14248000	4.88095200
H	3.34225600	-1.81272700	3.40757700
C	0.19826900	-0.35929500	5.14056500
H	0.47022300	1.34830100	3.85206300
C	0.66662600	-1.62343400	5.49785700
H	2.16665900	-3.13079000	5.14238700
H	-0.69743000	0.03984000	5.60485900
H	0.13939100	-2.20642200	6.24566000
N	1.36100700	2.28615900	-0.27096600
H	1.06537300	1.77097800	0.55250800
C	0.35570700	2.43680500	-1.29228600



H	0.71153700	2.00521300	-2.24058000
H	-0.49967700	1.82752900	-0.97985900
C	-0.12108800	3.85832600	-1.53554400
C	0.44683700	4.95316500	-0.88715200
C	-1.16781500	4.07467200	-2.43660100
C	-0.01358600	6.24346100	-1.14598400
H	1.24603700	4.78517800	-0.17217800
C	-1.63750000	5.35894000	-2.68714200
H	-1.62280800	3.22139800	-2.93703700
C	-1.05564700	6.45117700	-2.04424400
H	0.44098800	7.08789900	-0.63725500
H	-2.45683800	5.50969200	-3.38309900
H	-1.41706800	7.45536900	-2.24078600

### TS1A

Value of imaginary frequency = -1179.88 cm<sup>-1</sup>

P	0.64559000	0.02187500	-0.76139700
O	0.47551600	-1.10354600	0.42070300
O	2.21341000	-0.17221400	-1.15190400
O	0.35018600	1.34637700	-0.15290900
C	0.94128700	-2.36569600	0.10102800
C	2.32030000	-2.59899900	0.12982100
C	0.02189300	-3.34836000	-0.26173100
C	0.53510200	-4.59282400	-0.61934600
C	1.90650900	-4.84758600	-0.67360800
H	-0.16168800	-5.37938800	-0.90041700
C	3.09034700	-0.25793800	-0.08558300
C	3.20064000	-1.47988800	0.58176700
C	3.79379900	0.88113900	0.30563800
C	4.68192200	0.73955400	1.36844900
C	4.81244300	-0.45708200	2.07616100
H	5.25294900	1.60871800	1.68719200
C	4.03405500	-1.56844500	1.71355600
C	3.99091200	-2.79614200	2.60693300
C	5.21284700	-2.92641800	3.51201800
H	6.09373000	-3.18529500	2.90935600
C	5.46938200	-1.61180300	4.24213800
H	6.28989500	-1.71308300	4.95885400
C	5.79215800	-0.51372600	3.23264500
H	5.82915900	0.46405000	3.72388000
H	3.09044800	-2.71137800	3.23245800
C	2.81483300	-3.83736900	-0.32084100
C	4.30435400	-4.03362700	-0.54044200
C	4.71262000	-5.50271500	-0.60420900

H	4.61941400	-5.95744000	0.39127700
C	3.81841300	-6.25151900	-1.58789400
H	4.15160500	-7.28602200	-1.71430900
C	2.37282900	-6.22698900	-1.09877500
H	2.27743800	-6.90533600	-0.23980300
H	4.55898300	-3.55048700	-1.49444200
H	6.79803000	-0.68995500	2.82734100
H	4.57392700	-1.33751400	4.81409700
H	5.05925800	-3.74534600	4.22122300
H	3.84993900	-3.70642200	2.02114100
H	4.88654300	-3.50348500	0.21622300
H	5.76488000	-5.58061400	-0.89386100
H	3.88493400	-5.76923200	-2.57123900
H	1.69851100	-6.61525400	-1.86905100
O	-0.12227300	-0.41994900	-2.00026600
H	-1.19021200	0.35578000	-2.14830000
C	-2.23130000	-2.87462200	3.36391600
C	-1.51116200	-2.95823500	2.20758200
C	-2.15978000	-2.97172000	0.93000800
C	-3.59323900	-2.87638400	0.90374300
C	-4.31063400	-2.81614500	2.14033300
C	-3.65538300	-2.81525100	3.33436200
C	-1.44784100	-3.09144400	-0.28077100
C	-4.26261000	-2.86804800	-0.32032300
C	-3.56464800	-2.93969300	-1.52502000
C	-2.13215200	-3.04676700	-1.51175700
C	-1.44693600	-3.07732300	-2.77084100
H	-0.36347500	-3.09451000	-2.77192000
C	-2.13668600	-3.03075600	-3.94511100
C	-3.56064100	-2.95690800	-3.95450800
C	-4.24997900	-2.90913400	-2.78125500
H	-1.71733200	-2.86757700	4.32012300
H	-0.42874200	-3.01979500	2.24448600
H	-5.39597300	-2.76500500	2.09605600
H	-4.20998400	-2.76717000	4.26625300
H	-5.34912000	-2.79124300	-0.33606700
H	-1.59783500	-3.03597400	-4.88689600
H	-4.08915800	-2.92965500	-4.90217900
H	-5.33417000	-2.84098100	-2.76883600
C	1.59537800	3.86996600	2.41670500
C	2.31344200	2.92723400	1.74376900
C	2.78530500	3.16411900	0.40986900
C	2.45434600	4.41838300	-0.20521400
C	1.70382100	5.38448200	0.53862300

C	1.28843600	5.12363500	1.80791000
C	3.50324500	2.20001200	-0.32497200
C	2.84799300	4.66628100	-1.51879500
C	3.55231800	3.71606100	-2.25752600
C	3.88272400	2.45573600	-1.65593000
C	4.58745500	1.49458200	-2.44988700
H	4.84087500	0.53799500	-2.00516000
C	4.93272400	1.76385100	-3.74062100
C	4.60545400	3.01773000	-4.33518600
C	3.94105700	3.96252900	-3.61262900
H	1.23658900	3.66825900	3.42199100
H	2.52338600	1.97041800	2.20901100
H	1.46567200	6.32883900	0.05690800
H	0.71170700	5.85694100	2.36292500
H	2.58446000	5.61371800	-1.98394100
H	5.46184800	1.01886800	-4.32597500
H	4.89193500	3.21457000	-5.36330700
H	3.68998700	4.92495700	-4.05152100
C	-7.67808100	-0.76675900	-0.70306200
C	-7.17181400	-0.51795800	0.55584400
C	-5.87193200	-0.00008500	0.71486200
C	-5.07533800	0.26769900	-0.41993400
C	-5.61079000	0.01912200	-1.69575100
C	-6.88760400	-0.49073400	-1.83128900
H	-5.95536200	0.04965100	2.88141200
H	-8.67842200	-1.16790700	-0.82331000
H	-7.76839400	-0.71967400	1.44172400
C	-5.32093100	0.24175100	2.01915600
C	-3.72304200	0.77226800	-0.23400100
H	-4.99660200	0.20790200	-2.57103900
H	-7.28173700	-0.68504100	-2.82415000
C	-3.18762200	0.92757500	1.09751700
C	-4.05254500	0.67583500	2.21765500
H	-3.67735300	0.84028700	3.22043400
C	-2.92337500	1.10703300	-1.28751700
C	-2.01497200	1.35087600	-2.13853600
C	-1.56945200	2.52011200	-2.90613700
C	-2.42346000	3.60857300	-3.12480500
C	-0.26277900	2.55909600	-3.40243500
C	-1.97343800	4.71858900	-3.82660600
H	-3.43894900	3.57174200	-2.74157200
C	0.18562700	3.67806500	-4.09617700
H	0.39743500	1.71373500	-3.23669300
C	-0.66661600	4.75714700	-4.31068500

H	-2.64158700	5.55751800	-3.99376400
H	1.20612000	3.70029600	-4.46601400
H	-0.31617200	5.62790400	-4.85597900
N	-1.92557500	1.27999600	1.28542600
H	-1.29470600	1.41242400	0.48311300
C	-1.23500600	1.29097700	2.56338800
H	-1.43099400	0.35490200	3.10003000
H	-0.17109500	1.30386900	2.30150800
C	-1.56236800	2.48614200	3.43298700
C	-1.76044100	3.74603000	2.86397700
C	-1.60940000	2.35109200	4.82026400
C	-1.99942400	4.85128900	3.67405800
H	-1.71380700	3.85566800	1.78397000
C	-1.84249900	3.45850900	5.63221900
H	-1.45953700	1.37126500	5.26786700
C	-2.03846100	4.71135200	5.05992200
H	-2.15404400	5.82611400	3.22174400
H	-1.87728900	3.34000900	6.71046900
H	-2.22499300	5.57491600	5.68999000

#### IM1A

P	-0.50566100	-0.26184000	0.74438100
O	-0.35043900	-1.21573200	-0.60749000
O	-2.13668600	-0.35386300	0.96931700
O	-0.15412300	1.12027500	0.26236700
C	-0.89560300	-2.47051700	-0.47130900
C	-2.27832300	-2.61366200	-0.61420600
C	-0.06871600	-3.55395000	-0.16706000
C	-0.67495100	-4.79648000	-0.00401800
C	-2.05809300	-4.96703800	-0.07441000
H	-0.04683600	-5.65461100	0.22568100
C	-2.97481000	-0.28573100	-0.11431800
C	-3.07465100	-1.39877700	-0.95832600
C	-3.74873800	0.86317600	-0.31888000
C	-4.61737600	0.85887800	-1.40944100
C	-4.67770000	-0.19552600	-2.31986200
H	-5.24526300	1.73233200	-1.57258700
C	-3.87650800	-1.32797100	-2.11383600
C	-3.79906200	-2.41310000	-3.17397400
C	-5.00557300	-2.42826300	-4.10852200
H	-5.89150000	-2.78235800	-3.56397400
C	-5.27175300	-1.02559400	-4.64617000
H	-6.07707700	-1.03341600	-5.38704000
C	-5.63115300	-0.09028800	-3.49521100

H	-5.66929500	0.94846400	-3.83990500
H	-2.89148400	-2.22652500	-3.76612700
C	-2.87678600	-3.86286300	-0.35473000
C	-4.38755800	-3.98672500	-0.25556600
C	-4.88540900	-5.42386200	-0.38295200
H	-4.75797100	-5.76935300	-1.41789300
C	-4.10184100	-6.33815000	0.55350600
H	-4.50474100	-7.35552600	0.53978200
C	-2.63103100	-6.35394200	0.14739200
H	-2.52708200	-6.92849000	-0.78345900
H	-4.68216000	-3.59135600	0.72724700
H	-6.64430500	-0.33252400	-3.14574700
H	-4.37033600	-0.65937200	-5.15381800
H	-4.83003600	-3.13464900	-4.92568800
H	-3.65165700	-3.39582300	-2.72193200
H	-4.88508100	-3.34508800	-0.98520300
H	-5.95678600	-5.46272900	-0.16344400
H	-4.19806900	-5.96673500	1.58157400
H	-2.02935300	-6.87822600	0.89717400
O	0.14562700	-0.91185100	1.90517200
C	2.48712800	-2.49053000	-3.45011500
C	1.67518000	-2.79517700	-2.39867900
C	2.21719100	-3.08514400	-1.10414700
C	3.64531500	-3.05628000	-0.94937200
C	4.46112200	-2.75841100	-2.08681900
C	3.90403100	-2.47398700	-3.29622100
C	1.40303900	-3.40191100	0.00312100
C	4.20929500	-3.32126400	0.29942300
C	3.41411800	-3.59746600	1.41226700
C	1.98417700	-3.63071400	1.26889500
C	1.19379100	-3.85523900	2.44434800
H	0.11516300	-3.79845800	2.36127300
C	1.78451800	-4.08020600	3.65240500
C	3.20463300	-4.08547000	3.78267600
C	3.99142900	-3.84012300	2.69913200
H	2.05387700	-2.26375600	-4.41885700
H	0.59921200	-2.81332400	-2.52950700
H	5.54039300	-2.75956900	-1.96083200
H	4.53547100	-2.23713800	-4.14659500
H	5.29219600	-3.31114800	0.40857100
H	1.16852600	-4.23465600	4.53241900
H	3.65326800	-4.26182600	4.75510100
H	5.07358900	-3.81318400	2.79049000
C	-2.61525200	4.70577600	-1.86452000

C	-2.93234200	3.47803200	-1.36138100
C	-3.28734900	3.30525100	0.01885500
C	-3.25302800	4.47026400	0.85963300
C	-2.91342600	5.73973500	0.29081100
C	-2.61359100	5.86188900	-1.03043400
C	-3.65239200	2.05618000	0.56843100
C	-3.54718000	4.34851600	2.21547800
C	-3.90380600	3.12187300	2.77373200
C	-3.97317700	1.95547000	1.93921000
C	-4.40236800	0.72920800	2.54318200
H	-4.48129600	-0.15902500	1.92768700
C	-4.71018600	0.66479200	3.86892300
C	-4.61499600	1.82010300	4.69770300
C	-4.22677700	3.00988300	4.16296500
H	-2.34723800	4.80497600	-2.91268700
H	-2.91129100	2.60784600	-2.00787400
H	-2.89153800	6.60501600	0.94773300
H	-2.34856900	6.82754800	-1.44813700
H	-3.50947500	5.23188600	2.84938900
H	-5.03013600	-0.27710600	4.30244800
H	-4.85906100	1.74579500	5.75264000
H	-4.15895100	3.90269800	4.77858700
C	7.59179000	0.84838900	-2.74714000
C	6.74859000	1.86415900	-3.15999300
C	5.46135400	1.98351900	-2.61474000
C	5.02000900	1.06328300	-1.64632400
C	5.88803700	0.05257200	-1.22262600
C	7.15674700	-0.05443800	-1.77141800
H	4.97487200	3.79325200	-3.71482500
H	8.58591800	0.75724700	-3.17045600
H	7.07492300	2.58312100	-3.90607000
C	4.58680700	3.06891900	-3.00282600
C	3.67254100	1.22375600	-1.06526200
H	5.54948500	-0.64868000	-0.46488700
H	7.81848900	-0.84708500	-1.43658700
C	2.78028500	2.27022800	-1.59204000
C	3.33462900	3.22883100	-2.52369400
H	2.73324500	4.07471600	-2.82939500
C	3.27779700	0.49007800	-0.02870100
C	2.94687000	-0.20486700	1.02086800
C	3.36735400	0.09652400	2.40514900
C	4.40537900	0.99674600	2.67041800
C	2.74776500	-0.58384100	3.45591000
C	4.81494400	1.22045900	3.97726200

H	4.89682400	1.50896700	1.84696200
C	3.16993900	-0.35934400	4.76253400
H	1.92100400	-1.25125100	3.23358100
C	4.19874100	0.53935000	5.02669200
H	5.62110100	1.91858800	4.17863700
H	2.68758200	-0.89114600	5.57667700
H	4.52493600	0.70960500	6.04798400
N	1.53165400	2.30164500	-1.23186900
C	0.53336100	3.28728600	-1.64728000
H	0.68198700	3.56095800	-2.69512000
H	-0.42205300	2.76697500	-1.55605300
C	0.53997200	4.50307000	-0.74866100
C	0.23694500	4.34547300	0.60657300
C	0.82456800	5.77036600	-1.25284700
C	0.23164100	5.45478200	1.44441200
H	-0.00387200	3.35350300	0.98482000
C	0.81394600	6.88061900	-0.41096500
H	1.03891500	5.89581200	-2.31242700
C	0.51987500	6.72193500	0.93910000
H	-0.01382600	5.33026500	2.49453400
H	1.03388900	7.86545400	-0.81088500
H	0.51119300	7.58517800	1.59728900
H	2.30558900	-1.07812300	0.87713200
H	1.09289900	1.60237200	-0.55700700

**COM1B**

P	0.86847200	-0.43099000	-0.11418200
O	2.12958900	-0.33581300	0.88317100
O	0.74019900	1.08052900	-0.67008900
O	-0.33498800	-0.99610400	0.51066100
C	3.30276400	0.12202000	0.28167400
C	3.41557200	1.48225800	0.00349400
C	4.28807500	-0.80775600	-0.05119000
C	5.40909000	-0.31618900	-0.71348000
C	5.52557800	1.02263800	-1.09606400
H	6.20264200	-1.01269500	-0.97463000
C	1.02029500	2.14779200	0.17879300
C	2.35333900	2.39479300	0.51958600
C	-0.03056600	2.94275100	0.64074100
C	0.31545300	4.02958800	1.44340300
C	1.62297200	4.28099200	1.85379100
H	-0.48276500	4.67716800	1.79842400
C	2.65468200	3.43331400	1.42406900
C	4.04577000	3.56430800	2.02083700

C	4.31947000	4.94252100	2.61700600
H	4.41223300	5.68233900	1.81057600
C	3.18320000	5.35043300	3.54890100
H	3.40463100	6.29801200	4.04861700
C	1.88500700	5.47115500	2.75640200
H	1.03199600	5.60934300	3.42846500
H	4.12944900	2.80815100	2.81499000
C	4.51383800	1.93250300	-0.75764100
C	4.54686400	3.35338800	-1.29144000
C	5.94640200	3.80925200	-1.69435900
H	6.56510000	3.94501800	-0.79701400
C	6.59376300	2.76927800	-2.60366400
H	7.56230600	3.11792600	-2.97379000
C	6.76983600	1.45499400	-1.84816400
H	7.58808500	1.56711400	-1.12391400
H	3.89257900	3.38490400	-2.17425100
H	1.93194200	6.37404900	2.13252100
H	3.07024200	4.59127000	4.33303200
H	5.27600200	4.92756400	3.14769000
H	4.81714900	3.30598000	1.29387600
H	4.10440700	4.05136300	-0.57780700
H	5.88730700	4.78190900	-2.19146200
H	5.95287700	2.61026400	-3.47996600
H	7.07581400	0.65538100	-2.53054300
O	1.46729600	-1.19475100	-1.36148200
H	0.84747800	-1.79034800	-1.81610200
C	4.18349100	-2.15744900	4.01478700
C	4.21082800	-1.73104700	2.72085200
C	4.12030000	-2.65855000	1.63250700
C	4.02013700	-4.05506400	1.95037200
C	3.99347700	-4.46069000	3.32204200
C	4.06856200	-3.54367600	4.32497100
C	4.14310000	-2.25218900	0.28203100
C	3.96285100	-4.99203600	0.91994200
C	3.98609800	-4.60388500	-0.41815300
C	4.06298700	-3.20801100	-0.75159200
C	4.03815100	-2.85022300	-2.14063300
H	4.03448200	-1.79981400	-2.41005100
C	3.99792300	-3.80751600	-3.11123000
C	3.95255100	-5.19267900	-2.77594400
C	3.93465800	-5.57354200	-1.46929800
H	4.25112500	-1.43527100	4.82189300
H	4.30642200	-0.67288600	2.50409400
H	3.91181000	-5.52149700	3.54169900



H	4.04581100	-3.86112700	5.36227400
H	3.89928200	-6.04960000	1.16575400
H	3.99476500	-3.51609500	-4.15722300
H	3.92300400	-5.93603000	-3.56605100
H	3.88433900	-6.62380200	-1.19595300
C	-2.76851800	2.16632600	3.83856800
C	-1.88629700	2.31438300	2.80811400
C	-2.33700300	2.41567800	1.44905000
C	-3.74523100	2.26669000	1.20659700
C	-4.63782500	2.11467700	2.31551600
C	-4.17102600	2.08737700	3.59560600
C	-1.46544900	2.65578100	0.36230900
C	-4.22508800	2.28084400	-0.10221000
C	-3.37084600	2.49094200	-1.18296700
C	-1.97077100	2.70950600	-0.95218100
C	-1.14961000	3.02226700	-2.08376000
H	-0.09629900	3.22916200	-1.92799700
C	-1.67645500	3.07826300	-3.34105300
C	-3.05712800	2.80408500	-3.57079800
C	-3.87692400	2.52196200	-2.52098400
H	-2.39876100	2.09651400	4.85671400
H	-0.82273000	2.35266100	3.01313700
H	-5.69893800	2.01979600	2.10348400
H	-4.85727800	1.98222700	4.42982800
H	-5.28732100	2.12578500	-0.28420800
H	-1.03675800	3.33066300	-4.18185600
H	-3.44955300	2.83192100	-4.58213500
H	-4.93367800	2.32038000	-2.67380200
C	-8.20916000	0.31652500	-3.00686400
C	-8.12158300	0.13568300	-1.64981900
C	-6.89834600	-0.24139500	-1.04260100
C	-5.74607300	-0.43795700	-1.85198800
C	-5.86551800	-0.24907400	-3.25490100
C	-7.06389500	0.12010000	-3.81334800
H	-7.66006500	-0.29623700	0.98205200
H	-9.14926300	0.60802700	-3.46301500
H	-8.99208700	0.28143400	-1.01526100
C	-6.77718700	-0.42898500	0.36151600
C	-4.50915600	-0.79468800	-1.23711800
H	-4.98472400	-0.39223300	-3.87363700
H	-7.13474000	0.26309400	-4.88728700
C	-4.40851800	-0.93931100	0.15590400
C	-5.58904600	-0.76869300	0.94372900
H	-5.52961200	-0.90442300	2.01781000

C	-3.32899100	-0.96948700	-2.01490600
C	-2.28527800	-1.14229000	-2.60928400
C	-1.05139400	-1.36671000	-3.29981600
C	-0.51315200	-2.66375800	-3.38778000
C	-0.34670900	-0.29247600	-3.86198800
C	0.70877400	-2.87225600	-4.02215500
H	-1.05977600	-3.49197100	-2.94936500
C	0.86584100	-0.51309900	-4.50394100
H	-0.75533200	0.70682400	-3.76321600
C	1.39726100	-1.79723100	-4.58363800
H	1.12917800	-3.87183200	-4.06674200
H	1.40811100	0.32572300	-4.92776200
H	2.35028900	-1.96036100	-5.07588300
N	-3.21344000	-1.22882600	0.73883200
H	-2.37898800	-1.16191700	0.16683800
C	-2.98632000	-1.17429000	2.16497800
H	-1.90027600	-1.16106500	2.29319900
H	-3.36834900	-0.23547400	2.58591000
C	-3.57698100	-2.33794600	2.93933100
C	-3.78823000	-3.58039600	2.34279800
C	-3.90466300	-2.16978600	4.28596200
C	-4.30761100	-4.63812300	3.08351700
H	-3.54786100	-3.70316700	1.29106400
C	-4.42036700	-3.22678100	5.02924200
H	-3.75497800	-1.19723800	4.75046900
C	-4.62336500	-4.46626000	4.42847600
H	-4.46980800	-5.60036500	2.60737300
H	-4.67146300	-3.08096000	6.07539900
H	-5.03133200	-5.29124600	5.00381300

### TS1B

Value of imaginary frequency = -1215.02 cm<sup>-1</sup>

P	-0.71911900	0.21092200	0.16144400
O	-2.15500000	0.26929300	0.92425500
O	-0.82654500	-1.21850400	-0.62634300
O	0.36001600	0.23024700	1.18181400
C	-3.26405900	-0.03107000	0.15410500
C	-3.53010000	-1.36987400	-0.14046000
C	-4.06435800	1.01146900	-0.31226100
C	-5.15388400	0.66654500	-1.10712900
C	-5.41981100	-0.65169300	-1.47976400
H	-5.79624500	1.46217200	-1.47788600
C	-1.25344900	-2.31706700	0.08751700
C	-2.61172100	-2.41598500	0.40095600

C	-0.33048100	-3.30786700	0.43350000
C	-0.82072900	-4.39748700	1.15213600
C	-2.14814600	-4.48407000	1.57351400
H	-0.13004600	-5.19445600	1.41890400
C	-3.05452400	-3.47429000	1.21754200
C	-4.46293900	-3.47075300	1.78415000
C	-4.92401900	-4.84773500	2.25367800
H	-5.08845200	-5.50003200	1.38527800
C	-3.86890400	-5.47173600	3.16207900
H	-4.21990000	-6.41999600	3.58004700
C	-2.57686600	-5.69480800	2.38090800
H	-1.76472600	-5.98720200	3.05462600
H	-4.46764600	-2.78125400	2.64042100
C	-4.58915500	-1.68338100	-1.01704300
C	-4.75178800	-3.09459500	-1.55582900
C	-6.13582700	-3.36215400	-2.14080200
H	-6.87692400	-3.40673500	-1.33137400
C	-6.51969800	-2.25396800	-3.11583500
H	-7.47081300	-2.47515900	-3.60938500
C	-6.61486200	-0.92461000	-2.37308700
H	-7.52025200	-0.92992500	-1.75075200
H	-3.99733000	-3.23062200	-2.34425600
H	-2.71976800	-6.53835900	1.69173700
H	-3.67951500	-4.79789200	4.00714500
H	-5.88355200	-4.75805800	2.77171400
H	-5.17236200	-3.04925800	1.06890800
H	-4.51093700	-3.83902200	-0.79498700
H	-6.14287300	-4.33887900	-2.63392800
H	-5.75672900	-2.18579900	-3.90152500
H	-6.73512400	-0.09563800	-3.07808700
O	-0.71667300	1.23275600	-0.97349100
H	0.44387800	1.65651000	-1.22253900
C	-4.59234300	2.60076300	3.63661900
C	-4.39445800	2.09249100	2.38773300
C	-3.98834500	2.93457900	1.30261700
C	-3.80856900	4.33465000	1.56644800
C	-4.02924100	4.82731400	2.89118500
C	-4.40644300	3.98998600	3.89624700
C	-3.77551600	2.43980700	0.00100700
C	-3.44095600	5.18914800	0.52725800
C	-3.21007400	4.70819600	-0.76106800
C	-3.35473700	3.30386500	-1.02879800
C	-3.02710300	2.83106400	-2.34239800
H	-3.06659900	1.76527500	-2.53483900

C	-2.62456000	3.69307600	-3.31840600
C	-2.53117500	5.09290100	-3.06352200
C	-2.81495100	5.58155600	-1.82488200
H	-4.89416700	1.94363300	4.44577200
H	-4.53940100	1.03389100	2.20185200
H	-3.88673700	5.88873000	3.07457800
H	-4.56906100	4.37431200	4.89803400
H	-3.33027000	6.25311000	0.72699000
H	-2.36109300	3.31198400	-4.29951000
H	-2.21973300	5.76319300	-3.85805100
H	-2.73631300	6.64524200	-1.61502400
C	2.76773200	-3.42920500	3.40097900
C	1.79064100	-3.28651400	2.45900500
C	2.10022000	-3.28172700	1.05777400
C	3.48637900	-3.33741100	0.68468500
C	4.48175900	-3.48468700	1.70316000
C	4.13622000	-3.55407400	3.02020400
C	1.10765500	-3.22356200	0.05313800
C	3.84115600	-3.24784100	-0.66082500
C	2.87604600	-3.13360900	-1.65950200
C	1.48312300	-3.15653900	-1.30665700
C	0.52948300	-3.13723300	-2.37671100
H	-0.52649300	-3.19874200	-2.14271800
C	0.92834000	-3.04130200	-3.67597200
C	2.31066700	-2.96017200	-4.01429100
C	3.25408100	-3.01388200	-3.03520700
H	2.50469900	-3.43389100	4.45388500
H	0.75805500	-3.16457600	2.76507500
H	5.52213600	-3.55010700	1.39468700
H	4.89794200	-3.68158800	3.78307300
H	4.89207500	-3.27157900	-0.93994300
H	0.18474300	-3.02158400	-4.46607700
H	2.60613300	-2.85867200	-5.05369100
H	4.31331200	-2.95180200	-3.27507300
C	6.12803000	-0.70585800	-4.44374500
C	6.53486100	-0.88984200	-3.13778900
C	5.70732900	-0.49534800	-2.06916100
C	4.45089300	0.09301100	-2.33599900
C	4.06080200	0.29208100	-3.67031500
C	4.88512800	-0.10610300	-4.70483500
H	7.11954700	-1.04450200	-0.51407000
H	6.76504600	-1.01734100	-5.26438500
H	7.49882900	-1.34107000	-2.91819800
C	6.11657300	-0.66651900	-0.69924800

C	3.60483000	0.47192900	-1.21577300
H	3.09140800	0.73747500	-3.87167300
H	4.56411600	0.03961100	-5.73140500
C	3.95524700	0.04924700	0.11732100
C	5.30202200	-0.40751300	0.35275800
H	5.63589700	-0.57329900	1.37028200
C	2.59525700	1.38379700	-1.32088300
C	1.64779400	2.22369900	-1.24264300
C	1.61712400	3.66404700	-0.94277400
C	2.80744700	4.38285900	-0.75609500
C	0.38962000	4.31324000	-0.78075700
C	2.76846300	5.72682400	-0.41274200
H	3.75868200	3.87142500	-0.87673300
C	0.35826600	5.65926500	-0.42733200
H	-0.53334500	3.75480400	-0.91734200
C	1.54104100	6.36760700	-0.24404200
H	3.69480800	6.27523400	-0.27207600
H	-0.60036100	6.14762300	-0.28679700
H	1.51004000	7.41676900	0.03255500
N	3.06047500	0.11071300	1.08494700
H	2.07258700	0.30036500	0.85884100
C	3.34010100	-0.02829200	2.50284500
H	2.36036500	-0.11683200	2.98111500
H	3.87836500	-0.96173500	2.69348900
C	4.10664900	1.15881200	3.05174300
C	3.81251600	2.45084900	2.60914700
C	5.10710900	0.97578600	4.00463000
C	4.50806600	3.54133000	3.11773100
H	3.03732800	2.59867200	1.86051400
C	5.80222200	2.06858500	4.51730000
H	5.34476300	-0.02987000	4.34463200
C	5.50445700	3.35296100	4.07366700
H	4.27018300	4.53957900	2.76367100
H	6.58195000	1.91434900	5.25640100
H	6.04959900	4.20457600	4.46772000

#### IM1B

P	-0.77892000	0.30719100	-0.11613600
O	-2.17006900	0.11658800	0.74255800
O	-0.65128800	-1.19819800	-0.80308200
O	0.31147200	0.46922800	0.90491800
C	-3.24900300	-0.20795400	-0.05013500
C	-3.38948200	-1.53247300	-0.46623300
C	-4.13960100	0.79382800	-0.44083000

C	-5.17121100	0.42780400	-1.29906200
C	-5.29813300	-0.86836000	-1.80422500
H	-5.88008700	1.19069400	-1.61388200
C	-1.05412800	-2.31971800	-0.12948400
C	-2.42439800	-2.53849400	0.06850400
C	-0.09743500	-3.25381400	0.28800500
C	-0.56373500	-4.40680600	0.92022400
C	-1.91044200	-4.61512400	1.20923500
H	0.16227400	-5.15591600	1.22905300
C	-2.85344100	-3.65640000	0.80968500
C	-4.29881300	-3.77396800	1.26197500
C	-4.69497600	-5.19498800	1.65337500
H	-4.74793400	-5.82519000	0.75515800
C	-3.67076100	-5.78077000	2.62022000
H	-3.98554700	-6.76524800	2.97954500
C	-2.31316000	-5.88676400	1.93158200
H	-1.53452100	-6.15663600	2.65277200
H	-4.41978400	-3.11557300	2.13441000
C	-4.39109500	-1.85943800	-1.40314000
C	-4.41387700	-3.23023700	-2.05723800
C	-5.75339700	-3.56457100	-2.70770500
H	-6.51010900	-3.73548800	-1.92991700
C	-6.20329600	-2.41563500	-3.60463000
H	-7.11608700	-2.67496600	-4.14972800
C	-6.43578000	-1.16412200	-2.76318400
H	-7.35871000	-1.29463900	-2.18133000
H	-3.62990200	-3.23813800	-2.82809800
H	-2.34981700	-6.70685800	1.20131400
H	-3.59116200	-5.12728000	3.49819000
H	-5.69493100	-5.18866300	2.09776900
H	-4.98208400	-3.38091500	0.50718000
H	-4.12905700	-4.00984700	-1.34779600
H	-5.66461400	-4.49519100	-3.27661300
H	-5.42526700	-2.21924100	-4.35315000
H	-6.60239400	-0.29321200	-3.40571600
O	-0.96630000	1.25330900	-1.24746600
H	0.92915800	1.46822000	-2.06936900
C	-4.87832500	1.83992500	3.64601500
C	-4.61845800	1.50864100	2.34972900
C	-4.26912800	2.50854500	1.38533600
C	-4.21259700	3.87460800	1.82365100
C	-4.49382500	4.17951400	3.19278000
C	-4.81428300	3.19647700	4.07853600
C	-3.99570400	2.19759500	0.03799100

C	-3.89932600	4.87839400	0.90785500
C	-3.61114900	4.58141600	-0.42273800
C	-3.63977300	3.21566600	-0.86725900
C	-3.27339900	2.93932000	-2.22586000
H	-3.21116800	1.90539500	-2.54330200
C	-2.94855700	3.94813500	-3.08309600
C	-2.96548200	5.30773500	-2.65103700
C	-3.28118900	5.61123400	-1.36110400
H	-5.13601400	1.06469200	4.36049600
H	-4.67086400	0.47284800	2.03275600
H	-4.44371300	5.21830300	3.50776900
H	-5.02375000	3.43928400	5.11543400
H	-3.87396000	5.91378200	1.24060100
H	-2.65650100	3.71767900	-4.10244000
H	-2.70984000	6.09621900	-3.35221400
H	-3.28273700	6.64175200	-1.01487200
C	2.58194200	-3.27458200	3.63542600
C	1.73233600	-3.17854300	2.57146000
C	2.22423100	-3.10848100	1.22473600
C	3.64927600	-3.07826300	1.04158600
C	4.50682700	-3.17668900	2.18386200
C	3.99388900	-3.29025700	3.44216000
C	1.36862900	-3.06329000	0.09667500
C	4.17588200	-2.94715900	-0.24331100
C	3.34625900	-2.86419200	-1.36039200
C	1.91988000	-2.93754200	-1.19725200
C	1.11371500	-2.91607200	-2.38273400
H	0.03847800	-3.00044300	-2.28842200
C	1.67736200	-2.78263200	-3.61603300
C	3.09102700	-2.67556000	-3.76782500
C	3.89869000	-2.72656400	-2.67365200
H	2.18064400	-3.32504800	4.64239100
H	0.66213900	-3.13966900	2.73764300
H	5.58115100	-3.16914900	2.01793300
H	4.65389400	-3.37852300	4.29927700
H	5.25514000	-2.91980300	-0.38052400
H	1.04411200	-2.76006000	-4.49680800
H	3.51932600	-2.56296200	-4.75899100
H	4.97935800	-2.65452000	-2.77152600
C	7.41048000	-0.35786800	-3.30735800
C	7.45149800	-0.43126900	-1.92534700
C	6.31096100	-0.13321000	-1.16472500
C	5.11788600	0.23817200	-1.81199500
C	5.09157700	0.32461000	-3.20636200

C	6.22689000	0.02818600	-3.94537300
H	7.29688700	-0.39605000	0.75746100
H	8.29275300	-0.59383600	-3.89204400
H	8.36746300	-0.71752500	-1.41615000
C	6.34019800	-0.18814100	0.28407200
C	3.93150900	0.53446400	-0.99309300
H	4.16524500	0.60236900	-3.69957900
H	6.19246600	0.08926000	-5.02817900
C	3.95566300	0.21223500	0.44370800
C	5.24796700	-0.01781200	1.05858100
H	5.31496300	-0.08506500	2.13687400
C	2.88594300	1.21472100	-1.45199900
C	1.85514100	1.95359700	-1.74549700
C	1.80832300	3.42016600	-1.55270000
C	2.97705500	4.17512700	-1.40288100
C	0.55867700	4.04467000	-1.48586700
C	2.89836600	5.54247300	-1.18031100
H	3.94476900	3.68473400	-1.46888600
C	0.48994000	5.41696200	-1.26032900
H	-0.34111900	3.44105400	-1.58125100
C	1.65302300	6.16551500	-1.10719500
H	3.80757100	6.12405600	-1.06615100
H	-0.48288100	5.89424100	-1.20416200
H	1.59243500	7.23531400	-0.93298900
N	2.84925500	0.18117500	1.12250000
H	1.89693000	0.31833900	0.68434000
C	2.73892200	0.09377700	2.57961100
H	1.71539300	-0.24124300	2.75992500
H	3.42288500	-0.66645000	2.96466100
C	2.98225600	1.45127200	3.20213000
C	2.22190300	2.54208200	2.76815500
C	3.96370700	1.63489800	4.17271600
C	2.45654700	3.80412500	3.29913500
H	1.44779600	2.38533700	2.01914000
C	4.18985300	2.90041000	4.71150500
H	4.54993000	0.78457400	4.51478000
C	3.44042000	3.98545200	4.27096100
H	1.86962600	4.64838200	2.95183400
H	4.95515900	3.03651900	5.46894600
H	3.62136200	4.97285600	4.68361300
<b>R2</b>			
C	-1.96597400	1.61692000	-0.00003700
C	-1.67281800	0.24096800	0.00013900



C	-0.36347200	-0.17723800	0.00021000
C	0.69813600	0.74996600	0.00013300
C	0.40390900	2.14536500	-0.00000900
C	-0.95748800	2.54468800	-0.00011200
H	-3.00162100	1.94357400	-0.00008200
H	-0.15818800	-1.24019300	0.00035300
H	-1.18750800	3.60547100	-0.00022000
N	1.36660600	3.08726300	-0.00003000
H	2.33779200	2.81383400	0.00009700
H	1.11304600	4.06048300	-0.00030100
C	-2.80586700	-0.73483600	0.00002300
F	-3.59750500	-0.57377100	1.07387500
F	-3.59585300	-0.57549100	-1.07530200
F	-2.38019200	-2.00501600	0.00133400
C	2.08899600	0.30474200	0.00018100
O	3.06593700	1.03263900	0.00019100
C	2.37166200	-1.21738900	-0.00005900
F	1.83968400	-1.80259200	1.08270000
F	3.67447600	-1.45125900	-0.00024500
F	1.83941500	-1.80234000	-1.08280400

#### IM2-I

P	1.34225600	0.32397200	0.67091600
O	1.49924100	1.27710200	-0.67691200
O	2.80983100	0.51828700	1.37033200
O	1.16529900	-1.06250600	0.13505900
C	1.90193800	2.57880600	-0.47694600
C	3.23664100	2.81875400	-0.13636700
C	0.98687800	3.62238300	-0.66224700
C	1.44130700	4.91481600	-0.40764500
C	2.72726300	5.17898100	0.06551100
H	0.75357700	5.74428000	-0.55815200
C	3.91769300	0.52144900	0.54993000
C	4.18817700	1.66928800	-0.20201300
C	4.73325900	-0.60826800	0.49250800
C	5.85255100	-0.54545200	-0.33417300
C	6.13365800	0.56103800	-1.13391300
H	6.50233100	-1.41606600	-0.38759900
C	5.27658400	1.67135400	-1.09900000
C	5.45065700	2.79722200	-2.10540400
C	6.85180600	2.86185600	-2.70747700
H	7.56365600	3.21196400	-1.94779100
C	7.28084100	1.48464800	-3.20206000
H	8.24670900	1.53253600	-3.71400500

C	7.36142600	0.51978600	-2.02315200
H	7.51959300	-0.50578400	-2.37226000
H	4.72228000	2.62918400	-2.91232000
C	3.63596500	4.12239200	0.21745900
C	5.00207400	4.36428100	0.83357600
C	5.45073000	5.82028600	0.74393300
H	5.68486900	6.07346500	-0.29916600
C	4.34433900	6.74049500	1.25101000
H	4.68010400	7.78141900	1.28139900
C	3.11453700	6.61689400	0.35561000
H	3.31780800	7.12158300	-0.59886600
H	4.93880600	4.07433700	1.89191700
H	8.24104100	0.77516000	-1.41636100
H	6.54678600	1.11889700	-3.93125900
H	6.86735200	3.59413900	-3.52045100
H	5.18302500	3.76243700	-1.67319600
H	5.75070600	3.70074600	0.39508000
H	6.37064300	5.95892600	1.31991700
H	4.08464400	6.45580200	2.27842300
H	2.26087500	7.13961700	0.79964000
O	0.33937700	0.93984000	1.59799300
C	0.19390900	1.65829900	-4.40337900
C	0.44268300	2.30472000	-3.22881100
C	-0.62630700	2.74384100	-2.37919200
C	-1.97042700	2.52675300	-2.83744900
C	-2.19040600	1.81429700	-4.05992200
C	-1.14361600	1.38903600	-4.82093400
C	-0.40437900	3.38111000	-1.13685600
C	-3.04230500	3.00114800	-2.08104800
C	-2.83990200	3.65230100	-0.86598200
C	-1.50306700	3.82011900	-0.36371200
C	-1.35317700	4.38761400	0.94557600
H	-0.35932900	4.46042600	1.37155300
C	-2.43739300	4.79501000	1.66615600
C	-3.75892400	4.65313600	1.15013700
C	-3.94952900	4.09040700	-0.07478800
H	1.02270300	1.34840200	-5.03259100
H	1.46558200	2.50056600	-2.92916500
H	-3.21604900	1.62017800	-4.36009600
H	-1.32050000	0.85606700	-5.75000600
H	-4.05848100	2.83693800	-2.43516600
H	-2.29688200	5.20811700	2.66010100
H	-4.60936800	4.95080500	1.75521200
H	-4.95081300	3.93425900	-0.46835200

C	3.32326000	-3.99854100	-1.65540700
C	3.70172600	-2.90021000	-0.94417600
C	4.00324500	-2.99210600	0.45478800
C	3.86347000	-4.27049100	1.09394400
C	3.44724700	-5.39617700	0.31358300
C	3.19387300	-5.26837800	-1.01770100
C	4.42841300	-1.88092800	1.20756000
C	4.15944600	-4.39593900	2.44976300
C	4.55810300	-3.29710000	3.21018900
C	4.67018100	-2.00829000	2.58838100
C	5.04139500	-0.89369800	3.40698700
H	5.11375800	0.08677500	2.94802400
C	5.28722000	-1.04987700	4.73956300
C	5.20078800	-2.33632500	5.34990600
C	4.85050100	-3.42261800	4.60509200
H	3.10148900	-3.91142600	-2.71504900
H	3.76682600	-1.93221700	-1.42820600
H	3.34405100	-6.35614400	0.81222800
H	2.88498900	-6.12802900	-1.60463200
H	4.07117200	-5.36983000	2.92679900
H	5.55699400	-0.19035200	5.34466100
H	5.41517800	-2.44272900	6.40854500
H	4.78236800	-4.40866800	5.05793400
C	-6.82360100	-3.66990000	-0.05355600
C	-6.11523100	-3.63835500	-1.24043000
C	-4.77010400	-3.23668700	-1.25415500
C	-4.13458400	-2.87390100	-0.05091400
C	-4.86830600	-2.88816600	1.13963100
C	-6.19725200	-3.28175900	1.13571900
H	-4.54288800	-3.46794700	-3.40108300
H	-7.86348300	-3.97695200	-0.04628400
H	-6.59218300	-3.91400000	-2.17656600
C	-4.02300600	-3.18239700	-2.49019800
C	-2.71294400	-2.48979200	-0.08223100
H	-4.38523100	-2.58317800	2.06323400
H	-6.75546200	-3.28488200	2.06602800
C	-2.02248000	-2.39030900	-1.37807500
C	-2.73356900	-2.78527200	-2.56888100
H	-2.22146800	-2.75362600	-3.52209900
C	-2.02138100	-2.16859900	1.00877100
C	-1.21560600	-1.76144600	1.94626300
C	-0.33339500	-2.56416300	2.80749000
C	-0.48804700	-3.94470800	2.95487400
C	0.68974700	-1.89652000	3.48840300

C	0.37550900	-4.65157200	3.78179400
H	-1.29046700	-4.45544700	2.42911600
C	1.55116900	-2.60869900	4.31199200
H	0.80742600	-0.82468800	3.35024800
C	1.39255900	-3.98424900	4.46166700
H	0.25334900	-5.72357600	3.89908100
H	2.35841100	-2.09358100	4.82388000
H	2.07006000	-4.53677200	5.10597700
N	-0.79713600	-1.93509900	-1.43343800
C	-0.05623400	-1.65679400	-2.65464700
H	-0.68302800	-1.05048500	-3.32149200
H	0.78308900	-1.03009300	-2.33631700
C	0.45557500	-2.88515100	-3.38277600
C	1.17067000	-2.69130000	-4.56772300
C	0.25391100	-4.18302100	-2.91856500
C	1.67541600	-3.77524300	-5.27566900
H	1.33495000	-1.67965200	-4.93109100
C	0.74754300	-5.27182300	-3.63579900
H	-0.26990200	-4.35228600	-1.98341300
C	1.46109700	-5.07300900	-4.81209700
H	2.23323900	-3.60915100	-6.19155500
H	0.57835600	-6.27745800	-3.26397000
H	1.84916400	-5.92091900	-5.36668300
H	-1.15279800	-0.67574300	2.07426000
H	-0.25814400	-1.67251800	-0.57648200
C	-3.90966300	1.70743100	2.84327100
C	-5.23262000	1.54921800	2.37474100
C	-5.46010000	1.05343200	1.11550400
C	-4.38482800	0.70903800	0.26579100
C	-3.04715700	0.92195000	0.71764200
C	-2.84379300	1.40319800	2.04398500
H	-3.74217100	2.09621000	3.84373300
H	-6.48227500	0.93815900	0.77793700
H	-1.81897400	1.55737700	2.37105700
N	-1.96572500	0.68177700	-0.03757800
H	-2.08037600	0.51967000	-1.02765900
H	-1.06987800	0.98276500	0.34437800
C	-6.35754300	1.99184900	3.24928300
F	-7.55708800	1.66845300	2.74526200
F	-6.27879300	1.45357600	4.47883100
F	-6.35236900	3.32815100	3.42803200
C	-4.60936700	0.18622400	-1.06881100
O	-3.74467100	-0.08307500	-1.89142500
C	-6.06483900	-0.01002000	-1.55197700

F	-6.80334800	-0.72208200	-0.69150300
F	-6.08971000	-0.63656600	-2.72336000
F	-6.65709800	1.18667300	-1.70374300

**IM2-I'**

P	1.33265500	-0.24328800	-0.39582100
O	1.46130100	-1.66540600	0.43792500
O	2.88363100	-0.01629600	-0.87803000
O	0.97038700	0.77492000	0.64808300
C	2.19739200	-2.67716500	-0.13982400
C	3.59104800	-2.56698900	-0.15076100
C	1.54195900	-3.79453800	-0.66199400
C	2.32909800	-4.76613500	-1.27489100
C	3.71315200	-4.63849200	-1.40179600
H	1.83757500	-5.64431300	-1.68804700
C	3.82357600	-0.11999700	0.12688400
C	4.20215200	-1.39603400	0.54488000
C	4.34787300	1.03869500	0.69876200
C	5.25757400	0.87711000	1.73965700
C	5.60859200	-0.37999500	2.23620500
H	5.68531200	1.76643100	2.19743700
C	5.06606900	-1.53287700	1.64925100
C	5.30863000	-2.89822500	2.26839200
C	6.54170000	-2.94173300	3.16678500
H	7.44948800	-2.87638400	2.55200000
C	6.51640800	-1.77799200	4.15269600
H	7.34592100	-1.84521800	4.86309500
C	6.58668900	-0.45638000	3.39306200
H	6.41287500	0.38718400	4.06916300
H	4.42040800	-3.14952200	2.86606900
C	4.35647100	-3.52435400	-0.84357900
C	5.83969500	-3.29545400	-1.07431000
C	6.59124600	-4.56732600	-1.45765200
H	6.65835800	-5.23433300	-0.58754300
C	5.86308300	-5.28653800	-2.58904500
H	6.43550100	-6.15064200	-2.93962400
C	4.48322600	-5.73372900	-2.11458000
H	4.60223500	-6.58153800	-1.42597500
H	5.93524300	-2.56328000	-1.88898600
H	7.60428700	-0.32730200	2.99938400
H	5.58795400	-1.82125600	4.73604400
H	6.58039700	-3.90077500	3.69216500
H	5.36866600	-3.67246800	1.50060000
H	6.30246100	-2.82297400	-0.20504200

H	7.61613400	-4.31648400	-1.74741500
H	5.75841500	-4.60233900	-3.44055100
H	3.88818800	-6.10595900	-2.95503100
O	0.52138700	-0.42581500	-1.63476000
C	-0.32282300	-4.52515700	3.12807500
C	0.26711200	-4.29058700	1.92044900
C	-0.50032000	-4.28786600	0.71111600
C	-1.90454700	-4.57433200	0.80507900
C	-2.48148100	-4.82362900	2.08927600
C	-1.72000800	-4.79092700	3.21850800
C	0.06707800	-3.98396200	-0.54464000
C	-2.69150300	-4.54897600	-0.34650100
C	-2.15034100	-4.21308700	-1.58598800
C	-0.74870600	-3.91053600	-1.68987100
C	-0.24047000	-3.49592500	-2.96523900
H	0.80459000	-3.21695900	-3.04171000
C	-1.06003000	-3.41127200	-4.05189500
C	-2.44625300	-3.73327200	-3.94999600
C	-2.97227600	-4.11676300	-2.75382500
H	0.27578200	-4.50744100	4.03321000
H	1.33106900	-4.08709900	1.86602300
H	-3.55031000	-5.01170000	2.14525300
H	-2.17404900	-4.95758900	4.18978500
H	-3.75627900	-4.75844100	-0.26871900
H	-0.65885900	-3.08221200	-5.00519700
H	-3.08222100	-3.65193400	-4.82566500
H	-4.03121900	-4.34172200	-2.65777900
C	1.81223700	3.65434700	2.96824200
C	2.57290800	2.80541900	2.22095800
C	3.17057500	3.24000200	0.99069700
C	2.91446300	4.58338000	0.55152300
C	2.10649600	5.44124200	1.36550300
C	1.58539400	4.99924800	2.54254800
C	3.97711400	2.39547200	0.20573800
C	3.45969100	5.03239100	-0.64914300
C	4.24610600	4.19803400	-1.44350800
C	4.49999600	2.85051900	-1.02218900
C	5.29844100	2.01927700	-1.87374200
H	5.49852100	0.99781600	-1.56905100
C	5.79917900	2.49127600	-3.05051000
C	5.55537400	3.83505300	-3.45978200
C	4.80663300	4.65982200	-2.67621700
H	1.36472400	3.31297400	3.89732000
H	2.71899700	1.77659200	2.52990600

H	1.92951500	6.45642100	1.02005800
H	0.98266100	5.65688300	3.16158300
H	3.25849300	6.04881400	-0.98053100
H	6.39548700	1.84169300	-3.68315000
H	5.97431700	4.19555000	-4.39392000
H	4.61482800	5.68826500	-2.96969400
C	-5.71200900	2.11230400	-3.38676700
C	-5.81780100	2.15116600	-2.00846200
C	-4.66604000	2.10664400	-1.20566200
C	-3.39516700	2.05095900	-1.80725100
C	-3.30209500	2.00641600	-3.20050800
C	-4.44877700	2.03218500	-3.97961900
H	-5.76179900	2.06906000	0.66892600
H	-6.60440400	2.12693800	-4.00224100
H	-6.79178700	2.19393100	-1.53141600
C	-4.76392400	2.06657000	0.23736000
C	-2.19820600	2.07774500	-0.94063700
H	-2.32250800	1.94317800	-3.66380700
H	-4.36140600	1.98138000	-5.05969100
C	-2.35958700	1.93641600	0.51593300
C	-3.69555700	1.97442500	1.06221800
H	-3.83154000	1.89164300	2.13345200
C	-0.99628700	2.31226500	-1.45647800
C	0.12190600	2.63178600	-2.04613100
C	0.52314200	4.02136900	-2.34952300
C	-0.02086200	5.11048700	-1.65883200
C	1.43522800	4.25075400	-3.38148500
C	0.32609200	6.40683600	-2.01286400
H	-0.70903800	4.93129600	-0.83759200
C	1.76686800	5.55201600	-3.74644800
H	1.88509200	3.40723100	-3.89716500
C	1.21369100	6.63194000	-3.06573600
H	-0.09778900	7.24526900	-1.46938800
H	2.46717400	5.71738600	-4.55879700
H	1.47575900	7.64656200	-3.34822700
N	-1.30437400	1.77923100	1.26775500
C	-1.34733300	1.59279300	2.71264800
H	-1.98114300	0.72988200	2.94976600
H	-0.32029900	1.33734700	2.99259600
C	-1.83231000	2.80320400	3.48238800
C	-2.52707600	2.61686700	4.67852100
C	-1.58641200	4.09950600	3.02899200
C	-2.95740500	3.71317900	5.42013200
H	-2.74197200	1.60796600	5.02109100

C	-2.02179000	5.19482500	3.76928400
H	-1.04606500	4.24810600	2.09852400
C	-2.70540300	5.00490600	4.96716900
H	-3.49890900	3.55690000	6.34741100
H	-1.82876800	6.19970000	3.40618400
H	-3.04668700	5.85993700	5.54135400
H	0.75876500	1.80342400	-2.36450700
H	-0.36021100	1.52091200	0.83795500
C	-2.44189200	-1.49344300	1.59052700
C	-3.83711400	-1.47805900	1.81511700
C	-4.69763000	-1.36164000	0.75059600
C	-4.21558600	-1.21344000	-0.56885600
C	-2.80338100	-1.16969900	-0.79494900
C	-1.94218600	-1.33451800	0.33044300
H	-1.75784100	-1.67180700	2.41772000
H	-5.76338000	-1.37738100	0.94255300
H	-0.88064100	-1.41400000	0.14505500
N	-2.24955800	-0.98411900	-1.99503000
H	-2.83684800	-0.97020500	-2.81477700
H	-1.23277900	-0.90836900	-2.05698600
C	-4.33646600	-1.50366400	3.21702300
F	-5.66518000	-1.65202000	3.29388300
F	-3.77569200	-2.47697100	3.95058800
F	-4.04009400	-0.34232500	3.86068800
C	-5.12233600	-1.06509500	-1.69510200
O	-4.80287400	-0.99690200	-2.87043400
C	-6.64332700	-1.01010700	-1.40419000
F	-7.07338400	-2.18763100	-0.92726400
F	-7.32727100	-0.73099400	-2.50446800
F	-6.95518200	-0.07551900	-0.48314700

### TS2-I

Value of imaginary frequency = -313.14 cm<sup>-1</sup>

P	1.36538600	0.43103600	0.60825000
O	1.55055600	1.24915200	-0.81831900
O	2.73919300	0.87204900	1.38201200
O	1.38542300	-1.01664800	0.23933500
C	1.85620100	2.58782900	-0.71803000
C	3.16563100	2.95047900	-0.38481600
C	0.86165200	3.53923600	-0.95725400
C	1.22149700	4.87994800	-0.82678400
C	2.49248800	5.27785100	-0.41293400
H	0.46766600	5.63968800	-1.02169100
C	3.90322600	0.81687600	0.64325500



C	4.17281900	1.85697400	-0.25159500
C	4.76191500	-0.27187000	0.79567600
C	5.93209500	-0.26882900	0.03997100
C	6.21996600	0.72826600	-0.89160900
H	6.61993600	-1.10418400	0.15070400
C	5.31594000	1.78642900	-1.07222200
C	5.50486600	2.76272000	-2.22129000
C	6.94236500	2.82446400	-2.73045200
H	7.57840700	3.31721200	-1.98275300
C	7.46989800	1.41770400	-2.99262400
H	8.46769300	1.44793200	-3.44077100
C	7.50822600	0.63004500	-1.68633600
H	7.73595600	-0.42382500	-1.87684800
H	4.84978800	2.43270800	-3.04077500
C	3.47246300	4.30585800	-0.16096700
C	4.80644200	4.70187000	0.44646200
C	5.15887200	6.16867000	0.21554300
H	5.39317400	6.33160700	-0.84523900
C	3.98586700	7.05825500	0.61632400
H	4.25094800	8.11727500	0.54248300
C	2.78122100	6.76053300	-0.27229400
H	2.96792000	7.17438900	-1.27278800
H	4.73872600	4.51688500	1.52798600
H	8.33044300	1.01289300	-1.06620200
H	6.80946900	0.91407200	-3.70992600
H	6.98468600	3.43502300	-3.63754900
H	5.15263900	3.76095900	-1.95578300
H	5.60828300	4.05123700	0.09147600
H	6.05768700	6.42573800	0.78412800
H	3.72994700	6.86257300	1.66526000
H	1.88826200	7.26952600	0.10528300
O	0.22140000	1.03007500	1.37497300
C	-0.04988700	1.22081000	-4.47896400
C	0.24084800	1.96340500	-3.37289600
C	-0.79662500	2.43491600	-2.50298000
C	-2.15589200	2.15617400	-2.87570300
C	-2.41845200	1.34827400	-4.02802800
C	-1.39843900	0.88586300	-4.80256200
C	-0.53227300	3.16334500	-1.32175900
C	-3.20044700	2.67111300	-2.10686300
C	-2.95602200	3.38268000	-0.93414000
C	-1.60132900	3.59419400	-0.50439200
C	-1.39739200	4.21592200	0.77285200
H	-0.38533200	4.31358100	1.14777300

C	-2.45287900	4.64044300	1.52475600
C	-3.79480000	4.47303600	1.06936400
C	-4.03490600	3.85579800	-0.11983400
H	0.75409800	0.87576600	-5.12227700
H	1.27122300	2.20455100	-3.13964900
H	-3.45218500	1.10402500	-4.25577500
H	-1.60587900	0.27262800	-5.67387600
H	-4.22826700	2.49536300	-2.41889800
H	-2.27401600	5.09388800	2.49466500
H	-4.62093600	4.79768800	1.69404800
H	-5.05076500	3.67810800	-0.46395500
C	3.83799000	-4.06753100	-0.91477200
C	4.08313500	-2.84712200	-0.36117100
C	4.15769100	-2.67901600	1.06113600
C	3.92722700	-3.83086600	1.88658100
C	3.66167700	-5.09307200	1.26608700
C	3.62632400	-5.21156900	-0.08927700
C	4.42613500	-1.43418100	1.66459800
C	3.96103700	-3.69951300	3.27327700
C	4.18665500	-2.46501400	3.88194500
C	4.41856100	-1.30611500	3.06685800
C	4.64851900	-0.05552900	3.72567300
H	4.82795600	0.82667700	3.12085400
C	4.63254600	0.03820400	5.08557600
C	4.39773300	-1.11325000	5.89226500
C	4.18804700	-2.32496300	5.30610700
H	3.78024900	-4.17421100	-1.99428800
H	4.20777400	-1.97741600	-0.99597700
H	3.48253400	-5.95173500	1.90764000
H	3.42330100	-6.17138100	-0.55430300
H	3.79265400	-4.57724700	3.89409500
H	4.80002300	0.99803100	5.56339300
H	4.39234700	-1.01869800	6.97344100
H	4.02124100	-3.21362900	5.91029200
C	-6.44490500	-3.60751400	-0.85669800
C	-5.60921000	-3.68070000	-1.95095700
C	-4.24867400	-3.33702200	-1.83611100
C	-3.73291800	-2.91819500	-0.59152500
C	-4.59321700	-2.87143300	0.52045300
C	-5.92717300	-3.20282300	0.38523900
H	-3.78429800	-3.69861700	-3.92238900
H	-7.49580700	-3.85713500	-0.95168000
H	-5.99251500	-3.99063100	-2.91902800
C	-3.37219500	-3.35990000	-2.97518000

C	-2.34287500	-2.49737500	-0.51260900
H	-4.20177400	-2.54539600	1.48007900
H	-6.58301200	-3.14359900	1.24785200
C	-1.51134200	-2.49672800	-1.68750700
C	-2.07179300	-2.97842100	-2.92138100
H	-1.44727900	-3.02333400	-3.80517300
C	-1.84280800	-1.87104300	0.59493300
C	-1.18587000	-1.76365800	1.72342500
C	-0.66656700	-2.92213300	2.47758200
C	-1.10934200	-4.23043800	2.25266300
C	0.29926400	-2.67887600	3.45746100
C	-0.58518000	-5.27848400	2.99679000
H	-1.87136600	-4.42009900	1.50194200
C	0.81094500	-3.73058700	4.20901500
H	0.65624300	-1.66514300	3.61773800
C	0.37292800	-5.03103800	3.97889600
H	-0.93272900	-6.29092800	2.81859400
H	1.55790300	-3.52611100	4.96912400
H	0.77243500	-5.85204100	4.56611900
N	-0.27181500	-2.03016700	-1.62298100
C	0.65976100	-1.96814700	-2.72961500
H	0.18746300	-1.46695200	-3.58333500
H	1.46947900	-1.31656300	-2.38480200
C	1.22020700	-3.31311700	-3.15760900
C	2.06952400	-3.35625300	-4.26661500
C	0.93748800	-4.49532500	-2.47632700
C	2.62851900	-4.55768900	-4.68600800
H	2.29791500	-2.43642100	-4.80034600
C	1.48555000	-5.70313500	-2.90509400
H	0.30736100	-4.47494900	-1.59289200
C	2.33370200	-5.73911600	-4.00628300
H	3.29049700	-4.57446400	-5.54589500
H	1.25263100	-6.61645400	-2.36659600
H	2.76344800	-6.67936800	-4.33585500
H	-0.94807500	-0.77674100	2.11587500
H	0.14765000	-1.72118500	-0.72458600
C	-3.94463300	1.67026200	2.90498900
C	-5.27254000	1.55564300	2.47258100
C	-5.55442400	1.03656000	1.22568200
C	-4.52159300	0.59887900	0.37860000
C	-3.17825700	0.70640600	0.82532700
C	-2.91122600	1.25580400	2.09517000
H	-3.73209900	2.10380600	3.87753700
H	-6.58821000	0.97630200	0.90938900

H	-1.87190400	1.38033800	2.38762900
N	-2.09999100	0.25936800	0.09041600
H	-2.25129400	0.19415500	-0.91276700
H	-1.19971200	0.67135300	0.39676700
C	-6.36530400	2.10204600	3.33658100
F	-7.57561800	1.66952500	2.95791500
F	-6.19498700	1.76423700	4.62375700
F	-6.39893500	3.44768600	3.29855500
C	-4.81594200	0.13331100	-0.98389900
O	-4.00371200	-0.28140500	-1.78641900
C	-6.27030500	0.25320600	-1.50048000
F	-7.13306900	-0.44513700	-0.75159300
F	-6.35767600	-0.18004600	-2.74854400
F	-6.65746900	1.54156300	-1.47736300

### TS2-I'

Value of imaginary frequency = -257.02 cm<sup>-1</sup>

P	1.51009900	-0.17084700	-0.63267700
O	1.70858000	-1.44030200	0.41426700
O	3.06733200	0.13751000	-1.04191300
O	0.90994300	0.92536100	0.18493000
C	2.41780000	-2.50530800	-0.09884700
C	3.80701600	-2.39280100	-0.19751500
C	1.73754300	-3.65397300	-0.50757000
C	2.49355100	-4.66833600	-1.08859200
C	3.86841800	-4.54882800	-1.30070100
H	1.98438100	-5.57358500	-1.41234700
C	4.02282700	0.07491500	-0.05188800
C	4.44381800	-1.18036000	0.39618100
C	4.54890900	1.25868400	0.46474800
C	5.52150100	1.14830500	1.45501400
C	5.92872400	-0.08338600	1.96803100
H	5.94701600	2.06103400	1.86632000
C	5.36602900	-1.26343800	1.45810300
C	5.65356900	-2.59778100	2.12525200
C	6.93648500	-2.59580700	2.95221300
H	7.80685400	-2.55518700	2.28349300
C	6.96172900	-1.38963400	3.88544700
H	7.83281800	-1.42122300	4.54691300
C	6.97667600	-0.10366300	3.06425500
H	6.84037800	0.76947200	3.71072700
H	4.80271900	-2.82264600	2.78484900
C	4.53680400	-3.39650800	-0.86310800
C	6.00213700	-3.18223200	-1.19765100

C	6.73889300	-4.47858700	-1.52312100
H	6.85818800	-5.07672400	-0.60954600
C	5.95305200	-5.28317000	-2.55415900
H	6.50935300	-6.17153300	-2.86820300
C	4.60279800	-5.69334700	-1.97277900
H	4.76227200	-6.48829900	-1.23132200
H	6.04372000	-2.51730300	-2.07206000
H	7.96712400	0.01009000	2.60248200
H	6.07023200	-1.41082600	4.52501200
H	7.01112300	-3.53040500	3.51641700
H	5.67414700	-3.40861300	1.39474600
H	6.51082100	-2.64014400	-0.39738900
H	7.74460800	-4.24950300	-1.88828800
H	5.79919200	-4.66644100	-3.44860400
H	3.96422200	-6.12622700	-2.74984600
O	0.84227000	-0.66563200	-1.88274600
C	0.04158800	-4.15922300	3.39868200
C	0.57385500	-3.97608100	2.15664800
C	-0.24288700	-4.06033200	0.98211400
C	-1.63626900	-4.36945600	1.15289000
C	-2.15020000	-4.57085500	2.47262800
C	-1.34275700	-4.45993800	3.56360900
C	0.26880400	-3.82887700	-0.31141100
C	-2.47205800	-4.41985400	0.03847200
C	-1.98882400	-4.14061300	-1.23978000
C	-0.59690300	-3.83265000	-1.42332300
C	-0.14905300	-3.47852600	-2.73855500
H	0.88660700	-3.18835600	-2.87226100
C	-1.02145500	-3.43621200	-3.78658600
C	-2.39990800	-3.75392000	-3.60393600
C	-2.86533600	-4.09658000	-2.36952700
H	0.67641600	-4.07713800	4.27510900
H	1.62859300	-3.75005100	2.04450900
H	-3.20950000	-4.78589600	2.58510600
H	-1.74987600	-4.59151800	4.56074600
H	-3.53048500	-4.63647500	0.17173200
H	-0.66879200	-3.14217000	-4.76974900
H	-3.08037800	-3.70095000	-4.44765600
H	-3.91855300	-4.31838600	-2.21247900
C	2.07898600	3.65307100	2.98636400
C	2.82692700	2.87341900	2.15528000
C	3.27540700	3.36841300	0.88647900
C	2.88193900	4.69469000	0.50016300
C	2.08536500	5.47326800	1.39954900

C	1.70256900	4.97617000	2.60762100
C	4.06907300	2.59648800	0.01752800
C	3.28971700	5.19854900	-0.73400900
C	4.06927600	4.43896200	-1.60634400
C	4.45547900	3.10711400	-1.23578800
C	5.24115200	2.34867600	-2.16274500
H	5.53021800	1.33804700	-1.89468100
C	5.61773500	2.87517900	-3.36230800
C	5.24873900	4.20515300	-3.72098900
C	4.50228200	4.96031500	-2.86695800
H	1.74494800	3.26353100	3.94384000
H	3.08076700	1.85754900	2.43680800
H	1.78798700	6.47179300	1.09055100
H	1.08578000	5.56677900	3.27890200
H	2.99454100	6.20501300	-1.02270400
H	6.20783400	2.28171700	-4.05302200
H	5.56919400	4.61156100	-4.67503600
H	4.21716700	5.97699700	-3.12671200
C	-7.23440600	1.77666000	-2.04079900
C	-6.87433600	1.93857500	-0.71905100
C	-5.51802400	1.94101300	-0.34352100
C	-4.51518400	1.77834600	-1.32533800
C	-4.89925900	1.62730500	-2.66834300
C	-6.23703800	1.62128800	-3.01601100
H	-5.90580400	2.19005500	1.77533000
H	-8.28041600	1.76570900	-2.32608200
H	-7.63219400	2.05682200	0.05030800
C	-5.12170100	2.09256000	1.02847800
C	-3.11720000	1.76241800	-0.91399400
H	-4.13395800	1.48874900	-3.42572000
H	-6.51680400	1.48950300	-4.05593400
C	-2.76393600	1.97128200	0.47013700
C	-3.82517200	2.12594500	1.42896400
H	-3.58099000	2.25576500	2.47593600
C	-2.10520000	1.43501900	-1.76989100
C	-1.05324700	1.65807700	-2.52033400
C	-0.63990300	3.01830600	-2.92794100
C	-1.51122700	4.11325200	-2.90136600
C	0.68463400	3.19828100	-3.33586100
C	-1.05613100	5.37174000	-3.27095100
H	-2.54619300	3.97107100	-2.60287800
C	1.13324400	4.45982600	-3.71182600
H	1.36337900	2.34922800	-3.34101800
C	0.26585400	5.54729500	-3.67772300

H	-1.73673200	6.21683100	-3.25182600
H	2.16372300	4.58629100	-4.02612400
H	0.61601900	6.53141900	-3.97293700
N	-1.49295400	2.01860200	0.84528000
C	-1.04637100	2.17860800	2.21398200
H	-1.50644300	1.40853800	2.85076800
H	0.03084400	1.98357100	2.18776000
C	-1.31585100	3.55552300	2.78973700
C	-1.29182000	3.72860700	4.17494900
C	-1.54334700	4.66226000	1.97187400
C	-1.48376100	4.98766000	4.73550200
H	-1.12028100	2.86897800	4.81903300
C	-1.74735900	5.92033500	2.53219900
H	-1.54394500	4.54086500	0.89276800
C	-1.71692900	6.08838400	3.91356700
H	-1.46188600	5.10741200	5.81397900
H	-1.92491900	6.77309700	1.88458200
H	-1.87644800	7.06956300	4.34868700
H	-0.39746700	0.83578400	-2.80275100
H	-0.74074300	1.75511500	0.19608700
C	-2.32461800	-1.27707500	2.07890800
C	-3.71056800	-1.48347600	2.16931100
C	-4.48036900	-1.52876200	1.02942000
C	-3.89614300	-1.33908200	-0.23932300
C	-2.49923100	-1.10713800	-0.33064700
C	-1.72961100	-1.08834400	0.85389600
H	-1.71535600	-1.28425900	2.97852500
H	-5.54551000	-1.69517700	1.12519400
H	-0.66227300	-0.89942800	0.79523600
N	-1.88883700	-0.79817600	-1.51810100
H	-2.39390000	-1.08543500	-2.35158600
H	-0.85647200	-0.89564500	-1.57116600
C	-4.33314200	-1.57576600	3.52611400
F	-5.63855800	-1.87125400	3.47025400
F	-3.74117000	-2.50580600	4.29183800
F	-4.21634200	-0.40881600	4.18851700
C	-4.70810200	-1.44433300	-1.45840000
O	-4.32156800	-1.23814700	-2.59194800
C	-6.17263600	-1.92438700	-1.31994900
F	-6.19885500	-3.14790100	-0.76381000
F	-6.75649500	-1.99364300	-2.50546900
F	-6.90067800	-1.10889100	-0.54382600

IM3-I

P	1.44466400	0.34594000	0.28135800
O	1.74858900	1.02712900	-1.15696200
O	2.59401200	0.97885400	1.22025100
O	1.45467500	-1.12371700	0.17262100
C	1.96109900	2.40225800	-1.14909800
C	3.19029000	2.87815100	-0.68841100
C	0.93873200	3.24741200	-1.57598400
C	1.20406500	4.61656000	-1.53803900
C	2.39313000	5.13817900	-1.02970700
H	0.43170800	5.30042600	-1.88235400
C	3.87438500	0.91943800	0.66557700
C	4.21727800	1.87006400	-0.29900300
C	4.73671200	-0.10345100	1.04929000
C	5.99514700	-0.12101800	0.44897900
C	6.36939200	0.78635600	-0.54087700
H	6.68975200	-0.90600400	0.73815000
C	5.46097900	1.77438500	-0.95149900
C	5.76396000	2.63443000	-2.16617500
C	7.25362800	2.71786300	-2.48749900
H	7.76426600	3.31709000	-1.72183000
C	7.86335200	1.32024500	-2.52548900
H	8.91106900	1.35628700	-2.83805500
C	7.75372800	0.67052800	-1.14898000
H	8.04026500	-0.38497200	-1.19472200
H	5.23807900	2.18610100	-3.02149200
C	3.38958800	4.26548100	-0.56572000
C	4.60977300	4.80738700	0.15646800
C	4.90538700	6.26624100	-0.18075000
H	5.26359100	6.34252300	-1.21620000
C	3.64267700	7.10719500	-0.01842000
H	3.85487100	8.16939000	-0.17128500
C	2.57762000	6.64344400	-1.00856100
H	2.86417200	6.96921000	-2.01770300
H	4.41360500	4.72277800	1.23480100
H	8.47004600	1.15288100	-0.47005000
H	7.32693500	0.71348200	-3.26575700
H	7.39396700	3.23304100	-3.44233500
H	5.34082900	3.63474300	-2.05918500
H	5.48586100	4.18243000	-0.02850700
H	5.70829700	6.63700500	0.46312100
H	3.26823900	6.99823600	1.00715300
H	1.61670200	7.12285000	-0.79557700
O	0.16662800	1.05401000	0.84699200
C	0.47070900	0.53694100	-4.90333500



C	0.62474200	1.39798900	-3.85879200
C	-0.50832100	1.88909800	-3.13044300
C	-1.81369900	1.49462600	-3.58300100
C	-1.93154600	0.57304700	-4.67233200
C	-0.82572900	0.09913300	-5.30810800
C	-0.39055000	2.74510200	-2.01664300
C	-2.94603200	2.02882200	-2.97183200
C	-2.84532300	2.87057600	-1.86263600
C	-1.54811100	3.19094600	-1.33646600
C	-1.49214700	3.93437800	-0.11107100
H	-0.52621000	4.11270600	0.34763400
C	-2.63021000	4.38561100	0.49350100
C	-3.90989800	4.14009100	-0.08163400
C	-4.01128800	3.39520000	-1.21892000
H	1.34489800	0.17401000	-5.43492000
H	1.61800300	1.72040800	-3.56915800
H	-2.92728500	0.25947500	-4.97198200
H	-0.92309100	-0.60175300	-6.13119400
H	-3.92932900	1.75681000	-3.34571300
H	-2.56608900	4.93028600	1.43036500
H	-4.79896300	4.51651600	0.41522300
H	-4.98358800	3.16217900	-1.64686000
C	4.07417900	-4.08019200	-0.33844200
C	4.20114800	-2.79862600	0.10430000
C	4.22095700	-2.49856300	1.50736800
C	4.05946000	-3.58437800	2.43263600
C	3.98939500	-4.92231000	1.92560300
C	3.99534700	-5.16356200	0.58665600
C	4.35807200	-1.18591200	2.00017200
C	3.95834900	-3.31386800	3.79700700
C	4.00914000	-2.00769100	4.28726500
C	4.22818500	-0.91928700	3.37646900
C	4.31930000	0.40394300	3.91611600
H	4.49577800	1.23358900	3.23977500
C	4.17970400	0.62880400	5.25327400
C	3.95001600	-0.45216600	6.15355000
C	3.87211400	-1.72788200	5.68322800
H	4.00737200	-4.28802700	-1.40264400
H	4.24220000	-1.97875400	-0.60397000
H	3.91164300	-5.73911600	2.63899300
H	3.91725300	-6.17791800	0.20876300
H	3.83286400	-4.13855400	4.49609500
H	4.24411600	1.64031100	5.64107100
H	3.84176500	-0.25173500	7.21452600

H	3.70280100	-2.56101900	6.35981100
C	-6.57526700	-3.55510200	-0.87490500
C	-5.73653700	-3.74756000	-1.94312500
C	-4.39232100	-3.30258500	-1.90834000
C	-3.90379400	-2.63459900	-0.75159200
C	-4.79014500	-2.46698700	0.34984600
C	-6.08746300	-2.91482000	0.28734700
H	-3.86928000	-4.02692000	-3.87748800
H	-7.60388000	-3.89671000	-0.91340400
H	-6.09223600	-4.24809100	-2.84002800
C	-3.50397200	-3.50386000	-2.99774700
C	-2.56403100	-2.16016800	-0.72788300
H	-4.41798100	-1.99359200	1.25582900
H	-6.74532700	-2.77481700	1.13913600
C	-1.71410800	-2.36801400	-1.81555900
C	-2.21057300	-3.06988600	-2.95533900
H	-1.54692900	-3.25834700	-3.79152500
C	-2.05214800	-1.33460200	0.40169100
C	-1.34338500	-1.77143000	1.44990500
C	-0.99203100	-3.16870100	1.75788400
C	-1.84433400	-4.25009200	1.49887000
C	0.26302500	-3.41860300	2.33012900
C	-1.44138000	-5.54938600	1.78682400
H	-2.83068500	-4.07484800	1.08657000
C	0.65493100	-4.71760100	2.62879100
H	0.94161800	-2.58956800	2.51400200
C	-0.19269600	-5.78806000	2.35428400
H	-2.11346700	-6.37565100	1.57806100
H	1.62706400	-4.88872800	3.07562800
H	0.11606700	-6.80233400	2.58865100
N	-0.43673800	-1.85784900	-1.79058400
C	0.60119100	-2.28078800	-2.70228800
H	0.29073300	-2.09077700	-3.73623800
H	1.45179500	-1.61605400	-2.51327000
C	1.05218700	-3.72539000	-2.54768700
C	1.79508400	-4.32556700	-3.56766000
C	0.78067600	-4.45672300	-1.39123400
C	2.25958700	-5.63051400	-3.43785900
H	2.01023300	-3.76224400	-4.47339900
C	1.23465000	-5.76762300	-1.26412000
H	0.21686100	-4.00525300	-0.57958100
C	1.97563700	-6.35836200	-2.28324000
H	2.83370100	-6.08314900	-4.24066000
H	1.01145000	-6.31681000	-0.35427600

H	2.32799900	-7.38056000	-2.18288700
H	-0.90941700	-1.02662400	2.11504900
H	-0.06269900	-1.66805700	-0.86543400
C	-3.34277400	2.01722500	3.19217000
C	-4.68924600	2.22309100	2.91437600
C	-5.25898200	1.68532900	1.77128900
C	-4.47999400	0.96060400	0.86427800
C	-3.10186600	0.78581200	1.12258500
C	-2.55846600	1.29969600	2.30029300
H	-2.90371100	2.43675400	4.09092600
H	-6.31073700	1.86198900	1.57986200
H	-1.49707000	1.18193100	2.48620300
N	-2.21708600	0.11232100	0.21087500
H	-2.54503500	0.26367800	-0.74420400
H	-0.73559000	0.71575200	0.47294000
C	-5.50755300	3.13054600	3.78464900
F	-6.80084200	2.78340800	3.79321800
F	-5.07305400	3.13434900	5.05076200
F	-5.44578100	4.39930200	3.34267500
C	-5.10241500	0.47969000	-0.39753000
O	-4.50277500	0.19808900	-1.40724300
C	-6.64643900	0.41054800	-0.46813400
F	-7.18992400	-0.10301100	0.64026600
F	-7.03448900	-0.30781800	-1.50611500
F	-7.13098600	1.66016800	-0.61253100

### IM3-I'

P	1.31028300	-0.50720700	-0.27541700
O	1.22456900	-1.78082400	0.72020500
O	2.79162600	-0.62003500	-0.90251400
O	1.00577100	0.73456200	0.46068600
C	1.75797800	-2.97713400	0.24729800
C	3.14746200	-3.10992500	0.22007700
C	0.90109300	-3.98136100	-0.19508600
C	1.49825200	-5.14680300	-0.67501500
C	2.87985700	-5.30210700	-0.77132900
H	0.85070100	-5.94979800	-1.01915300
C	3.81357800	-0.73660700	0.04019000
C	3.97964700	-1.96279100	0.68440800
C	4.62788600	0.36443200	0.29653400
C	5.59550900	0.20900000	1.28692600
C	5.72797200	-0.96523800	2.02974900
H	6.24997000	1.05023100	1.50355300
C	4.90544200	-2.06378600	1.74033100

C	4.94082700	-3.30558300	2.61245300
C	6.24024100	-3.44562700	3.40077300
H	7.06415300	-3.69126000	2.71730700
C	6.55614100	-2.14069300	4.12558900
H	7.43524900	-2.24971700	4.76732200
C	6.79044600	-1.02544900	3.11019000
H	6.85181000	-0.05372700	3.61070200
H	4.10042800	-3.23449400	3.31747400
C	3.72262500	-4.26423600	-0.34551100
C	5.21718000	-4.33574400	-0.60625800
C	5.72230400	-5.75885500	-0.82901900
H	5.69280900	-6.31374500	0.11820900
C	4.85354200	-6.47256400	-1.85962300
H	5.25435400	-7.46302000	-2.09406000
C	3.42752600	-6.60025500	-1.33196400
H	3.40913400	-7.35605100	-0.53508000
H	5.41970200	-3.73840700	-1.50710600
H	7.76446400	-1.18195800	2.62712700
H	5.71289200	-1.87844300	4.77675200
H	6.15358300	-4.27575300	4.10787300
H	4.74880900	-4.20394000	2.02163500
H	5.78191200	-3.85342500	0.19358700
H	6.76785800	-5.72972900	-1.14942200
H	4.85369500	-5.89556600	-2.79287500
H	2.75580100	-6.96638700	-2.11492900
O	0.44107000	-0.85579900	-1.53124800
C	-1.38545500	-3.94618300	3.45335200
C	-0.66171700	-3.86590700	2.29998900
C	-1.30112500	-3.94187900	1.02057600
C	-2.72653200	-4.11128700	0.99024800
C	-3.44289600	-4.22131600	2.22264100
C	-2.79782600	-4.13622500	3.41915300
C	-0.58665200	-3.88390400	-0.19272800
C	-3.38976700	-4.17765000	-0.23474400
C	-2.70170300	-4.05012700	-1.44109200
C	-1.27379500	-3.89063700	-1.42484300
C	-0.60185100	-3.72675200	-2.68092600
H	0.46909400	-3.55754200	-2.68056700
C	-1.29603900	-3.74203600	-3.85449300
C	-2.70874300	-3.93219900	-3.86748600
C	-3.38778900	-4.07908200	-2.69670300
H	-0.88151700	-3.87427700	4.41181000
H	0.41383300	-3.73423700	2.34243600
H	-4.51959900	-4.35611600	2.18031200

H	-3.35529300	-4.20186300	4.34741100
H	-4.46799300	-4.31964100	-0.24822600
H	-0.77014300	-3.59868200	-4.79278100
H	-3.24027000	-3.94064200	-4.81315700
H	-4.46815400	-4.19953000	-2.68929000
C	3.33273700	3.97458000	2.20418300
C	3.69277200	2.81596300	1.58242800
C	4.12364400	2.81784600	0.21460900
C	4.14413000	4.07351400	-0.48380900
C	3.75333000	5.26376200	0.20863200
C	3.36011200	5.22056500	1.51067700
C	4.51054000	1.64274200	-0.45843100
C	4.52969400	4.10445200	-1.82344700
C	4.86886300	2.94050200	-2.51403900
C	4.86558100	1.68177500	-1.82296600
C	5.25266300	0.51425700	-2.55739700
H	5.27454400	-0.44384400	-2.04997400
C	5.59206900	0.59113900	-3.87516800
C	5.58015700	1.84065100	-4.56037500
C	5.23384900	2.97765900	-3.89665300
H	2.99796400	3.95543100	3.23733400
H	3.63471700	1.87081700	2.11084700
H	3.76250700	6.20438300	-0.33588700
H	3.03478100	6.12209500	2.02100500
H	4.56971700	5.05882800	-2.34464700
H	5.87696200	-0.30782200	-4.41206400
H	5.85204100	1.87929100	-5.61011100
H	5.22492700	3.93833700	-4.40392800
C	-6.84498800	2.58097200	-1.06649600
C	-6.29226400	3.19406600	0.03020300
C	-4.89327300	3.18441800	0.24604900
C	-4.04198300	2.52037000	-0.68008300
C	-4.63822600	1.95134300	-1.83920700
C	-6.00027900	1.96724400	-2.01847300
H	-4.93517100	4.36128200	2.06098300
H	-7.91935700	2.58095600	-1.21491000
H	-6.92423200	3.69580000	0.75841000
C	-4.29629400	3.82719900	1.36280600
C	-2.64185300	2.44060100	-0.43281000
H	-4.00460600	1.50670700	-2.60013500
H	-6.42915000	1.50786500	-2.90481300
C	-2.08666400	3.06368200	0.68967500
C	-2.94822800	3.79382000	1.56886000
H	-2.51800300	4.31638300	2.41546000

C	-1.78022900	1.60561400	-1.31078100
C	-0.77202900	2.07022200	-2.06311800
C	-0.43989600	3.49848900	-2.22852500
C	-1.43150700	4.47071000	-2.41608600
C	0.90249900	3.89664900	-2.20786300
C	-1.08890800	5.80917500	-2.56993900
H	-2.47288400	4.16768200	-2.45435400
C	1.24106400	5.23715700	-2.36159200
H	1.68270500	3.15350800	-2.05723200
C	0.24916600	6.19666900	-2.54521200
H	-1.86881300	6.54906800	-2.71875700
H	2.28490900	5.52863900	-2.33742700
H	0.51789200	7.24051900	-2.67541500
N	-0.75595100	2.95856400	0.96961500
C	-0.14138800	3.44040700	2.17833400
H	-0.72092100	3.14222500	3.06502600
H	0.82600000	2.93149600	2.24861900
C	0.08833700	4.94193200	2.20764500
C	0.40074300	5.57051800	3.41521500
C	0.03903000	5.70113200	1.03953500
C	0.67168300	6.93511000	3.45537400
H	0.43167500	4.98473400	4.33199100
C	0.30616800	7.06715700	1.07915500
H	-0.20250400	5.21487800	0.09865300
C	0.62474600	7.68882900	2.28345400
H	0.91199900	7.41168800	4.40079200
H	0.26348500	7.64297300	0.15934300
H	0.83014800	8.75427600	2.31271700
H	-0.12111100	1.35622800	-2.56469200
H	-0.19231000	2.32999400	0.40972500
C	-2.82870500	-0.54386400	2.20901000
C	-4.11472700	-1.07542800	2.12136100
C	-4.69778500	-1.28818100	0.88530500
C	-4.02293300	-0.93519300	-0.29278800
C	-2.74445200	-0.34087200	-0.19826000
C	-2.15270000	-0.17844800	1.05794500
H	-2.36079600	-0.41449300	3.17859600
H	-5.68197900	-1.73962700	0.84274400
H	-1.16234200	0.26571900	1.12060500
N	-2.04459900	0.16658300	-1.32418900
H	-2.48539800	-0.13625200	-2.19170400
H	-0.52126600	-0.54183100	-1.44448600
C	-4.90110800	-1.35827600	3.36744800
F	-5.70249900	-2.42846000	3.22816800

F	-4.10691400	-1.57993200	4.42425100
F	-5.69738700	-0.32709600	3.68895900
C	-4.65044900	-1.16510800	-1.60785700
O	-4.09626300	-1.06062000	-2.68203000
C	-6.13560300	-1.60188400	-1.65006000
F	-6.26301100	-2.85129600	-1.16173000
F	-6.58153700	-1.60299300	-2.89700300
F	-6.91668800	-0.80146600	-0.92125300

**IM4a**

C	3.93099200	-4.59728600	0.84689300
C	4.41833300	-3.82123200	-0.17251500
C	3.64278200	-2.77092500	-0.72161600
C	2.33746400	-2.51461700	-0.21658900
C	1.86350900	-3.33293200	0.84485200
C	2.63829600	-4.34313400	1.35690500
H	5.14878900	-2.12817500	-2.13412800
H	4.53059300	-5.39975700	1.26317200
H	5.41125700	-3.99757500	-0.57767000
C	4.14285000	-1.94745500	-1.76499900
C	1.57006700	-1.44294200	-0.77393100
H	0.87637100	-3.14767600	1.25365500
H	2.25234600	-4.95432000	2.16666800
C	2.06901300	-0.68898500	-1.83615500
C	3.39125100	-0.94728400	-2.30716900
H	3.79890700	-0.33278000	-3.10159200
C	0.24393200	-1.09718700	-0.19692200
C	0.02742700	-0.60378500	1.03946200
H	-1.00910800	-0.52416400	1.36215200
C	0.98792900	-0.16521300	2.06174700
C	0.47910700	0.07370300	3.34894600
C	2.35415200	0.07491800	1.84009600
C	1.29785800	0.51214200	4.38131200
H	-0.57964700	-0.08593800	3.53440200
C	3.16913800	0.51989700	2.87437000
H	2.78160000	-0.06245900	0.85430500
C	2.65148400	0.73627100	4.14900700
H	0.87587400	0.68451800	5.36632400
H	4.21969800	0.70609300	2.67358500
H	3.29545800	1.08278900	4.95076000
N	1.31509900	0.29897300	-2.43602100
C	1.93065800	1.49206100	-2.98871300
H	1.10611800	2.13858600	-3.30527600
H	2.49342400	1.24959100	-3.89804400

H	0.40893700	0.46561600	-2.02062300
N	-0.81586100	-1.35438700	-1.10089800
C	-2.16703000	-1.07982700	-0.93873600
C	-3.10527400	-2.06555400	-1.28582200
C	-2.65034200	0.15458600	-0.45364900
C	-4.46163300	-1.84741700	-1.13070500
H	-2.74775500	-3.02024200	-1.65874600
C	-4.01826600	0.34467400	-0.24680900
C	-4.92275400	-0.64693300	-0.58910000
H	-5.17040400	-2.62225400	-1.40587500
H	-4.37995700	1.28766000	0.14988200
C	-1.75050300	1.32216100	-0.27202600
O	-0.91028800	1.67320500	-1.06258600
C	-1.94373900	2.18278100	0.99778400
F	-0.83539900	2.84489600	1.28509300
F	-2.28245900	1.42610200	2.04783400
F	-2.93372400	3.06731700	0.79894600
H	-0.61451400	-2.11923700	-1.73191300
C	2.82626200	2.24130600	-2.01730200
C	4.03368700	2.79320300	-2.44228000
C	2.44664600	2.38701900	-0.68101400
C	4.84794000	3.48943900	-1.55259400
H	4.34226800	2.67245100	-3.47840900
C	3.26101500	3.07660000	0.21104200
H	1.51028400	1.95349400	-0.33582100
C	4.46318000	3.63115200	-0.22307700
H	5.78746100	3.91075500	-1.89627500
H	2.95602400	3.17010200	1.24890400
H	5.09998500	4.16623400	0.47416500
C	-6.39492800	-0.46237100	-0.37503000
F	-6.86765200	-1.30812000	0.55323200
F	-6.69053600	0.78064800	0.02621200
F	-7.08682900	-0.70329400	-1.49892300

**IM5a**

P	-0.98095800	-0.69498400	0.26449700
O	-0.85409600	-1.95396200	-0.73460300
O	-2.56748900	-0.51091800	0.48114000
O	-0.22845000	0.44937700	-0.26894500
C	-1.56989000	-3.08955700	-0.37651900
C	-2.94828900	-3.08153000	-0.56873700
C	-0.88513500	-4.16605000	0.18210000
C	-1.65396600	-5.26655500	0.55424500
C	-3.04470600	-5.28200600	0.44242400



H	-1.14853500	-6.12802700	0.98437800
C	-3.43862600	-0.63406500	-0.59675100
C	-3.58687300	-1.88757600	-1.19932900
C	-4.19528500	0.47582500	-0.98508400
C	-5.03272800	0.29559200	-2.08735200
C	-5.09046800	-0.89194900	-2.81400000
H	-5.64784100	1.13414300	-2.40420600
C	-4.35507800	-2.00065700	-2.37558000
C	-4.32549900	-3.27731500	-3.19702700
C	-5.50849700	-3.40223700	-4.15333900
H	-6.42836600	-3.58950100	-3.58287800
C	-5.66713400	-2.11891000	-4.96250300
H	-6.45222500	-2.22329300	-5.71698400
C	-5.99417100	-0.95579500	-4.03058100
H	-5.94266800	-0.00348000	-4.56817900
H	-3.39358700	-3.26853900	-3.78012600
C	-3.71074600	-4.17174000	-0.09823000
C	-5.22792200	-4.10321300	-0.07357900
C	-5.89235900	-5.47060400	0.06197700
H	-5.77039100	-6.03470400	-0.87246300
C	-5.26340500	-6.25254200	1.21021300
H	-5.78608900	-7.19914300	1.37516700
C	-3.79193000	-6.51750900	0.90690600
H	-3.72213700	-7.27966300	0.11901000
H	-5.51185900	-3.47936800	0.78631600
H	-7.03196100	-1.05551400	-3.68483900
H	-4.73164700	-1.91383700	-5.49786700
H	-5.35936800	-4.26430900	-4.80999600
H	-4.25789200	-4.15709000	-2.55401300
H	-5.61404000	-3.58026800	-0.94998300
H	-6.96724400	-5.34024600	0.21766000
H	-5.35274100	-5.66941800	2.13532900
H	-3.28535200	-6.93689500	1.78205400
O	-0.64296200	-1.21862900	1.72010100
H	0.32267100	-1.28168900	1.85667900
C	1.96584700	-3.97198200	-3.05291700
C	1.06348900	-3.98916900	-2.03117100
C	1.48731300	-4.15943500	-0.67342900
C	2.88954900	-4.35422100	-0.42944400
C	3.80049300	-4.35294000	-1.53294100
C	3.35783800	-4.15155100	-2.80435000
C	0.58705600	-4.17019800	0.41324000
C	3.34034500	-4.55629200	0.87613100
C	2.46425700	-4.53974000	1.96232400

C	1.06599200	-4.30414100	1.73523200
C	0.20919600	-4.20638400	2.88217400
H	-0.83627800	-3.96059500	2.73370000
C	0.69914900	-4.38881500	4.14161300
C	2.07476900	-4.69581700	4.35459700
C	2.92978300	-4.75964000	3.29776000
H	1.62239500	-3.82441600	-4.07147300
H	0.00785900	-3.86185900	-2.24123600
H	4.85693500	-4.51085500	-1.33143500
H	4.06286300	-4.13104600	-3.62868300
H	4.39628200	-4.75595400	1.04985100
H	0.03568200	-4.29784300	4.99534700
H	2.43773900	-4.85767100	5.36413800
H	3.98672800	-4.96115100	3.44602400
C	-3.54307000	4.13784500	-3.09924400
C	-3.58712800	2.98443000	-2.37319000
C	-4.04768100	2.97559900	-1.01424700
C	-4.34792600	4.24435700	-0.41087000
C	-4.31136600	5.43067000	-1.21273300
C	-3.94674400	5.37866000	-2.52394500
C	-4.22394700	1.78580800	-0.27089800
C	-4.69945400	4.29771400	0.93594700
C	-4.81997100	3.13828300	1.70014000
C	-4.61090600	1.85417500	1.08780400
C	-4.86398400	0.69438600	1.89263100
H	-4.76005700	-0.28981400	1.45342700
C	-5.24418900	0.80443900	3.19768600
C	-5.41848200	2.08146200	3.80620100
C	-5.21601800	3.21080100	3.07346400
H	-3.17994200	4.11675900	-4.12159200
H	-3.25544400	2.05395300	-2.81891900
H	-4.58372700	6.37296200	-0.74547300
H	-3.93295100	6.28124500	-3.12696800
H	-4.90991300	5.26074500	1.39508200
H	-5.42607900	-0.09254000	3.78061300
H	-5.72222600	2.14547000	4.84620100
H	-5.35571700	4.19478500	3.51237000
C	0.66754400	5.43506000	-4.19371400
C	-0.22080100	5.40764400	-3.15043500
C	0.05406000	4.65930000	-1.97856100
C	1.26780800	3.92580800	-1.87651200
C	2.17323200	3.98265700	-2.97199000
C	1.87863900	4.71154800	-4.09545000
H	-1.77665400	5.19069800	-0.96561500

H	0.45122600	6.01094900	-5.08759600
H	-1.15483700	5.96203700	-3.19717300
C	-0.85430300	4.62417800	-0.89122700
C	1.53550600	3.18525700	-0.68814600
H	3.11648900	3.45146600	-2.90189500
H	2.58709100	4.73907500	-4.91765600
C	0.61817500	3.16123300	0.35659100
C	-0.59468100	3.89810400	0.23521300
H	-1.31081600	3.89654200	1.04984400
C	2.82116000	2.44825000	-0.54668700
C	4.01312500	3.03731900	-0.31441600
N	0.89708400	2.48157300	1.53579900
C	-0.18847600	2.06960100	2.40553700
H	0.15533500	1.18914000	2.95950800
H	-1.06311900	1.74578200	1.82207800
H	1.61407300	1.77799400	1.43269900
N	2.68579200	1.04820700	-0.62737800
C	3.74742200	0.18451900	-0.85834900
C	4.63946300	0.44701900	-1.91719400
C	4.01543300	-0.93699200	-0.03452500
C	5.69335500	-0.39747900	-2.19251800
H	4.44991100	1.31493300	-2.53858500
C	5.11643000	-1.76314800	-0.29646900
C	5.92895400	-1.51498300	-1.38237600
H	6.33545300	-0.20646600	-3.04672200
H	5.31100300	-2.61811500	0.33804300
C	3.13317800	-1.20548400	1.10435000
O	1.93009600	-1.04215600	1.06004800
C	3.74687500	-1.46118000	2.49810600
F	4.32369300	-0.32074500	2.89578200
F	4.68445300	-2.41490800	2.51682500
F	2.79733400	-1.77703900	3.36798600
H	1.74493700	0.66640200	-0.51261600
C	-0.62303800	3.13102500	3.39721000
C	-1.88870700	3.03738000	3.97862300
C	0.21217000	4.18995500	3.74881800
C	-2.30652600	3.97857900	4.91354100
H	-2.55366400	2.22510500	3.69032100
C	-0.20856200	5.13506500	4.68095100
H	1.18629900	4.26712600	3.27535000
C	-1.46581100	5.03073100	5.26896700
H	-3.29436700	3.89144500	5.35630000
H	0.44754800	5.95869000	4.94557000
H	-1.79235300	5.76929400	5.99435300

C	6.99858700	-2.48965200	-1.76445800
F	8.14286400	-1.87720300	-2.09529100
F	7.26721900	-3.35664900	-0.77589600
F	6.63210100	-3.22261400	-2.83335400
C	4.32609300	4.47046600	-0.20620700
C	5.64731300	4.86278800	-0.47239800
C	3.41403500	5.46512500	0.18214400
C	6.04207100	6.19165000	-0.38525800
H	6.37247200	4.10479500	-0.75812600
C	3.81121000	6.79386300	0.26965700
H	2.39395800	5.19774900	0.43020500
C	5.12137800	7.16789300	-0.01720500
H	7.07013000	6.46366900	-0.60361900
H	3.08689100	7.54361900	0.57254100
H	5.42306100	8.20797200	0.05377700
H	4.88262500	2.38972700	-0.22440100

### TS3a

Value of imaginary frequency = -207.66 cm<sup>-1</sup>

P	1.31464000	-0.14089900	-0.30817100
O	2.73745100	0.60868100	-0.45650900
O	1.75199500	-1.60643200	0.22265400
O	0.58056400	-0.10594900	-1.58257300
C	3.66214300	0.42650300	0.56434100
C	4.33862800	-0.79107400	0.64591500
C	3.86639600	1.46909500	1.46631700
C	4.77693600	1.24343400	2.49354600
C	5.42424200	0.01599500	2.65801600
H	4.96230000	2.04216000	3.20798900
C	2.72420400	-2.22147100	-0.55986500
C	4.04960700	-1.82217700	-0.39539000
C	2.32658100	-3.18092300	-1.48896300
C	3.32506800	-3.74185300	-2.27845500
C	4.65802100	-3.32912200	-2.19447500
H	3.04915400	-4.50345100	-3.00414000
C	5.02762100	-2.34423400	-1.26460900
C	6.42928700	-1.76115700	-1.27780700
C	7.45552900	-2.68084500	-1.93350300
H	7.63670000	-3.55245600	-1.29042700
C	6.94455800	-3.15124700	-3.29180000
H	7.70283800	-3.74120300	-3.81490700
C	5.67600600	-3.98031200	-3.11113200
H	5.20930600	-4.18801900	-4.07939800
H	6.38344800	-0.81716000	-1.83941700

C	5.19131000	-1.02285400	1.74329800
C	5.74868500	-2.41199000	1.99895200
C	6.95155200	-2.41299100	2.93803200
H	7.81877900	-1.97065300	2.42980300
C	6.63592300	-1.60691700	4.19417000
H	7.45385600	-1.66938700	4.91791300
C	6.38023500	-0.14854500	3.82411400
H	7.33555800	0.32352100	3.55711300
H	4.94253100	-3.00869400	2.44941100
H	5.94651500	-4.95692900	-2.68707500
H	6.72938500	-2.27605000	-3.91752900
H	8.40920600	-2.15451800	-2.03448900
H	6.74819800	-1.48375000	-0.27099100
H	5.99306600	-2.91633800	1.06172200
H	7.21995600	-3.44311800	3.19030000
H	5.74547400	-2.02837200	4.67723800
H	5.99678200	0.40697400	4.68598600
O	0.62050000	0.39974200	0.98305700
H	-0.20335500	0.98688900	0.91039000
C	4.94650600	4.26344300	-1.57483400
C	4.60552500	3.38222200	-0.59231800
C	3.50868100	3.64771500	0.28947900
C	2.78027300	4.87171300	0.11173900
C	3.17305200	5.77033700	-0.92968500
C	4.21947800	5.47629800	-1.74997200
C	3.12603400	2.75364300	1.30846000
C	1.69819800	5.15341400	0.94691400
C	1.30694300	4.27076300	1.95341800
C	2.03278100	3.04535200	2.14507300
C	1.57473500	2.14225900	3.16030100
H	2.09676600	1.20140000	3.29401900
C	0.47623600	2.43023200	3.91338100
C	-0.23870600	3.64943400	3.72290200
C	0.17275900	4.54288600	2.78206900
H	5.77946700	4.04161500	-2.23426500
H	5.16747300	2.46274000	-0.46703100
H	2.60419200	6.68560500	-1.05991400
H	4.50196300	6.16130600	-2.54271700
H	1.14164700	6.07643500	0.80137200
H	0.12878700	1.71885600	4.65566900
H	-1.11911700	3.85444100	4.32346000
H	-0.36953800	5.47026500	2.62126900
C	-0.24659200	-1.63852400	-4.57166300
C	0.58060900	-2.16255200	-3.62305200

C	0.08014000	-3.05474100	-2.61934000
C	-1.31562700	-3.39502900	-2.65576100
C	-2.15862000	-2.79500300	-3.64680100
C	-1.64169500	-1.94346100	-4.57696600
C	0.89100700	-3.57233800	-1.59168200
C	-1.83439700	-4.28145700	-1.71439400
C	-1.03322500	-4.81700200	-0.70602500
C	0.34768100	-4.43586000	-0.62112600
C	1.12457900	-4.95511400	0.46581100
H	2.16873900	-4.67160500	0.54484200
C	0.57200300	-5.79199300	1.39014900
C	-0.79585800	-6.18446700	1.29200200
C	-1.56867000	-5.71359600	0.27263600
H	0.15532400	-0.96746900	-5.32472500
H	1.62880700	-1.88683800	-3.59904900
H	-3.21905800	-3.03312600	-3.63271000
H	-2.28653600	-1.49490100	-5.32617200
H	-2.89116300	-4.53663400	-1.75096100
H	1.17739500	-6.17030000	2.20750100
H	-1.21407500	-6.86114800	2.03036500
H	-2.61350000	-5.99879900	0.18593500
C	-7.23301300	-2.85570000	-2.30853900
C	-6.57657600	-3.51693900	-1.30248700
C	-5.38564100	-2.99287000	-0.74442800
C	-4.85817800	-1.76322000	-1.22384900
C	-5.56269700	-1.10055300	-2.26580200
C	-6.71338300	-1.63411800	-2.79076600
H	-5.12964600	-4.55951700	0.72605400
H	-8.14352700	-3.26370500	-2.73384100
H	-6.95890800	-4.45789400	-0.91577300
C	-4.69788900	-3.65331000	0.30824900
C	-3.64164000	-1.25436600	-0.67024600
H	-5.17698000	-0.16465000	-2.65764400
H	-7.22954300	-1.11015500	-3.58897000
C	-2.92946800	-1.98302000	0.28354200
C	-3.51872200	-3.17951200	0.80080700
H	-3.02249200	-3.70620500	1.60558200
C	-3.25888200	0.13580300	-1.02344200
C	-4.02043800	1.23232700	-0.60369300
N	-1.70789300	-1.56692600	0.74980700
C	-1.05134800	-2.17594900	1.89396800
H	-0.04772100	-1.74627200	1.93573600
H	-0.91882500	-3.24826500	1.70698100
H	-1.46010500	-0.60488900	0.56762500

N	-2.12853400	0.33047500	-1.72688800
C	-1.59083300	1.60954200	-1.98581300
C	-0.91546800	1.84744900	-3.17795000
C	-1.69815600	2.61719500	-1.01608100
C	-0.35304100	3.09331700	-3.41524400
H	-0.81807200	1.03928500	-3.89455100
C	-1.11660900	3.85769800	-1.25201800
C	-0.46606900	4.09712000	-2.45908800
H	0.17901300	3.28592900	-4.34064700
H	-1.16857900	4.63713900	-0.50113100
C	-2.29737100	2.28108400	0.32547800
O	-1.62571700	1.58311800	1.11609200
C	-3.18637800	3.34311100	0.99420500
F	-4.09107000	3.88304100	0.17229900
F	-2.39369300	4.35493000	1.40643200
F	-3.79683700	2.86167000	2.06676000
H	-1.55723100	-0.46494700	-2.00877700
C	-1.76667200	-1.95709500	3.21461600
C	-1.92601000	-3.00773900	4.11701700
C	-2.26373200	-0.69374100	3.54751000
C	-2.57396800	-2.80728200	5.33369000
H	-1.54352600	-3.99317400	3.85696100
C	-2.91780900	-0.49448200	4.75951400
H	-2.14117300	0.13829100	2.85673400
C	-3.07486600	-1.54994800	5.65586200
H	-2.69596600	-3.63574100	6.02449800
H	-3.30709100	0.49025100	5.00084400
H	-3.58766800	-1.39307000	6.59948100
C	0.06095600	5.46627300	-2.77128800
F	1.24912800	5.41650700	-3.38640400
F	-0.76749500	6.13757600	-3.58894400
F	0.20301400	6.21636300	-1.66515800
C	-5.21759100	1.08488200	0.24888400
C	-6.39443500	1.76016800	-0.08922300
C	-5.19561600	0.32951600	1.42959300
C	-7.52966400	1.65737900	0.70844200
H	-6.41775500	2.36656700	-0.99116100
C	-6.32861600	0.22517200	2.22396100
H	-4.27653500	-0.16005200	1.73717600
C	-7.50314700	0.88405800	1.86426400
H	-8.43604600	2.18266100	0.42419500
H	-6.28628000	-0.36475100	3.13434700
H	-8.38822000	0.80259400	2.48700300
H	-4.03515800	2.08503900	-1.27796500

**IM6a**

P	1.29096000	-0.05644200	-0.27507500
O	2.54057700	0.90310600	-0.61373000
O	2.01604100	-1.38451600	0.29741400
O	0.73793600	-0.40390900	-1.68966100
C	3.46953700	1.02202700	0.42064500
C	4.38409700	-0.01441000	0.60538600
C	3.41893800	2.14302500	1.24431500
C	4.34613600	2.20175700	2.28136600
C	5.24819700	1.16687600	2.53615800
H	4.33542500	3.07047000	2.93542000
C	3.10443600	-1.85419200	-0.43705000
C	4.31877700	-1.17415800	-0.33017100
C	2.93377400	-2.96682900	-1.25785800
C	4.04103200	-3.37998700	-1.99425800
C	5.25516600	-2.69150500	-1.97001700
H	3.93817200	-4.25276800	-2.63491800
C	5.39544700	-1.56064300	-1.15102200
C	6.64282000	-0.69954200	-1.23721400
C	7.84863500	-1.44733000	-1.79940600
H	8.19735800	-2.19018800	-1.06953300
C	7.46891400	-2.15246800	-3.09790500
H	8.34196100	-2.62176600	-3.56073000
C	6.39830400	-3.20528500	-2.82403500
H	5.99793700	-3.60260200	-3.76226900
H	6.40848400	0.14844100	-1.89645400
C	5.25337900	0.03024200	1.71227500
C	6.08870500	-1.18262100	2.08215700
C	7.25449100	-0.84843700	3.00868700
H	8.01376900	-0.27785700	2.45734400
C	6.76315800	-0.02351200	4.19404900
H	7.56927000	0.15188100	4.91243000
C	6.20641400	1.30995200	3.70299700
H	7.04160100	1.94942400	3.38639200
H	5.42177700	-1.89500600	2.58875100
H	6.86019900	-4.05606700	-2.30489400
H	7.08632500	-1.41118200	-3.81060300
H	8.67298200	-0.74657000	-1.96086000
H	6.88197900	-0.25582900	-0.26860100
H	6.44461700	-1.70281100	1.19065600
H	7.73207800	-1.77311400	3.34574100
H	5.97870200	-0.58161900	4.72036800
H	5.70606500	1.84369300	4.51731100



O	0.33459300	0.48360100	0.72018100
H	-1.32403500	1.49446000	1.08511800
C	3.69809200	4.90743900	-2.01329200
C	3.60202200	4.02364100	-0.97965200
C	2.53591100	4.11377600	-0.02741700
C	1.57776500	5.17084000	-0.18413100
C	1.72699700	6.08959100	-1.27045800
C	2.74715300	5.95830900	-2.16354700
C	2.39831700	3.20893900	1.04195400
C	0.51292200	5.27254000	0.71137000
C	0.34856800	4.35842200	1.75130900
C	1.30586200	3.30191200	1.92514300
C	1.07508400	2.35134300	2.97362000
H	1.76934900	1.52725000	3.09418800
C	-0.01872400	2.44885700	3.78166500
C	-0.96147900	3.50555500	3.61132000
C	-0.77560100	4.43327000	2.63299600
H	4.50856200	4.81534200	-2.72920600
H	4.33638700	3.23256500	-0.87023400
H	1.00084900	6.88946000	-1.37048600
H	2.84259300	6.65525100	-2.98996400
H	-0.21674300	6.06732300	0.58024100
H	-0.18335200	1.70530700	4.55555200
H	-1.83444200	3.55546100	4.25395000
H	-1.49072200	5.23665400	2.48460500
C	0.37435000	-2.55715700	-4.67261000
C	1.18672500	-2.68536700	-3.58628000
C	0.83229900	-3.54963000	-2.49849000
C	-0.40290300	-4.27726400	-2.59155300
C	-1.22884100	-4.10942800	-3.74843700
C	-0.85408100	-3.27749000	-4.75802300
C	1.63075700	-3.68418700	-1.34727700
C	-0.78255000	-5.12121200	-1.55060500
C	-0.00129100	-5.25735100	-0.40312900
C	1.22424200	-4.51947000	-0.28847700
C	1.99307900	-4.67384600	0.91117800
H	2.92521900	-4.12726600	1.00936900
C	1.57040000	-5.48846000	1.92031700
C	0.34994300	-6.21750900	1.80491700
C	-0.40680500	-6.10551800	0.67590600
H	0.65659600	-1.88973100	-5.48063700
H	2.10255900	-2.10937700	-3.51725800
H	-2.16941600	-4.65144400	-3.79095900
H	-1.49077100	-3.14996300	-5.62729900

H	-1.71967000	-5.66727900	-1.62464000
H	2.16533400	-5.58584700	2.82249300
H	0.03256800	-6.86410700	2.61688800
H	-1.33770700	-6.65743400	0.57158800
C	-6.37874500	-3.32835600	-2.89299000
C	-5.73305000	-4.04073400	-1.91367400
C	-4.62666600	-3.49208800	-1.22340800
C	-4.17431300	-2.18340100	-1.54391500
C	-4.85275500	-1.47682500	-2.57324100
C	-5.92547000	-2.03290500	-3.22507500
H	-4.31971300	-5.18382400	0.09080800
H	-7.22673300	-3.75652700	-3.41654300
H	-6.06350500	-5.04199200	-1.64967100
C	-3.95235500	-4.20078000	-0.19364100
C	-3.06735200	-1.62726000	-0.84022000
H	-4.49606200	-0.49419000	-2.87038900
H	-6.42408600	-1.47516900	-4.01164400
C	-2.37423700	-2.37398400	0.11319600
C	-2.86723500	-3.67526400	0.44220300
H	-2.37995500	-4.23701400	1.22954900
C	-2.82134900	-0.16973800	-0.96849500
C	-3.87718200	0.79394400	-0.39720100
N	-1.27088600	-1.86776400	0.74849100
C	-0.64366100	-2.47448400	1.91039500
H	0.34048900	-2.00516500	1.99987900
H	-0.46352100	-3.53629700	1.72189400
H	-1.10864500	-0.87073100	0.67378900
N	-1.74485500	0.28645700	-1.50543700
C	-1.58905300	1.68951900	-1.65024000
C	-0.75025400	2.14241500	-2.66700000
C	-2.27703900	2.59746600	-0.82753600
C	-0.65860300	3.50309600	-2.93383700
H	-0.20088800	1.41800800	-3.25796200
C	-2.17957500	3.95622900	-1.10095300
C	-1.39923300	4.39552800	-2.17020000
H	-0.02571800	3.86798800	-3.73449700
H	-2.71820400	4.68560400	-0.50955700
C	-3.08661000	1.94888000	0.28684400
O	-2.26926100	1.45955100	1.32295800
C	-4.05958000	2.93017200	0.95012300
F	-4.97434700	3.35656300	0.06222200
F	-3.42302700	4.01546700	1.42270700
F	-4.70022700	2.39299400	1.98220900
H	-0.29190600	-0.35047900	-1.71814200

C	-1.42302100	-2.28797900	3.19701900
C	-1.86796800	-3.37694700	3.94304100
C	-1.71321800	-0.99450600	3.64255900
C	-2.60184000	-3.18343100	5.11276500
H	-1.63312500	-4.38437600	3.60442100
C	-2.45340200	-0.79791200	4.80253100
H	-1.37313300	-0.13892400	3.06086400
C	-2.89926900	-1.89410700	5.54191200
H	-2.94550300	-4.04014400	5.68404800
H	-2.68821300	0.21171500	5.12642300
H	-3.47709400	-1.74123000	6.44795000
C	-1.45674100	5.84931300	-2.53830500
F	-0.46925700	6.20882700	-3.36728300
F	-2.61356600	6.14775300	-3.15034400
F	-1.38975100	6.64965300	-1.45600200
C	-4.91291700	0.11303200	0.47048500
C	-6.25644400	0.15249800	0.10583000
C	-4.54039500	-0.56738400	1.63272400
C	-7.21715100	-0.49203200	0.88206600
H	-6.55289200	0.67720600	-0.79901700
C	-5.49613900	-1.20967300	2.40756700
H	-3.49848200	-0.58780600	1.93061800
C	-6.83818200	-1.17646500	2.03123400
H	-8.25964300	-0.46222100	0.58214900
H	-5.18292900	-1.73793200	3.30351000
H	-7.58569300	-1.68446100	2.63239500
H	-4.39385800	1.25056200	-1.25378600

#### IM7a

C	3.42218500	-4.52723600	-1.29976500
C	4.15004200	-3.37827200	-1.47545000
C	3.51243100	-2.11582900	-1.54118400
C	2.09961800	-2.03113000	-1.41408100
C	1.37234200	-3.24115700	-1.25416200
C	2.01528900	-4.45188400	-1.19549800
H	5.32754200	-0.96729900	-1.79155800
H	3.91789100	-5.49082400	-1.25166600
H	5.23189600	-3.41773500	-1.57108700
C	4.24422400	-0.91428500	-1.72580500
C	1.46009100	-0.75885700	-1.46199400
H	0.28741500	-3.20744400	-1.20645500
H	1.43664500	-5.36261300	-1.07671000
C	2.19747100	0.39629600	-1.73879500
C	3.61901300	0.29384700	-1.83491300

H	4.20850200	1.19224200	-1.97281200
C	0.03793800	-0.61711900	-1.07152200
C	-0.39672500	-1.03351800	0.35245600
H	-1.00030200	-1.94804000	0.25880900
C	0.75744800	-1.31568500	1.29241400
C	0.83611600	-2.54955900	1.93517900
C	1.75261100	-0.36264300	1.52566100
C	1.89520900	-2.83671000	2.79181100
H	0.06695100	-3.29739400	1.75683300
C	2.81084600	-0.64887900	2.37859000
H	1.70608800	0.59811000	1.02511300
C	2.88614300	-1.88706600	3.01299500
H	1.94704800	-3.80516500	3.27848200
H	3.58171700	0.09832200	2.53922900
H	3.71732500	-2.11141100	3.67380500
N	1.58600700	1.62157100	-1.84214900
C	2.29771900	2.86793200	-1.99160900
H	1.55247600	3.62414100	-2.25700200
H	3.00988200	2.83218000	-2.82865800
H	-1.32504700	1.96668500	1.15323000
N	-0.77920800	-0.06817100	-1.89506600
C	-2.11875800	0.10771000	-1.50836500
C	-3.05785700	0.25981800	-2.52787300
C	-2.52205500	0.13518900	-0.16078100
C	-4.40377100	0.41139000	-2.22532500
H	-2.70284500	0.24503600	-3.55223900
C	-3.87125700	0.29505500	0.13621400
C	-4.80228800	0.42321600	-0.89411900
H	-5.14004100	0.52600000	-3.01285100
H	-4.22451500	0.31966700	1.15944200
C	-1.38309100	0.04851700	0.85178800
O	-0.68803700	1.27827800	0.91963800
C	-1.89584300	-0.26056100	2.26351500
F	-0.93080500	-0.34202700	3.17052100
F	-2.59780200	-1.39976000	2.29036900
F	-2.71046800	0.73901800	2.67407100
H	0.59612200	1.60619500	-2.02863300
C	3.02031400	3.29902900	-0.72691800
C	4.29984200	3.84740100	-0.78316100
C	2.39509900	3.15622500	0.51349200
C	4.95048900	4.24772400	0.38194000
H	4.79559200	3.95511700	-1.74552100
C	3.04461500	3.55027000	1.67835100
H	1.39970700	2.71993500	0.55627100

C	4.32526100	4.09690600	1.61520200
H	5.94974200	4.66757000	0.32552100
H	2.55117300	3.42706500	2.63760100
H	4.83394100	4.40021300	2.52454000
C	-6.25634500	0.52957900	-0.53674400
F	-6.78675400	-0.67021100	-0.25271500
F	-6.44278800	1.29879000	0.54695800
F	-6.97964800	1.05365100	-1.53581800

**IM2-II**

P	-0.71829600	-0.73531900	-0.98304500
O	-1.89149800	-0.35575100	0.13385100
O	-0.94023200	-2.35774700	-1.12168800
O	0.58455000	-0.47625900	-0.27934800
C	-3.07851400	-1.05435800	0.15787300
C	-3.08151400	-2.38423600	0.59457200
C	-4.26253200	-0.41505800	-0.21629900
C	-5.44303900	-1.15066500	-0.16663700
C	-5.47134700	-2.49781900	0.18839400
H	-6.36968300	-0.65660400	-0.45014500
C	-0.76963100	-3.06057200	0.05371600
C	-1.79306100	-3.01566500	1.00192400
C	0.39376900	-3.81031800	0.25202700
C	0.53666700	-4.43145700	1.49093400
C	-0.40745800	-4.30514300	2.51198500
H	1.43076400	-5.02433000	1.67131300
C	-1.58781300	-3.59035300	2.27305800
C	-2.59500100	-3.39555900	3.39098800
C	-2.52039900	-4.50333300	4.43858100
H	-2.83232000	-5.45662600	3.99067400
C	-1.09221500	-4.62516500	4.96134200
H	-1.02759600	-5.36852900	5.76159800
C	-0.13028700	-5.00092500	3.83302700
H	0.90418700	-4.79616300	4.13233800
H	-2.38528000	-2.43054700	3.87639300
C	-4.27523900	-3.13447400	0.54865800
C	-4.25435400	-4.63783700	0.77132100
C	-5.62579700	-5.21942900	1.10382000
H	-5.92646200	-4.90347200	2.11203000
C	-6.66257300	-4.73914300	0.09377000
H	-7.63223000	-5.21575000	0.26626100
C	-6.80334100	-3.22268200	0.18395100
H	-7.33923000	-2.97069600	1.10940000
H	-3.88628500	-5.09950600	-0.15649800

H	-0.18833800	-6.08400100	3.66215400
H	-0.80043000	-3.66470800	5.40578100
H	-3.21517700	-4.29067800	5.25662700
H	-3.60709600	-3.30455600	2.99132800
H	-3.53049500	-4.91660100	1.53824000
H	-5.56670000	-6.31196000	1.11645000
H	-6.33892500	-5.02236100	-0.91572700
H	-7.41894900	-2.84166000	-0.63737900
O	-1.01446600	-0.10239100	-2.29781800
C	-4.74363500	2.80382100	2.56033100
C	-4.50356400	1.79571300	1.67427200
C	-4.52173000	2.03445000	0.26178400
C	-4.75891300	3.37543900	-0.19676800
C	-5.02336600	4.40149700	0.76686100
C	-5.02871600	4.12369900	2.10105400
C	-4.32819600	1.00243600	-0.67638400
C	-4.76964800	3.64087500	-1.56657400
C	-4.56856000	2.62887800	-2.50501300
C	-4.33127300	1.28435200	-2.05682900
C	-4.10176700	0.26980500	-3.04280300
H	-3.86952200	-0.73639100	-2.71257200
C	-4.14262300	0.56838300	-4.37252200
C	-4.41224200	1.89709200	-4.81513000
C	-4.60777800	2.89587500	-3.90991800
H	-4.72542200	2.60433900	3.62666300
H	-4.29735100	0.79066100	2.02736200
H	-5.22984000	5.40549100	0.40500100
H	-5.24387500	4.90437500	2.82394900
H	-4.95644300	4.65532900	-1.91132200
H	-3.95604900	-0.21011400	-5.10467200
H	-4.44420400	2.11041100	-5.87899500
H	-4.78660800	3.91687500	-4.23497800
C	4.49107200	-2.72485300	0.86761400
C	3.17269700	-2.96137400	0.60726100
C	2.76735900	-3.70535200	-0.54946500
C	3.78935800	-4.12403100	-1.46859400
C	5.16325600	-3.89078600	-1.13728700
C	5.50697900	-3.22818400	0.00184700
C	1.41770900	-4.02407100	-0.80899800
C	3.42581800	-4.75010700	-2.65900400
C	2.08997800	-5.00985700	-2.96260900
C	1.06448400	-4.67099100	-2.01455400
C	-0.28191500	-5.04390600	-2.33416200
H	-1.07140500	-4.82964200	-1.62426300

C	-0.58552600	-5.65863500	-3.51193900
C	0.43148600	-5.96059100	-4.46285900
C	1.72802200	-5.65011400	-4.18994900
H	4.77081500	-2.14380000	1.74143800
H	2.40688000	-2.56966300	1.26837100
H	5.92590000	-4.24314000	-1.82674300
H	6.54907300	-3.04124100	0.23459500
H	4.19990900	-5.05251600	-3.36080200
H	-1.61492100	-5.92370900	-3.73033400
H	0.16724300	-6.44599800	-5.39679800
H	2.51878900	-5.88681900	-4.89647700
C	-1.36682800	6.40109500	3.84692300
C	-0.16086800	5.77881000	4.11544600
C	0.28409900	4.71805200	3.31218900
C	-0.49686800	4.28516600	2.22451800
C	-1.71587900	4.91616000	1.96643400
C	-2.14356300	5.96129700	2.77053900
H	2.12082600	4.40985200	4.42980800
H	-1.70863200	7.22137600	4.46838100
H	0.45471300	6.10352900	4.94944900
C	1.53770600	4.05333000	3.58435500
C	0.00954900	3.19559200	1.36570300
H	-2.33171200	4.57513100	1.13965800
H	-3.09547900	6.43657700	2.55632800
C	1.24702400	2.49909100	1.74570300
C	2.00361300	3.00855900	2.86429300
H	2.93161900	2.52340700	3.13588900
C	-0.61027200	2.89410500	0.22757400
C	-1.26666300	2.69473000	-0.88015500
C	-1.08022700	3.47138700	-2.12531900
C	-1.39001800	2.86736200	-3.34809600
C	-0.58680300	4.78079300	-2.09477700
C	-1.19829200	3.57467300	-4.53093700
H	-1.74842000	1.84017000	-3.35652300
C	-0.40199900	5.47896800	-3.28060600
H	-0.33945100	5.23806200	-1.14116100
C	-0.70757200	4.87678300	-4.50032600
H	-1.43923200	3.10268500	-5.47805700
H	-0.01781100	6.49326000	-3.25353800
H	-0.56195600	5.42463400	-5.42596400
N	1.62978800	1.43432800	1.09487200
C	2.77235100	0.59076800	1.44812000
H	2.91357600	-0.07809400	0.59180000
H	3.67270900	1.20330000	1.54863800

C	2.51225100	-0.22053000	2.69975600
C	1.28288400	-0.86379300	2.87578300
C	3.51010900	-0.36611400	3.66307600
C	1.06383600	-1.63309900	4.01272500
H	0.51525200	-0.77833100	2.10827700
C	3.29039700	-1.15021600	4.79398200
H	4.46742100	0.13191000	3.52345800
C	2.06364100	-1.78111000	4.97242500
H	0.10579600	-2.12636600	4.13917500
H	4.07451200	-1.25909600	5.53623600
H	1.88504900	-2.38573600	5.85649200
H	-1.98214700	1.86915000	-0.89901300
H	1.01132300	0.96149200	0.38994700
C	4.32091600	-0.53975900	-1.86950200
C	5.26845400	0.34942400	-1.31325300
C	4.91037300	1.64811100	-1.04954800
C	3.61325900	2.12221300	-1.33926600
C	2.66870400	1.24272700	-1.96324400
C	3.06054100	-0.10956900	-2.18312200
H	4.59854100	-1.57280700	-2.04981200
H	5.64431100	2.31119400	-0.60656700
H	2.32844400	-0.79374800	-2.59966600
N	1.44384700	1.63851300	-2.31798500
H	1.17203500	2.60001600	-2.17396700
H	0.72144400	0.95986500	-2.55800700
C	6.62653400	-0.12468200	-0.91296800
F	7.04250900	-1.16459400	-1.65130800
F	7.54991700	0.84530800	-1.02599700
F	6.66946600	-0.52521000	0.37713700
C	3.17761400	3.42310000	-0.86681000
O	2.09014500	3.94098400	-1.06895900
C	4.12614900	4.21588400	0.06759100
F	4.47281800	3.47856900	1.14295400
F	3.53857200	5.31703300	0.51049200
F	5.25895300	4.56718200	-0.55634800

**IM2-II'**

P	-1.36583400	-0.00304200	-0.95144000
O	-2.34342300	0.64534400	0.22149600
O	-2.46641700	-0.92330000	-1.74928500
O	-0.41341700	-0.85930000	-0.17109800
C	-3.53461800	1.21559600	-0.15158000
C	-4.58717500	0.38460400	-0.56180200
C	-3.68423400	2.60450400	-0.06347400



C	-4.90970600	3.13468900	-0.46753400
C	-5.92823500	2.35269700	-1.00955500
H	-5.05617800	4.20984400	-0.39167900
C	-3.32175700	-1.70925900	-1.01888200
C	-4.42682500	-1.09470500	-0.42214800
C	-3.08140300	-3.08796900	-0.90666900
C	-4.04580700	-3.83850600	-0.23799000
C	-5.13681400	-3.25853100	0.41052100
H	-3.91045000	-4.91568000	-0.17314700
C	-5.31208500	-1.86708400	0.36148800
C	-6.37868100	-1.20139900	1.21736900
C	-7.48109400	-2.15640600	1.66708300
H	-8.11600300	-2.41634300	0.80921500
C	-6.87599500	-3.42965200	2.24810700
H	-7.65106700	-4.08333400	2.65937500
C	-6.09394900	-4.16301100	1.16331100
H	-5.53630100	-5.00320400	1.59003600
H	-5.88222400	-0.78639200	2.10709000
C	-5.76147300	0.96288400	-1.08335600
C	-6.78885900	0.10859400	-1.80566300
C	-8.16286600	0.76707100	-1.89334700
H	-8.62499400	0.79779000	-0.89694300
C	-8.02833100	2.18800000	-2.43253600
H	-9.01004800	2.64622200	-2.58635200
C	-7.20435500	3.03460900	-1.46637000
H	-7.81529600	3.25756900	-0.58078400
H	-6.41006900	-0.06055700	-2.82365500
H	-6.80398400	-4.59877400	0.44699200
H	-6.20321000	-3.16629600	3.07477800
H	-8.12296700	-1.65547900	2.39809300
H	-6.81213200	-0.33848300	0.71049000
H	-6.86431100	-0.88365600	-1.35686700
H	-8.81918200	0.16674000	-2.53077200
H	-7.53225400	2.15351300	-3.41068400
H	-6.95756400	4.00194600	-1.91629600
O	-0.87335400	1.02418800	-1.90552200
C	-1.85602000	2.20250200	3.85337000
C	-2.41389700	2.30889400	2.61339300
C	-2.09106500	3.39877900	1.73896500
C	-1.19698300	4.40697600	2.24106200
C	-0.66040900	4.27651500	3.56227600
C	-0.96514800	3.20140500	4.34142600
C	-2.62086600	3.52522700	0.43353900
C	-0.87196600	5.50575500	1.44665000

C	-1.35689000	5.62654400	0.14736600
C	-2.22045500	4.60790100	-0.38315900
C	-2.60801800	4.72256200	-1.76015000
H	-3.18888500	3.92358400	-2.20591700
C	-2.22541700	5.79125300	-2.51651800
C	-1.42866300	6.83411200	-1.96070100
C	-0.99802700	6.74299500	-0.67272600
H	-2.09592400	1.34624000	4.47579300
H	-3.10000100	1.54268100	2.27472900
H	-0.00246200	5.06241700	3.92659300
H	-0.54510400	3.10671400	5.33789600
H	-0.21371100	6.27577400	1.84365100
H	-2.52269400	5.84571800	-3.55901400
H	-1.14795100	7.68296200	-2.57606600
H	-0.35875400	7.50889400	-0.24192000
C	-0.46579800	-5.20099800	1.79766100
C	-1.31208200	-4.56648900	0.93471500
C	-0.95145200	-4.32846600	-0.43511300
C	0.35898900	-4.75275200	-0.84692200
C	1.23234300	-5.37690400	0.09872600
C	0.83057200	-5.61564900	1.37814900
C	-1.79567400	-3.68027100	-1.37078600
C	0.77624300	-4.54205100	-2.15985000
C	-0.07138200	-3.97247100	-3.10597200
C	-1.38339700	-3.54294500	-2.71200600
C	-2.23819700	-2.99799200	-3.72468400
H	-3.23950600	-2.68678000	-3.44926800
C	-1.81635000	-2.87468000	-5.01358800
C	-0.50196400	-3.27700800	-5.39318500
C	0.34055200	-3.80910300	-4.46697500
H	-0.77504300	-5.36164500	2.82613700
H	-2.26850100	-4.21775000	1.30190700
H	2.22538700	-5.65828900	-0.23671000
H	1.49551400	-6.10685100	2.08195600
H	1.78127900	-4.84034900	-2.44977500
H	-2.48413200	-2.46176400	-5.76257000
H	-0.18196200	-3.16007900	-6.42359900
H	1.34234300	-4.12819300	-4.74090300
C	7.52547100	0.93461100	1.84030200
C	6.92289700	-0.24821300	2.23375700
C	5.52575400	-0.34650900	2.28297300
C	4.72858200	0.75189400	1.91492300
C	5.34645900	1.94315100	1.53109100
C	6.73122500	2.03308500	1.50142700

H	5.51452600	-2.39608300	3.00016700
H	8.60576500	1.00650700	1.78466600
H	7.52298200	-1.11353700	2.50030400
C	4.87858500	-1.57720900	2.67497700
C	3.25624400	0.59949200	1.92675800
H	4.73660500	2.78548800	1.21968100
H	7.19883500	2.95718100	1.18094600
C	2.67236600	-0.74181000	2.10339600
C	3.54392900	-1.77880600	2.61055800
H	3.13865100	-2.74946900	2.85760000
C	2.49312200	1.68378400	1.85882300
C	1.95116200	2.86563700	1.80739800
C	1.69821300	3.53132100	0.49790900
C	0.77456400	3.00266500	-0.39651200
C	2.43603200	4.66927700	0.15452400
C	0.60339800	3.58404200	-1.65269100
H	0.17253200	2.14623300	-0.11714000
C	2.26168200	5.25038300	-1.09646300
H	3.14852000	5.08793500	0.86039200
C	1.35184300	4.70362200	-2.00303400
H	-0.11859200	3.13842300	-2.32789300
H	2.83715500	6.13076200	-1.36496900
H	1.21367800	5.16515100	-2.97558200
N	1.42162300	-0.96222200	1.81711100
C	0.64634100	-2.18578000	2.05226000
H	0.29282600	-2.51026600	1.07435800
H	1.28933200	-2.95833800	2.46667300
C	-0.50782300	-1.89058100	2.98749600
C	-1.78713500	-1.65781800	2.48047600
C	-0.29918800	-1.84856400	4.36715500
C	-2.84662800	-1.40708200	3.34758100
H	-1.94024200	-1.67056200	1.40678100
C	-1.35787900	-1.59617700	5.23448500
H	0.69730100	-2.02520700	4.76713400
C	-2.63705500	-1.38091100	4.72452900
H	-3.83723200	-1.23817200	2.93558700
H	-1.18733300	-1.57617500	6.30613000
H	-3.46621300	-1.19209500	5.39965100
H	1.72264500	3.38872600	2.73736400
H	0.88137100	-0.27320200	1.27859700
C	5.07252000	1.80314600	-1.85677800
C	6.03224700	0.80187300	-1.58738300
C	5.61808100	-0.44863900	-1.20396100
C	4.24529000	-0.76099700	-1.07487100

C	3.26685900	0.24622900	-1.36409500
C	3.73576800	1.54008300	-1.74750500
H	5.40281600	2.79789000	-2.14180600
H	6.36920500	-1.19895500	-0.99051100
H	3.00064100	2.31405100	-1.94784800
N	1.95188300	0.03972500	-1.26345800
H	1.55790100	-0.86171200	-1.01831000
H	1.28012900	0.72930800	-1.59251900
C	7.48242700	1.11163700	-1.75804300
F	7.78975900	2.33656300	-1.28613500
F	8.27084500	0.22998800	-1.12307000
F	7.85826000	1.10984800	-3.04907100
C	3.81873900	-2.09296700	-0.67629300
O	2.67047300	-2.44877100	-0.46459600
C	4.89886600	-3.19887900	-0.54081900
F	5.52837600	-3.39445700	-1.70529200
F	4.34655200	-4.34813900	-0.16852500
F	5.83876000	-2.89123700	0.37421300

## TS2-II

Value of imaginary frequency = -279.12 cm<sup>-1</sup>

P	-1.19452400	-0.05928300	-0.88636700
O	-1.75372500	1.01069400	0.24873300
O	-2.57545100	-0.83669600	-1.30513800
O	-0.29482800	-0.98821300	-0.12819700
C	-3.04943300	1.46550300	0.30097000
C	-4.10461200	0.56202000	0.49490400
C	-3.28244800	2.84630600	0.24737400
C	-4.60914100	3.27367900	0.29468500
C	-5.68720600	2.39425000	0.34504700
H	-4.80356900	4.34328700	0.26141000
C	-3.11261300	-1.57206800	-0.26795700
C	-3.81283900	-0.88525000	0.71948100
C	-2.92828000	-2.95835800	-0.23558100
C	-3.41381600	-3.62664300	0.88388700
C	-4.01915200	-2.96023200	1.95368500
H	-3.29241700	-4.70649300	0.93802100
C	-4.22691700	-1.57694100	1.87911000
C	-4.83987800	-0.83642300	3.05397500
C	-5.69758800	-1.74342400	3.93237400
H	-6.58596500	-2.06474900	3.37168600
C	-4.89280800	-2.96630600	4.36021200
H	-5.46611000	-3.59418700	5.04891400
C	-4.47301000	-3.78874800	3.14236900

H	-3.67384400	-4.48688500	3.41529000
H	-4.02459000	-0.41508300	3.66099600
C	-5.43803700	1.01873000	0.43135400
C	-6.59115900	0.03163300	0.35691800
C	-7.93860800	0.64821000	0.72251000
H	-7.96771000	0.86058600	1.80003800
C	-8.15446300	1.94343100	-0.05348700
H	-9.15302000	2.35163300	0.12944900
C	-7.09276000	2.96440200	0.34396800
H	-7.31831900	3.33680300	1.35267200
H	-6.63644900	-0.33780000	-0.67801200
H	-5.32154600	-4.40690200	2.81987500
H	-4.00456000	-2.62959700	4.90924800
H	-6.05338300	-1.18725000	4.80488100
H	-5.41604300	0.02548100	2.71240000
H	-6.39977800	-0.85047400	0.96986400
H	-8.73813600	-0.07016100	0.51756800
H	-8.08381300	1.73373300	-1.12826700
H	-7.12848900	3.83654800	-0.31713200
O	-0.67211600	0.63308300	-2.10106500
C	-0.30018600	3.32561200	3.34434800
C	-1.20090100	3.13629000	2.33696300
C	-1.30870200	4.06475300	1.25015500
C	-0.45993900	5.22441900	1.27748400
C	0.46150100	5.39385800	2.35971600
C	0.54756600	4.47149600	3.36067800
C	-2.22108900	3.89336500	0.18491200
C	-0.54080500	6.16729400	0.25270200
C	-1.40388900	5.99013000	-0.82490500
C	-2.24224800	4.82457200	-0.87609200
C	-3.05845400	4.64374700	-2.04195100
H	-3.65431500	3.74204500	-2.12582700
C	-3.07298000	5.56875300	-3.04403000
C	-2.28030800	6.75098300	-2.96045500
C	-1.46629700	6.94691000	-1.88744100
H	-0.22799100	2.59712300	4.14531800
H	-1.83899800	2.26099800	2.34642500
H	1.09638100	6.27598300	2.35893900
H	1.25606600	4.60521100	4.17171300
H	0.09434100	7.04955500	0.28829700
H	-3.69087300	5.40265300	-3.92080300
H	-2.31684800	7.48004600	-3.76351400
H	-0.83210200	7.82677300	-1.82078500
C	0.62496600	-5.29983700	0.37409000

C	-0.47579400	-4.51975600	0.16635800
C	-1.11346800	-4.45987200	-1.11583600
C	-0.52515300	-5.21593300	-2.18834100
C	0.62811300	-6.02382500	-1.92675100
C	1.18226000	-6.07668900	-0.68302300
C	-2.26855300	-3.68500700	-1.35623600
C	-1.08146700	-5.14637700	-3.46404600
C	-2.21367800	-4.37519400	-3.71993300
C	-2.83141800	-3.64098000	-2.65080100
C	-4.02527300	-2.90781500	-2.95309800
H	-4.52612600	-2.36714000	-2.15865000
C	-4.54119200	-2.88484100	-4.21390300
C	-3.90895600	-3.59451700	-5.27565600
C	-2.78349700	-4.31919900	-5.03136700
H	1.09261200	-5.31385800	1.35498800
H	-0.86609300	-3.90859300	0.97427100
H	1.05663200	-6.58919200	-2.74989200
H	2.06405000	-6.68054500	-0.49905300
H	-0.62771700	-5.71203200	-4.27469900
H	-5.44561400	-2.31997700	-4.41513900
H	-4.33360200	-3.55869700	-6.27367100
H	-2.29430000	-4.87504400	-5.82645400
C	6.85414200	3.07784800	2.41061300
C	6.50029000	1.85245600	2.93467200
C	5.32592400	1.20409600	2.51349800
C	4.48016800	1.80609500	1.55380800
C	4.87094400	3.04691600	1.01976600
C	6.03278700	3.66678100	1.44088600
H	5.64416000	-0.53655800	3.76713400
H	7.76347000	3.57272000	2.73294500
H	7.12802700	1.36482700	3.67524000
C	4.98748400	-0.09579900	3.02134400
C	3.24603900	1.11400400	1.15184600
H	4.27555800	3.50102200	0.23786300
H	6.31576200	4.61653900	0.99875700
C	2.99102400	-0.21510700	1.64450100
C	3.90185300	-0.78637400	2.60506100
H	3.67088700	-1.75424900	3.03075300
C	2.35795600	1.79335800	0.34776200
C	1.74658800	2.94292700	0.17607200
C	1.48237800	3.74893600	-1.04619800
C	0.51375300	3.42392900	-1.99427300
C	2.23805200	4.91868600	-1.20263300
C	0.34735900	4.23248900	-3.11765500

H	-0.12214500	2.55592500	-1.85540900
C	2.06209700	5.72303600	-2.32190800
H	2.95772600	5.20136600	-0.43854400
C	1.12161900	5.37396500	-3.28913500
H	-0.41374700	3.97042800	-3.84535200
H	2.65901600	6.62215300	-2.43727400
H	0.97787300	6.00443200	-4.16083500
N	1.94877900	-0.90502700	1.23009300
C	1.69340000	-2.31280600	1.50497000
H	1.14937300	-2.66795400	0.62819000
H	2.63802400	-2.86292700	1.54678300
C	0.85808100	-2.55867500	2.74162000
C	-0.39039200	-1.93927200	2.87161500
C	1.28916900	-3.44606200	3.72686400
C	-1.18210900	-2.20800200	3.98145000
H	-0.73645500	-1.26987800	2.08668500
C	0.48918500	-3.71690800	4.83622500
H	2.25518300	-3.93661200	3.62221300
C	-0.74778300	-3.09546300	4.96568900
H	-2.14996100	-1.72456200	4.07070300
H	0.83494600	-4.41041400	5.59601000
H	-1.37337400	-3.30199600	5.82885200
H	1.54418300	3.43698000	1.13387600
H	1.22592600	-0.49881700	0.61773000
C	2.50358200	-2.78457500	-1.74082500
C	3.84321000	-2.96141000	-1.35563000
C	4.68239800	-1.87709000	-1.21698700
C	4.19260300	-0.56877500	-1.40150600
C	2.81917700	-0.39005700	-1.69268400
C	2.00075800	-1.51586700	-1.91285800
H	1.86297800	-3.65045500	-1.88849300
H	5.72317100	-2.04497100	-0.97015300
H	0.96267000	-1.35926800	-2.17907100
N	2.23184200	0.86455500	-1.65913200
H	2.78891800	1.61663700	-2.05499300
H	1.23438100	0.86935800	-1.92157000
C	4.32789200	-4.34252400	-1.04128200
F	3.92245100	-5.23907800	-1.95149100
F	5.66421900	-4.41025000	-0.97153800
F	3.85378800	-4.76595800	0.14978800
C	5.08251700	0.59762900	-1.34111000
O	4.78784800	1.72140200	-1.69803600
C	6.52630100	0.38188100	-0.82854600
F	6.54122700	-0.29429500	0.32857900

F	7.14220400	1.53798400	-0.64699800
F	7.22525900	-0.33678300	-1.72169800

### TS2-II'

Value of imaginary frequency = -300.34 cm<sup>-1</sup>

P	1.23869600	0.14756100	1.05008800
O	1.85850100	1.00007300	-0.23617000
O	2.61266500	-0.45467200	1.71120000
O	0.44630900	-0.94907100	0.39552800
C	2.96605100	1.79858100	-0.07659700
C	4.20472500	1.19179800	0.16885800
C	2.85719500	3.18628500	-0.24338000
C	4.01715400	3.93872800	-0.05048800
C	5.22554100	3.37910500	0.35781600
H	3.96023500	5.01518500	-0.19481200
C	3.50110700	-1.08769700	0.87163300
C	4.31181700	-0.29272800	0.06014100
C	3.60901100	-2.48507700	0.88797400
C	4.52800300	-3.05198800	0.00834700
C	5.27691700	-2.29773500	-0.89607400
H	4.64139100	-4.13375600	0.00695700
C	5.17709600	-0.90033900	-0.87677400
C	5.93809000	-0.06528700	-1.89394100
C	7.11096100	-0.81170600	-2.52427900
H	7.90501800	-0.94489800	-1.77703100
C	6.65877000	-2.17702100	-3.02929700
H	7.46386500	-2.68687900	-3.56693600
C	6.18945300	-3.03515400	-1.85833600
H	5.67136500	-3.92815200	-2.22430800
H	5.23770600	0.24081500	-2.68514100
C	5.32266900	1.98778400	0.48680400
C	6.58793700	1.35652500	1.04110200
C	7.81604800	2.25172600	0.90051300
H	8.10555500	2.32165100	-0.15714500
C	7.51118400	3.64814500	1.43430700
H	8.40586400	4.27798400	1.42507100
C	6.41068300	4.29515400	0.59784700
H	6.82869600	4.58528000	-0.37589300
H	6.41100100	1.15886800	2.10809700
H	7.06689200	-3.39369300	-1.30311100
H	5.83460000	-2.04159400	-3.74127800
H	7.53388800	-0.21208400	-3.33600700
H	6.28482400	0.86998400	-1.45263100
H	6.77036200	0.37838100	0.59162300



H	8.66083300	1.80449600	1.43305800
H	7.18442100	3.56830500	2.47879300
H	6.06397100	5.22151400	1.06769500
O	0.60709200	1.04667700	2.05167400
C	0.65845300	2.17517400	-3.83610900
C	1.33873200	2.47550800	-2.69356500
C	0.95334400	3.57858200	-1.86077000
C	-0.13698500	4.39976000	-2.31394400
C	-0.80663600	4.06825700	-3.53671300
C	-0.43660700	2.97953800	-4.26737200
C	1.61050400	3.89658900	-0.65004400
C	-0.53346600	5.50353900	-1.56135900
C	0.08201600	5.81216900	-0.35004000
C	1.15654700	4.98801600	0.12894300
C	1.69861000	5.29502900	1.42096900
H	2.45924000	4.64441800	1.83624300
C	1.25074700	6.36398700	2.14136900
C	0.22136200	7.20810100	1.63493200
C	-0.35271400	6.92781000	0.43249300
H	0.96002700	1.31811500	-4.42960400
H	2.18084000	1.86132100	-2.40153800
H	-1.62477000	4.70637500	-3.86134600
H	-0.95946200	2.72941900	-5.18491900
H	-1.35032300	6.12736600	-1.91782600
H	1.67357000	6.56708500	3.12028100
H	-0.11661600	8.05630200	2.22153200
H	-1.16240500	7.53984700	0.04458100
C	1.10862500	-5.63611700	-0.63625700
C	1.87632200	-4.61711500	-0.15269900
C	1.98912300	-4.36912000	1.25558200
C	1.23173700	-5.21498700	2.13687700
C	0.43080600	-6.26587600	1.58799000
C	0.37499100	-6.48099500	0.24502900
C	2.79433300	-3.34018200	1.79532200
C	1.29052700	-5.00428000	3.51262000
C	2.09075900	-4.00385300	4.06000000
C	2.86899300	-3.16292900	3.19410800
C	3.72692700	-2.19275500	3.80832500
H	4.34813300	-1.56626900	3.17943000
C	3.78032000	-2.05167500	5.16232700
C	2.98113700	-2.86769600	6.01449200
C	2.16647700	-3.81548000	5.47654000
H	1.04487900	-5.79027700	-1.70983800
H	2.39365000	-3.96557500	-0.84831700

H	-0.13260000	-6.89076500	2.27548500
H	-0.23306800	-7.28389100	-0.15900100
H	0.70867300	-5.64232400	4.17403600
H	4.43906900	-1.30888500	5.60032300
H	3.03315100	-2.73377400	7.09022200
H	1.55953700	-4.45532300	6.11124300
C	-7.14595900	0.15513300	-2.69574900
C	-6.34696200	-0.80163300	-3.28549500
C	-4.98043200	-0.89201500	-2.96423800
C	-4.40397800	0.01929600	-2.05206400
C	-5.23633200	0.98581200	-1.45879900
C	-6.58282700	1.04308800	-1.76734500
H	-4.61357600	-2.62093400	-4.22165400
H	-8.20268800	0.21062900	-2.93201900
H	-6.76572800	-1.51231200	-3.99259900
C	-4.16251400	-1.94564400	-3.49895000
C	-2.97792700	-0.10332300	-1.73271300
H	-4.82618500	1.66044300	-0.71290400
H	-7.21132600	1.77223400	-1.26715200
C	-2.24884100	-1.26499500	-2.16792500
C	-2.87953100	-2.14968800	-3.11575100
H	-2.30162100	-2.96146200	-3.53842000
C	-2.38532400	0.90890000	-1.01748300
C	-2.22647300	2.21160300	-0.97331000
C	-2.23569700	3.16763500	0.15723000
C	-1.26018000	3.19801700	1.14967800
C	-3.31435200	4.05970000	0.21403000
C	-1.40221200	4.06313000	2.23366900
H	-0.39216200	2.55015400	1.09559400
C	-3.44471400	4.92909000	1.29068800
H	-4.05810000	4.05615900	-0.57901200
C	-2.49426400	4.92192600	2.31141600
H	-0.63939500	4.06324900	3.00484300
H	-4.28909100	5.60957900	1.33460000
H	-2.59568300	5.60011900	3.15270400
N	-1.05476200	-1.52067500	-1.68121000
C	-0.34312500	-2.79138800	-1.76910200
H	0.05079800	-2.95169300	-0.76300400
H	-1.04831700	-3.60018700	-1.97423700
C	0.78729100	-2.75723100	-2.76904300
C	1.82436100	-1.83416400	-2.59215900
C	0.83229100	-3.64330900	-3.84313800
C	2.88041500	-1.80007000	-3.49497100
H	1.79935100	-1.15641500	-1.73952500

C	1.89800100	-3.61309800	-4.74179300
H	0.03149400	-4.36795600	-3.97559900
C	2.92101300	-2.68756500	-4.57074200
H	3.67979100	-1.08049700	-3.35184300
H	1.92412400	-4.30893300	-5.57425100
H	3.74923000	-2.65643800	-5.27221900
H	-2.23378900	2.64653700	-1.97878200
H	-0.62002200	-0.90313600	-0.97819300
C	-5.39790800	1.21149800	2.29613100
C	-6.18991500	0.12517700	1.90011500
C	-5.60639400	-0.99249600	1.33974800
C	-4.21906000	-1.04249200	1.12422900
C	-3.42693100	0.08320600	1.46496000
C	-4.03672100	1.19230200	2.08547800
H	-5.86110200	2.07453000	2.76415500
H	-6.23518900	-1.83262700	1.07207000
H	-3.42142900	2.03972800	2.37283800
N	-2.10999300	0.18149000	1.06172500
H	-1.58939300	-0.68979500	0.93115700
H	-1.51932800	0.85303700	1.55806100
C	-7.67739500	0.21817800	2.04808500
F	-8.21774200	1.01341000	1.10620400
F	-8.27260200	-0.97637500	1.94281700
F	-8.02344200	0.74514700	3.23242400
C	-3.58802300	-2.25481000	0.57422100
O	-2.39633400	-2.48406300	0.56286900
C	-4.50342200	-3.35952500	-0.00737500
F	-5.17464900	-3.97426700	0.97731700
F	-3.78117100	-4.26539100	-0.65225800
F	-5.40637300	-2.85911400	-0.86082100

### IM3-II

P	-1.43361300	-0.13907500	-0.55118600
O	-2.09448000	0.88688100	0.49927700
O	-2.65752400	-0.51268400	-1.52390300
O	-0.82400400	-1.26375900	0.18180000
C	-3.17409300	1.70179400	0.18590800
C	-4.40340300	1.11121200	-0.12064100
C	-2.99530500	3.08515500	0.25039800
C	-4.11501800	3.86846300	-0.02773000
C	-5.33466000	3.32613200	-0.43113600
H	-4.01274600	4.94933000	0.03419500
C	-3.66360400	-1.16293500	-0.79490900
C	-4.52963700	-0.37478900	-0.04063700

C	-3.68130400	-2.55702500	-0.77267200
C	-4.64113200	-3.15096600	0.04169000
C	-5.49210300	-2.40769900	0.86223400
H	-4.68569300	-4.23681600	0.07890500
C	-5.42652700	-1.00650000	0.84679500
C	-6.20472400	-0.18717200	1.86216400
C	-7.36251500	-0.94977000	2.50069700
H	-8.17265700	-1.07145000	1.76942700
C	-6.89762500	-2.32432800	2.96969200
H	-7.69286500	-2.84588400	3.51012900
C	-6.45534500	-3.15128000	1.76661400
H	-5.99216400	-4.08886100	2.08973200
H	-5.49583500	0.11370100	2.64682800
C	-5.47873900	1.93332900	-0.51135200
C	-6.73933000	1.32591100	-1.10099500
C	-7.94146400	2.26439900	-1.04133000
H	-8.27201300	2.37862100	-0.00009900
C	-7.56775200	3.63110300	-1.60681800
H	-8.43975200	4.28998500	-1.65254200
C	-6.47981100	4.26915700	-0.74756500
H	-6.92388900	4.60144500	0.20057100
H	-6.52434300	1.08868700	-2.15272700
H	-7.34110700	-3.43163100	1.18055100
H	-6.05671100	-2.20592200	3.66505100
H	-7.76868600	-0.36610100	3.33196700
H	-6.56271100	0.74684800	1.42531800
H	-6.97405500	0.36922300	-0.63021000
H	-8.77691400	1.82630800	-1.59519500
H	-7.20402900	3.50708900	-2.63453200
H	-6.08443200	5.16886800	-1.22998300
O	-0.45552300	0.64604500	-1.48821800
C	-0.86630300	2.32598300	3.93409400
C	-1.56020200	2.59401900	2.79126800
C	-1.02887600	3.46641100	1.78657900
C	0.22298400	4.11254000	2.06495600
C	0.92442600	3.79804500	3.27116300
C	0.40661900	2.91975300	4.17267000
C	-1.68235300	3.71750700	0.56016800
C	0.73995300	5.03149100	1.15296800
C	0.10018200	5.29909100	-0.05449500
C	-1.11475900	4.60579600	-0.38085700
C	-1.68065100	4.84028500	-1.67931100
H	-2.56183400	4.28505200	-1.97807400
C	-1.11772500	5.72919400	-2.54558800

C	0.06111400	6.44972200	-2.19450000
C	0.65401500	6.22930300	-0.99046400
H	-1.27914800	1.64195800	4.66835700
H	-2.52992700	2.13473300	2.63115200
H	1.88735600	4.27154800	3.44316200
H	0.95385900	2.67077000	5.07564600
H	1.67510100	5.53948500	1.38163900
H	-1.56205500	5.88046000	-3.52447700
H	0.49707000	7.14676200	-2.90252200
H	1.57318200	6.74145400	-0.72028700
C	-0.74220200	-4.91592000	1.26661500
C	-1.64334900	-4.12785800	0.61282200
C	-1.76505800	-4.16925600	-0.81644900
C	-0.86868500	-5.02709500	-1.54153300
C	0.05325900	-5.84917700	-0.81569100
C	0.11127600	-5.80324900	0.54515200
C	-2.69267000	-3.37837400	-1.52657100
C	-0.90055900	-5.03604000	-2.93516200
C	-1.78736000	-4.22971700	-3.64760000
C	-2.70880300	-3.38926900	-2.93575200
C	-3.62379400	-2.59768500	-3.70279000
H	-4.33808300	-1.96894700	-3.18256600
C	-3.60888600	-2.62633100	-5.06519400
C	-2.68424800	-3.45271900	-5.76792200
C	-1.80591300	-4.23107600	-5.07811900
H	-0.65943400	-4.84936100	2.34761100
H	-2.25124300	-3.42579700	1.17260400
H	0.71754000	-6.49943500	-1.37925000
H	0.81837400	-6.42618100	1.08403600
H	-0.21557500	-5.68293000	-3.47863100
H	-4.30916300	-2.01543300	-5.62547400
H	-2.68887300	-3.45973700	-6.85294200
H	-1.09938900	-4.87055100	-5.59981700
C	7.13074000	2.18404300	2.52429700
C	6.38721800	1.36782400	3.33550100
C	5.10289100	0.91700100	2.94645300
C	4.53236800	1.32404600	1.70360200
C	5.34651400	2.15959900	0.88113100
C	6.59741100	2.56749200	1.27738500
H	4.78149100	-0.22290100	4.75584700
H	8.11639500	2.52042800	2.82717200
H	6.77419600	1.04025700	4.29696900
C	4.36314200	0.05092800	3.79105000
C	3.22651700	0.83827300	1.31971900

H	4.99105200	2.46805600	-0.09339900
H	7.18587400	3.18516100	0.60599400
C	2.56828100	-0.07161100	2.15647900
C	3.14975000	-0.42969300	3.41289700
H	2.57703100	-1.05932600	4.08475300
C	2.63057700	1.34203200	0.04616800
C	2.58798600	2.66445200	-0.19432900
C	2.44288500	3.36066100	-1.48835800
C	1.45473300	3.08692000	-2.44058700
C	3.39857600	4.34675700	-1.78488200
C	1.45830000	3.74147600	-3.67091500
H	0.64693100	2.40263400	-2.20909300
C	3.40195100	4.99402300	-3.01230100
H	4.15581700	4.58702800	-1.04221800
C	2.43545900	4.68389000	-3.96771800
H	0.67721900	3.51919400	-4.39125500
H	4.16102500	5.73997500	-3.22625000
H	2.43620100	5.18760100	-4.92913000
N	1.35880000	-0.63322800	1.84592000
C	0.96985900	-1.94751600	2.33064800
H	0.52260700	-2.48559000	1.49047900
H	1.86291200	-2.50951700	2.62786900
C	-0.04175900	-1.94585000	3.45707900
C	-1.15596600	-1.10395200	3.40205000
C	0.08086800	-2.84018900	4.52035900
C	-2.12943800	-1.16818100	4.39369800
H	-1.24865300	-0.40343200	2.57723500
C	-0.89396000	-2.90350400	5.51482500
H	0.94906300	-3.49461000	4.57001000
C	-2.00328700	-2.06733300	5.45200500
H	-2.99449400	-0.51245200	4.34068000
H	-0.78265600	-3.60174300	6.33845900
H	-2.76515800	-2.11287200	6.22375200
H	2.89500800	3.29106100	0.63774600
H	0.90997100	-0.36531300	0.98499400
C	2.66174500	-3.27177100	-0.71668300
C	4.03848800	-3.40926700	-0.84537700
C	4.83860800	-2.30017100	-1.08394800
C	4.26091600	-1.03060100	-1.18055700
C	2.87020000	-0.88330500	-0.99937200
C	2.08385300	-2.00991500	-0.79416000
H	2.03433900	-4.14258300	-0.55201600
H	5.90550000	-2.43375800	-1.21818200
H	1.01008000	-1.89905100	-0.67805300

N	2.21658800	0.40802400	-0.99731600
H	2.43597200	0.87882300	-1.88257100
H	0.52143300	0.46735700	-1.25975400
C	4.65411400	-4.77022800	-0.68894600
F	3.87094100	-5.72459300	-1.21475000
F	5.85091800	-4.84964400	-1.28589200
F	4.83392500	-5.08433900	0.60217300
C	5.09389400	0.13167100	-1.58059300
O	4.66728300	1.11084900	-2.14558900
C	6.61624600	0.05676800	-1.31666300
F	6.88138300	-0.39185200	-0.09016100
F	7.17941200	1.24444200	-1.47949600
F	7.18142400	-0.79332500	-2.19430600

**IM3-II'**

P	1.15027600	-0.18016700	0.48843900
O	2.34929300	0.53042400	-0.32152600
O	1.93736600	-1.08189500	1.56376900
O	0.27955800	-0.88689300	-0.47030900
C	3.59757900	0.79982600	0.21164300
C	4.41106400	-0.26390200	0.61844900
C	4.01938200	2.13297800	0.25901700
C	5.31001500	2.35754100	0.73872300
C	6.11143600	1.34059000	1.25553200
H	5.68234900	3.37913400	0.75308700
C	2.70966800	-2.05144900	0.91922200
C	3.94058700	-1.66495700	0.39581400
C	2.17299900	-3.33066500	0.76662200
C	2.93368800	-4.23554100	0.03446600
C	4.14498100	-3.88128400	-0.56725600
H	2.54740500	-5.24216300	-0.10751400
C	4.66037100	-2.58729800	-0.39768900
C	5.91103600	-2.14994200	-1.14318700
C	6.73884600	-3.31397800	-1.68190100
H	7.25245800	-3.81593900	-0.85119700
C	5.84295300	-4.31872100	-2.39748200
H	6.43477500	-5.10818500	-2.86966400
C	4.86450900	-4.92605600	-1.39799400
H	4.12294800	-5.54735600	-1.91009600
H	5.59672700	-1.51153600	-1.98020400
C	5.64411500	0.01855400	1.23921600
C	6.40847800	-1.06935600	1.97292800
C	7.88820300	-0.74303000	2.15544800
H	8.40095600	-0.78247100	1.18473000

C	8.04531700	0.65083600	2.75590200
H	9.09512400	0.87058600	2.97102200
C	7.48173600	1.69829000	1.79936200
H	8.16936200	1.81131600	0.95019800
H	5.94405900	-1.17413600	2.96396500
H	5.41312300	-5.59627200	-0.72236500
H	5.28779200	-3.80888100	-3.19543900
H	7.51494800	-2.92955600	-2.35014900
H	6.53449100	-1.50655800	-0.52048000
H	6.28112200	-2.03985100	1.48982800
H	8.35525600	-1.49866800	2.79388600
H	7.50603400	0.69238000	3.71050900
H	7.43494400	2.67841000	2.28494100
O	0.44320000	0.88581600	1.39180100
C	2.11129900	2.39137100	-3.61313700
C	2.77106000	2.34659500	-2.42181100
C	2.54998300	3.33715200	-1.40960400
C	1.68636200	4.43813100	-1.73960900
C	1.00432300	4.44501700	-2.99853300
C	1.19166800	3.44294200	-3.89958700
C	3.14119900	3.27392100	-0.12777900
C	1.52398700	5.48126800	-0.83106900
C	2.13595300	5.45738300	0.42058100
C	2.91847700	4.31550900	0.80651600
C	3.40867700	4.28353000	2.15599000
H	3.93936500	3.40556100	2.50343100
C	3.19925900	5.32428400	3.01402100
C	2.47139400	6.47739000	2.60266900
C	1.94608800	6.52981400	1.34766300
H	2.28758600	1.61748500	-4.35251100
H	3.46936700	1.53925800	-2.23361400
H	0.32921300	5.26968300	-3.20963400
H	0.65690600	3.44098800	-4.84369100
H	0.88930500	6.32401600	-1.09535700
H	3.57964700	5.26726100	4.02896800
H	2.31854500	7.29539200	3.29891600
H	1.35405600	7.38233600	1.02692200
C	-1.18687600	-4.29597300	-1.73596800
C	-0.13128100	-3.95481500	-0.94429200
C	-0.23008800	-4.00571000	0.48557000
C	-1.49638100	-4.37794300	1.05414300
C	-2.57890600	-4.73025700	0.18581800
C	-2.42995800	-4.70111100	-1.16686000
C	0.84342800	-3.68309200	1.34037600



C	-1.65540900	-4.38326300	2.43810600
C	-0.60744900	-4.04427500	3.29300300
C	0.67090700	-3.69602300	2.74073900
C	1.72927200	-3.38360300	3.65427800
H	2.70890700	-3.13624700	3.26028100
C	1.52585400	-3.39775700	5.00195300
C	0.25055400	-3.72899000	5.54441100
C	-0.77981400	-4.04545200	4.71292000
H	-1.08980200	-4.23721600	-2.81550800
H	0.79489700	-3.61402500	-1.39398300
H	-3.52579000	-5.01454200	0.63578500
H	-3.26068100	-4.95752900	-1.81617400
H	-2.61936300	-4.65727100	2.86127400
H	2.34346500	-3.15550800	5.67313900
H	0.10910100	-3.73136600	6.62023800
H	-1.75674700	-4.30616300	5.11050000
C	-7.43547200	1.54499600	-2.12340300
C	-6.76269500	0.94430200	-3.15460300
C	-5.34821500	0.86429600	-3.15428300
C	-4.59894000	1.44159800	-2.08909500
C	-5.33213900	2.05545900	-1.03213200
C	-6.70341800	2.09480000	-1.04716100
H	-5.21375200	-0.23204500	-5.01328700
H	-8.51920900	1.59150600	-2.12385900
H	-7.30389300	0.50109100	-3.98639300
C	-4.64851700	0.18537700	-4.18443200
C	-3.16868000	1.31634800	-2.07969900
H	-4.79642100	2.47681300	-0.18805100
H	-7.23220200	2.55313400	-0.21718600
C	-2.52229500	0.58380700	-3.07195500
C	-3.29339000	0.04823500	-4.14696300
H	-2.78109800	-0.45518300	-4.95881500
C	-2.40647100	1.87618800	-0.92448100
C	-2.33979000	3.19643600	-0.71772000
C	-1.87380600	3.88141000	0.50480600
C	-0.60142300	3.68176700	1.04244600
C	-2.78001400	4.70348700	1.18765200
C	-0.26517300	4.23218200	2.27623000
H	0.13345600	3.10290000	0.49145400
C	-2.43931300	5.26420200	2.41328600
H	-3.76536500	4.87755300	0.76270100
C	-1.18490300	5.01567300	2.96770900
H	0.72499600	4.05596500	2.68546500
H	-3.15431000	5.88974000	2.93829400

H	-0.91657900	5.44706500	3.92683800
N	-1.15144500	0.37596500	-3.07329800
C	-0.59816800	-0.95100100	-3.36760300
H	-0.50462800	-1.53106300	-2.44595000
H	-1.30492100	-1.47824000	-4.01140900
C	0.74195500	-0.85900800	-4.05542000
C	1.91316200	-1.13496600	-3.35025800
C	0.82826100	-0.49895200	-5.40282300
C	3.15014500	-1.06908700	-3.99033000
H	1.84478700	-1.38812300	-2.29473500
C	2.06017900	-0.43859100	-6.04470500
H	-0.08328800	-0.26632900	-5.94861900
C	3.22757500	-0.72681600	-5.33688900
H	4.05471200	-1.29012100	-3.43255700
H	2.11379700	-0.16785200	-7.09462200
H	4.19121900	-0.68102600	-5.83434300
H	-2.81292400	3.81501800	-1.47852500
H	-0.63908600	0.84544300	-2.33422800
C	-4.23379800	0.97217300	2.94836800
C	-5.08113400	-0.10016000	2.67281400
C	-4.87938400	-0.88102900	1.54823100
C	-3.82299600	-0.59996400	0.67303200
C	-2.97506400	0.49377600	0.94148800
C	-3.18838100	1.26445000	2.08795300
H	-4.38835800	1.56956500	3.84130500
H	-5.54415700	-1.71471200	1.35681100
H	-2.51434800	2.08897300	2.29597500
N	-1.91831400	0.89869100	0.05594300
H	-1.58501900	0.07075700	-0.45066900
H	-0.47296200	1.07433800	0.99840000
C	-6.22694100	-0.37372300	3.60270900
F	-7.16335800	0.58388500	3.52119800
F	-6.82499000	-1.54189900	3.33627700
F	-5.82187100	-0.40614700	4.88126100
C	-3.62584800	-1.44661800	-0.53335200
O	-2.58107500	-1.58859600	-1.11933600
C	-4.86816900	-2.17917600	-1.09700800
F	-5.20356400	-3.22529100	-0.31759300
F	-4.62282400	-2.63832700	-2.31542300
F	-5.92434600	-1.36450600	-1.14537100

**IM4b**

C	-6.14452400	0.92709400	2.56528700
C	-6.35048500	0.11338100	1.48092200

C	-5.32041400	-0.11351400	0.53561000
C	-4.05626300	0.51932300	0.70492500
C	-3.87175700	1.35254400	1.84218600
C	-4.88790300	1.54786900	2.74377000
H	-6.48179100	-1.44039700	-0.71763200
H	-6.93872000	1.09500100	3.28488500
H	-7.30966000	-0.37458800	1.32948500
C	-5.51253800	-0.96752000	-0.58406900
C	-3.01643100	0.26331900	-0.24356700
H	-2.91465200	1.84296400	1.98549200
H	-4.72521400	2.18978200	3.60384500
C	-3.24179500	-0.56265600	-1.33676500
C	-4.51820000	-1.18018500	-1.49369800
H	-4.69934300	-1.79727700	-2.36763100
C	-1.63631100	0.78766200	0.00546500
C	-1.31749600	2.07144500	-0.25495200
H	-2.08802300	2.62760200	-0.78192600
C	-0.11883900	2.83957800	0.10642400
C	0.32223500	3.86108900	-0.74913300
C	0.55691600	2.65467600	1.32161700
C	1.39981000	4.66746800	-0.40465100
H	-0.19091700	4.01184600	-1.69473400
C	1.63663900	3.46075900	1.66478100
H	0.21299300	1.89021800	2.01266700
C	2.06025200	4.47069500	0.80551600
H	1.72731500	5.44762900	-1.08418800
H	2.14248800	3.30415000	2.61208200
H	2.90253800	5.09884800	1.07613200
N	-2.26954200	-0.73322600	-2.31527600
C	-1.88254400	-2.07704000	-2.73727700
H	-1.33216000	-1.98282300	-3.67785500
H	-2.78256800	-2.66020600	-2.95007400
H	-1.44748800	-0.16067000	-2.14966500
N	-0.83272300	-0.21274100	0.56695400
C	0.52127100	-0.42749900	0.73750600
C	0.85706800	-1.21733600	1.86083300
C	1.57547300	0.04117500	-0.08353800
C	2.15730900	-1.55125500	2.15462000
H	0.05240800	-1.56019500	2.50419100
C	2.90125700	-0.29316500	0.24848100
C	3.19364100	-1.08589000	1.33733300
H	2.38323400	-2.16079100	3.02361500
H	3.71636200	0.04832700	-0.37803200
C	1.34890300	0.71094900	-1.37463500

O	0.36375300	0.58878200	-2.06868700
C	2.49730900	1.56754600	-1.96089900
F	2.03070500	2.40829700	-2.87370900
F	3.39578100	0.76354300	-2.56060200
F	3.14420000	2.26517100	-1.02535200
H	-1.39009100	-0.95444000	0.97284300
C	-1.02873500	-2.79109900	-1.70973000
C	-1.62203000	-3.41336400	-0.60648800
C	0.36385000	-2.78353800	-1.81056700
C	-0.83734700	-4.02973300	0.36485800
H	-2.70620800	-3.42250000	-0.51750900
C	1.15219800	-3.40696500	-0.84548700
H	0.83246600	-2.28744800	-2.65729600
C	0.55125300	-4.03531400	0.24087700
H	-1.31002500	-4.52135100	1.20981300
H	2.23478600	-3.39391400	-0.93292600
H	1.16368900	-4.52056400	0.99444200
C	4.59802100	-1.53247100	1.59826100
F	4.82024400	-2.76401200	1.10481200
F	5.50018400	-0.71730500	1.03645100
F	4.86173700	-1.59301200	2.91226900

**IM5b**

P	1.04143700	0.64010400	-0.98558300
O	2.10227600	1.85239800	-0.83699000
O	1.89925000	-0.64799700	-0.49508600
O	0.47591400	0.61104300	-2.34328200
C	2.92615800	1.85610700	0.27846000
C	3.99768000	0.96350400	0.30895500
C	2.63987200	2.73286200	1.32446600
C	3.48899200	2.69126900	2.42702100
C	4.54223200	1.78085500	2.52606600
H	3.29253900	3.36678800	3.25637500
C	3.11913300	-0.85126600	-1.12289200
C	4.17606900	0.00907100	-0.82802400
C	3.25162000	-1.94247300	-1.98438500
C	4.46409400	-2.07629700	-2.64983200
C	5.50039100	-1.14823400	-2.49820000
H	4.60201900	-2.92321400	-3.31804300
C	5.36337300	-0.09670300	-1.58074600
C	6.43872800	0.96692100	-1.45577000
C	7.79871700	0.50586100	-1.97216200
H	8.21970700	-0.24609500	-1.29114600
C	7.64901800	-0.09950900	-3.36472400

H	8.62406400	-0.35191500	-3.79157900
C	6.77324700	-1.34777900	-3.29916100
H	6.51531700	-1.69019700	-4.30657600
H	6.10939000	1.83635200	-2.04187500
C	4.78748300	0.88370000	1.47460200
C	5.79056100	-0.24388900	1.64936200
C	6.80759100	0.01332600	2.75821200
H	7.51105300	0.79428100	2.44006600
C	6.10032600	0.46076400	4.03297200
H	6.80897900	0.56648500	4.85967400
C	5.38799900	1.78679500	3.78475800
H	6.13945200	2.58325900	3.69613800
H	5.21643400	-1.15038600	1.89103800
H	7.34742100	-2.16288800	-2.83796300
H	7.18866600	0.64147900	-4.03014900
H	8.49387900	1.35042000	-1.98444100
H	6.51440000	1.32245200	-0.42538400
H	6.30385500	-0.46665100	0.71232500
H	7.39488200	-0.89320600	2.93197900
H	5.36971500	-0.30259700	4.32849100
H	4.75878300	2.05424900	4.63962500
O	0.01367500	0.74623200	0.18779400
H	-0.90273800	0.95234000	-0.23519000
C	2.42537300	6.09167000	-1.34103400
C	2.49114100	5.02593900	-0.49424300
C	1.43131300	4.74937000	0.42937100
C	0.30629800	5.64234600	0.45183400
C	0.27745500	6.75062500	-0.45357900
C	1.30028800	6.96791300	-1.32618700
C	1.45590000	3.63977100	1.29692300
C	-0.74862200	5.40240500	1.33228400
C	-0.75342500	4.28612900	2.16878000
C	0.36420200	3.38089300	2.15173900
C	0.27978000	2.19529600	2.95342000
H	1.09713300	1.48351700	2.92410000
C	-0.83038000	1.92883600	3.69776300
C	-1.93850400	2.82722400	3.70977600
C	-1.89408500	3.97339700	2.97525200
H	3.23589700	6.27840900	-2.03798200
H	3.35174800	4.36607200	-0.51532400
H	-0.58938000	7.40558400	-0.43140900
H	1.26728000	7.80840500	-2.01185900
H	-1.60954300	6.06810800	1.32607400
H	-0.88269200	1.01325900	4.27723900

H	-2.81803500	2.58091300	4.29521200
H	-2.73524400	4.66111800	2.95867300
C	-0.11269400	-1.62346300	-4.66046300
C	0.98461200	-1.76203500	-3.86453700
C	1.08238400	-2.84124800	-2.92996100
C	0.00626200	-3.79603900	-2.87616200
C	-1.12549800	-3.61321200	-3.73272300
C	-1.18590700	-2.55856500	-4.59438600
C	2.16824100	-2.96958600	-2.04354200
C	0.06945600	-4.85039000	-1.96386400
C	1.14521100	-4.99225500	-1.08688300
C	2.21599800	-4.03345400	-1.11907800
C	3.27893700	-4.17997500	-0.16630300
H	4.09378400	-3.46379600	-0.17782400
C	3.27099500	-5.19326900	0.74736200
C	2.20236600	-6.13703700	0.78086700
C	1.17787800	-6.03894000	-0.11166100
H	-0.18660500	-0.77561600	-5.33301600
H	1.77865700	-1.02553500	-3.89626000
H	-1.94233600	-4.32734400	-3.67178000
H	-2.05771400	-2.41798600	-5.22652100
H	-0.75062300	-5.56355000	-1.91857400
H	4.08138300	-5.28112700	1.46363600
H	2.20916300	-6.92759500	1.52369900
H	0.35532900	-6.74836200	-0.09312900
C	-4.66026700	-1.65281800	-5.93271400
C	-4.03803100	-0.43307500	-5.87660700
C	-3.57750200	0.09466900	-4.64208300
C	-3.76698300	-0.64856200	-3.44212000
C	-4.40180700	-1.91992200	-3.53745200
C	-4.83712900	-2.40244800	-4.74529900
H	-2.77463100	1.91223800	-5.49003300
H	-5.01164900	-2.04768400	-6.88020000
H	-3.88618500	0.15355000	-6.77871000
C	-2.91690400	1.34594700	-4.57388900
C	-3.28611800	-0.10910500	-2.20863700
H	-4.53598200	-2.51089600	-2.63867100
H	-5.31934900	-3.37382900	-4.79215400
C	-2.65055900	1.12431400	-2.18326600
C	-2.46745900	1.85161900	-3.38635400
H	-1.98302800	2.81910100	-3.36577900
C	-3.37294600	-0.90894500	-0.95126300
C	-4.56880300	-1.19479200	-0.39632000
N	-2.18132300	1.62438000	-0.94469600

C	-1.67758800	2.99741600	-0.85478000
H	-0.90830400	3.13475000	-1.62139200
H	-1.15899300	3.05924500	0.10606300
H	-2.82013800	1.39158100	-0.18306900
N	-2.10041500	-1.30789300	-0.52450000
C	-1.54058500	-1.67539200	0.68314400
C	-0.35509800	-2.43350400	0.56558100
C	-2.00958400	-1.36803000	1.98343800
C	0.31230600	-2.91637100	1.66159800
H	0.03011800	-2.62784800	-0.42924600
C	-1.33260800	-1.91039900	3.09694300
C	-0.19546900	-2.66947200	2.94586700
H	1.22272500	-3.49497500	1.52936900
H	-1.69176900	-1.70519200	4.09810200
C	-3.06015700	-0.37787800	2.24761000
O	-3.36160300	0.55250000	1.52824500
C	-3.82690500	-0.47310800	3.59181100
F	-4.97267400	0.19198100	3.51751700
F	-3.10408600	0.07715900	4.59079400
F	-4.08330400	-1.73350100	3.94283800
H	-1.44364800	-1.36743200	-1.29925400
C	-2.71903900	4.08951900	-0.91303400
C	-2.54114900	5.20372200	-1.73175200
C	-3.83135800	4.03720600	-0.06794500
C	-3.45788400	6.25250700	-1.71088900
H	-1.66521000	5.25953200	-2.37425100
C	-4.74930400	5.08181200	-0.04805700
H	-3.96933200	3.18271700	0.59242400
C	-4.56390300	6.19311200	-0.86879200
H	-3.30722700	7.11439400	-2.35351500
H	-5.60864000	5.03213500	0.61323600
H	-5.27985800	7.00843600	-0.85089900
C	0.54022200	-3.22063100	4.12536300
F	1.78584600	-2.72378300	4.21038000
F	-0.07714500	-2.94731400	5.28419900
F	0.67267700	-4.55550300	4.04512600
H	-5.41120900	-0.68010400	-0.85099500
C	-4.91177400	-2.13009500	0.67988300
C	-6.05157100	-1.88108300	1.46037700
C	-4.20070300	-3.31947200	0.90285500
C	-6.46444500	-2.78387800	2.43221800
H	-6.61070000	-0.96423500	1.29565300
C	-4.61345000	-4.22022300	1.87729700
H	-3.33522600	-3.54826400	0.28773500

C	-5.74577600	-3.95758100	2.64396500
H	-7.34604600	-2.56909600	3.02749400
H	-4.05131200	-5.13545500	2.03263700
H	-6.06531200	-4.66358300	3.40348200

### TS3b

Value of imaginary frequency = -288.46 cm<sup>-1</sup>

P	0.97695300	0.08409800	-0.30007900
O	2.21806400	1.05814500	-0.64328200
O	1.68070400	-1.35297100	-0.05867800
O	-0.02700500	0.14471200	-1.37712800
C	3.28510100	1.00695900	0.24795500
C	4.13442500	-0.09503800	0.19371200
C	3.44726300	2.05055200	1.15873400
C	4.48551300	1.92446600	2.07484900
C	5.30516000	0.79226700	2.12137100
H	4.64501300	2.72567700	2.79279100
C	2.66597900	-1.72982300	-0.96371900
C	3.91031300	-1.10156100	-0.88783900
C	2.38547000	-2.73215200	-1.89266000
C	3.39345400	-3.05398000	-2.79637500
C	4.61895800	-2.38513600	-2.81860200
H	3.20435500	-3.84046900	-3.52322100
C	4.88218700	-1.38812300	-1.86743900
C	6.14702800	-0.55285200	-1.95880600
C	7.25420800	-1.22384500	-2.76717000
H	7.65902200	-2.07561800	-2.20444600
C	6.70610300	-1.71501100	-4.10319800
H	7.50489900	-2.11927400	-4.73174100
C	5.64240700	-2.78287500	-3.86475000
H	5.12636000	-3.02971700	-4.79809000
H	5.87507700	0.39702400	-2.44120100
C	5.12853900	-0.23563900	1.18333500
C	5.91543300	-1.52880300	1.29730300
C	7.19677900	-1.38176600	2.11299800
H	7.92926800	-0.78900100	1.54886700
C	6.89741300	-0.68805900	3.43831400
H	7.78668200	-0.65402700	4.07448100
C	6.38977500	0.72781400	3.17970900
H	7.23071800	1.35393300	2.85171100
H	5.26217200	-2.26652300	1.78471500
H	6.13395700	-3.70775900	-3.53359100
H	6.26674100	-0.86835000	-4.64533100
H	8.07769600	-0.51933000	-2.91602300



H	6.50950700	-0.28024200	-0.96558600
H	6.13483900	-1.94170100	0.31011100
H	7.64237200	-2.36715500	2.27796500
H	6.13510600	-1.26162600	3.98022200
H	6.01725500	1.17898700	4.10497800
O	0.52765600	0.40684300	1.16238500
H	-0.35324300	0.87073800	1.28847400
C	4.09225200	4.99072400	-1.85168600
C	3.87983000	4.05545300	-0.88285200
C	2.81781900	4.20328900	0.06800500
C	1.98276800	5.36598100	-0.03216200
C	2.24302600	6.32588800	-1.06075000
C	3.26347500	6.14649300	-1.94491800
C	2.57335500	3.25753000	1.08533100
C	0.91961700	5.52970800	0.85661900
C	0.66004000	4.59242400	1.85528900
C	1.51276600	3.44206300	1.99196400
C	1.21683000	2.50462100	3.03670700
H	1.85165800	1.63251800	3.14739200
C	0.13260200	2.67568700	3.84392300
C	-0.72969300	3.80194500	3.68512300
C	-0.46554200	4.73372900	2.72940300
H	4.90272000	4.85817800	-2.56123800
H	4.52299600	3.18415000	-0.81963700
H	1.59607900	7.19666500	-1.11888100
H	3.45229600	6.88014300	-2.72194800
H	0.26051600	6.38942300	0.74519200
H	-0.09019300	1.94213700	4.61221000
H	-1.59958900	3.90013100	4.32555900
H	-1.11080900	5.59708800	2.59191500
C	-1.06153100	-1.44835800	-4.14246100
C	0.03967500	-1.86963400	-3.45684800
C	0.00733600	-3.07142100	-2.67788000
C	-1.20618400	-3.84644300	-2.67792100
C	-2.33379000	-3.37293500	-3.42135500
C	-2.26868200	-2.20811100	-4.12573100
C	1.09671000	-3.48846400	-1.88779000
C	-1.27418100	-5.01548300	-1.91771700
C	-0.20741100	-5.42734300	-1.11733200
C	0.99925300	-4.64640800	-1.09031900
C	2.05596200	-5.06781900	-0.21766400
H	2.97007000	-4.48460500	-0.18506300
C	1.91905300	-6.17338100	0.56904400
C	0.72120000	-6.94696800	0.53778300

C	-0.30497100	-6.58510700	-0.28181100
H	-1.03057300	-0.51263100	-4.69086900
H	0.94278900	-1.27033200	-3.45342900
H	-3.25140500	-3.95420400	-3.39629500
H	-3.13790400	-1.84714300	-4.66814500
H	-2.19201200	-5.59899000	-1.92213600
H	2.72710100	-6.47035000	1.22946700
H	0.63274600	-7.82233800	1.17255800
H	-1.22381000	-7.16389600	-0.31135100
C	-5.88305600	-0.93148700	-4.91918900
C	-5.14240000	0.20477700	-5.12977200
C	-4.35042700	0.76149000	-4.09569500
C	-4.31640800	0.13227500	-2.81924800
C	-5.09949400	-1.04120200	-2.62759600
C	-5.86070800	-1.55221300	-3.64872300
H	-3.61203200	2.42646500	-5.26222800
H	-6.48625000	-1.35079900	-5.71728000
H	-5.15013400	0.69807100	-6.09831400
C	-3.57166900	1.93338100	-4.29456200
C	-3.47152500	0.66657500	-1.80422500
H	-5.09388100	-1.53896000	-1.66187100
H	-6.45259000	-2.44617000	-3.47826800
C	-2.71500900	1.81517000	-2.02550800
C	-2.79213100	2.45234400	-3.30291300
H	-2.23348800	3.36713600	-3.46726100
C	-3.39864300	-0.08784500	-0.51845400
C	-4.32793000	0.10960300	0.51529200
N	-1.95356000	2.34826300	-1.02956300
C	-0.89144700	3.30413800	-1.25315700
H	-0.35738800	3.09111900	-2.18796800
H	-0.15846300	3.16654700	-0.44548300
H	-1.86429500	1.79963800	-0.18752200
N	-2.39582700	-0.97179200	-0.43604500
C	-1.91117200	-1.52995700	0.76995100
C	-1.17204800	-2.70197100	0.71404600
C	-2.11816100	-0.87637600	1.99177200
C	-0.62311700	-3.23918100	1.87269200
H	-1.03322500	-3.18766800	-0.24114100
C	-1.56306200	-1.41167000	3.14523700
C	-0.83260200	-2.59882300	3.08649200
H	-0.04499200	-4.15754600	1.82051400
H	-1.69217100	-0.90373400	4.09600500
C	-2.63692300	0.53432400	2.01154000
O	-1.85205100	1.43259400	1.63352000

C	-3.55971100	0.95719100	3.16673100
F	-4.43543200	1.89498000	2.80656800
F	-2.78282300	1.48340700	4.13335800
F	-4.21523600	-0.06318300	3.71596800
H	-1.73798200	-0.97958600	-1.21988500
C	-1.37453400	4.73992800	-1.21621800
C	-0.86095000	5.69766600	-2.08726800
C	-2.29976800	5.12812100	-0.24358500
C	-1.25157400	7.03218500	-1.98126700
H	-0.13292400	5.40195600	-2.83943500
C	-2.68742000	6.45861400	-0.13342600
H	-2.69722400	4.37276100	0.42985500
C	-2.16067100	7.41649100	-1.00049200
H	-0.84535800	7.76993400	-2.66686300
H	-3.40242000	6.75215500	0.62935000
H	-2.46557000	8.45473400	-0.91636300
C	-0.20626900	-3.14516400	4.33588000
F	1.03861400	-2.67740600	4.51345800
F	-0.90762800	-2.81058000	5.42952200
F	-0.11835700	-4.48247700	4.30174700
H	-4.90166400	1.02194600	0.37474100
C	-5.11417200	-0.96708200	1.16235100
C	-6.25341700	-0.59008200	1.89336800
C	-4.86366700	-2.33888000	1.00692000
C	-7.08611900	-1.53644700	2.47004800
H	-6.47254700	0.46704000	2.01333200
C	-5.70447900	-3.28688100	1.58384000
H	-4.02834300	-2.68249500	0.40701800
C	-6.81275300	-2.89523700	2.32471300
H	-7.95560100	-1.21214800	3.03298900
H	-5.48697200	-4.34117000	1.44472400
H	-7.46264200	-3.63774300	2.77553100

**IM6b**

P	-1.09982500	0.06735700	0.20306700
O	-2.14118400	1.18214100	0.72115800
O	-2.03418800	-1.21300900	-0.13212100
O	-0.33936400	-0.24766300	1.53310400
C	-3.19416900	1.40459800	-0.16802900
C	-4.22672300	0.46812000	-0.19892900
C	-3.15805200	2.52121100	-1.00209900
C	-4.20453900	2.65656000	-1.90972800
C	-5.22057000	1.70541700	-2.02928700
H	-4.20852600	3.52298100	-2.56698100

C	-3.06406000	-1.50433500	0.75621700
C	-4.17911700	-0.66430500	0.77397100
C	-2.95266300	-2.61990000	1.58649900
C	-3.99886100	-2.85224700	2.47473500
C	-5.09324700	-1.99191100	2.58363100
H	-3.93879400	-3.72012000	3.12737900
C	-5.18140100	-0.87353300	1.74124200
C	-6.27907100	0.15637400	1.94210000
C	-7.48488600	-0.39087800	2.70073500
H	-8.03324900	-1.09803100	2.06408800
C	-7.02804700	-1.10271800	3.97007700
H	-7.88368600	-1.42357000	4.57133900
C	-6.16797100	-2.30956000	3.60568600
H	-5.70091400	-2.73558100	4.49944300
H	-5.84393200	0.98933500	2.51271600
C	-5.22991100	0.58830300	-1.18069100
C	-6.23362200	-0.53101900	-1.39122300
C	-7.46914300	-0.09047600	-2.17143700
H	-8.08438000	0.57163700	-1.54754900
C	-7.05354900	0.65060300	-3.43847900
H	-7.92379200	0.89645100	-4.05398000
C	-6.30146900	1.92635500	-3.06974600
H	-7.01671800	2.66013700	-2.67388800
H	-5.72139400	-1.32761900	-1.94949200
H	-6.81449800	-3.09659900	3.19430500
H	-6.44605300	-0.40460100	4.58466900
H	-8.17255100	0.42687800	2.93539700
H	-6.59025200	0.58901800	0.98903100
H	-6.52257100	-0.98277100	-0.43992000
H	-8.08248200	-0.96397400	-2.41121900
H	-6.40677700	-0.00010800	-4.04015200
H	-5.85692100	2.38385000	-3.95939100
O	-0.31898600	0.43996100	-0.99038300
H	1.23638700	1.06264900	-1.74185500
C	-3.18277500	5.43622200	2.11204300
C	-3.16313300	4.50208300	1.11928600
C	-2.13608400	4.50696600	0.12027100
C	-1.13469500	5.53378100	0.18784700
C	-1.19419200	6.49692400	1.24424700
C	-2.18328300	6.45027100	2.18004000
C	-2.07639400	3.54538400	-0.90880100
C	-0.10593200	5.55630200	-0.75458100
C	-0.02185300	4.59203500	-1.75822900
C	-1.02917200	3.57029800	-1.84985300

C	-0.90100900	2.58923600	-2.88861900
H	-1.64361500	1.80237800	-2.95662700
C	0.16129200	2.60788400	-3.74280900
C	1.16991900	3.61243700	-3.63609900
C	1.07378500	4.57655900	-2.68053000
H	-3.96702300	5.41088900	2.86176200
H	-3.93100800	3.73685300	1.07751900
H	-0.42062700	7.25901100	1.28250800
H	-2.21769700	7.18359100	2.97921800
H	0.67200800	6.31417200	-0.67612600
H	0.25563800	1.83863200	-4.50311900
H	2.01870400	3.58853200	-4.31113800
H	1.83631100	5.34362500	-2.57741100
C	0.37796900	-2.16456200	4.24645700
C	-0.70420100	-2.34760000	3.43890100
C	-0.71576300	-3.38124600	2.44543500
C	0.42062600	-4.26014900	2.37044000
C	1.53395000	-4.03168200	3.24070700
C	1.52178400	-3.00962800	4.14049600
C	-1.77381800	-3.53484100	1.52836700
C	0.42931900	-5.28930500	1.42860700
C	-0.62019300	-5.45962900	0.52356300
C	-1.73677300	-4.55560500	0.55716100
C	-2.76615000	-4.71744800	-0.42592000
H	-3.61069000	-4.03641300	-0.41362700
C	-2.69256000	-5.70356000	-1.36557300
C	-1.58697600	-6.60387100	-1.39191200
C	-0.58540200	-6.48319200	-0.47556000
H	0.38355700	-1.35329600	4.96712000
H	-1.55623100	-1.68081700	3.50578100
H	2.40152600	-4.67963600	3.15051200
H	2.38656000	-2.82288000	4.77071200
H	1.28688600	-5.95638500	1.37877000
H	-3.48039900	-5.80629200	-2.10457400
H	-1.54665600	-7.38035200	-2.14863500
H	0.26568800	-7.15827200	-0.49000700
C	5.19560700	-2.02651100	5.02548900
C	4.65624800	-0.79012800	5.27678700
C	3.97820900	-0.06921800	4.26224400
C	3.84626500	-0.63966400	2.96406700
C	4.41367700	-1.92409600	2.73405800
C	5.07175800	-2.59242200	3.73442000
H	3.55101000	1.66657900	5.47778300
H	5.71704900	-2.56839400	5.80738300

H	4.74409600	-0.33860900	6.26167400
C	3.42595700	1.21796700	4.49582100
C	3.15283100	0.08590300	1.95975200
H	4.31347700	-2.37952000	1.75458000
H	5.49979700	-3.56990900	3.53368000
C	2.57204100	1.32713600	2.22781000
C	2.75346100	1.90049100	3.52303500
H	2.36019700	2.89028000	3.72490500
C	2.94321500	-0.46674400	0.59431400
C	3.85853200	-0.00735800	-0.53414400
N	1.81553600	1.95135700	1.27687300
C	1.14214400	3.21514800	1.44589500
H	0.63450200	3.25404300	2.41687800
H	0.34867200	3.24571200	0.68874800
H	1.76798900	1.55143200	0.34844300
N	1.93169400	-1.22947000	0.40230300
C	1.64758600	-1.70091300	-0.90202900
C	0.76129900	-2.76377500	-1.00240200
C	2.17285500	-1.08807200	-2.05058500
C	0.39055800	-3.24920100	-2.25033800
H	0.36279100	-3.18467000	-0.08896900
C	1.79668200	-1.56948500	-3.29658900
C	0.91736900	-2.65084900	-3.38840600
H	-0.30483100	-4.07937800	-2.32935100
H	2.17818000	-1.11806700	-4.20565200
C	3.00084500	0.15786300	-1.81216400
O	2.17614800	1.28410600	-1.58744800
C	3.88076500	0.53558000	-3.00709600
F	4.72106400	1.52548800	-2.67730700
F	3.13252200	0.97546200	-4.03247000
F	4.60882600	-0.49068900	-3.45803000
H	0.51883400	-0.73776300	1.36543700
C	2.04040800	4.42263300	1.26261100
C	1.92585700	5.53772500	2.08963100
C	2.94452000	4.45332000	0.19682200
C	2.69013700	6.67924300	1.85047100
H	1.21709700	5.51986900	2.91474400
C	3.70820500	5.59035700	-0.04242400
H	3.02135200	3.58877600	-0.46049100
C	3.58012200	6.70884600	0.78132100
H	2.59219300	7.54239900	2.50188500
H	4.40279700	5.60758600	-0.87706000
H	4.17670000	7.59576700	0.59311000
C	0.49096600	-3.10960700	-4.75213400

F	-0.44970600	-2.30656100	-5.27451800
F	1.51814000	-3.10892100	-5.61710700
F	-0.01758300	-4.34907700	-4.72908000
H	4.19237300	1.00185500	-0.27136800
C	5.08638700	-0.89414300	-0.66362600
C	6.35123600	-0.30603900	-0.68322400
C	4.98417200	-2.28417600	-0.78020100
C	7.49479700	-1.08804700	-0.81325400
H	6.43787500	0.77317000	-0.59864300
C	6.12688700	-3.06500800	-0.91222200
H	4.00932800	-2.76329200	-0.76073700
C	7.38530300	-2.46944800	-0.92910200
H	8.47141900	-0.61530500	-0.82236200
H	6.03254400	-4.14238400	-1.00092200
H	8.27603000	-3.08083600	-1.02979600

**IM7b**

C	2.75070500	4.75453500	-2.19535600
C	3.71458100	4.00911200	-1.56950000
C	3.39992000	2.75886600	-0.98056700
C	2.06695300	2.26207800	-1.04022600
C	1.08949300	3.06117200	-1.69550600
C	1.42472200	4.26802500	-2.25358700
H	5.40877900	2.35612700	-0.29439000
H	2.99806600	5.71092700	-2.64363000
H	4.74008100	4.36429800	-1.51119000
C	4.38972000	1.98037100	-0.32837100
C	1.76206900	1.01424900	-0.41510500
H	0.07072300	2.69965600	-1.76307900
H	0.65992700	4.85780100	-2.74918000
C	2.76660000	0.26005600	0.19444400
C	4.09691500	0.77072200	0.23231700
H	4.88507900	0.17848100	0.68227200
C	0.37330900	0.49324100	-0.38526300
C	-0.27473600	0.35423900	0.99047800
H	0.50566000	0.10037200	1.71174900
C	-0.89754200	1.67373100	1.42677700
C	-0.63924700	2.14574600	2.71531400
C	-1.72035600	2.42687200	0.58492100
C	-1.19379600	3.34169800	3.15818900
H	-0.00068400	1.56703000	3.37610300
C	-2.27574600	3.62255600	1.02822600
H	-1.93228900	2.08399200	-0.42308700
C	-2.01518400	4.08301600	2.31517200

H	-0.98033100	3.69458200	4.16181700
H	-2.91166200	4.19677600	0.36250300
H	-2.44734000	5.01757300	2.65746400
N	2.48237100	-0.97291400	0.74381900
C	3.45880300	-1.80848400	1.39598600
H	2.90074800	-2.58711500	1.92683900
H	3.98037900	-1.23177700	2.17059800
H	1.61146800	-1.41929800	0.48942600
N	-0.23774100	0.22878400	-1.48033800
C	-1.55801400	-0.25702900	-1.42238200
C	-2.30369300	-0.20581300	-2.60055400
C	-2.13958900	-0.77176800	-0.24776700
C	-3.61786700	-0.65264600	-2.62151900
H	-1.82559400	0.19816200	-3.48600900
C	-3.45195800	-1.22897200	-0.27571900
C	-4.18610100	-1.16168600	-1.45858300
H	-4.20449000	-0.60249100	-3.53226000
H	-3.92686900	-1.61950700	0.61724500
C	-1.22883000	-0.84929700	0.96061000
O	-0.37361900	-1.98307600	0.86652300
C	-1.98849600	-0.98673100	2.28297900
F	-1.16519700	-0.85702100	3.32728800
F	-2.54090600	-2.21541300	2.36623000
F	-2.97212100	-0.09693700	2.41299000
C	4.48570600	-2.46527700	0.48437600
C	5.61373000	-3.06380500	1.04979800
C	4.32198100	-2.50014200	-0.89871800
C	6.55714800	-3.69609700	0.24830500
H	5.75259500	-3.03318000	2.12832300
C	5.26835900	-3.13038600	-1.70348300
H	3.45477500	-2.02367700	-1.34617000
C	6.38589400	-3.73099800	-1.13379600
H	7.42906600	-4.15749100	0.70107900
H	5.13154200	-3.14752000	-2.78009000
H	7.12316900	-4.21995400	-1.76215700
C	-5.58528400	-1.70490800	-1.48280200
F	-5.60104700	-3.02146800	-1.74626300
F	-6.20241500	-1.53820100	-0.30422400
F	-6.33294500	-1.10968900	-2.42248600
H	-0.91559100	-2.75916800	0.67294900

#### IM2-III

P	1.23884800	0.11867500	0.67618000
O	1.55958700	1.06806800	-0.65793100



O	2.68076700	0.21130800	1.45644100
O	1.05922200	-1.24599400	0.08004100
C	2.10822900	2.30319000	-0.41181500
C	3.46364800	2.36409100	-0.08367800
C	1.31012500	3.44439500	-0.52316100
C	1.91076500	4.66423100	-0.22278200
C	3.23769500	4.75775900	0.20533300
H	1.31692900	5.57197000	-0.30723500
C	3.78946400	0.01819200	0.66129400
C	4.23012400	1.08132900	-0.13360600
C	4.41609600	-1.22960500	0.65011600
C	5.50063300	-1.38956600	-0.20820400
C	5.93385500	-0.37374600	-1.06261900
H	6.00388500	-2.35369800	-0.23390100
C	5.28235800	0.86970600	-1.04691800
C	5.61949400	1.92216400	-2.08895600
C	7.00537200	1.73878600	-2.70086100
H	7.77353000	1.97352500	-1.95196200
C	7.18408100	0.30011200	-3.17473100
H	8.13873900	0.17096900	-3.69342800
C	7.10715900	-0.65268000	-1.98419800
H	7.05924700	-1.69311400	-2.32447400
H	4.86403100	1.84829800	-2.88591200
C	4.02563000	3.59941100	0.28791700
C	5.42926400	3.65616100	0.86174200
C	6.03864800	5.05474000	0.81771700
H	6.27117400	5.32539300	-0.22108100
C	5.05830900	6.07080100	1.39640300
H	5.51244800	7.06428300	1.45901800
C	3.79958400	6.12790900	0.53489400
H	4.03636400	6.64363600	-0.40588400
H	5.37022600	3.32333600	1.90775900
H	8.03471200	-0.56675200	-1.40201400
H	6.39328600	0.06283200	-3.89860600
H	7.13891400	2.44259900	-3.52777400
H	5.51179100	2.92883200	-1.68047200
H	6.08166000	2.93418600	0.36415400
H	6.98360300	5.06338800	1.36920500
H	4.79411500	5.77232500	2.41875100
H	3.02550600	6.72835100	1.02406200
O	0.21203600	0.79363200	1.51629400
C	0.38930900	2.00278500	-4.44786300
C	0.67642100	2.48883600	-3.20590000
C	-0.36481900	2.86824200	-2.29415100

C	-1.72250500	2.76304600	-2.75160800
C	-1.98393400	2.21680300	-4.04930900
C	-0.96337900	1.84964200	-4.87480800
C	-0.10159300	3.34448400	-0.99027600
C	-2.76172500	3.20706900	-1.93313200
C	-2.51345100	3.71935500	-0.66102300
C	-1.16641900	3.74884000	-0.15834300
C	-0.96830700	4.16742300	1.19862700
H	0.03131100	4.12097900	1.61553100
C	-2.01700200	4.58628600	1.96370100
C	-3.34490500	4.60484300	1.44353000
C	-3.58363000	4.17056800	0.17557700
H	1.19637200	1.71965800	-5.11613500
H	1.71017100	2.59653400	-2.89526900
H	-3.01988900	2.10753400	-4.35745200
H	-1.17230900	1.44618500	-5.86072900
H	-3.78652100	3.14430600	-2.29315700
H	-1.84489900	4.89025900	2.99140800
H	-4.16895900	4.91675900	2.07763700
H	-4.59503600	4.13613500	-0.22068500
C	2.36401900	-4.59488900	-1.01796600
C	2.99802100	-3.51827200	-0.47403700
C	3.33343000	-3.47955800	0.91763300
C	2.97084800	-4.60572800	1.73340200
C	2.32190300	-5.72647700	1.12048300
C	2.02688400	-5.72225300	-0.21062400
C	3.94906200	-2.35733700	1.50787700
C	3.21874000	-4.56780100	3.10567700
C	3.78188700	-3.44290100	3.70957700
C	4.15501000	-2.31429700	2.90163000
C	4.71790400	-1.17279500	3.55984700
H	5.00723500	-0.31541400	2.96226600
C	4.88054700	-1.14993700	4.91343600
C	4.50218200	-2.26877900	5.71245600
C	3.97429700	-3.37881100	5.12599800
H	2.10574000	-4.58583100	-2.07278300
H	3.22158400	-2.65375300	-1.08554100
H	2.06354500	-6.57640200	1.74641300
H	1.52903100	-6.57518400	-0.66146400
H	2.93838100	-5.41848800	3.72267000
H	5.30087600	-0.27141400	5.39209200
H	4.63736600	-2.22917800	6.78842700
H	3.68047400	-4.23752100	5.72310800
H	-0.17333900	-1.70225400	-0.89066200

C	-6.51737800	-4.27108500	-0.82059700
C	-5.91435800	-3.74335400	-1.94882400
C	-4.57390900	-3.33377800	-1.91023700
C	-3.83699600	-3.45338100	-0.71736100
C	-4.45477000	-3.99384000	0.41328700
C	-5.78032500	-4.39839700	0.36012800
H	-4.51268000	-2.74591900	-4.00154300
H	-7.55645500	-4.57943100	-0.85067500
H	-6.47376300	-3.62854500	-2.87268300
C	-3.93101100	-2.78348600	-3.08453200
C	-2.44214200	-2.97333500	-0.68622400
H	-3.88881600	-4.08312200	1.33570000
H	-6.24925900	-4.80905700	1.24812200
C	-1.89136800	-2.28368800	-1.87178400
C	-2.67261100	-2.29757700	-3.08730300
H	-2.26062200	-1.86730100	-3.99020700
C	-1.65416100	-3.12437300	0.37265600
C	-0.77497300	-3.24049000	1.32692600
C	-0.62984600	-2.32474700	2.47730000
C	0.64361900	-2.14901300	3.02437400
C	-1.71700300	-1.63707400	3.01515300
C	0.83553400	-1.28435200	4.09218100
H	1.48348300	-2.66236000	2.57411500
C	-1.52546200	-0.79098100	4.10304500
H	-2.70929100	-1.77020300	2.59090100
C	-0.25407700	-0.60905000	4.63804400
H	1.83723000	-1.13710400	4.48705800
H	-2.37677300	-0.26599700	4.52537600
H	-0.11146500	0.06225100	5.47873900
N	-0.73160700	-1.69848800	-1.78622300
C	-0.08579100	-0.84876100	-2.78528500
H	-0.80635200	-0.55437400	-3.54978500
H	0.21770000	0.05809200	-2.25365300
C	1.13619600	-1.51123200	-3.38090600
C	1.00026700	-2.58459500	-4.26373300
C	2.41151400	-1.06314000	-3.03528500
C	2.12501600	-3.20241200	-4.80062600
H	0.00803200	-2.94304700	-4.52951500
C	3.53797100	-1.68248200	-3.57374600
H	2.51469100	-0.24755700	-2.32274900
C	3.39774400	-2.75162000	-4.45369800
H	2.00993400	-4.03452700	-5.48785800
H	4.52545600	-1.33697100	-3.28033700
H	4.27644000	-3.23551300	-4.86792500

H	-0.06733300	-4.07214600	1.25174500
C	-4.05664700	1.59730000	2.73432300
C	-5.36914700	1.56424200	2.20868700
C	-5.58156400	1.13686900	0.92245000
C	-4.49730500	0.75750700	0.09902900
C	-3.16799800	0.83666900	0.61285800
C	-2.98431000	1.23857900	1.96828900
H	-3.90273900	1.93772500	3.75502600
H	-6.59395100	1.11048100	0.53700400
H	-1.96481600	1.28094600	2.34096700
N	-2.07834600	0.52736200	-0.10310700
H	-2.15783600	0.49174200	-1.10871600
H	-1.17958600	0.70479500	0.35394800
C	-6.48934400	2.06503800	3.05604900
F	-7.69204300	1.82504100	2.51358300
F	-6.48091200	1.50779700	4.28005300
F	-6.40759400	3.39674100	3.25551700
C	-4.70628700	0.30327800	-1.26159800
O	-3.84101100	0.16098900	-2.11450500
C	-6.14504300	-0.06345400	-1.69752600
F	-6.73021100	-0.89249700	-0.82578900
F	-6.13632300	-0.66118600	-2.88778600
F	-6.91186800	1.03458000	-1.79534700

### IM2-III'

P	1.29236000	0.13711700	-0.45328900
O	1.95378200	-1.28739800	0.07943700
O	2.60168400	0.81347700	-1.18372400
O	0.99423400	0.89170900	0.81168000
C	2.60298900	-2.03541700	-0.87750100
C	3.88031100	-1.63424600	-1.26886100
C	1.97089800	-3.15856200	-1.40998300
C	2.64547500	-3.84211700	-2.41839000
C	3.88389100	-3.41757500	-2.90701100
H	2.17790500	-4.72287900	-2.85324100
C	3.79637300	0.72273200	-0.49761300
C	4.48779700	-0.49287200	-0.52150000
C	4.27058300	1.82791300	0.21192000
C	5.46073400	1.67290000	0.91763000
C	6.14663500	0.45868900	0.96968400
H	5.84638300	2.52413900	1.47428300
C	5.64814100	-0.64653400	0.26273800
C	6.27189300	-2.01930800	0.44843000
C	7.70175200	-1.96653700	0.97955000

H	8.37239500	-1.58787800	0.19672400
C	7.78038000	-1.04977300	2.19598900
H	8.77953800	-1.07053600	2.64128300
C	7.41982500	0.37630200	1.78994300
H	7.32317000	1.01748000	2.67236000
H	5.64395300	-2.56934200	1.16504800
C	4.50942300	-2.29726700	-2.33838000
C	5.79190300	-1.74227300	-2.92999900
C	6.55602900	-2.76397200	-3.76757200
H	6.99006100	-3.53106500	-3.11215300
C	5.61457300	-3.42861300	-4.76776300
H	6.16184200	-4.09636100	-5.43984100
C	4.53430000	-4.21026200	-4.02499600
H	4.98367400	-5.11549000	-3.59411400
H	5.51731900	-0.88965200	-3.56714500
H	8.24495600	0.79501800	1.19771200
H	7.07967600	-1.40738100	2.96163200
H	8.03890700	-2.97748400	1.22728600
H	6.23069200	-2.59945600	-0.47544500
H	6.43198200	-1.32579600	-2.14828000
H	7.38890600	-2.27284400	-4.27959900
H	5.14923100	-2.65469200	-5.39104500
H	3.76202100	-4.55553300	-4.72018000
O	0.26095600	-0.13289600	-1.49197800
C	1.46221700	-4.43198500	2.65821900
C	1.62713100	-4.05300700	1.35815600
C	0.53442000	-4.08208400	0.42959100
C	-0.72777900	-4.58496400	0.89800600
C	-0.85382000	-4.99304200	2.26477200
C	0.20019100	-4.90550900	3.12446700
C	0.64864400	-3.61491300	-0.89736100
C	-1.80957900	-4.65424000	0.01964500
C	-1.72065900	-4.15767700	-1.28039600
C	-0.48225000	-3.59172400	-1.73822500
C	-0.46459400	-2.95982800	-3.02435600
H	0.44134500	-2.45699200	-3.34241400
C	-1.58233300	-2.93368000	-3.80424300
C	-2.79579600	-3.54156900	-3.36661900
C	-2.86279200	-4.13226800	-2.14198700
H	2.29825100	-4.37475400	3.34763400
H	2.59591600	-3.70416300	1.01733200
H	-1.81674600	-5.36923200	2.60062800
H	0.09034400	-5.20578800	4.16156100
H	-2.75672200	-5.06376900	0.36754900

H	-1.55794200	-2.42637900	-4.76303100
H	-3.67361900	-3.50324800	-4.00344900
H	-3.79543100	-4.55052300	-1.77231800
C	1.95658200	3.02081100	3.60913500
C	2.68285800	2.64561100	2.51943200
C	2.82481800	3.51045300	1.38649800
C	2.16321600	4.78506100	1.42040400
C	1.43160400	5.15536300	2.59580700
C	1.33041900	4.30246000	3.65485700
C	3.53612300	3.12534600	0.23336500
C	2.22230800	5.61948600	0.30465700
C	2.89707000	5.23536100	-0.85424500
C	3.56890200	3.96695500	-0.89594300
C	4.23516700	3.59583900	-2.10889800
H	4.75182400	2.64287800	-2.15002800
C	4.21703700	4.41502500	-3.19935000
C	3.53888300	5.66840700	-3.15791300
C	2.90507800	6.06471400	-2.01927300
H	1.84603400	2.33229600	4.44227200
H	3.13130700	1.66072400	2.47925400
H	0.95401100	6.13160000	2.61769600
H	0.76771400	4.59249700	4.53690400
H	1.71057700	6.57902400	0.32805100
H	4.72167200	4.11226100	-4.11122900
H	3.53126000	6.30255500	-4.03844700
H	2.38122400	7.01546500	-1.97627500
H	-0.25789900	0.50715100	1.64156100
C	-7.03185600	1.59144800	1.85177300
C	-6.39982300	0.55253800	2.51054000
C	-4.99888400	0.47902000	2.53672400
C	-4.22884000	1.45551300	1.88223600
C	-4.88069100	2.50950100	1.23494700
C	-6.26436300	2.57765700	1.22287200
H	-4.94357300	-1.31096900	3.76707500
H	-8.11462600	1.63987700	1.81677600
H	-6.97610800	-0.22914800	2.99648900
C	-4.32793600	-0.61040400	3.21115400
C	-2.75761400	1.31625100	1.85270900
H	-4.29097900	3.26179700	0.72167700
H	-6.75514000	3.39096000	0.69918900
C	-2.14426300	0.08856000	2.40289300
C	-2.99415300	-0.80674000	3.15938800
H	-2.55371100	-1.65232200	3.67031600
C	-1.98980200	2.27586300	1.34249600

C	-1.25245200	3.24831000	0.89257400
C	-1.00506700	3.50853700	-0.55884500
C	0.25213900	3.27415800	-1.11310300
C	-2.03786500	3.99579500	-1.36214600
C	0.46780400	3.49666500	-2.46996500
H	1.04684800	2.89109200	-0.48448500
C	-1.81767700	4.22704300	-2.71726000
H	-3.02112700	4.17433000	-0.93917700
C	-0.56573900	3.97190100	-3.27301600
H	1.44947000	3.29196400	-2.88823100
H	-2.63455400	4.58374800	-3.33581900
H	-0.39691100	4.14297200	-4.33141600
N	-0.87673900	-0.13750700	2.22607300
C	-0.10212800	-1.30275800	2.65569600
H	-0.75816000	-2.10013200	3.00635600
H	0.41541500	-1.67167700	1.76594900
C	0.91321700	-0.91478800	3.70753600
C	0.50932000	-0.64851400	5.01669400
C	2.26136200	-0.80028200	3.36701000
C	1.44233200	-0.28123500	5.98106000
H	-0.54245900	-0.72858700	5.28343300
C	3.19605600	-0.43382500	4.33305600
H	2.56563600	-0.98503100	2.33944800
C	2.78964800	-0.17477800	5.63941700
H	1.12031900	-0.08045500	6.99780300
H	4.24281100	-0.34152600	4.05809600
H	3.51910500	0.11155000	6.39031000
H	-0.79851500	3.91965500	1.62800400
C	-3.74585400	-1.86246300	0.04503300
C	-5.13497100	-1.65068300	-0.09152900
C	-5.59252200	-0.57734400	-0.81637300
C	-4.69470600	0.32353500	-1.42588600
C	-3.28221800	0.10468000	-1.30174900
C	-2.84334400	-1.02703800	-0.55022600
H	-3.38746700	-2.71168400	0.61939500
H	-6.66123200	-0.42703200	-0.90852400
H	-1.77180600	-1.20710700	-0.48706100
N	-2.35866700	0.90172800	-1.83864300
H	-2.63687600	1.72310400	-2.35512900
H	-1.36973900	0.64336200	-1.76655600
C	-6.06975400	-2.60596800	0.56238800
F	-7.34779100	-2.39599600	0.22396400
F	-5.77323300	-3.88498100	0.25462100
F	-6.01412000	-2.54308800	1.91486300

C	-5.18427700	1.47295000	-2.16565800
O	-4.50131100	2.37822100	-2.61792700
C	-6.70503000	1.57092600	-2.45496300
F	-7.14874400	0.47127100	-3.07949600
F	-6.96636300	2.61738600	-3.22662400
F	-7.42383700	1.70744900	-1.32588300

### TS2-III

Value of imaginary frequency = -330.56 cm<sup>-1</sup>

P	1.29581800	0.18015200	0.42013600
O	1.90806200	0.81988900	-0.97666100
O	2.59935300	0.32966200	1.40518300
O	1.01437800	-1.24789100	0.07798300
C	2.44564600	2.07936000	-0.83804500
C	3.73039600	2.18841500	-0.30547000
C	1.67415000	3.18248900	-1.20575500
C	2.24062200	4.43752100	-1.00542900
C	3.49927000	4.59832900	-0.41707000
H	1.67209100	5.32058200	-1.28914500
C	3.82332900	0.00209100	0.86754800
C	4.44667700	0.91164300	0.00567400
C	4.38400100	-1.23522600	1.18673000
C	5.61211800	-1.54563100	0.61050000
C	6.24446800	-0.69071900	-0.29560300
H	6.07188300	-2.50282700	0.84630400
C	5.64738300	0.53665300	-0.62802500
C	6.21487300	1.38404700	-1.75364400
C	7.68397500	1.09243800	-2.04616500
H	8.30598300	1.46469400	-1.22114400
C	7.90101600	-0.40921800	-2.20344800
H	8.93139900	-0.62966000	-2.49823000
C	7.57082000	-1.12032300	-0.89401000
H	7.56938700	-2.20641000	-1.03419200
H	5.62103000	1.16915500	-2.65440000
C	4.24700500	3.47089300	-0.04065900
C	5.53563800	3.62640700	0.74579200
C	6.17486400	5.00254000	0.58339100
H	6.57784000	5.10693100	-0.43298600
C	5.13603800	6.09264600	0.82950200
H	5.59445100	7.08591000	0.80653100
C	4.03141000	6.00561300	-0.22041300
H	4.42582100	6.36570200	-1.18060900
H	5.29270400	3.46736100	1.80602800
H	8.36632200	-0.90825600	-0.16654100



H	7.25098900	-0.78316400	-3.00501600
H	7.99366000	1.62974100	-2.94760400
H	6.06727300	2.44801500	-1.55828200
H	6.24609500	2.83670400	0.49028400
H	7.01814000	5.10188900	1.27347400
H	4.70671100	5.95902900	1.83043800
H	3.20255900	6.67321200	0.03702200
O	0.24311600	1.07192700	0.99855000
C	1.15977600	1.31815700	-5.02456000
C	1.31590100	1.93592400	-3.81809500
C	0.18402200	2.35944700	-3.04606200
C	-1.12296100	2.12537700	-3.59378000
C	-1.24435300	1.47969800	-4.86562500
C	-0.14064000	1.08593300	-5.56175600
C	0.31320500	2.97391400	-1.78173900
C	-2.25108000	2.53409000	-2.88262700
C	-2.13836900	3.14721800	-1.63595900
C	-0.83670400	3.35305300	-1.06007500
C	-0.77028500	3.91081000	0.25920100
H	0.19849700	3.99587600	0.73724600
C	-1.90157000	4.28867700	0.91872400
C	-3.18966800	4.12747200	0.32531500
C	-3.30124700	3.56054600	-0.90769500
H	2.03282100	0.99891100	-5.58447000
H	2.31203400	2.11158100	-3.42599900
H	-2.24301900	1.31150900	-5.26004500
H	-0.24338800	0.59655100	-6.52511700
H	-3.23806900	2.35648500	-3.30308200
H	-1.82849300	4.69836700	1.92130500
H	-4.07682900	4.42079400	0.87907400
H	-4.27680000	3.39809800	-1.36152400
C	2.25212100	-4.56565600	-0.43300600
C	2.94980200	-3.52335300	0.09710300
C	2.98766800	-3.29505700	1.50997200
C	2.26773400	-4.20131500	2.36125200
C	1.56101200	-5.29683600	1.76771000
C	1.54960900	-5.47173600	0.41645200
C	3.65006100	-2.18701400	2.07274200
C	2.24360000	-3.97881200	3.73730600
C	2.88099800	-2.87551300	4.30521100
C	3.58840200	-1.95379700	3.46084300
C	4.19417100	-0.80880300	4.07273900
H	4.72743300	-0.10371200	3.44388500
C	4.10200700	-0.59757300	5.41728500

C	3.40209900	-1.51700500	6.25283000
C	2.81364600	-2.61969100	5.71102800
H	2.21873700	-4.69537400	-1.51112300
H	3.45641300	-2.82375000	-0.55585600
H	1.02884500	-5.98060200	2.42397200
H	1.00253100	-6.30077900	-0.02180600
H	1.69442100	-4.66379000	4.37951500
H	4.56380800	0.27929900	5.85965300
H	3.33846900	-1.33000100	7.31989900
H	2.26935100	-3.32308700	6.33501700
H	-0.26177700	-1.78036800	-0.96369100
C	-6.83994300	-3.65878400	-1.07971100
C	-6.09217300	-3.42744200	-2.21404500
C	-4.73284400	-3.07286800	-2.11730000
C	-4.12149300	-2.95454700	-0.84947300
C	-4.90203800	-3.19492200	0.29683700
C	-6.23405700	-3.53922300	0.18110300
H	-4.43688600	-2.90741800	-4.25762800
H	-7.88839700	-3.92396100	-1.15760700
H	-6.54324200	-3.50446400	-3.19939400
C	-3.94839700	-2.80698100	-3.29168900
C	-2.72014100	-2.56046700	-0.77887900
H	-4.44521800	-3.10144000	1.27674700
H	-6.81935000	-3.71446400	1.07797200
C	-1.98040700	-2.27278100	-1.98103400
C	-2.64505900	-2.43940500	-3.24657500
H	-2.10378100	-2.24806000	-4.16444100
C	-2.14126000	-2.23515500	0.42151600
C	-1.54029100	-2.55144900	1.54026900
C	-1.25797900	-1.74301900	2.75289000
C	0.05139700	-1.37997600	3.07695200
C	-2.30498500	-1.40854800	3.61474300
C	0.30077300	-0.63874000	4.22798400
H	0.86501900	-1.66219700	2.41586100
C	-2.04755800	-0.69277900	4.78035300
H	-3.32120200	-1.70028800	3.36491000
C	-0.74657500	-0.29723900	5.08087900
H	1.31976800	-0.33550900	4.45171600
H	-2.86691000	-0.43377000	5.44382100
H	-0.54688300	0.27163200	5.98351200
N	-0.73899400	-1.82319800	-1.88327500
C	0.10578800	-1.29004600	-2.94523400
H	-0.50499200	-1.03828300	-3.81358000
H	0.52613100	-0.35380200	-2.56554000

C	1.23625200	-2.22347500	-3.31617500
C	0.98838700	-3.41102400	-4.00785200
C	2.54556700	-1.89814000	-2.96293900
C	2.03629900	-4.25630400	-4.35711200
H	-0.03239800	-3.67720500	-4.27340400
C	3.59644400	-2.74373300	-3.31365300
H	2.72896300	-0.98674900	-2.39753200
C	3.34513900	-3.92123800	-4.01197200
H	1.83416000	-5.17487600	-4.89884000
H	4.61201800	-2.48451300	-3.02862300
H	4.16410300	-4.57966900	-4.28345700
H	-1.23491400	-3.60296800	1.55854500
C	-3.89368400	1.88989700	2.82921700
C	-5.18397900	1.95026400	2.28599500
C	-5.45129200	1.37760900	1.05814100
C	-4.43429700	0.72719600	0.33998200
C	-3.13768100	0.64192900	0.90479400
C	-2.88536100	1.23907300	2.15293000
H	-3.68926600	2.36280300	3.78501800
H	-6.44950900	1.46442200	0.64672800
H	-1.87213800	1.19749400	2.54358800
N	-2.09440500	-0.03307800	0.29242800
H	-2.15279700	0.00376100	-0.72327000
H	-1.16563500	0.30731100	0.63651900
C	-6.23322400	2.75248600	2.98871700
F	-7.47090900	2.43188200	2.58787900
F	-6.17881700	2.58806800	4.31905000
F	-6.07764900	4.07137700	2.76107100
C	-4.66803600	0.31502600	-1.05404600
O	-3.80654200	0.07360600	-1.87500300
C	-6.12666000	0.24795500	-1.56437500
F	-6.90447800	-0.45044900	-0.73260400
F	-6.17729400	-0.31449900	-2.76404200
F	-6.63886800	1.48740600	-1.66748600

### TS2-III'

Value of imaginary frequency = -297.98 cm<sup>-1</sup>

P	1.28076600	0.14668500	-0.35421900
O	1.85588800	-1.34634600	0.08429500
O	2.59138800	0.73910600	-1.15908700
O	1.12212800	0.89071300	0.93294700
C	2.44141100	-2.09821400	-0.90851000
C	3.72935800	-1.75803800	-1.32535100
C	1.74670300	-3.18305200	-1.44293400

C	2.36047200	-3.87829500	-2.48232900
C	3.60298400	-3.50431800	-2.99845300
H	1.84045600	-4.72923600	-2.91710500
C	3.80070700	0.58051100	-0.50924900
C	4.42060600	-0.67118600	-0.57124300
C	4.35831100	1.64234200	0.20808600
C	5.55521900	1.40300100	0.87742600
C	6.16916100	0.14986600	0.89208700
H	6.00438000	2.21967800	1.43826300
C	5.58941700	-0.90958100	0.17834200
C	6.13638600	-2.31987700	0.31987600
C	7.57756100	-2.36173700	0.82087700
H	8.25327700	-2.00735400	0.03103300
C	7.73555400	-1.47576900	2.05240300
H	8.74040900	-1.56523900	2.47590000
C	7.45292000	-0.02302600	1.68065900
H	7.41381800	0.60531500	2.57661200
H	5.49271000	-2.85011900	1.03729200
C	4.29720500	-2.42862300	-2.42395400
C	5.59245100	-1.92768800	-3.03604400
C	6.28162400	-2.96851000	-3.91406100
H	6.69106000	-3.77133400	-3.28613400
C	5.28310100	-3.56164100	-4.90361700
H	5.77860000	-4.24092200	-5.60377700
C	4.18314700	-4.30408000	-4.14969500
H	4.59600000	-5.24061300	-3.75036900
H	5.34770900	-1.04768000	-3.64756100
H	8.28870700	0.35731500	1.07749600
H	7.02976800	-1.80563400	2.82580100
H	7.85934800	-3.39560200	1.04195600
H	6.04328200	-2.87462300	-0.61591000
H	6.27221300	-1.56301900	-2.26207200
H	7.12625900	-2.50956900	-4.43663100
H	4.84272300	-2.75123900	-5.49805200
H	3.37678600	-4.59369800	-4.83152200
O	0.15694900	-0.00746800	-1.32846200
C	1.28596200	-4.46990300	2.63156300
C	1.43496400	-4.07762800	1.33387200
C	0.32768100	-4.08438200	0.42239600
C	-0.93047100	-4.58579700	0.90315500
C	-1.04043500	-5.00664800	2.26735300
C	0.02650400	-4.93599800	3.11178800
C	0.42595200	-3.60688100	-0.90231500
C	-2.02277100	-4.64638100	0.03742000

C	-1.95113700	-4.13358100	-1.25785200
C	-0.71761400	-3.56673000	-1.72594200
C	-0.71313000	-2.92714400	-3.00851500
H	0.19267600	-2.43089500	-3.33724400
C	-1.83947700	-2.89150200	-3.77586900
C	-3.04959100	-3.49743300	-3.32731500
C	-3.10343500	-4.09748700	-2.10600500
H	2.13266100	-4.42759500	3.30885400
H	2.40179200	-3.73456200	0.98299900
H	-2.00128200	-5.37842200	2.61359100
H	-0.07103800	-5.24474000	4.14758600
H	-2.96372700	-5.06482900	0.39186000
H	-1.82308500	-2.38182600	-4.73359000
H	-3.93350000	-3.45723800	-3.95576700
H	-4.03104500	-4.52347700	-1.73263500
C	2.09637300	2.87008200	3.63193100
C	2.82640100	2.49340200	2.54574700
C	3.00817600	3.37356300	1.43085100
C	2.40408100	4.67544400	1.48909300
C	1.65035800	5.03847700	2.65210600
C	1.49962800	4.16522800	3.68798900
C	3.71254900	2.98542100	0.27464900
C	2.54471800	5.54753200	0.41004400
C	3.24602300	5.17677000	-0.73685800
C	3.83668600	3.87017700	-0.81399800
C	4.52360000	3.51006400	-2.01907400
H	4.97681800	2.52667700	-2.08626600
C	4.60574500	4.37834700	-3.06806200
C	4.01058700	5.67185100	-2.99094900
C	3.35588500	6.05594000	-1.85969400
H	1.95452200	2.17023300	4.45090600
H	3.24355600	1.49567900	2.49270200
H	1.20181300	6.02786100	2.68571000
H	0.92271100	4.45100900	4.56227200
H	2.08099700	6.53047300	0.45448500
H	5.12695100	4.08468700	-3.97362300
H	4.08183600	6.34567300	-3.83862400
H	2.89199100	7.03601000	-1.79133000
H	-0.27722200	0.60076000	1.83368700
C	-7.00457400	1.82474700	1.71166000
C	-6.43822000	0.75755700	2.37448400
C	-5.03774900	0.61778600	2.44069200
C	-4.20103500	1.56524400	1.81278600
C	-4.79944300	2.67100200	1.17539700

C	-6.17229000	2.79412000	1.12463000
H	-5.08298900	-1.19223900	3.63532100
H	-8.08263000	1.92266600	1.64619200
H	-7.06122900	-0.00079800	2.83984700
C	-4.43001900	-0.49088900	3.12299000
C	-2.76169700	1.34162600	1.77906100
H	-4.16806800	3.41132200	0.69484000
H	-6.61456500	3.64252600	0.61148500
C	-2.19573800	0.18832600	2.43151500
C	-3.09078100	-0.69078700	3.14802800
H	-2.68586700	-1.53577500	3.68961100
C	-2.00793600	2.10498000	0.91308600
C	-1.22180500	3.11737100	0.63610200
C	-0.79505800	3.60349000	-0.70409400
C	0.48948700	3.34982100	-1.18002400
C	-1.70616800	4.30673100	-1.49929900
C	0.84998400	3.76516400	-2.45944300
H	1.19567500	2.82010700	-0.55069400
C	-1.33751800	4.72884900	-2.77258500
H	-2.70822700	4.50342200	-1.12972300
C	-0.05969900	4.45408800	-3.25496300
H	1.84833800	3.54401500	-2.82537100
H	-2.05342000	5.26518300	-3.38696300
H	0.22704600	4.77823800	-4.25034600
N	-0.89560900	-0.04213500	2.36588500
C	-0.16718500	-1.24293300	2.76429200
H	-0.85450500	-2.00399300	3.13716800
H	0.30824600	-1.64970800	1.86577300
C	0.89854900	-0.92724800	3.78994400
C	0.54881400	-0.62597000	5.10724200
C	2.24279200	-0.91232700	3.41734400
C	1.52970200	-0.32497100	6.04661800
H	-0.49986200	-0.62492300	5.39692000
C	3.22623100	-0.61092700	4.35750100
H	2.50674300	-1.11828100	2.38254400
C	2.87268000	-0.31846900	5.67201700
H	1.24877500	-0.09622500	7.06979600
H	4.26960200	-0.59393500	4.05547200
H	3.63931600	-0.08220500	6.40311000
H	-0.87434500	3.66571700	1.51764000
C	-3.88044000	-1.86166600	0.08011000
C	-5.22959900	-1.61973400	-0.17691000
C	-5.61691400	-0.47925400	-0.85820600
C	-4.66454300	0.47722700	-1.23342400

C	-3.29562100	0.25632200	-0.91838300
C	-2.91957600	-0.94930200	-0.30761100
H	-3.58145100	-2.76464600	0.60024500
H	-6.66751000	-0.32708200	-1.07177900
H	-1.86130600	-1.13338300	-0.13387600
N	-2.31947900	1.22428500	-1.04641500
H	-2.55468300	2.01019500	-1.64527700
H	-1.35696600	0.84792200	-1.18258900
C	-6.24484500	-2.58537800	0.34485000
F	-7.42977300	-2.46023400	-0.26341300
F	-5.83967700	-3.85959500	0.19304600
F	-6.46129000	-2.41661800	1.66516900
C	-5.08670000	1.71585300	-1.90324400
O	-4.37901100	2.68066000	-2.10899800
C	-6.54153700	1.80627500	-2.43231000
F	-6.81572400	0.76916900	-3.23341800
F	-6.71326100	2.92471900	-3.11993700
F	-7.43401300	1.79362900	-1.43020200

### IM3-III

P	1.39952100	-0.01652800	-0.28242300
O	1.93560800	-0.94707900	0.92810000
O	2.61302900	-0.10778100	-1.34398600
O	1.07836300	1.32168800	0.24506300
C	2.47553600	-2.17790800	0.58287900
C	3.75985100	-2.20889400	0.04016900
C	1.69868900	-3.31647000	0.78554900
C	2.26792800	-4.53104100	0.41104400
C	3.52507700	-4.60953100	-0.19338600
H	1.69529200	-5.44299400	0.56394100
C	3.87429100	0.12274400	-0.79802100
C	4.48787900	-0.90970300	-0.08623300
C	4.43970200	1.38775100	-0.94424400
C	5.68275100	1.59159500	-0.35339100
C	6.31350000	0.60740800	0.41133200
H	6.15118900	2.56776000	-0.45389800
C	5.70272000	-0.64617200	0.57730300
C	6.27005800	-1.65154900	1.56443200
C	7.74506800	-1.42010500	1.88030800
H	8.35611800	-1.68173700	1.00620600
C	7.98225700	0.04256800	2.24227800
H	9.01730500	0.20791100	2.55528200
C	7.65204100	0.93136000	1.04657500
H	7.66853200	1.98768300	1.33344500

H	5.68681500	-1.56027600	2.49240500
C	4.27240600	-3.44030500	-0.41064000
C	5.55515800	-3.48581000	-1.22078600
C	6.19532100	-4.87082800	-1.25187900
H	6.60422000	-5.11298200	-0.26179000
C	5.15597600	-5.91802200	-1.64062900
H	5.61472500	-6.90464100	-1.75374600
C	4.05529400	-5.97583400	-0.58494400
H	4.45212000	-6.46256200	0.31635300
H	5.30230300	-3.18576800	-2.24765800
H	8.43512900	0.80899100	0.28596300
H	7.34237800	0.31138600	3.09259200
H	8.05374900	-2.08120600	2.69540100
H	6.10819300	-2.67536200	1.22163100
H	6.26823200	-2.73763700	-0.86770900
H	7.03464100	-4.87250500	-1.95349300
H	4.72341400	-5.65082500	-2.61292000
H	3.22461300	-6.60129000	-0.92750000
O	0.26177200	-0.77872400	-1.02646200
C	0.96442200	-1.74894400	4.72066000
C	1.19928600	-2.28846200	3.49021200
C	0.12059400	-2.71564700	2.64847200
C	-1.21336900	-2.60702600	3.16793000
C	-1.41808300	-2.04227600	4.46612800
C	-0.36521400	-1.61540400	5.21770600
C	0.32014000	-3.20544300	1.33982400
C	-2.29099400	-3.02737000	2.38946700
C	-2.11028500	-3.48264400	1.08529200
C	-0.78445700	-3.55170900	0.53475100
C	-0.65355300	-3.92099000	-0.84505200
H	0.33265200	-3.91983500	-1.29464900
C	-1.74747000	-4.22824800	-1.59803400
C	-3.05853400	-4.19907200	-1.03631200
C	-3.22929500	-3.83594900	0.26504800
H	1.79698600	-1.40993200	5.32855100
H	2.21808500	-2.38683300	3.13095700
H	-2.43856600	-1.94627300	4.82626100
H	-0.52988000	-1.17358800	6.19507100
H	-3.29881200	-2.95212000	2.79214600
H	-1.62453200	-4.48698100	-2.64496600
H	-3.91602700	-4.43973100	-1.65625100
H	-4.22262500	-3.78173500	0.70518800
C	2.36445000	4.41255800	1.24700800
C	3.05926400	3.47750600	0.54226800



C	3.04159200	3.46451000	-0.89018000
C	2.27560600	4.47488500	-1.56640900
C	1.56883400	5.44699600	-0.78908900
C	1.60796100	5.41558900	0.57137500
C	3.69307000	2.47141400	-1.64632500
C	2.20859200	4.47013400	-2.95900700
C	2.85377700	3.49261000	-3.71644000
C	3.60350600	2.46488400	-3.05111500
C	4.22200900	1.45313700	-3.85539600
H	4.79512800	0.67340100	-3.36429600
C	4.09765000	1.46085400	-5.21407500
C	3.34984600	2.48157500	-5.87122700
C	2.75144500	3.46510900	-5.14262600
H	2.37021400	4.37960000	2.33226600
H	3.60229600	2.70172800	1.07033800
H	0.99051100	6.20208900	-1.31443400
H	1.05557900	6.14797400	1.15138900
H	1.62088300	5.23201800	-3.46619500
H	4.57180400	0.68345300	-5.80465600
H	3.25921100	2.46767100	-6.95250400
H	2.17071900	4.24305900	-5.63036100
H	-0.43189100	2.12123300	1.15357500
C	-7.17562000	3.10512200	0.71476100
C	-6.48283500	3.10463200	1.89713700
C	-5.08770600	2.85671100	1.92677900
C	-4.37832300	2.62967700	0.70952200
C	-5.13627100	2.60699000	-0.49721400
C	-6.48854000	2.83751300	-0.49118000
H	-4.91817600	2.97096500	4.07853900
H	-8.24401400	3.29192400	0.70131200
H	-6.99408900	3.28574100	2.83902300
C	-4.37323300	2.80488000	3.15315900
C	-2.97396900	2.36665000	0.76015800
H	-4.62879400	2.39549500	-1.43258300
H	-7.03857900	2.81180000	-1.42676300
C	-2.30234400	2.33204800	1.98264800
C	-3.03250000	2.56053500	3.18645800
H	-2.50504800	2.54342600	4.13426100
C	-2.25248300	1.86080200	-0.44060300
C	-1.98267900	2.59786400	-1.52130100
C	-1.38949100	2.11859000	-2.79348000
C	-0.04937900	1.73297200	-2.87063900
C	-2.19374100	2.02337900	-3.93590000
C	0.46061800	1.19404500	-4.05024700

H	0.59397900	1.87970400	-2.00740200
C	-1.68057000	1.49882600	-5.11700300
H	-3.23304700	2.33798900	-3.88566900
C	-0.35554600	1.06799800	-5.17044300
H	1.50040100	0.88125600	-4.08779400
H	-2.31589400	1.42068600	-5.99384600
H	0.04593500	0.65138900	-6.08887700
N	-0.95557000	2.06711000	2.02241600
C	-0.29696600	1.25431400	3.03238900
H	-1.02179800	1.00591300	3.81304300
H	0.02248600	0.29754000	2.59266200
C	0.91435400	1.93762400	3.62997100
C	0.76747500	3.08430100	4.41368400
C	2.19542200	1.44121700	3.39129000
C	1.87722400	3.71009100	4.97140700
H	-0.22691300	3.49260400	4.57874500
C	3.31136300	2.07122400	3.94101200
H	2.31221600	0.56288900	2.76129500
C	3.15530800	3.20289300	4.73598900
H	1.74873300	4.59598800	5.58569100
H	4.30430800	1.67818700	3.74000000
H	4.02321300	3.69261800	5.16628200
H	-2.29348200	3.64014000	-1.46985700
C	-3.91755700	-1.39395400	-2.94607700
C	-5.09381400	-1.69227600	-2.26402500
C	-5.23514900	-1.36207600	-0.92535900
C	-4.20237800	-0.70372700	-0.24769000
C	-3.03236800	-0.35605800	-0.95479900
C	-2.89184300	-0.72787100	-2.29073800
H	-3.80554600	-1.67617000	-3.98794700
H	-6.14897200	-1.63553400	-0.41182900
H	-1.96714500	-0.48961200	-2.80621700
N	-1.96258500	0.41436400	-0.37016400
H	-1.91118300	0.18043500	0.62499700
H	-0.62421000	-0.26127700	-0.87340700
C	-6.17321900	-2.46584600	-2.96278600
F	-7.36581400	-2.30391100	-2.37730900
F	-6.29059300	-2.09839000	-4.24549700
F	-5.91262100	-3.78674500	-2.96273100
C	-4.30829300	-0.49580700	1.22140900
O	-3.37079400	-0.35622600	1.97245100
C	-5.70658800	-0.59192100	1.86960200
F	-6.63966100	0.04705100	1.16505600
F	-5.68975200	-0.10842400	3.10109400

F	-6.06028500	-1.89311600	1.93726400
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**IM3-III'**

P	-1.19123200	0.07199500	-0.22456600
O	-1.32656500	1.41202900	0.67325000
O	-2.60156800	0.00973600	-1.01248900
O	-0.88614200	-1.07115600	0.65362800
C	-1.91253500	2.51698800	0.06732900
C	-3.29618200	2.51125500	-0.10330200
C	-1.10266300	3.56869800	-0.35455200
C	-1.73951700	4.63358400	-0.98692300
C	-3.11355500	4.64528600	-1.23383100
H	-1.13330500	5.47210100	-1.32167400
C	-3.72115900	0.07850700	-0.18435000
C	-4.05890600	1.31558000	0.36400900
C	-4.45262000	-1.08289000	0.06512700
C	-5.49853400	-0.97998600	0.97714900
C	-5.79518200	0.21244600	1.64329100
H	-6.08591800	-1.86952400	1.19284900
C	-5.07266700	1.37588000	1.33971000
C	-5.29841400	2.65657500	2.12247600
C	-6.64577700	2.69232800	2.83845000
H	-7.45326900	2.80905400	2.10339500
C	-6.85864000	1.39952700	3.62028300
H	-7.77534300	1.44566400	4.21525900
C	-6.92257100	0.21678500	2.65792100
H	-6.91585800	-0.73022000	3.20765900
H	-4.49373900	2.73120900	2.86781500
C	-3.90543700	3.56775200	-0.80749400
C	-5.36781800	3.48113000	-1.20684700
C	-5.96618600	4.82973000	-1.59806000
H	-6.07971000	5.45687800	-0.70385900
C	-5.05969500	5.53813700	-2.59955300
H	-5.51726100	6.46525700	-2.95691000
C	-3.71133400	5.83975900	-1.95189000
H	-3.83953200	6.65309900	-1.22476500
H	-5.43168400	2.79705700	-2.06551900
H	-7.87780800	0.24830100	2.11660800
H	-6.02601700	1.26227000	4.32214400
H	-6.68760700	3.56251900	3.49992400
H	-5.17986700	3.53171100	1.47907100
H	-5.96330300	3.01442600	-0.41935200
H	-6.96757600	4.67989800	-2.01218800
H	-4.91451300	4.89204800	-3.47442500

H	-2.99765100	6.20637300	-2.69661000
O	-0.20000200	0.40930400	-1.38437400
C	0.52824700	4.23792600	3.54414500
C	0.01277800	4.00206800	2.30378600
C	0.86758900	3.86166600	1.16332400
C	2.28134200	4.00782800	1.36019600
C	2.78169800	4.26910100	2.67461000
C	1.93381200	4.37122600	3.73675400
C	0.37138000	3.58487900	-0.12737100
C	3.14637100	3.86048100	0.27497100
C	2.67074800	3.52216100	-0.98907900
C	1.25695900	3.37826900	-1.20163100
C	0.81082300	2.98023700	-2.50597000
H	-0.25096700	2.83554600	-2.67114100
C	1.70170800	2.72709700	-3.50572500
C	3.10512200	2.88453600	-3.29378800
C	3.57038400	3.28068200	-2.07715600
H	-0.13691800	4.32701700	4.39696200
H	-1.05959600	3.90716800	2.17055300
H	3.85456600	4.37300800	2.80484100
H	2.32353700	4.55872200	4.73199400
H	4.21614400	3.97310200	0.42999500
H	1.34397700	2.39168200	-4.47359800
H	3.79702800	2.67679300	-4.10423600
H	4.63592700	3.39648100	-1.89754100
C	-2.35166100	-4.34045500	1.91248200
C	-3.02279800	-3.31171700	1.32253800
C	-3.49160800	-3.41130400	-0.02449300
C	-3.22716400	-4.62428600	-0.74870700
C	-2.51925400	-5.68169500	-0.09425700
C	-2.09560600	-5.54526000	1.19301900
C	-4.16252200	-2.35222700	-0.66327300
C	-3.63775200	-4.73325000	-2.07638000
C	-4.30233200	-3.68967500	-2.72035500
C	-4.57725200	-2.47508700	-2.00422600
C	-5.25610600	-1.42226500	-2.70119600
H	-5.48331400	-0.50372900	-2.17048400
C	-5.61318500	-1.56070000	-4.01036600
C	-5.32309800	-2.76131900	-4.72231300
C	-4.69214900	-3.79148700	-4.09281900
H	-2.00036400	-4.23726400	2.93376200
H	-3.19059500	-2.39019200	1.86527700
H	-2.32413500	-6.59252700	-0.65351100
H	-1.55375200	-6.35037200	1.67868700

H	-3.42298100	-5.64599700	-2.62736600
H	-6.12311600	-0.74938500	-4.51976300
H	-5.60901900	-2.84828400	-5.76534100
H	-4.46441800	-4.71156000	-4.62357900
H	0.30055700	-2.47405900	1.32647300
C	6.84721500	-3.31959600	-0.38083800
C	6.37759300	-3.44489700	0.90234500
C	4.99789700	-3.31151200	1.19103000
C	4.07662600	-3.05369500	0.14053400
C	4.58870100	-2.98236200	-1.18361900
C	5.93478000	-3.09514900	-1.43490500
H	5.18576200	-3.65215500	3.32207200
H	7.90824600	-3.40249200	-0.59013600
H	7.06189400	-3.63588700	1.72475900
C	4.49568400	-3.41698500	2.51636200
C	2.69466200	-2.80938800	0.43748000
H	3.90238100	-2.83937800	-2.01164700
H	6.29769100	-3.01477500	-2.45581700
C	2.24011500	-2.89357500	1.74900900
C	3.17075300	-3.24368800	2.77815900
H	2.79731800	-3.36625600	3.78948400
C	1.86052900	-2.28565100	-0.68575700
C	0.93863800	-2.99280500	-1.35150600
C	0.27214100	-2.50147300	-2.58393600
C	-1.11135100	-2.31447400	-2.64008900
C	1.04301400	-2.17150100	-3.70624200
C	-1.70325300	-1.77049200	-3.77699700
H	-1.71657400	-2.55228500	-1.76977700
C	0.45112900	-1.63923800	-4.84615800
H	2.11777400	-2.34336700	-3.69241300
C	-0.92449900	-1.43137600	-4.87930200
H	-2.77413400	-1.59567300	-3.79376800
H	1.06623600	-1.38652700	-5.70397100
H	-1.39058800	-1.00511800	-5.76193200
N	0.92191800	-2.65417000	2.11113800
C	0.62786100	-1.73631200	3.21362300
H	1.50566900	-1.67607700	3.86320000
H	0.43778600	-0.72490000	2.82923000
C	-0.57619100	-2.15698000	4.02126700
C	-0.50098000	-3.23587200	4.90540400
C	-1.78541300	-1.47803200	3.88062100
C	-1.61547400	-3.63029200	5.63702600
H	0.43750200	-3.77549800	5.00809900
C	-2.90715300	-1.87553800	4.60694200

H	-1.84840500	-0.65242200	3.17462000
C	-2.82457200	-2.95132300	5.48503300
H	-1.54586700	-4.46890000	6.32270300
H	-3.84772400	-1.34768900	4.47621200
H	-3.69743800	-3.26259300	6.04986200
H	0.69986500	-3.98689800	-0.98163900
C	3.34188600	0.81946200	1.85715600
C	4.61969600	1.23192800	1.48000200
C	5.07770500	1.00936300	0.19194400
C	4.28810100	0.31965500	-0.73818900
C	3.01594400	-0.14868000	-0.33625700
C	2.54789600	0.14461700	0.94721500
H	2.96968300	1.04189300	2.85153000
H	6.06206500	1.37152400	-0.08335300
H	1.54966800	-0.19298000	1.20943300
N	2.19958000	-0.94736300	-1.15823400
H	2.51229900	-0.93374600	-2.12567100
H	0.66608400	-0.09614200	-1.34414600
C	5.51973000	1.94954400	2.44057000
F	6.68449200	1.30706500	2.60259700
F	5.83584000	3.18738200	2.00079300
F	4.96276700	2.09195200	3.64850800
C	4.78393000	0.06412700	-2.10313300
O	4.11974100	-0.35196800	-3.02980800
C	6.27145500	0.36520900	-2.40882600
F	6.48414700	1.69328400	-2.38471500
F	6.59822300	-0.08443600	-3.61073700
F	7.08933100	-0.19344800	-1.51218200

#### IM4c

C	-4.64107900	4.68076100	-0.01115400
C	-5.14394600	3.58148800	-0.65610100
C	-4.35071900	2.42339700	-0.85049000
C	-3.01302200	2.38687100	-0.36134200
C	-2.51819600	3.55034400	0.29429600
C	-3.30923300	4.65841400	0.46155200
H	-5.88380500	1.30717600	-1.88600600
H	-5.25395900	5.56408300	0.13308800
H	-6.16283800	3.57868000	-1.03443900
C	-4.85828900	1.28527300	-1.52722300
C	-2.22614100	1.21028600	-0.56400800
H	-1.49944300	3.55561800	0.66511300
H	-2.90451200	5.53197700	0.96312900
C	-2.75008600	0.11663300	-1.25747400

C	-4.09486500	0.17233700	-1.72873400
H	-4.52141900	-0.68893400	-2.22904600
C	-0.82804000	1.14088400	-0.04770000
C	-0.58644100	1.16371800	1.27946500
H	-1.48061400	1.09864400	1.89381300
C	0.67030000	1.30992000	2.02098100
C	0.76433300	0.75021600	3.30539900
C	1.75383100	2.06458700	1.54561300
C	1.90028500	0.93095900	4.08377400
H	-0.06924700	0.16640800	3.68563900
C	2.89074800	2.24377300	2.32494700
H	1.68833800	2.53956200	0.57120000
C	2.96835900	1.67939400	3.59537200
H	1.95304400	0.48509300	5.07166700
H	3.71550800	2.83540500	1.94092300
H	3.85695100	1.82210200	4.20140700
N	-1.97534500	-0.99981100	-1.49392700
C	-2.55771900	-2.27891700	-1.84045100
H	-1.71947200	-2.96760700	-1.98897100
H	-3.06696800	-2.21200300	-2.80915600
H	-1.13760600	-1.06531500	-0.92820300
N	0.11260700	1.09187500	-1.09219600
C	1.40812900	0.64552600	-1.23951600
C	2.12693100	1.23345400	-2.30856900
C	2.08073200	-0.31208700	-0.43980900
C	3.44571900	0.93520100	-2.54805700
H	1.61787000	1.96298900	-2.93148800
C	3.44294200	-0.57602900	-0.68272100
C	4.12016600	0.03225400	-1.71464600
H	3.97031400	1.40956800	-3.37147200
H	3.96792400	-1.29928000	-0.07094200
C	1.38156400	-1.16493900	0.53254900
O	0.20785200	-1.46792600	0.47893300
C	2.21174600	-1.81827300	1.66225500
F	1.42386100	-2.19524900	2.65971300
F	3.15226100	-1.00236600	2.14166800
F	2.83093600	-2.91331000	1.18527700
H	-0.25824100	1.50384000	-1.93886700
C	-3.50647500	-2.85609400	-0.80258800
C	-4.61178700	-3.60873100	-1.19731700
C	-3.26954900	-2.65880600	0.55891600
C	-5.46569000	-4.16599000	-0.24951200
H	-4.80787500	-3.75702700	-2.25704900
C	-4.12279400	-3.21356300	1.50682500

H	-2.41322300	-2.06683200	0.87299800
C	-5.22226100	-3.96876900	1.10605000
H	-6.32480500	-4.74659000	-0.57047200
H	-3.92986300	-3.05404600	2.56302200
H	-5.88891100	-4.39739800	1.84738700
C	5.56864900	-0.24752600	-1.97001800
F	6.32289200	0.84716600	-1.77939900
F	6.04644400	-1.20845400	-1.16913100
F	5.77700500	-0.63478300	-3.23871300

**IM5c**

P	-0.94888300	-0.66682200	0.27696300
O	-0.61359100	-1.88714900	-0.72188600
O	-2.54243800	-0.75838000	0.50279700
O	-0.40699700	0.59040400	-0.25822000
C	-1.11280400	-3.13185000	-0.35571200
C	-2.47350600	-3.36650300	-0.52759600
C	-0.24154100	-4.07423200	0.18569900
C	-0.80134700	-5.29049700	0.57004700
C	-2.17018600	-5.54689400	0.48546300
H	-0.14573400	-6.05095000	0.98774600
C	-3.39182700	-1.04543500	-0.56200800
C	-3.31993600	-2.30946600	-1.15617300
C	-4.34686300	-0.09694500	-0.94249100
C	-5.15170100	-0.43527600	-2.03182200
C	-4.99988300	-1.61659800	-2.75466700
H	-5.91638100	0.27293300	-2.34086300
C	-4.06942300	-2.56928800	-2.32143700
C	-3.82022500	-3.82635300	-3.13574500
C	-4.97273100	-4.17012400	-4.07571700
H	-5.83632100	-4.51684300	-3.49205400
C	-5.37162700	-2.94276300	-4.88906500
H	-6.13428200	-3.19332000	-5.63207100
C	-5.89228200	-1.85137800	-3.95822300
H	-6.02082900	-0.90927400	-4.50089600
H	-2.91199700	-3.65510300	-3.73101900
C	-3.02747900	-4.57147200	-0.04475600
C	-4.53283900	-4.76930100	0.00118400
C	-4.94543900	-6.23138400	0.14829700
H	-4.73880100	-6.76911400	-0.78681800
C	-4.17374400	-6.88621500	1.28894800
H	-4.52067700	-7.90877600	1.46350600
C	-2.68296900	-6.89136000	0.96494400
H	-2.49162100	-7.63418800	0.17874100



H	-4.91040000	-4.20110100	0.86363500
H	-6.89041000	-2.13490800	-3.59792300
H	-4.49566500	-2.57548600	-5.43822900
H	-4.67795800	-4.99572800	-4.72999600
H	-3.58809500	-4.67452700	-2.48863400
H	-5.01609800	-4.32587200	-0.87089700
H	-6.02434400	-6.29088600	0.31859200
H	-4.35087200	-6.32343000	2.21402400
H	-2.09866800	-7.21033600	1.83397800
O	-0.51001200	-1.11998000	1.72877200
H	0.43596200	-0.93893800	1.89092000
C	2.44957800	-3.38412700	-3.11606400
C	1.59011800	-3.56410600	-2.07342100
C	2.07135300	-3.66313500	-0.72760800
C	3.49181900	-3.61320700	-0.51924700
C	4.36018000	-3.44107200	-1.64359000
C	3.85707800	-3.31365000	-2.90200900
C	1.21470100	-3.82955300	0.38099700
C	4.00373100	-3.74289000	0.77245100
C	3.16598400	-3.87788900	1.88028700
C	1.74268200	-3.88267800	1.68958300
C	0.91093600	-3.93400700	2.85777200
H	-0.16444100	-3.86808100	2.73630200
C	1.45620200	-4.03432400	4.10354700
C	2.86895400	-4.10371000	4.28063800
C	3.69539500	-4.01820500	3.20274800
H	2.06022900	-3.29461800	-4.12484300
H	0.52349800	-3.62272500	-2.25727000
H	5.43228400	-3.40496500	-1.46768700
H	4.52622700	-3.15926300	-3.74176500
H	5.08235100	-3.75492300	0.91819500
H	0.80875800	-4.05914900	4.97395100
H	3.27955200	-4.20345400	5.27993200
H	4.77464000	-4.03637000	3.32390500
C	-4.45988700	3.60678500	-3.07857700
C	-4.26053500	2.47377700	-2.34637400
C	-4.68938400	2.38339600	-0.98011200
C	-5.22769600	3.57106100	-0.37723700
C	-5.43770800	4.73588800	-1.18387000
C	-5.09177000	4.74738000	-2.50123200
C	-4.61844300	1.18627100	-0.23085300
C	-5.57094200	3.56030100	0.97282100
C	-5.45547300	2.40304800	1.74102500
C	-5.00054000	1.18293500	1.13098500

C	-5.01603100	-0.00095200	1.94055300
H	-4.72150400	-0.94705700	1.50432300
C	-5.40686900	0.03648700	3.24664800
C	-5.82798700	1.25600500	3.85209200
C	-5.85317600	2.40075700	3.11583000
H	-4.11716400	3.64997400	-4.10727600
H	-3.75752500	1.62450000	-2.79382000
H	-5.88428500	5.60886300	-0.71598300
H	-5.26706400	5.63037000	-3.10794000
H	-5.96495700	4.46452900	1.43066200
H	-5.40652200	-0.87677500	3.83267600
H	-6.13574600	1.26231100	4.89286000
H	-6.18125500	3.33962700	3.55312700
C	-0.59159100	5.60625300	-4.30497800
C	-1.43572200	5.45118200	-3.23634700
C	-1.00722800	4.79625700	-2.05479500
C	0.32404500	4.30136800	-1.96106600
C	1.17339600	4.47507700	-3.09060000
C	0.72767600	5.10399100	-4.22494700
H	-2.89142500	5.00098500	-1.02157000
H	-0.92746300	6.10834200	-5.20634700
H	-2.45501200	5.82792900	-3.27114300
C	-1.87910000	4.61701900	-0.95261400
C	0.74487000	3.65385300	-0.76247500
H	2.19213200	4.10609300	-3.04391700
H	1.39700700	5.21862800	-5.07217900
C	-0.14016700	3.48770700	0.29955900
C	-1.47199200	3.97741000	0.18170300
H	-2.16179300	3.86191100	1.01112200
C	2.15324000	3.18605400	-0.60473800
C	3.14986600	4.09123200	-0.49057900
H	2.85983800	5.12241200	-0.67404400
C	4.56289700	3.85435400	-0.14857600
C	5.58260500	4.48036400	-0.87452800
C	4.92250300	3.00295000	0.90444100
C	6.92037600	4.22968600	-0.58529200
H	5.31772200	5.15476500	-1.68483800
C	6.25694300	2.74670200	1.19166400
H	4.13946900	2.53894800	1.49714400
C	7.26228200	3.35322500	0.44068700
H	7.69772900	4.71549500	-1.16674000
H	6.50904500	2.07116400	2.00317800
H	8.30537600	3.15010500	0.66012800
N	0.26165000	2.89451500	1.48970300

C	-0.71952000	2.26469200	2.35345000
H	-0.21042500	1.45349900	2.88610900
H	-1.51663400	1.79178400	1.76183400
H	1.12214700	2.37204600	1.41968400
N	2.30235700	1.79158700	-0.49406200
C	3.44898300	1.09218600	-0.84320800
C	4.21842900	1.50311200	-1.94741100
C	3.93713700	0.01458300	-0.05823900
C	5.38171500	0.85126300	-2.29142300
H	3.86615500	2.34456600	-2.53234300
C	5.14035300	-0.61856400	-0.40223300
C	5.84192700	-0.22282500	-1.52012200
H	5.94294500	1.16630600	-3.16551300
H	5.51016800	-1.43772800	0.19940200
C	3.21403000	-0.35842000	1.15619100
O	2.00354800	-0.29053900	1.26253600
C	3.99136200	-0.60795100	2.47217600
F	4.46898900	0.57696800	2.88914600
F	5.03489100	-1.43604900	2.36243700
F	3.17530000	-1.07559200	3.40425700
H	1.44219600	1.25318400	-0.36513900
C	-1.34547400	3.19788400	3.37155600
C	-2.55449000	2.83756100	3.96932800
C	-0.73661400	4.39766600	3.73505500
C	-3.13618900	3.65580500	4.93187200
H	-3.04576000	1.91222100	3.67307700
C	-1.32193000	5.21938900	4.69480600
H	0.19180100	4.67960700	3.24821100
C	-2.51995200	4.84989400	5.29912200
H	-4.07688300	3.36117900	5.38752100
H	-0.84174000	6.15389600	4.96876600
H	-2.97556400	5.49188500	6.04647900
C	7.05094400	-0.98330400	-1.96524000
F	8.05621500	-0.16976400	-2.31318900
F	7.50600300	-1.81243500	-1.01175700
F	6.78515900	-1.74544700	-3.04431500

### TS3c

Value of imaginary frequency = -230.88 cm<sup>-1</sup>

P	-1.25928200	-0.01058300	-0.28736700
O	-2.45403900	-1.04637900	-0.59921000
O	-2.06239500	1.35177200	0.05201700
O	-0.33105500	0.06739100	-1.42552000
C	-3.58117700	-0.99963200	0.21366500

C	-4.47833200	0.05773400	0.05628400
C	-3.75901400	-2.01253800	1.15394800
C	-4.88568900	-1.92641000	1.96531800
C	-5.77543700	-0.85173100	1.89171500
H	-5.05476100	-2.70706000	2.70331600
C	-2.95369500	1.71917200	-0.95481700
C	-4.18639800	1.07001800	-1.00303900
C	-2.55640700	2.67568900	-1.88778100
C	-3.46210200	2.97400800	-2.90097400
C	-4.68638900	2.31084800	-3.02424800
H	-3.18970300	3.72701800	-3.63689000
C	-5.04848700	1.33106900	-2.08617700
C	-6.28577300	0.47865700	-2.30275100
C	-7.30975900	1.13142500	-3.22717200
H	-7.77580200	1.98626600	-2.71918800
C	-6.63039600	1.61150400	-4.50607800
H	-7.36281500	2.00459400	-5.21715400
C	-5.60026500	2.68778700	-4.17446800
H	-4.99382700	2.92628200	-5.05412400
H	-5.95334900	-0.46966000	-2.74858900
C	-5.56289100	0.16627400	0.94875200
C	-6.41241000	1.42460400	0.97133400
C	-7.75964500	1.22761600	1.66107800
H	-8.40602500	0.59530400	1.03783700
C	-7.56023900	0.56334600	3.01998900
H	-8.50564100	0.49298100	3.56585400
C	-6.96290100	-0.82870800	2.83477700
H	-7.73630500	-1.49704600	2.43238900
H	-5.84223500	2.19247000	1.51366100
H	-6.12682400	3.61392700	-3.90659900
H	-6.13502600	0.76106200	-4.99098300
H	-8.10874000	0.41881800	-3.45177000
H	-6.74577700	0.20553000	-1.35083200
H	-6.55055300	1.82381200	-0.03571300
H	-8.26298600	2.19314500	1.76671100
H	-6.88385700	1.17947600	3.62558500
H	-6.66600100	-1.25293000	3.79929200
O	-0.69061700	-0.35369100	1.13103600
H	0.24849900	-0.69504300	1.21617200
C	-3.60592200	-5.16363400	-1.72791100
C	-3.66097700	-4.17006700	-0.79625900
C	-2.73517900	-4.13016400	0.29570800
C	-1.74789400	-5.16846900	0.38312500
C	-1.72700900	-6.19409800	-0.61392700

C	-2.62347000	-6.19188200	-1.63896900
C	-2.76017900	-3.11334400	1.26944900
C	-0.82029500	-5.14741700	1.42540900
C	-0.83187100	-4.13990900	2.38964900
C	-1.82336000	-3.10200900	2.31959900
C	-1.77981800	-2.06059600	3.30414500
H	-2.50323200	-1.25510500	3.24349000
C	-0.82194400	-2.04881100	4.27308000
C	0.15729700	-3.08294800	4.34145200
C	0.14600300	-4.09689000	3.43331500
H	-4.31533400	-5.17410400	-2.54920200
H	-4.41445400	-3.39313100	-0.87223700
H	-0.96643800	-6.96516600	-0.54213600
H	-2.59084300	-6.96950400	-2.39508900
H	-0.06399200	-5.92700900	1.47829200
H	-0.78819200	-1.23476700	4.98986600
H	0.92160500	-3.04714300	5.11082700
H	0.89662500	-4.88173900	3.46690100
C	0.79722900	1.56830600	-4.35604200
C	-0.27675500	1.94559500	-3.60508700
C	-0.15581000	2.96326600	-2.60275600
C	1.12847800	3.58487300	-2.42824600
C	2.23975800	3.13594900	-3.21371700
C	2.08125500	2.15777200	-4.14887700
C	-1.22680900	3.34260500	-1.77026400
C	1.28304100	4.59549300	-1.48154200
C	0.22184500	4.99558900	-0.67016000
C	-1.05068500	4.34328800	-0.79485100
C	-2.10124100	4.74177300	0.09532900
H	-3.06823000	4.25690800	0.01440500
C	-1.90107100	5.71309400	1.03172000
C	-0.63930900	6.36873600	1.14393300
C	0.38516200	6.02123200	0.31470700
H	0.68023000	0.79916800	-5.11361000
H	-1.23532300	1.45702600	-3.73795900
H	3.21102100	3.59127200	-3.03791100
H	2.92777100	1.82338500	-4.74048800
H	2.25841200	5.06065800	-1.35542500
H	-2.70966300	5.99663700	1.69769800
H	-0.50271300	7.14523800	1.88972200
H	1.35417300	6.50690100	0.38962500
C	6.84232200	4.35277400	-1.06258100
C	5.91923600	4.86196000	-0.18527500
C	4.77988700	4.11030000	0.18891900

C	4.58513300	2.80016600	-0.32650300
C	5.55053500	2.30911500	-1.24908000
C	6.64315400	3.06380100	-1.60129900
H	3.97494100	5.61081100	1.52608300
H	7.71110200	4.93509000	-1.34984500
H	6.04160700	5.85740400	0.23336500
C	3.80436100	4.63420300	1.07953200
C	3.40927800	2.05493400	0.03488200
H	5.42058900	1.33027700	-1.69765700
H	7.35938100	2.66081800	-2.31029700
C	2.41208500	2.65170100	0.81786600
C	2.66834400	3.94695500	1.37625000
H	1.94551200	4.37541500	2.05847000
C	3.37848000	0.63159500	-0.37845800
C	4.37323500	-0.23609100	0.12511100
H	4.92267000	0.21894100	0.94424800
C	5.21955400	-1.13451700	-0.69288200
C	5.05275400	-1.33371800	-2.07220600
C	6.33820500	-1.72425400	-0.08160500
C	5.93751300	-2.13038900	-2.79290800
H	4.24691000	-0.83620100	-2.60095300
C	7.21929200	-2.51755400	-0.80086300
H	6.50263700	-1.55799000	0.97926800
C	7.01808700	-2.73587900	-2.16237000
H	5.78132400	-2.26742900	-3.85832700
H	8.07025800	-2.96492100	-0.29701600
H	7.70505500	-3.35789200	-2.72641200
N	1.21405600	2.04210900	1.07495100
C	0.24594900	2.57657200	2.01722300
H	-0.65624600	1.97078500	1.90835500
H	-0.03163800	3.59097800	1.71022500
H	1.20280400	1.03937800	0.95945300
N	2.38265100	0.17854600	-1.15674300
C	2.12475100	-1.20726400	-1.34094400
C	1.65411400	-1.68404300	-2.55632900
C	2.35869300	-2.08432000	-0.27615000
C	1.43313200	-3.04650000	-2.71992400
H	1.44785000	-0.97866500	-3.35407500
C	2.13050100	-3.44273300	-0.43909100
C	1.68771300	-3.92153600	-1.67043100
H	1.06190600	-3.43017200	-3.66383700
H	2.29257300	-4.12870600	0.38558200
C	2.70851500	-1.49334200	1.05531300
O	1.83411200	-0.81709000	1.64291500

C	3.64086400	-2.27446100	1.99168200
F	4.45864500	-3.10611200	1.34391700
F	2.88117900	-3.02996000	2.80182700
F	4.37200500	-1.47087900	2.76578600
H	1.65504300	0.81304500	-1.48773200
C	0.67982600	2.57876600	3.47160000
C	0.25717100	3.60864200	4.31302700
C	1.46191600	1.54773000	3.99582200
C	0.59903500	3.60881700	5.66219500
H	-0.34321700	4.41752300	3.90061200
C	1.80438300	1.54955400	5.34502200
H	1.80096700	0.74198100	3.34926400
C	1.37438900	2.57640900	6.18181400
H	0.26614700	4.41778400	6.30511400
H	2.41308500	0.74339100	5.74334700
H	1.64664200	2.57486100	7.23251400
C	1.55681100	-5.39881400	-1.89346700
F	0.53442900	-5.69488700	-2.70642400
F	2.66092200	-5.91234000	-2.45909800
F	1.36981300	-6.06656900	-0.74088600

**IM6c**

P	1.37341900	0.03338600	-0.23925200
O	2.36962700	1.22325400	-0.66405100
O	2.36631000	-1.04336100	0.42966900
O	0.89522800	-0.52238900	-1.61003000
C	3.24807800	1.62888000	0.34047900
C	4.37547600	0.84418000	0.58353300
C	2.94033900	2.76944400	1.07607000
C	3.83493700	3.12033300	2.08469900
C	4.95250600	2.34436900	2.39648800
H	3.62728900	4.01208200	2.67140800
C	3.54117500	-1.32369000	-0.26440400
C	4.56981800	-0.38162500	-0.24541300
C	3.62861100	-2.53107800	-0.95269300
C	4.80426600	-2.76426700	-1.66071000
C	5.83001000	-1.81918500	-1.73499100
H	4.90539500	-3.70197500	-2.20227200
C	5.70880100	-0.60370300	-1.04353500
C	6.72999500	0.50134400	-1.24488300
C	8.07547000	-0.01119300	-1.75115400
H	8.58154900	-0.57382100	-0.95521700
C	7.86810300	-0.91898900	-2.95980200
H	8.82571300	-1.22603400	-3.39035000

C	7.06321500	-2.15047000	-2.55350200
H	6.76687900	-2.72653700	-3.43600900
H	6.31262300	1.19955200	-1.98440200
C	5.21557200	1.17549000	1.66432400
C	6.30666400	0.21918500	2.11311100
C	7.36831100	0.88530000	2.98392200
H	7.97557200	1.56556800	2.37198100
C	6.70582100	1.67237200	4.10998600
H	7.45298600	2.08567100	4.79381300
C	5.85765200	2.79846600	3.52576500
H	6.52381700	3.58182300	3.13942600
H	5.82077800	-0.58070900	2.69031500
H	7.70431200	-2.81389000	-1.95719600
H	7.32884400	-0.36371100	-3.73747400
H	8.72021300	0.83582800	-2.00331700
H	6.85852500	1.08831300	-0.33302900
H	6.76956200	-0.28029500	1.25997300
H	8.04535500	0.12436600	3.38311800
H	6.07144700	0.99622700	4.69674800
H	5.25203900	3.27125400	4.30553800
O	0.32844800	0.40900300	0.74654400
H	-1.21909300	1.27099200	1.12386500
C	2.41288300	5.03388900	-2.53186600
C	2.57156500	4.30104100	-1.39323600
C	1.58143600	4.31793400	-0.35811700
C	0.42723500	5.15012600	-0.54527000
C	0.30990800	5.92073600	-1.74456800
C	1.26455800	5.85794000	-2.71425100
C	1.70335100	3.56016800	0.82317900
C	-0.55880000	5.19335700	0.44068100
C	-0.46458800	4.42037800	1.59716100
C	0.67711900	3.56983800	1.78906600
C	0.70177500	2.73340600	2.95380800
H	1.52863600	2.04411900	3.08429400
C	-0.30979700	2.77323300	3.86699900
C	-1.41609700	3.65574600	3.69653800
C	-1.48877900	4.45033500	2.59493600
H	3.17098200	4.99624800	-3.30759000
H	3.45641100	3.68729500	-1.26353100
H	-0.56061200	6.55729600	-1.86229400
H	1.15825200	6.43983900	-3.62427000
H	-1.42669200	5.83193000	0.29495300
H	-0.28175500	2.11751500	4.73176400
H	-2.20996500	3.66925000	4.43606800



H	-2.33929600	5.10690800	2.43636000
C	1.19686200	-3.17899400	-4.41856500
C	1.97005700	-2.97158700	-3.31547700
C	1.74278500	-3.70816100	-2.10670200
C	0.66776500	-4.66008300	-2.09112400
C	-0.11928000	-4.84711800	-3.27070000
C	0.13647900	-4.13179500	-4.40029400
C	2.49948800	-3.50155900	-0.93713100
C	0.38903200	-5.36412300	-0.92103900
C	1.11208400	-5.14369600	0.25025800
C	2.18611500	-4.19232000	0.25031500
C	2.89867700	-3.98561300	1.47646100
H	3.72101000	-3.27824700	1.49266600
C	2.55855900	-4.65861600	2.61197900
C	1.48650000	-5.59961300	2.60923400
C	0.79185300	-5.83491500	1.46137900
H	1.37817200	-2.60115800	-5.31931600
H	2.75178000	-2.22066100	-3.33120000
H	-0.94411000	-5.55330800	-3.23114900
H	-0.47783600	-4.26947200	-5.28442200
H	-0.42773900	-6.08165800	-0.91794400
H	3.10958600	-4.48196900	3.53011300
H	1.23435700	-6.12845800	3.52299000
H	-0.02682900	-6.54940800	1.44029000
C	-3.75350100	-5.07515600	-3.13237000
C	-3.46066600	-5.46028400	-1.84802900
C	-2.92307800	-4.53899800	-0.91591200
C	-2.67507200	-3.19403400	-1.31371700
C	-2.98445200	-2.82716600	-2.65125200
C	-3.50751900	-3.74227100	-3.53050400
H	-2.86381900	-5.94112600	0.72804100
H	-4.17001500	-5.78538600	-3.83886200
H	-3.64567900	-6.48015100	-1.51955600
C	-2.64542400	-4.91958300	0.42510300
C	-2.18912600	-2.27101100	-0.33619600
H	-2.78444300	-1.81376700	-2.98105300
H	-3.73065600	-3.43740000	-4.54824200
C	-1.83066300	-2.70208200	0.94489300
C	-2.10306600	-4.04970200	1.32558200
H	-1.88062000	-4.37668500	2.33420700
C	-2.32238200	-0.81276200	-0.55023500
C	-3.42676800	-0.15860700	0.25952800
H	-3.41988300	-0.62587900	1.24678700
C	-4.76326900	-0.48399300	-0.39462500

C	-5.02111100	-0.20925800	-1.74005700
C	-5.75465200	-1.09278500	0.37614800
C	-6.25164600	-0.53418700	-2.30005900
H	-4.26063100	0.26060600	-2.35761600
C	-6.98468500	-1.41907100	-0.18533500
H	-5.55439200	-1.31147800	1.42174900
C	-7.23617700	-1.13973300	-1.52473100
H	-6.43908300	-0.31715700	-3.34663400
H	-7.74489700	-1.89571400	0.42492600
H	-8.19418000	-1.39655500	-1.96495900
N	-1.23964800	-1.81733700	1.80335900
C	-1.00686200	-2.06894000	3.20935200
H	-0.31147500	-1.29251800	3.54257200
H	-0.50134800	-3.03169000	3.36413000
H	-0.76835000	-1.01018200	1.40954900
N	-1.63523200	-0.17096100	-1.42887600
C	-1.88732100	1.20504800	-1.66006200
C	-1.32901300	1.76338500	-2.80979800
C	-2.67219300	1.98733800	-0.79447600
C	-1.60970200	3.07975000	-3.15119100
H	-0.69577600	1.14362900	-3.43600800
C	-2.94253400	3.30552900	-1.14047700
C	-2.43864200	3.83319000	-2.32797500
H	-1.19354500	3.51862400	-4.05054300
H	-3.55369800	3.92940800	-0.49779800
C	-3.10368500	1.33359600	0.50495600
O	-2.10848000	1.44024000	1.49139200
C	-4.31589000	2.01967800	1.14523400
F	-5.32128800	2.18941900	0.28028500
F	-4.00515100	3.22899700	1.62951500
F	-4.77598700	1.28879300	2.17295400
H	-0.14097600	-0.54685600	-1.67835700
C	-2.28529200	-1.99937900	4.02194100
C	-2.69637000	-3.05759400	4.82755400
C	-3.08170000	-0.85159300	3.94124300
C	-3.89085400	-2.98036900	5.54298700
H	-2.07949500	-3.95131900	4.89495300
C	-4.27552400	-0.77581700	4.64942300
H	-2.75672000	-0.01787400	3.32067500
C	-4.68363000	-1.84220700	5.45103600
H	-4.20352800	-3.81371500	6.16426600
H	-4.88655200	0.11818600	4.57398200
H	-5.61710500	-1.78359400	6.00167900
C	-2.87516400	5.20692200	-2.74346000

F	-2.08140000	5.73351700	-3.68590500
F	-4.12098000	5.19470700	-3.24120700
F	-2.89330900	6.06606000	-1.70521800

**IM7c**

H	1.50049100	-1.99276500	-2.00505700
C	-3.38147100	4.93029000	0.62058800
C	-4.20483400	4.04349900	-0.02247700
C	-3.69100700	2.84549300	-0.57759400
C	-2.30180000	2.55551100	-0.47245700
C	-1.47454300	3.49394900	0.20292900
C	-2.00195100	4.64454600	0.73156400
H	-5.59469800	2.13732500	-1.31687300
H	-3.78146800	5.84592100	1.04311200
H	-5.26905800	4.24283700	-0.11671300
C	-4.53410100	1.91416400	-1.23792200
C	-1.80825800	1.32539200	-1.00735800
H	-0.41214200	3.29809600	0.28527900
H	-1.34933800	5.34647900	1.24114600
C	-2.65245800	0.45460600	-1.69326600
C	-4.04094500	0.76506900	-1.78320700
H	-4.70571500	0.09263500	-2.31187700
C	-0.39523500	0.92195900	-0.80117300
C	-0.18000000	-0.28716400	0.10443400
H	-1.01308700	-0.97814800	-0.05002600
C	-0.21624500	0.13530100	1.56609500
C	0.58586600	1.16495700	2.06565700
C	-1.08884500	-0.52727400	2.43107100
C	0.51973200	1.51670200	3.40935300
H	1.26646100	1.69691100	1.40721200
C	-1.15599000	-0.17207600	3.77443500
H	-1.72010500	-1.32327400	2.04344900
C	-0.35023900	0.84921400	4.26685600
H	1.14758500	2.31774500	3.78552400
H	-1.84208200	-0.69281200	4.43438100
H	-0.40250600	1.12831900	5.31416100
N	-2.15032900	-0.65546900	-2.35039900
C	-2.92717600	-1.86999300	-2.54901400
H	-2.31189400	-2.53044100	-3.16650800
H	-3.82500900	-1.64904100	-3.13499400
H	-1.15177400	-0.80863000	-2.28084400
N	0.55981900	1.60469300	-1.31311500
C	1.88688000	1.19799500	-1.07696100
C	2.89038900	2.12400700	-1.36468500

C	2.22976800	-0.07026400	-0.56958400
C	4.22456300	1.80749700	-1.14970100
H	2.58996100	3.09119300	-1.75195900
C	3.56843400	-0.38672100	-0.36549400
C	4.55732400	0.55282300	-0.65035900
H	5.00553400	2.52941400	-1.36140600
H	3.86087200	-1.35072900	0.03542500
C	1.08175300	-1.03535200	-0.34762300
O	0.70442300	-1.65419800	-1.57398300
C	1.43536600	-2.16748900	0.62273200
F	0.35007400	-2.87530100	0.95861400
F	2.00923400	-1.73314700	1.74296400
F	2.29358200	-3.02508100	0.03197100
C	-3.30202100	-2.57334900	-1.25922300
C	-4.61082700	-2.57387600	-0.78023400
C	-2.30391900	-3.19488900	-0.50301900
C	-4.91982900	-3.17842400	0.43666600
H	-5.39666900	-2.09976900	-1.36256200
C	-2.60771200	-3.79743400	0.71325200
H	-1.27991800	-3.19588400	-0.87017400
C	-3.91944300	-3.78790900	1.18634800
H	-5.94267200	-3.16983300	0.79926000
H	-1.82070800	-4.27356200	1.28959600
H	-4.15951400	-4.25782800	2.13462300
C	5.99788100	0.17172200	-0.46884000
F	6.77562300	1.24576200	-0.27542700
F	6.16513200	-0.64741000	0.57958400
F	6.47868900	-0.47260500	-1.54420000

#### IM2-IV

P	1.27919000	-0.12950200	0.05065800
O	2.65803000	-0.94597400	0.43209600
O	1.86242200	0.96647700	-1.02493800
O	0.84489900	0.53750800	1.32245300
C	3.38020500	-1.41034900	-0.64727200
C	4.18453800	-0.50778100	-1.34997700
C	3.27062800	-2.75442700	-1.00907700
C	4.01694300	-3.18222300	-2.10329700
C	4.80044900	-2.30698700	-2.85740800
H	3.95897200	-4.22839300	-2.39603200
C	3.03748900	1.60658000	-0.69605000
C	4.24239700	0.90279200	-0.85957800
C	2.98927300	2.91934800	-0.22727300
C	4.20763500	3.53786000	0.07427500

C	5.41410400	2.85845400	-0.02917700
H	4.19708200	4.56681400	0.42545800
C	5.43750700	1.52831700	-0.47770300
C	6.77839500	0.83495500	-0.41583600
C	7.93374000	1.67114300	-1.01278000
H	8.04838300	1.44042600	-2.07686400
C	7.73350600	3.18967600	-0.83444400
H	7.33161000	3.62086800	-1.75727600
C	6.73990700	3.49864700	0.29385500
H	7.13178700	3.10541900	1.24259400
H	6.99251900	0.66822000	0.64838900
C	4.86524500	-0.95067800	-2.50114100
C	5.57048900	0.04210200	-3.40638300
C	6.61430000	-0.60677500	-4.31032200
H	7.46603200	-0.94894900	-3.70660300
C	6.00179800	-1.79725900	-5.04215600
H	6.70685600	-2.22392500	-5.76182800
C	5.57837500	-2.86335100	-4.03532600
H	6.47747400	-3.36317700	-3.64957000
H	4.80256700	0.51879100	-4.03244000
H	6.61929500	4.57796100	0.42378600
H	8.69254300	3.68071800	-0.64651500
H	8.86376000	1.35445300	-0.53115800
H	6.74239800	-0.15584500	-0.87314100
H	6.01394300	0.85224400	-2.82648400
H	7.00013400	0.13275600	-5.01867900
H	5.12782600	-1.45605300	-5.61109300
H	4.98505200	-3.64224100	-4.52552600
O	0.34729100	-1.00766500	-0.71540500
C	4.14786500	-4.04360900	2.98744300
C	3.86565300	-3.63452700	1.71816400
C	2.68276400	-4.08250300	1.04435600
C	1.80636100	-4.97886800	1.74621900
C	2.13345300	-5.37229600	3.08276800
C	3.26836300	-4.92338800	3.68495500
C	2.36435600	-3.67937100	-0.26917100
C	0.65024800	-5.44141500	1.11786400
C	0.32595700	-5.05533200	-0.18277000
C	1.19116400	-4.15355200	-0.89224600
C	0.79607300	-3.73830600	-2.20651300
H	1.41259200	-3.01685500	-2.73015400
C	-0.34928600	-4.20715000	-2.77933100
C	-1.19863700	-5.11472700	-2.07842100
C	-0.86758100	-5.52288300	-0.82126600

H	5.04975500	-3.69308000	3.47935300
H	4.53933300	-2.96259600	1.19731200
H	1.44838400	-6.03311400	3.60638400
H	3.50341600	-5.22110600	4.70161500
H	-0.01344100	-6.11546200	1.65543800
H	-0.63842900	-3.86429400	-3.76743000
H	-2.11153200	-5.46747200	-2.54856300
H	-1.50385200	-6.21528900	-0.27501600
C	1.82720100	4.18027000	3.68203500
C	2.12955600	3.69329300	2.44544500
C	1.39408300	4.11111100	1.28659700
C	0.28154800	4.99920800	1.48534500
C	0.00971800	5.50009600	2.79870900
C	0.76700800	5.11729800	3.86199000
C	1.71425100	3.66673400	-0.01576200
C	-0.51843100	5.35105100	0.39945400
C	-0.24868800	4.87596500	-0.88461700
C	0.88936300	4.02401600	-1.10464400
C	1.15086800	3.59437900	-2.44676700
H	2.00666400	2.95590300	-2.63360600
C	0.34263100	3.97136500	-3.47920600
C	-0.78856500	4.80959400	-3.25438200
C	-1.07332300	5.24557200	-1.99527400
H	2.38948100	3.84079200	4.54614400
H	2.91753900	2.95933600	2.32446100
H	-0.82835900	6.17925900	2.92628000
H	0.54575400	5.49423700	4.85526600
H	-1.36589400	6.01563800	0.55390200
H	0.55807500	3.62675800	-4.48528900
H	-1.43076700	5.08261100	-4.08509200
H	-1.94297800	5.86830600	-1.80644400
H	-0.81289500	0.39665800	1.30704400
C	-6.06308100	-3.87451300	0.33056500
C	-6.21802000	-2.51888100	0.56181300
C	-5.10171700	-1.71374500	0.83785500
C	-3.82431900	-2.29866200	0.91293500
C	-3.67882500	-3.66771900	0.67976400
C	-4.78838200	-4.44513300	0.38363300
H	-6.22951000	0.14160900	0.95313500
H	-6.92560300	-4.48671800	0.09227800
H	-7.19999800	-2.05999600	0.50320800
C	-5.22851800	-0.27942900	0.99873100
C	-2.66789400	-1.44502300	1.22963200
H	-2.68457800	-4.10476100	0.71016700

H	-4.66140300	-5.50391200	0.18175200
C	-2.83161500	0.01858200	1.20525700
C	-4.17334900	0.55236300	1.14978500
H	-4.31770600	1.62293700	1.23102800
C	-1.48665700	-1.94612100	1.57345200
C	-0.29665700	-2.31973200	1.94149200
C	0.15580600	-2.48293900	3.33945000
C	-0.64246000	-3.09089200	4.31027300
C	1.42211800	-1.99555800	3.67270300
C	-0.17399300	-3.21119600	5.61394900
H	-1.61884500	-3.47830500	4.03268300
C	1.87780900	-2.10979300	4.98114300
H	2.02991400	-1.52470500	2.90412900
C	1.08494800	-2.71898400	5.95087500
H	2.86131100	-1.73055700	5.24038000
H	1.44872800	-2.81448100	6.96904500
N	-1.78348900	0.78845300	1.25210100
C	-1.77956200	2.24875400	1.24386900
H	-0.78646200	2.52454400	0.87194800
H	-2.52158800	2.62634300	0.53590500
C	-2.00334000	2.80697600	2.62972600
C	-1.23821100	2.32925600	3.69593900
C	-2.95463200	3.80121600	2.84838900
C	-1.43811700	2.83832600	4.97347000
H	-0.47777100	1.57298100	3.51141900
C	-3.14550000	4.31752400	4.12859200
H	-3.54012100	4.17422700	2.01015300
C	-2.39048600	3.83289600	5.19208000
H	-0.84073700	2.46614000	5.79994300
H	-3.88826200	5.09149000	4.29453100
H	-2.54317400	4.22912400	6.19103400
H	0.43739300	-2.44717200	1.14147800
C	-2.40750700	1.89303200	-2.03599600
C	-3.80957100	2.05699200	-2.12202200
C	-4.61916600	0.95674100	-2.25769300
C	-4.08028000	-0.35029200	-2.26040700
C	-2.66817200	-0.52194500	-2.10722000
C	-1.85057100	0.64731400	-2.04118200
H	-1.76593700	2.76619200	-1.95929000
H	-5.68811700	1.10579300	-2.34478400
H	-0.77780700	0.51415800	-1.96167500
N	-2.07107000	-1.71657400	-2.02195100
H	-2.63095100	-2.55645800	-2.01832900
H	-1.10090200	-1.73643600	-1.71245100

C	-4.36949600	3.43317800	-2.01182300
F	-3.91925500	4.25987500	-2.97078200
F	-5.70815400	3.45417800	-2.06500900
F	-4.01546600	4.01166900	-0.83581400
C	-4.93637400	-1.52203900	-2.35915900
O	-4.56516100	-2.68404700	-2.37916900
C	-6.46519700	-1.29982500	-2.49040800
F	-6.75426800	-0.66627400	-3.63531600
F	-7.11503900	-2.45486200	-2.47721800
H	-0.79094300	-3.69080700	6.36704100
F	-6.96040100	-0.54450900	-1.48750300

#### IM2-IV'

P	1.32706900	0.01414400	-0.24396800
O	2.45489800	-0.96949800	0.45277100
O	2.26263300	0.81924900	-1.32389000
O	0.85141000	0.91690500	0.85735200
C	3.28171000	-1.64835500	-0.41850400
C	4.34374100	-0.95891200	-1.01086900
C	3.03141700	-2.99733400	-0.67570000
C	3.87857700	-3.64677000	-1.56775400
C	4.91834400	-2.98289200	-2.22146900
H	3.70849900	-4.70122600	-1.77400900
C	3.44170300	1.34760300	-0.85002900
C	4.52710500	0.48164200	-0.65964600
C	3.51214000	2.71798100	-0.60205400
C	4.71775100	3.22139400	-0.10804100
C	5.79304100	2.38168800	0.16373300
H	4.80276600	4.28844900	0.08323000
C	5.70234100	1.00631800	-0.10268300
C	6.87871400	0.16508700	0.33320400
C	8.24714900	0.75298000	-0.08197600
H	8.54071900	0.35658400	-1.05935500
C	8.25226000	2.29436600	-0.12993100
H	8.12270700	2.63286900	-1.16322800
C	7.10675700	2.88955200	0.70073100
H	7.22782700	2.59427400	1.75261300
H	6.84321900	0.12414500	1.43014900
C	5.14574400	-1.62265100	-1.96067900
C	6.16720300	-0.84953900	-2.77428400
C	7.22550100	-1.74183800	-3.41616500
H	7.88641600	-2.14946900	-2.63909000
C	6.55657200	-2.89067900	-4.16463900
H	7.29341600	-3.49126200	-4.70633800



C	5.78908500	-3.77073400	-3.18202700
H	6.50884900	-4.35779600	-2.59521200
H	5.62127800	-0.31505900	-3.56519500
H	7.13218000	3.98271800	0.67339200
H	9.21587900	2.68245300	0.21230400
H	8.99836300	0.39561700	0.62873900
H	6.78160100	-0.86764000	-0.00911100
H	6.63709500	-0.07149100	-2.17165100
H	7.85091200	-1.14659800	-4.08852200
H	5.86585200	-2.47791500	-4.91062200
H	5.16975000	-4.49750900	-3.71787100
O	0.35984100	-0.78185800	-1.05844600
C	3.33859700	-4.08716600	3.43849800
C	3.23835400	-3.75217800	2.12129600
C	2.05708100	-4.05975000	1.36950600
C	0.99103800	-4.74858700	2.04098600
C	1.12951900	-5.06300400	3.43052100
C	2.26490600	-4.74359100	4.10973900
C	1.91655600	-3.71239300	0.00989300
C	-0.15998800	-5.08910300	1.33106000
C	-0.30117600	-4.77281000	-0.02012700
C	0.74487900	-4.05447400	-0.69467300
C	0.53761700	-3.68895100	-2.06507000
H	1.29103200	-3.08710800	-2.56010800
C	-0.59491200	-4.06190500	-2.72727000
C	-1.61202500	-4.81425200	-2.06663800
C	-1.47337900	-5.14588400	-0.75240800
H	4.24128200	-3.84431100	3.99033000
H	4.05786100	-3.24632300	1.62209200
H	0.30204800	-5.55885900	3.93020900
H	2.35662000	-4.97930200	5.16494400
H	-0.96374000	-5.61492200	1.84217200
H	-0.73436100	-3.77459700	-3.76485700
H	-2.49553000	-5.12382600	-2.61738700
H	-2.24335200	-5.71400700	-0.23611500
C	1.41125800	4.66972000	2.58540700
C	2.04334300	4.01121700	1.57288000
C	1.69583900	4.25285500	0.20107300
C	0.61274500	5.15937500	-0.06782700
C	-0.01333800	5.84250900	1.02522500
C	0.38001300	5.61727200	2.30922300
C	2.34081800	3.60094000	-0.86792000
C	0.17206800	5.33505200	-1.37762900
C	0.77416200	4.66246700	-2.44145900

C	1.88819600	3.79188000	-2.19091300
C	2.49853700	3.14755700	-3.31533800
H	3.34946700	2.49695100	-3.14766800
C	2.02488400	3.33654900	-4.57924500
C	0.90771500	4.18761300	-4.82047600
C	0.30627600	4.83164300	-3.78281600
H	1.66961500	4.45507600	3.61730500
H	2.79955000	3.26641700	1.79263900
H	-0.81736300	6.53858400	0.80131400
H	-0.10630200	6.12982200	3.13293200
H	-0.66208200	6.00467100	-1.57433400
H	2.50070900	2.83287900	-5.41441400
H	0.54329800	4.32048000	-5.83396700
H	-0.54330400	5.48771300	-3.95058900
H	-0.83322800	0.93456700	1.02836700
C	-6.62185800	-2.58951200	0.49457400
C	-6.57453600	-1.26620200	0.89902000
C	-5.34062200	-0.64514200	1.13970700
C	-4.14873400	-1.37032800	0.95756500
C	-4.20527400	-2.70744900	0.56129000
C	-5.43386500	-3.31012800	0.33461300
H	-6.19967100	1.25294400	1.75865900
H	-7.57522300	-3.06136300	0.28473800
H	-7.48922000	-0.69305300	1.02181800
C	-5.26440900	0.74030300	1.55256900
C	-2.86893400	-0.68741700	1.18773900
H	-3.27784500	-3.25040700	0.39720500
H	-5.47111600	-4.34229800	0.00259300
C	-2.85275300	0.77624600	1.34445200
C	-4.10452000	1.42890700	1.65256400
H	-4.10008700	2.47461700	1.93371300
C	-1.72896000	-1.32904600	1.41913800
C	-0.56903100	-1.78580300	1.79115300
C	-0.17844300	-1.89046100	3.21649400
C	-1.07538600	-2.31609600	4.19917400
C	1.11391000	-1.49336300	3.56964200
C	-0.68141400	-2.34359300	5.53167400
H	-2.07320500	-2.63345100	3.90885500
C	1.49680500	-1.51475000	4.90736900
H	1.80005800	-1.16454300	2.79331800
C	0.60401700	-1.94038400	5.88823400
H	2.50155800	-1.20759700	5.18090200
H	0.90992300	-1.96324100	6.92944500
N	-1.72753900	1.42384800	1.26271300

C	-1.50360600	2.82031700	1.63394900
H	-0.54790200	3.08492200	1.17223000
H	-2.28103900	3.45699200	1.20351200
C	-1.40734500	2.94619600	3.13801000
C	-0.52286100	2.11075100	3.82784900
C	-2.17022800	3.87456100	3.84047900
C	-0.41451900	2.20348200	5.20973800
H	0.08448300	1.39984300	3.26940300
C	-2.05084400	3.97550200	5.22598100
H	-2.84960100	4.53115600	3.30124100
C	-1.17653700	3.13837800	5.91078200
H	0.26602600	1.54376000	5.73873500
H	-2.64626200	4.70325900	5.76805300
H	-1.08934100	3.21129700	6.99009700
H	0.16785500	-2.01856000	1.02031200
C	-3.68777900	-1.84951200	-2.54454800
C	-4.99286100	-1.30272900	-2.53013400
C	-5.17341600	0.01458700	-2.19342600
C	-4.07186300	0.85035800	-1.88988200
C	-2.74776100	0.31469300	-1.97733600
C	-2.59727800	-1.07617700	-2.26673500
H	-3.55540800	-2.90621500	-2.75616200
H	-6.18223500	0.40774100	-2.15459700
H	-1.59386000	-1.49331200	-2.23887400
N	-1.64409500	1.04361200	-1.79491100
H	-1.71291700	2.02080300	-1.55474700
H	-0.75481700	0.54548100	-1.75883200
C	-6.15758100	-2.14628700	-2.93149100
F	-5.99427700	-3.43489400	-2.57572900
F	-7.30838000	-1.72067400	-2.38346800
F	-6.34971600	-2.15227500	-4.26366000
C	-4.25934000	2.22166400	-1.45772500
O	-3.37740900	2.99709800	-1.11425000
C	-5.70107400	2.79099700	-1.42751800
F	-6.51602900	2.07562500	-0.62851300
F	-5.70289400	4.04023200	-0.98374600
H	-1.37747100	-2.68022900	6.29317800
F	-6.23904100	2.77781100	-2.65392200

#### TS2-IV

Value of imaginary frequency = -278.65 cm<sup>-1</sup>

P	1.38381800	-0.24031800	-0.20812900
O	2.54640100	-1.09881000	0.58343500
O	2.31828400	0.81851200	-1.04220500

O	0.56057100	0.44569000	0.83264300
C	3.44812300	-1.69589700	-0.27541100
C	4.48389000	-0.91220800	-0.79280300
C	3.25963800	-3.03229800	-0.63958900
C	4.18358600	-3.58365700	-1.52190800
C	5.21610800	-2.83106300	-2.08562400
H	4.07156100	-4.62702400	-1.80904600
C	3.44710000	1.33488100	-0.45272400
C	4.57975600	0.50916300	-0.33635200
C	3.43308800	2.66260800	-0.02254400
C	4.62268800	3.17769500	0.50464800
C	5.74938400	2.38361300	0.66939000
H	4.64484300	4.21636400	0.82552600
C	5.72499700	1.03505200	0.27821600
C	6.94037900	0.21875700	0.65289800
C	8.28090800	0.90350200	0.29847000
H	8.60401600	0.59551400	-0.70122800
C	8.20701900	2.44179100	0.36397100
H	8.04986600	2.84806300	-0.64078900
C	7.03994400	2.91106400	1.24291300
H	7.18302300	2.53880000	2.26734900
H	6.90166800	0.09046500	1.74296600
C	5.35181100	-1.47499300	-1.75020500
C	6.34314900	-0.60230900	-2.49749200
C	7.48558900	-1.39443900	-3.12589100
H	8.13907500	-1.79174600	-2.33710900
C	6.92589300	-2.55020900	-3.94979800
H	7.72308300	-3.07993600	-4.47995200
C	6.17338000	-3.51859800	-3.04133000
H	6.90303800	-4.08752200	-2.44883400
H	5.78839300	-0.08424500	-3.29289300
H	7.01016000	4.00276100	1.30377300
H	9.15282700	2.85298200	0.72821000
H	9.04263500	0.53359900	0.99145900
H	6.89703300	-0.78738600	0.23128300
H	6.73079200	0.18837200	-1.85454400
H	8.09760100	-0.73167900	-3.74546800
H	6.24426200	-2.14946600	-4.71054900
H	5.62417400	-4.25637100	-3.63556000
O	0.77365400	-1.11859300	-1.25497100
C	2.94736200	-4.18988800	3.47561000
C	3.04677500	-3.83280900	2.16425600
C	2.02259000	-4.18181300	1.22396000
C	0.89418000	-4.92961300	1.70546600

C	0.82562100	-5.27730000	3.09212600
C	1.81809700	-4.92008100	3.95153300
C	2.09172300	-3.81457900	-0.13552200
C	-0.12679700	-5.27778700	0.82277000
C	-0.07900600	-4.91241300	-0.52279400
C	1.05015200	-4.17439000	-1.01935500
C	1.03123100	-3.76766900	-2.39489200
H	1.85027400	-3.16395000	-2.76670500
C	-0.01971000	-4.07546400	-3.20722600
C	-1.13829400	-4.80973600	-2.71024800
C	-1.16480900	-5.21115900	-1.40808300
H	3.73350400	-3.91350900	4.17121900
H	3.90887100	-3.27603700	1.81339400
H	-0.04618700	-5.82257900	3.44245100
H	1.75100100	-5.17768200	5.00351100
H	-0.98949200	-5.82520500	1.19650300
H	-0.01894300	-3.74137600	-4.23960400
H	-1.97067400	-5.03508100	-3.36964700
H	-2.01271800	-5.76467500	-1.01342100
C	1.79815900	4.17334900	3.61427300
C	2.25318200	3.62099400	2.45483300
C	1.71075100	4.00968700	1.18380600
C	0.61728100	4.94254500	1.18638600
C	0.18174600	5.51056700	2.42662900
C	0.76227600	5.15297500	3.60335800
C	2.19957000	3.50403700	-0.04245300
C	-0.00622600	5.27391300	-0.01509900
C	0.42791000	4.73973900	-1.22867900
C	1.56001900	3.85348600	-1.25203600
C	2.00775200	3.38015100	-2.52832300
H	2.86944800	2.72414200	-2.56844400
C	1.36878500	3.73721500	-3.67956600
C	0.23240600	4.59864300	-3.64823400
C	-0.22195900	5.08200700	-2.45767900
H	2.21658900	3.85291900	4.56326600
H	3.02289600	2.85919900	2.48341600
H	-0.63611500	6.22517800	2.40383300
H	0.41654800	5.58146100	4.53817400
H	-0.84589300	5.96603300	-0.00799000
H	1.72628400	3.36172900	-4.63283800
H	-0.27437300	4.85730000	-4.57249800
H	-1.09352600	5.72938400	-2.41685800
H	-1.26399700	0.47616300	0.65896500
C	-7.24721900	-2.78620700	1.21959700

C	-7.10916500	-1.41782600	1.32068300
C	-5.84437400	-0.81512000	1.18865500
C	-4.70642700	-1.61481100	0.95140100
C	-4.86469400	-3.00844300	0.84897300
C	-6.11497200	-3.58069100	0.97967500
H	-6.57901300	1.21306900	1.41180900
H	-8.22420800	-3.24677300	1.31483200
H	-7.97552900	-0.78591200	1.49518700
C	-5.68685600	0.61399600	1.24715500
C	-3.40947800	-0.97134900	0.81698700
H	-3.99422900	-3.62421000	0.64002600
H	-6.22268100	-4.65631600	0.88638000
C	-3.29579900	0.46605300	0.87879800
C	-4.49282700	1.23696500	1.09804900
H	-4.42217000	2.31577700	1.15631400
C	-2.24480100	-1.66884900	0.64158900
C	-1.11391900	-2.13195600	1.12125300
C	-0.91096500	-2.18166000	2.59302200
C	-1.94368100	-2.55131500	3.45918800
C	0.33855400	-1.82639200	3.11104200
C	-1.73395600	-2.55219400	4.83347900
H	-2.90720800	-2.84400700	3.05098600
C	0.53551300	-1.81855900	4.48771800
H	1.14171600	-1.54052900	2.43924000
C	-0.49572500	-2.18014000	5.35066200
H	1.50676700	-1.53808200	4.88321300
H	-0.33393800	-2.17891000	6.42404500
N	-2.11843000	1.04580100	0.72993200
C	-1.83224600	2.46933600	0.86542300
H	-0.81903500	2.59398800	0.46935200
H	-2.51154100	3.05727400	0.23923900
C	-1.88709600	2.90040300	2.31496700
C	-1.10070200	2.22083500	3.24885000
C	-2.72099300	3.93403700	2.73579100
C	-1.16558400	2.56860400	4.59250200
H	-0.44051100	1.42565900	2.90712600
C	-2.77908000	4.28715700	4.08268700
H	-3.32381600	4.46936100	2.00418600
C	-2.00528100	3.60007400	5.01238200
H	-0.55643000	2.03272300	5.31404800
H	-3.43354600	5.09135800	4.40426700
H	-2.05592900	3.86669200	6.06359100
H	-0.28892000	-2.42470400	0.47498800
C	-1.91288000	1.84515400	-2.61516600

C	-3.29700600	2.09042000	-2.66012400
C	-4.19212000	1.05663700	-2.50637300
C	-3.73559900	-0.25026300	-2.22314000
C	-2.34349500	-0.47278100	-2.06571900
C	-1.44511900	0.58774400	-2.33170900
H	-1.21254900	2.65491900	-2.79722900
H	-5.25126500	1.25917700	-2.60191600
H	-0.38175800	0.38696900	-2.28559200
N	-1.84531100	-1.65162600	-1.55537700
H	-2.36868100	-2.49506300	-1.76724300
H	-0.81297000	-1.70251900	-1.55972500
C	-3.76039400	3.50017000	-2.84749600
F	-3.11865000	4.11087800	-3.85555200
F	-5.07432900	3.58127900	-3.09286800
F	-3.52021000	4.24498300	-1.74609200
C	-4.66436700	-1.38598900	-2.16575000
O	-4.34022200	-2.55333500	-2.06342700
C	-6.17948700	-1.11293900	-2.33965400
F	-6.42251000	-0.71782800	-3.59843400
F	-6.88050800	-2.20862000	-2.09731600
H	-2.53883700	-2.84422400	5.50025800
F	-6.62552300	-0.14355900	-1.52604500

#### TS2-IV'

Value of imaginary frequency = -317.79 cm<sup>-1</sup>

P	1.42930500	-0.20612400	-0.48679300
O	2.24363900	-1.05211200	0.67615200
O	2.67194900	0.18397800	-1.48222600
O	0.85657500	0.99642300	0.19407000
C	3.03926600	-2.07224800	0.19550600
C	4.29087000	-1.74552600	-0.33262400
C	2.56902900	-3.38595200	0.23338600
C	3.40078200	-4.37747600	-0.27919000
C	4.63701300	-4.08798400	-0.85811800
H	3.05874400	-5.40970500	-0.24699700
C	3.84608000	0.62905200	-0.91648400
C	4.69881200	-0.31046800	-0.31696600
C	4.16693500	1.98453700	-0.99814500
C	5.37204200	2.39983600	-0.42409100
C	6.20159000	1.50954100	0.24640100
H	5.64724800	3.44980300	-0.48991000
C	5.86416900	0.14914700	0.31300000
C	6.76430000	-0.71765200	1.16220600
C	8.27119700	-0.49784400	0.89365200

H	8.61804500	-1.19745500	0.12630200
C	8.60401900	0.94443800	0.46207500
H	8.69332500	0.99335600	-0.62827900
C	7.50263800	1.92740500	0.88228400
H	7.40983500	1.92413400	1.97761700
H	6.56083100	-0.44615500	2.20681200
C	5.08210500	-2.75838400	-0.90986500
C	6.34241200	-2.40519700	-1.67768600
C	7.29317000	-3.58639000	-1.84765700
H	7.73724900	-3.84663100	-0.87708100
C	6.53612700	-4.79177700	-2.39664400
H	7.21632700	-5.62192300	-2.60964300
C	5.47234700	-5.23464300	-1.39580600
H	5.96696500	-5.72956300	-0.54875800
H	6.03304700	-2.04859600	-2.67081400
H	7.75856400	2.94958800	0.58882900
H	9.57001100	1.25120100	0.87329600
H	8.81781900	-0.75308200	1.80652000
H	6.50641300	-1.77493000	1.07136700
H	6.85764800	-1.56223700	-1.21615000
H	8.11642000	-3.30457600	-2.51131200
H	6.06009200	-4.51364100	-3.34533900
H	4.81152200	-5.98502400	-1.84213200
O	0.56004200	-1.16078200	-1.25278800
C	1.89716600	-3.19730300	4.44763800
C	2.10265700	-3.24733000	3.10215400
C	1.05193400	-3.64148400	2.20970200
C	-0.21718200	-4.00149500	2.77754600
C	-0.40336500	-3.88859700	4.19276300
C	0.61992800	-3.50549800	5.00368900
C	1.24065400	-3.72511500	0.81598600
C	-1.22735400	-4.48974300	1.94964200
C	-1.02963500	-4.64159000	0.57635700
C	0.20867500	-4.21221200	-0.01213200
C	0.34885400	-4.31021900	-1.43605200
H	1.23732300	-3.89482800	-1.89706700
C	-0.61972200	-4.89566400	-2.19728100
C	-1.81112100	-5.40270400	-1.59729800
C	-2.02140100	-5.25018300	-0.25896600
H	2.70766700	-2.90474600	5.10793800
H	3.07345500	-2.99846400	2.68750700
H	-1.38001700	-4.12828600	4.60385100
H	0.46919500	-3.42716400	6.07544300
H	-2.17477100	-4.79404200	2.38906000



H	-0.49250700	-4.96850500	-3.27226700
H	-2.55653400	-5.89111200	-2.21806600
H	-2.93745000	-5.60505700	0.20642500
C	2.34631000	5.18698100	1.18162700
C	2.86315100	4.12887900	0.49493600
C	2.71121000	4.02096300	-0.92914600
C	1.93242600	5.02721300	-1.59783600
C	1.40862900	6.12331000	-0.83859900
C	1.62295900	6.21305100	0.50306000
C	3.27168000	2.96423800	-1.67461000
C	1.70070600	4.92031900	-2.96715800
C	2.22313300	3.86276700	-3.71109900
C	3.03485800	2.87183300	-3.06246900
C	3.59149200	1.82986200	-3.87264600
H	4.22016400	1.08105100	-3.40474900
C	3.34117900	1.76719900	-5.21083100
C	2.51890900	2.74225100	-5.84634200
C	1.98152000	3.75835700	-5.11720000
H	2.45066100	5.23816100	2.26115500
H	3.37928400	3.33656500	1.02480700
H	0.83879900	6.88470300	-1.36473700
H	1.22578500	7.04819600	1.07111000
H	1.10394000	5.67960000	-3.46763500
H	3.77079700	0.96544900	-5.80262300
H	2.32886000	2.67148700	-6.91246700
H	1.35857700	4.51378300	-5.58813900
H	-0.79029000	1.67641500	0.45584200
C	-7.36167000	0.18258700	1.57192700
C	-6.85876700	1.46476100	1.61880500
C	-5.48203800	1.70033000	1.43574100
C	-4.60856500	0.61235700	1.22330000
C	-5.13600900	-0.69152100	1.18866000
C	-6.49175800	-0.89909200	1.34878400
H	-5.63100900	3.85692000	1.58505600
H	-8.42443000	0.00661100	1.69571700
H	-7.51935200	2.31236000	1.77863200
C	-4.94336600	3.03241400	1.41410200
C	-3.19354800	0.88638800	1.03183000
H	-4.46933400	-1.52824800	0.99241900
H	-6.88832300	-1.90658100	1.28015000
C	-2.70795600	2.23734400	0.92773700
C	-3.63491900	3.30692400	1.17577600
H	-3.28194700	4.33002400	1.16807900
C	-2.25200800	-0.09609100	0.93800000

C	-1.30680400	-0.85549600	1.43037900
C	-1.05799500	-0.73302400	2.89493700
C	-2.10239700	-0.77752600	3.82212500
C	0.24537800	-0.46229800	3.31924800
C	-1.84712300	-0.54055100	5.16777100
H	-3.11110600	-0.99427400	3.48128400
C	0.48825000	-0.21286300	4.66711300
H	1.05125200	-0.42992300	2.59100500
C	-0.55277200	-0.24824700	5.59123200
H	1.50186100	-0.00074900	4.99433100
H	-0.35565800	-0.05470000	6.64104000
N	-1.44515400	2.46097000	0.59829800
C	-0.78405300	3.75791500	0.66283200
H	0.17386600	3.62637000	0.15005000
H	-1.35788600	4.50719000	0.10877400
C	-0.54768700	4.18416900	2.09552500
C	0.07693100	3.29161500	2.97110800
C	-0.91366800	5.44832900	2.54933300
C	0.33080900	3.66610800	4.28449600
H	0.37087900	2.30819800	2.60861900
C	-0.64908000	5.82863800	3.86425700
H	-1.39490900	6.14544400	1.86638000
C	-0.02744300	4.93761200	4.73279000
H	0.80900300	2.96326800	4.95951400
H	-0.93541400	6.81699200	4.20965300
H	0.17362400	5.22980300	5.75848900
H	-0.64639700	-1.46248700	0.81009500
C	-4.25703600	-2.89854000	-1.81741000
C	-5.44853400	-2.19728700	-2.07093900
C	-5.43862700	-0.82336100	-2.16542000
C	-4.24631200	-0.09827800	-1.97663200
C	-3.05321200	-0.80665200	-1.67233600
C	-3.07938800	-2.21781600	-1.62834300
H	-4.26693300	-3.98254700	-1.76223900
H	-6.36809500	-0.31020300	-2.37709000
H	-2.15244300	-2.74411200	-1.41724300
N	-1.90067800	-0.18141600	-1.28545200
H	-1.84297600	0.80790800	-1.51069100
H	-0.98447500	-0.69022600	-1.35498800
C	-6.73089400	-2.96176800	-2.16335800
F	-7.14701100	-3.37524800	-0.94975300
F	-7.72292500	-2.23217700	-2.68927000
F	-6.59703100	-4.06868500	-2.91063200
C	-4.23666800	1.36740500	-2.06247200

O	-3.25301800	2.07931900	-1.98699900
C	-5.58470500	2.09374000	-2.29690200
F	-6.49290100	1.75791200	-1.37059500
F	-5.41900000	3.40730000	-2.25488900
H	-2.66095800	-0.57685500	5.88467700
F	-6.08904800	1.76868200	-3.49631900

#### IM3-IV

P	1.35053300	-0.02809200	-0.24736400
O	2.45427900	-0.84844500	0.60849800
O	2.24626400	0.65609800	-1.39334700
O	0.61091200	0.88363300	0.64512700
C	3.34647700	-1.62182800	-0.12708300
C	4.38270600	-0.98725400	-0.81815700
C	3.15002200	-3.00216700	-0.14811800
C	4.04202400	-3.75360100	-0.90672900
C	5.05890400	-3.16229900	-1.65941200
H	3.92235700	-4.83432700	-0.93096500
C	3.40138000	1.29377800	-0.96471200
C	4.51825200	0.49653500	-0.68782600
C	3.38124200	2.67986000	-0.82558700
C	4.57492600	3.28880900	-0.42745800
C	5.70194400	2.53629400	-0.11509000
H	4.60373000	4.37104700	-0.32825300
C	5.67422900	1.13495700	-0.21470000
C	6.89319300	0.41093100	0.30520200
C	8.22538800	0.99970600	-0.21292000
H	8.51773300	0.49780300	-1.14082500
C	8.15813300	2.52192600	-0.45016600
H	7.99821200	2.72446400	-1.51422500
C	6.99965100	3.16425100	0.32551600
H	7.14988600	3.00688500	1.40284100
H	6.87474800	0.51794100	1.39801100
C	5.22124400	-1.76788200	-1.63944800
C	6.21176400	-1.10210400	-2.57630700
C	7.32718700	-2.03752700	-3.03289900
H	7.99038300	-2.26466200	-2.18716000
C	6.72988700	-3.33356800	-3.57241500
H	7.50634300	-3.98408600	-3.98532200
C	5.98004100	-4.06281700	-2.46105300
H	6.71039200	-4.50649600	-1.77084900
H	5.64978900	-0.75987500	-3.45703500
H	6.97288400	4.24544900	0.16373900
H	9.10689200	2.99210700	-0.17750700

H	9.00441400	0.76522500	0.51834400
H	6.84060700	-0.66172000	0.10771200
H	6.62606200	-0.19830800	-2.12842200
H	7.93635700	-1.54016600	-3.79356500
H	6.04011300	-3.09583800	-4.39178500
H	5.40207100	-4.89809700	-2.86949200
O	0.57816500	-1.06119000	-1.12381400
C	3.25485100	-3.20952400	4.12545000
C	3.21639600	-3.14409900	2.76390600
C	2.11248600	-3.68773600	2.02977100
C	1.05143500	-4.30680900	2.77349900
C	1.13088100	-4.35398200	4.20061100
C	2.19780800	-3.82367200	4.85857900
C	2.03649200	-3.63054400	0.62190500
C	-0.04714400	-4.83232500	2.09461000
C	-0.14287300	-4.76621400	0.70620300
C	0.91605200	-4.15739400	-0.05225000
C	0.74898300	-4.05187200	-1.47337900
H	1.52016500	-3.55596100	-2.05208800
C	-0.37588900	-4.52014100	-2.08513200
C	-1.41560700	-5.14313300	-1.33064700
C	-1.30128600	-5.25552000	0.02173700
H	4.10047500	-2.79005900	4.66125200
H	4.03047800	-2.67831800	2.21902500
H	0.30895800	-4.80890400	4.74599300
H	2.24350900	-3.85342000	5.94229000
H	-0.85777300	-5.28172200	2.66356700
H	-0.49377400	-4.41077100	-3.15823700
H	-2.30466100	-5.49794200	-1.83924000
H	-2.08960300	-5.71552800	0.61136500
C	1.56000200	4.75834900	2.44240800
C	2.10627100	4.05581200	1.40880900
C	1.55626600	4.12984200	0.08580000
C	0.35776600	4.90236800	-0.09314600
C	-0.16998800	5.64304500	1.01269000
C	0.41948000	5.58912400	2.23948200
C	2.11874200	3.45137400	-1.01738400
C	-0.27996600	4.90410000	-1.33330300
C	0.23625900	4.19382400	-2.41718300
C	1.47226200	3.47686800	-2.27031600
C	1.99220700	2.80217800	-3.42235200
H	2.94192000	2.28497600	-3.34178800
C	1.31019600	2.79240500	-4.60195800
C	0.05768500	3.46147500	-4.72765000

C	-0.45357400	4.15208300	-3.67156200
H	1.98655600	4.67612700	3.43658800
H	2.96021500	3.41260400	1.58599500
H	-1.05912700	6.24617900	0.84698000
H	0.01032900	6.14819400	3.07437200
H	-1.20100200	5.47031600	-1.45860800
H	1.71912000	2.26359400	-5.45663500
H	-0.48568900	3.41851300	-5.66539700
H	-1.40597800	4.66980400	-3.75548500
H	-1.04720900	0.84547500	1.69024900
C	-7.15633100	-1.93307800	0.45170600
C	-6.98943700	-0.68322300	0.99403200
C	-5.70122100	-0.18725100	1.30581900
C	-4.55412300	-0.99055600	1.05450700
C	-4.76441700	-2.30221000	0.54431700
C	-6.02613200	-2.75288200	0.23789100
H	-6.37966500	1.71353100	2.08580700
H	-8.14654300	-2.29807900	0.20148400
H	-7.84892200	-0.04650900	1.18756000
C	-5.50722800	1.10321700	1.86788200
C	-3.24975100	-0.47002700	1.30271100
H	-3.91703000	-2.96860500	0.41340700
H	-6.15275700	-3.75242500	-0.16702800
C	-3.09139900	0.81833000	1.82901000
C	-4.26061700	1.58476300	2.13781600
H	-4.14244200	2.56529000	2.58489200
C	-2.05989200	-1.23392600	0.85414600
C	-1.03435900	-1.63033700	1.62272600
C	-0.92079000	-1.45732400	3.08169800
C	-1.98796900	-1.68023300	3.95895700
C	0.31942700	-1.06099200	3.59972600
C	-1.81533600	-1.50893800	5.32856900
H	-2.94661000	-1.99931000	3.56185400
C	0.48429100	-0.88050200	4.96878000
H	1.15194100	-0.89706100	2.91858300
C	-0.58064600	-1.10896600	5.83741800
H	1.45052000	-0.57307500	5.35631200
H	-0.44883600	-0.98094300	6.90749700
N	-1.85567700	1.36356500	2.01153400
C	-1.61627300	2.76069300	2.28048400
H	-0.56956600	2.94469800	2.01176900
H	-2.22388700	3.40226500	1.62461700
C	-1.84330500	3.15072100	3.72939500
C	-1.61700800	2.22484600	4.74800800

C	-2.26326200	4.43896800	4.06233100
C	-1.79054300	2.58969600	6.07884700
H	-1.31403500	1.21479600	4.48544500
C	-2.43538200	4.80598500	5.39461900
H	-2.46139400	5.15625800	3.26852000
C	-2.19614300	3.88116200	6.40731300
H	-1.61230000	1.85701400	6.86050200
H	-2.76638500	5.81027500	5.64096600
H	-2.33486800	4.16326500	7.44624500
H	-0.16157500	-2.07016000	1.14112100
C	-2.55013900	1.79220200	-2.11762400
C	-3.47299000	1.49874000	-3.12328400
C	-3.95316900	0.21117000	-3.26852600
C	-3.48961800	-0.81968800	-2.43474500
C	-2.52624600	-0.53092000	-1.44504400
C	-2.08718600	0.79070800	-1.28773700
H	-2.18583400	2.80586000	-1.98891600
H	-4.68962100	0.00248500	-4.03585900
H	-1.36396000	1.02621100	-0.51216700
N	-1.96844700	-1.50489900	-0.58260100
H	-2.21195900	-2.46031700	-0.84499700
H	-0.38684400	-1.29139000	-0.88910000
C	-3.89632100	2.57897300	-4.07243400
F	-3.04102500	2.70722100	-5.10158400
F	-5.10440500	2.33889400	-4.59990400
F	-3.94568500	3.77671500	-3.46625200
C	-4.03983300	-2.17973100	-2.57251900
O	-3.48052700	-3.19780700	-2.22696300
C	-5.44809300	-2.32651900	-3.19646400
F	-5.38024800	-2.14323400	-4.52703200
F	-5.93018900	-3.54121700	-2.97251700
H	-2.64727600	-1.69144100	6.00134200
F	-6.30088800	-1.42873900	-2.70319900

#### IM3-IV'

P	1.50434500	-0.12442500	-0.48963200
O	2.19337000	-1.01131400	0.68664800
O	2.72517600	0.08883200	-1.51973900
O	0.91675200	1.09754800	0.09143300
C	2.98696700	-2.08198800	0.29242900
C	4.25362800	-1.81998700	-0.23508500
C	2.49401000	-3.37643500	0.45550500
C	3.31322000	-4.42180700	0.03665600
C	4.55491200	-4.20442300	-0.56155200

H	2.95733700	-5.44154800	0.16555900
C	3.91008100	0.53811100	-0.94416300
C	4.71295500	-0.40115300	-0.28711100
C	4.23651400	1.88782100	-1.04415000
C	5.42886200	2.29860900	-0.44105100
C	6.22798200	1.40975800	0.26826300
H	5.71606200	3.34446000	-0.51479900
C	5.86942600	0.05577400	0.36199000
C	6.73378500	-0.79729300	1.25973900
C	8.24786400	-0.61281500	1.00880000
H	8.58775800	-1.32723900	0.25213900
C	8.61603400	0.81857700	0.56746500
H	8.74636400	0.84913000	-0.51921200
C	7.51544200	1.82464800	0.93264100
H	7.38801200	1.84674000	2.02399400
H	6.51737000	-0.48401500	2.28989200
C	5.02822300	-2.89284700	-0.71879400
C	6.30942600	-2.62912600	-1.48738400
C	7.23815400	-3.83870600	-1.53563100
H	7.65562100	-4.02558600	-0.53684400
C	6.46627600	-5.06970200	-2.00095400
H	7.13204900	-5.92819300	-2.12854800
C	5.37168500	-5.40797800	-0.99255600
H	5.83486200	-5.84625300	-0.09813500
H	6.02651800	-2.35405600	-2.51359300
H	7.79357600	2.83653200	0.62509500
H	9.56987000	1.11988000	1.00913600
H	8.77634500	-0.87200000	1.93088100
H	6.45895200	-1.85251300	1.20257800
H	6.83115200	-1.75882400	-1.08748400
H	8.08097300	-3.62945100	-2.20118100
H	6.01767500	-4.86199200	-2.98042400
H	4.70084700	-6.17462300	-1.39366000
O	0.57860200	-1.08689800	-1.29598300
C	1.82622400	-2.64154300	4.61792000
C	2.03332200	-2.86676800	3.29034900
C	0.98771500	-3.38636300	2.45872000
C	-0.27724300	-3.67951200	3.07287600
C	-0.46174100	-3.39550900	4.46378600
C	0.55645900	-2.89602600	5.21529700
C	1.16922000	-3.64213100	1.08378600
C	-1.29194800	-4.26162400	2.31424300
C	-1.10527600	-4.57235900	0.96686800
C	0.13133900	-4.22059100	0.32408400

C	0.25729000	-4.48464300	-1.08027400
H	1.15162700	-4.15052600	-1.59411200
C	-0.72524900	-5.13943400	-1.76370000
C	-1.91422500	-5.56598900	-1.10086000
C	-2.10850100	-5.26450100	0.21452600
H	2.63239300	-2.25040600	5.23061400
H	3.00248600	-2.66166300	2.84883700
H	-1.43538100	-3.59160600	4.90352000
H	0.40644800	-2.68086400	6.26794500
H	-2.23765800	-4.50795600	2.79185700
H	-0.60639700	-5.33706900	-2.82382600
H	-2.66740800	-6.11767100	-1.65533600
H	-3.02267900	-5.55644400	0.72475400
C	2.24020500	5.03875300	1.05915700
C	2.79882200	3.98710400	0.39526800
C	2.75348700	3.90613500	-1.03730700
C	2.02960500	4.92598500	-1.74445600
C	1.47079300	6.02125300	-1.00969500
C	1.59074000	6.08989600	0.34467100
C	3.36808300	2.86453300	-1.76032200
C	1.89142700	4.83622700	-3.12789900
C	2.45278000	3.78242600	-3.84840600
C	3.21943500	2.78256400	-3.15998900
C	3.81931000	1.74306800	-3.94198900
H	4.41631600	0.98789600	-3.44280500
C	3.64958400	1.69050400	-5.29333100
C	2.87392200	2.67580200	-5.97040200
C	2.29888500	3.69001700	-5.26750900
H	2.26295300	5.07315600	2.14381600
H	3.26804300	3.18101800	0.94791900
H	0.95097600	6.79810500	-1.56397100
H	1.16807800	6.92308100	0.89576600
H	1.33469000	5.60561900	-3.65807900
H	4.10974500	0.89038100	-5.86404700
H	2.74934800	2.61405000	-7.04658800
H	1.71029900	4.45238400	-5.77026500
H	-0.83360200	1.80187700	0.55182200
C	-7.17819400	-0.40696100	1.68483700
C	-6.83907300	0.92165800	1.67089700
C	-5.50213100	1.33208500	1.44529200
C	-4.49127500	0.35134200	1.23796300
C	-4.86898100	-1.02118000	1.28368800
C	-6.17593100	-1.38564700	1.48877100
H	-5.91237600	3.45276900	1.52008500



H	-8.20714400	-0.71080700	1.84432100
H	-7.59668500	1.68684600	1.81939000
C	-5.14146400	2.70273700	1.36436000
C	-3.16004900	0.77003600	0.96020300
H	-4.10423100	-1.78102500	1.14667600
H	-6.44484000	-2.43765600	1.49611200
C	-2.83906000	2.12617300	0.86536900
C	-3.86296800	3.09640600	1.08574300
H	-3.61699900	4.15090100	1.03899200
C	-2.08455400	-0.19040700	0.60401000
C	-1.21959000	-0.76316000	1.44431800
C	-1.13410700	-0.43950100	2.88456800
C	-2.23121900	-0.46681700	3.75119800
C	0.11157700	-0.02079700	3.36662300
C	-2.08580800	-0.06598400	5.07486000
H	-3.19602800	-0.80396600	3.38537400
C	0.24759200	0.39528100	4.68789400
H	0.96310600	-0.00487700	2.69073700
C	-0.85030000	0.37409900	5.54448700
H	1.21621800	0.72902000	5.04830800
H	-0.74342500	0.69522100	6.57614900
N	-1.57538900	2.49389500	0.48989600
C	-1.11161000	3.86051700	0.47054200
H	-0.11490500	3.83655900	0.01493500
H	-1.74467200	4.46688600	-0.18915900
C	-1.01520300	4.50398300	1.84257100
C	-0.62776200	3.74607400	2.94929900
C	-1.26865300	5.86528200	2.01054800
C	-0.48119300	4.34420600	4.19637300
H	-0.44495300	2.68056100	2.83331400
C	-1.11756600	6.46799500	3.25718000
H	-1.58106000	6.45846700	1.15338000
C	-0.71971700	5.70795600	4.35348900
H	-0.18443800	3.73802000	5.04701400
H	-1.31899000	7.52853400	3.37369000
H	-0.60638100	6.17412500	5.32711700
H	-0.42915000	-1.39777500	1.04310000
C	-4.18773100	-3.01683800	-1.82086300
C	-5.25709900	-2.29950100	-2.35820800
C	-5.19302300	-0.92205500	-2.47853500
C	-4.05264300	-0.23095400	-2.04814000
C	-2.99076900	-0.95524300	-1.47530400
C	-3.06212000	-2.34378700	-1.38067500
H	-4.24128500	-4.09761100	-1.73858200

H	-6.03242300	-0.38807200	-2.90763700
H	-2.22679200	-2.87611200	-0.93579500
N	-1.87060200	-0.32426300	-0.85126600
H	-1.77701400	0.63176100	-1.21298200
H	-0.42879000	-0.87369300	-1.16173700
C	-6.50097900	-3.04462300	-2.74383100
F	-7.17026900	-3.46673600	-1.65970300
F	-7.34043300	-2.28968900	-3.46315100
F	-6.21361600	-4.13791900	-3.46704900
C	-3.97772200	1.24608000	-2.17413800
O	-2.95208200	1.88508100	-2.23171300
C	-5.30767700	2.02544300	-2.29272400
F	-6.22422100	1.58195900	-1.43099200
F	-5.11317500	3.31796600	-2.08582600
H	-2.94360300	-0.08942500	5.73938600
F	-5.80606300	1.86655500	-3.53275800

**IM4d**

C	-5.23260600	-0.91963100	3.15898300
C	-5.43048800	-1.56598400	1.96624600
C	-4.49036200	-1.45124400	0.91298300
C	-3.32621900	-0.65215900	1.09062900
C	-3.14884000	0.00407000	2.33828700
C	-4.07647900	-0.12871500	3.34089900
H	-5.57963800	-2.71532400	-0.46402600
H	-5.95802700	-1.01116800	3.96042100
H	-6.31404500	-2.17854600	1.80788300
C	-4.68242000	-2.11771100	-0.32744000
C	-2.37540800	-0.56249500	0.02380300
H	-2.27075000	0.62269500	2.48722800
H	-3.92204000	0.38463400	4.28465600
C	-2.60328000	-1.20925100	-1.18191700
C	-3.78133100	-1.99542800	-1.34414400
H	-3.96948900	-2.46872900	-2.30222000
C	-1.08142800	0.15447400	0.23325100
C	-0.94441900	1.48894800	0.33076300
H	0.02475900	1.89539200	0.61724200
C	-2.01830500	2.47731800	0.14266300
C	-2.05922600	3.60156600	0.97767100
C	-2.98709400	2.35524300	-0.86235100
C	-3.05688400	4.55872200	0.83821600
H	-1.30249400	3.71516800	1.74966500
C	-3.98511100	3.31265600	-0.99905800
H	-2.93898000	1.51789600	-1.55156100

C	-4.02852900	4.41408500	-0.14807800
H	-3.07537700	5.41869000	1.50022300
H	-4.72677400	3.20284400	-1.78390300
H	-4.80803900	5.16065000	-0.26048200
N	-1.74691700	-1.03119000	-2.27008600
C	-1.21256900	-2.21828800	-2.94360500
H	-0.73816300	-1.88480300	-3.87052200
H	-2.03929400	-2.87693300	-3.22198300
H	-0.99049200	-0.38481000	-2.06095800
N	-0.01795600	-0.75582800	0.38287200
C	1.32379400	-0.51575400	0.60826200
C	1.95807200	-1.29648600	1.59721700
C	2.10368600	0.43413900	-0.09361800
C	3.28813700	-1.12341800	1.90678600
H	1.36513700	-2.03488200	2.12772200
C	3.44765500	0.62987100	0.26898900
C	4.03671800	-0.13822100	1.25144600
H	3.75274300	-1.73261200	2.67608200
H	4.04933900	1.36580300	-0.25057400
C	1.60543000	1.11157500	-1.30783800
O	0.74796300	0.69231600	-2.04845200
C	2.23117900	2.48079000	-1.67100200
F	1.48177400	3.11222400	-2.55944200
F	3.46000000	2.33093700	-2.19197700
F	2.33963400	3.24689700	-0.57874100
H	-0.32231500	-1.68595900	0.64697100
C	-0.21396900	-2.95076100	-2.07447900
C	-0.65234000	-3.82841300	-1.07861800
C	1.14832400	-2.65647900	-2.16406100
C	0.25483900	-4.39374700	-0.18395000
H	-1.71104300	-4.06280100	-0.99885900
C	2.05795000	-3.22707300	-1.27901900
H	1.49325800	-1.96226800	-2.92612700
C	1.61202200	-4.09346100	-0.28341200
H	-0.09700900	-5.07683900	0.58304800
H	3.11376200	-2.98484200	-1.35485000
H	2.32030400	-4.53385600	0.41148300
C	5.47270500	0.05237800	1.63328900
F	6.16975900	-1.08708000	1.49583400
F	6.07383100	0.98669200	0.88587200
F	5.59676400	0.42083300	2.91787800

**IM5d**

P	1.10898000	0.20313600	-0.39516700
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O	1.87599400	1.47610700	-1.02092300
O	2.30264200	-0.79557000	0.02182100
O	0.09431500	-0.29511400	-1.33535400
C	2.90318100	1.98581300	-0.23260300
C	4.10985200	1.29111600	-0.20179800
C	2.65772400	3.13701600	0.51533000
C	3.69164100	3.57560600	1.33605100
C	4.89658700	2.87559700	1.45505200
H	3.54143300	4.47689900	1.92591400
C	3.32602200	-0.95721300	-0.90575700
C	4.24482700	0.08055000	-1.07025600
C	3.39362600	-2.15385900	-1.61702500
C	4.41364600	-2.26795500	-2.55636300
C	5.30484300	-1.22412200	-2.81841200
H	4.50025700	-3.19467600	-3.11868000
C	5.21546600	-0.03033600	-2.08538500
C	6.07474300	1.16539500	-2.45453700
C	7.32819500	0.78477800	-3.23731800
H	8.03341400	0.26289400	-2.57676300
C	6.96001200	-0.12490700	-4.40531100
H	7.83291600	-0.33737000	-5.02933100
C	6.36797200	-1.43013900	-3.88056700
H	5.94818200	-2.02101400	-4.70093400
H	5.45587800	1.83293700	-3.07109900
C	5.10873700	1.71223900	0.69892600
C	6.33704800	0.85187700	0.93505300
C	7.48413200	1.60983000	1.59766600
H	7.91708100	2.32402600	0.88462000
C	6.97620900	2.36326600	2.82303800
H	7.80043900	2.84123100	3.36040800
C	5.95482800	3.41457400	2.39854300
H	6.47929700	4.23834300	1.89549400
H	6.03150000	0.02131400	1.58734900
H	7.17387500	-2.03823600	-3.44767100
H	6.22628900	0.38586200	-5.04131200
H	7.83057100	1.69055000	-3.58911500
H	6.33629200	1.74827000	-1.56893100
H	6.67220900	0.38399500	0.00680200
H	8.27847500	0.90864700	1.86968600
H	6.50950500	1.65157600	3.51544500
H	5.46665700	3.85420600	3.27422700
O	0.64869900	0.61474900	1.05356600
H	-0.28869200	0.89063700	1.13574600
C	1.70467400	5.37933200	-2.98731400

C	2.00307400	4.66886300	-1.86282700
C	1.07327800	4.57799400	-0.77631900
C	-0.18122400	5.26350900	-0.90762100
C	-0.45255600	6.00327600	-2.10201800
C	0.45818200	6.05884100	-3.11315100
C	1.35012300	3.84909700	0.39948900
C	-1.12413800	5.18033200	0.11715000
C	-0.87036800	4.44629900	1.27510200
C	0.39436800	3.77886600	1.43384200
C	0.60992600	3.03314400	2.64137800
H	1.55302000	2.51364200	2.77054800
C	-0.36234100	2.94114400	3.59357700
C	-1.62119000	3.59282200	3.42401700
C	-1.86154000	4.32377900	2.30131300
H	2.42398900	5.43245100	-3.79817100
H	2.95920000	4.16363400	-1.77941200
H	-1.40958400	6.51147200	-2.17884700
H	0.24296700	6.62124300	-4.01588600
H	-2.08827700	5.67146100	-0.00460800
H	-0.18109300	2.36133700	4.49372500
H	-2.38386100	3.49100600	4.18883500
H	-2.81611400	4.81922400	2.14695600
C	-0.32881600	-2.64014900	-3.73626900
C	0.86706400	-2.50701400	-3.09506100
C	1.26901600	-3.43902400	-2.08386800
C	0.39453600	-4.54648400	-1.79858000
C	-0.84508000	-4.65492600	-2.50598400
C	-1.20283500	-3.72748200	-3.43802100
C	2.45182600	-3.27995300	-1.33545000
C	0.74498500	-5.45987400	-0.80298800
C	1.90017000	-5.29520300	-0.03717900
C	2.76714600	-4.17887900	-0.29694600
C	3.91705900	-4.00918100	0.54208200
H	4.57887200	-3.16941200	0.35841200
C	4.17747300	-4.87562000	1.56272200
C	3.31557300	-5.98314700	1.81669900
C	2.21609300	-6.18563800	1.03769700
H	-0.63627700	-1.89812600	-4.46560900
H	1.50981500	-1.66037000	-3.30918300
H	-1.50817900	-5.48133000	-2.26570700
H	-2.15941100	-3.80570700	-3.94727500
H	0.08118800	-6.29497900	-0.59134000
H	5.04766500	-4.72299400	2.19261800
H	3.53944100	-6.65934700	2.63504200

H	1.54910200	-7.02266800	1.22397100
C	-5.10452300	-4.14895200	-4.11533100
C	-4.88058200	-2.87047800	-4.55665000
C	-4.35631900	-1.87939100	-3.68762600
C	-4.06030500	-2.21577800	-2.33434000
C	-4.32000600	-3.54727200	-1.90169900
C	-4.82198300	-4.48332100	-2.76860200
H	-4.36865100	-0.29032400	-5.15170800
H	-5.50072300	-4.90178400	-4.78857600
H	-5.09709000	-2.59464200	-5.58554700
C	-4.10724100	-0.55573900	-4.13073000
C	-3.48905000	-1.22954300	-1.48447300
H	-4.10588200	-3.81375500	-0.87199400
H	-5.00644800	-5.49453600	-2.41890400
C	-3.18083300	0.03697900	-1.97596700
C	-3.54335500	0.37967500	-3.30813000
H	-3.37411500	1.38990200	-3.66392100
C	-3.15711700	-1.56667500	-0.06698900
C	-4.05927600	-1.67637700	0.93264300
N	-2.59274700	0.94652600	-1.12462000
C	-2.09071200	2.23146600	-1.56101700
H	-1.63335200	2.18642200	-2.55891700
H	-1.28256400	2.51016000	-0.87004100
H	-2.00840400	0.50264600	-0.43368100
N	-1.79535600	-1.80190100	0.12367500
C	-1.09486700	-1.91537300	1.31731700
C	0.00949900	-2.77338900	1.35759600
C	-1.39648300	-1.16292500	2.47404700
C	0.77172700	-2.90929700	2.50551900
H	0.25341700	-3.33862000	0.46711100
C	-0.66028100	-1.34160200	3.64388700
C	0.41797900	-2.21737300	3.66271800
H	1.62898400	-3.57841500	2.50431700
H	-0.90261800	-0.76382200	4.53028200
C	-2.25915600	0.04410300	2.39567400
O	-2.03192500	0.96150200	1.63391200
C	-3.36031000	0.27520400	3.44772800
F	-4.28436200	1.10672500	2.99587000
F	-2.77959100	0.83198200	4.52944500
F	-3.93681400	-0.85762700	3.84409100
H	-1.24301900	-1.92134400	-0.72124800
C	-3.15567000	3.30599800	-1.49842100
C	-3.28741700	4.25907100	-2.50494100
C	-3.98005400	3.38450800	-0.37092600

C	-4.21970200	5.29016400	-2.38654600
H	-2.64344800	4.20491400	-3.37998100
C	-4.91118000	4.41011000	-0.25258400
H	-3.86842600	2.64126100	0.41557100
C	-5.03044400	5.36977500	-1.25890400
H	-4.31443900	6.02690600	-3.17863200
H	-5.54522200	4.46388300	0.62750200
H	-5.75795500	6.16986800	-1.16629100
C	1.25537800	-2.36583300	4.89558700
F	2.40803200	-1.68412000	4.80415200
F	0.61897900	-1.91623600	5.98840700
F	1.58585000	-3.64733700	5.11670100
C	-5.46743800	-1.25886300	0.87189300
C	-6.44490900	-2.00338600	1.54392600
C	-5.85497500	-0.07891400	0.22039700
C	-7.77662600	-1.60515200	1.53244300
H	-6.15193900	-2.90670600	2.07265800
C	-7.18688300	0.31603700	0.20824100
H	-5.09724100	0.54182400	-0.24877700
C	-8.15419400	-0.44679900	0.85841100
H	-8.52124500	-2.19947100	2.05291000
H	-7.46488000	1.23493900	-0.29901500
H	-9.19329100	-0.13345500	0.85191600
H	-3.73284800	-2.12684100	1.86728000

### TS3d

Value of imaginary frequency = -259.27 cm<sup>-1</sup>

P	1.01917600	0.20822600	-0.30901900
O	1.69342600	1.51733000	-0.97618500
O	2.29412900	-0.70437400	0.09351900
O	0.05629700	-0.39384800	-1.24914300
C	2.69043100	2.11606400	-0.21420500
C	3.94198300	1.50567000	-0.17737700
C	2.38470600	3.27646600	0.49641100
C	3.39518400	3.80329000	1.29374000
C	4.64122100	3.18274600	1.42570400
H	3.19350300	4.71322900	1.85430100
C	3.31375300	-0.80259400	-0.84359700
C	4.15581400	0.29598400	-1.02911700
C	3.46648800	-1.99612300	-1.54816200
C	4.48431200	-2.04338900	-2.49601800
C	5.29442500	-0.94100700	-2.77655800
H	4.63199800	-2.96635300	-3.05187400
C	5.12319300	0.24876700	-2.05234000

C	5.88858000	1.50155700	-2.44006200
C	7.15541400	1.20886200	-3.23922100
H	7.90742000	0.74744600	-2.58525900
C	6.84090300	0.26338000	-4.39420200
H	7.71840700	0.11235300	-5.02965400
C	6.35793600	-1.07779400	-3.84912100
H	5.97520000	-1.70826400	-4.65811400
H	5.21410300	2.11918300	-3.05039200
C	4.92018800	2.01467500	0.70031300
C	6.20576100	1.24447300	0.94279500
C	7.30736100	2.09676100	1.56661300
H	7.67968200	2.81942000	0.82816700
C	6.76597500	2.84660700	2.77978500
H	7.56289700	3.39315000	3.29257700
C	5.66968200	3.81489000	2.34418500
H	6.13063900	4.66130700	1.81700300
H	5.96553000	0.41471100	1.62275000
H	7.21370400	-1.61692600	-3.42049700
H	6.06092700	0.71055500	-5.02307900
H	7.58309100	2.14676300	-3.60544700
H	6.12048100	2.10710700	-1.56157800
H	6.55952800	0.77342400	0.02301600
H	8.15221400	1.45960500	1.84418200
H	6.35793200	2.12340500	3.49688300
H	5.16154000	4.23969100	3.21587000
O	0.52788600	0.61612700	1.11304000
H	-0.47300200	0.72738500	1.24540700
C	1.34053800	5.41482100	-3.04433300
C	1.66746100	4.73498700	-1.90869400
C	0.74020100	4.61933700	-0.82242700
C	-0.54258600	5.24761600	-0.96472800
C	-0.84384000	5.95617900	-2.17067900
C	0.06537500	6.03636200	-3.18186500
C	1.04375300	3.91795500	0.36327400
C	-1.48383600	5.13353600	0.05890200
C	-1.20511000	4.41727600	1.22210500
C	0.08821500	3.81152300	1.39297100
C	0.33510300	3.08682300	2.60650700
H	1.30325400	2.61872400	2.74491000
C	-0.64037000	2.94211700	3.54702300
C	-1.93154100	3.52105600	3.36103500
C	-2.19776700	4.24434500	2.23971900
H	2.05813100	5.48684600	-3.85533200
H	2.64398000	4.27177600	-1.81642100



H	-1.82281100	6.41927400	-2.25754200
H	-0.17348600	6.57407900	-4.09374400
H	-2.46808000	5.58039500	-0.07166800
H	-0.44004700	2.37150700	4.44847800
H	-2.69779700	3.37036400	4.11410000
H	-3.17504600	4.69078200	2.07765900
C	-0.21425800	-2.74997000	-3.65495900
C	0.96442100	-2.52350900	-3.00755300
C	1.45331100	-3.44322000	-2.02366200
C	0.68939700	-4.63799000	-1.77496000
C	-0.53549000	-4.84147000	-2.48676700
C	-0.98051500	-3.92397500	-3.39072200
C	2.61930000	-3.19607500	-1.27250900
C	1.13047800	-5.54692300	-0.81157800
C	2.26716200	-5.29662000	-0.04115600
C	3.02256900	-4.09413400	-0.26433300
C	4.15509600	-3.84282400	0.57767200
H	4.73091900	-2.93687000	0.42111800
C	4.50157600	-4.71370900	1.56842700
C	3.75069200	-5.90675500	1.78589200
C	2.67200600	-6.18803300	1.00267900
H	-0.58959300	-2.01937800	-4.36390400
H	1.52333600	-1.61363600	-3.19385900
H	-1.11570200	-5.73499300	-2.27368700
H	-1.92554700	-4.07692400	-3.90442300
H	0.55272900	-6.45016700	-0.62940300
H	5.35587200	-4.49959000	2.20216400
H	4.04301400	-6.58580800	2.57996400
H	2.08989400	-7.09143700	1.16133500
C	-4.80622600	-4.55627800	-3.93654900
C	-4.66083000	-3.28670400	-4.43681300
C	-4.18080500	-2.23184100	-3.62152300
C	-3.84160600	-2.49471500	-2.26385100
C	-4.01605600	-3.81691300	-1.76831000
C	-4.48328500	-4.81596500	-2.58370900
H	-4.30604000	-0.70325900	-5.14516200
H	-5.17211200	-5.35789400	-4.56907600
H	-4.91046200	-3.06878400	-5.47198200
C	-4.01863200	-0.91102200	-4.11792400
C	-3.32244200	-1.43935000	-1.46817700
H	-3.76694700	-4.03327300	-0.73351400
H	-4.60738000	-5.81881400	-2.18692900
C	-3.12252000	-0.16457600	-1.99335200
C	-3.51799400	0.09321800	-3.33942300

H	-3.42632500	1.09886300	-3.73418400
C	-2.92305800	-1.72877600	-0.06012300
C	-3.74150000	-1.60208500	1.06788100
N	-2.62479000	0.82032800	-1.19039900
C	-2.21760000	2.13320800	-1.63969000
H	-1.77507800	2.09705900	-2.64288200
H	-1.41635600	2.46629400	-0.96595500
H	-2.17447700	0.51574600	-0.34035500
N	-1.64659400	-2.11733800	0.07934500
C	-0.95591100	-2.17853200	1.30526300
C	0.18579700	-2.96827400	1.38080800
C	-1.33908800	-1.36768000	2.38583300
C	0.96257400	-2.96503800	2.53036600
H	0.45626900	-3.57849400	0.52944000
C	-0.54735600	-1.35954500	3.52894500
C	0.58286100	-2.17058700	3.60607600
H	1.85524300	-3.58266700	2.58266700
H	-0.80595000	-0.71811300	4.36340500
C	-2.37842400	-0.28956100	2.17578500
O	-1.99486700	0.74282400	1.56982700
C	-3.37574700	-0.01158300	3.30689800
F	-4.33985600	0.81172500	2.92093800
F	-2.70429500	0.60097000	4.30746700
F	-3.91745000	-1.11611600	3.82781800
H	-1.06311900	-2.08084800	-0.75837400
C	-3.35091300	3.13633300	-1.57794000
C	-3.57645000	4.04500800	-2.60795900
C	-4.15170900	3.18881000	-0.43169200
C	-4.58348500	5.00451400	-2.49790000
H	-2.94803100	4.01462900	-3.49532300
C	-5.15920000	4.14056700	-0.32304100
H	-3.95971700	2.49052600	0.38099900
C	-5.37550900	5.05455000	-1.35559900
H	-4.75095600	5.70775700	-3.30805200
H	-5.77502700	4.17313800	0.57098100
H	-6.16190000	5.79769300	-1.27008400
C	1.44845500	-2.13071300	4.83148700
F	2.49807800	-1.31167100	4.67156600
F	0.77236000	-1.69782000	5.90634600
F	1.94426600	-3.34219800	5.12474500
C	-5.16025500	-1.19607900	1.00833600
C	-6.09385300	-1.88464400	1.79206900
C	-5.59983300	-0.10225500	0.25143400
C	-7.43337900	-1.51321500	1.79762700

H	-5.76165000	-2.72088400	2.40153800
C	-6.93878300	0.26818300	0.25929600
H	-4.88469500	0.48119400	-0.31737500
C	-7.86242300	-0.43659400	1.02729000
H	-8.14181200	-2.06477600	2.40760600
H	-7.25555100	1.12281300	-0.33065100
H	-8.90707000	-0.14253600	1.03349800
H	-3.50731100	-2.29960400	1.87005800

**IM6d**

P	1.01251000	0.24419500	-0.18446000
O	1.79905800	1.59138400	-0.58726000
O	2.18808500	-0.85768200	-0.00682900
O	0.28653300	-0.07656300	-1.53464700
C	2.83275200	1.91689600	0.29374600
C	4.01961500	1.19410600	0.19790300
C	2.63299300	2.92580400	1.23456900
C	3.67212800	3.16145900	2.12895900
C	4.84572200	2.40256800	2.12817300
H	3.54958800	3.95016100	2.86757800
C	3.21322800	-0.85036500	-0.95065000
C	4.14267600	0.18931100	-0.89959300
C	3.28846000	-1.87377000	-1.89826700
C	4.31086400	-1.78751700	-2.83877100
C	5.20359800	-0.71450200	-2.88127000
H	4.39502300	-2.57768000	-3.58131900
C	5.11721400	0.29467000	-1.91134200
C	5.98442500	1.53710300	-2.01153600
C	7.22554800	1.33622600	-2.87697600
H	7.93870700	0.68395300	-2.35549300
C	6.84137500	0.70070000	-4.20926400
H	7.70545200	0.63255000	-4.87653000
C	6.25920300	-0.68940900	-3.96973600
H	5.83394800	-1.09515900	-4.89325300
H	5.36497200	2.33286500	-2.44959200
C	5.02452600	1.39975100	1.16365200
C	6.22772400	0.47601700	1.22320300
C	7.39127700	1.05787400	2.02119600
H	7.84503800	1.88755400	1.46279100
C	6.89818300	1.56722100	3.37191800
H	7.73241100	1.90525700	3.99350000
C	5.90886700	2.71063000	3.16503700
H	6.45902800	3.60443900	2.84084700
H	5.89868100	-0.45954500	1.69759700

H	7.07075100	-1.37125000	-3.68147000
H	6.09721900	1.33327700	-4.70914500
H	7.72506300	2.29731300	-3.02995200
H	6.26486800	1.90015000	-1.02050500
H	6.55396200	0.19410400	0.21965200
H	8.16649400	0.29656900	2.14807600
H	6.40811800	0.74572500	3.90920100
H	5.42387700	2.97760300	4.10943300
O	0.18556200	0.32965400	1.03455300
H	-1.51441500	0.34591500	1.96835700
C	2.21885400	6.13505000	-1.52553700
C	2.34371200	5.10833900	-0.63744700
C	1.29975500	4.81020700	0.29832600
C	0.12000500	5.62657200	0.27404300
C	0.03043000	6.69561200	-0.67258800
C	1.04505300	6.94381900	-1.54673700
C	1.39193900	3.75279900	1.22596300
C	-0.92856100	5.34659300	1.15029900
C	-0.85615600	4.28842800	2.05555000
C	0.33298500	3.48209600	2.11229900
C	0.36889500	2.39772200	3.05008300
H	1.25572700	1.77552000	3.09323800
C	-0.70941400	2.11325200	3.83376300
C	-1.90117400	2.89469500	3.75071000
C	-1.96431300	3.95545500	2.89977500
H	3.02092100	6.34276500	-2.22655400
H	3.24388900	4.50286700	-0.62991900
H	-0.87627300	7.29398600	-0.68087800
H	0.96671900	7.75566800	-2.26252500
H	-1.83795400	5.94207300	1.09555300
H	-0.67772900	1.26610400	4.51214000
H	-2.75740600	2.62424800	4.35976600
H	-2.86383300	4.56027800	2.82312100
C	-0.33077300	-1.97180500	-4.22711200
C	0.85353600	-1.97505200	-3.55191500
C	1.20461300	-3.06104600	-2.68465900
C	0.30591900	-4.18236100	-2.60976300
C	-0.92406200	-4.13854100	-3.34085600
C	-1.24312200	-3.06263100	-4.11204300
C	2.36132800	-3.04485500	-1.88080000
C	0.62915000	-5.26645900	-1.79392000
C	1.78678800	-5.27399800	-1.01384900
C	2.66390100	-4.13605200	-1.03979400
C	3.80501400	-4.14530700	-0.17314900

H	4.47157500	-3.28932300	-0.17737700
C	4.05595200	-5.20530300	0.64815300
C	3.18815800	-6.33645100	0.66513500
C	2.09048000	-6.36672200	-0.14185400
H	-0.59582000	-1.12245200	-4.84853500
H	1.52788700	-1.12947800	-3.62503900
H	-1.60915900	-4.97677400	-3.24861200
H	-2.19414100	-3.02513200	-4.63606900
H	-0.05128600	-6.11325600	-1.74186700
H	4.92367300	-5.19048700	1.29948900
H	3.40438800	-7.16765100	1.32801900
H	1.41644500	-7.21863700	-0.13224500
C	-5.16523700	-2.88759300	-4.68737200
C	-4.82249800	-1.57761000	-4.91094600
C	-4.18257700	-0.80944200	-3.90701200
C	-3.88505400	-1.40735700	-2.65083500
C	-4.25346300	-2.76613900	-2.44732700
C	-4.87783300	-3.48267800	-3.43631600
H	-4.04818000	1.01161700	-5.06542300
H	-5.65618000	-3.46705700	-5.46188300
H	-5.03770500	-1.10583700	-5.86621600
C	-3.81016400	0.54482200	-4.11340400
C	-3.20682000	-0.64863800	-1.66144000
H	-4.01878700	-3.24548000	-1.50076200
H	-5.15080200	-4.51848900	-3.26010700
C	-2.84264700	0.67812800	-1.88873300
C	-3.17269600	1.26860700	-3.14669000
H	-2.92648200	2.30966400	-3.32177400
C	-2.78758000	-1.30805600	-0.39359600
C	-3.73035600	-1.49655000	0.80007500
N	-2.21729900	1.41675300	-0.91695400
C	-1.59184800	2.69799500	-1.15958900
H	-1.02061900	2.68565700	-2.09774700
H	-0.85953100	2.84972900	-0.35560700
H	-1.94286300	0.94001400	-0.06871000
N	-1.56410500	-1.68365900	-0.32274000
C	-1.09969400	-2.26850500	0.87856700
C	0.04015900	-3.05461400	0.80026900
C	-1.71769200	-2.01067100	2.11282000
C	0.57661200	-3.62751500	1.94500700
H	0.49735800	-3.19176200	-0.16836400
C	-1.17521000	-2.57871200	3.25909100
C	-0.04212100	-3.38928900	3.16581400
H	1.46587300	-4.24770700	1.88239000

H	-1.62292400	-2.41591500	4.23107700
C	-2.90373400	-1.05545000	2.04699900
O	-2.48639600	0.28419100	1.90034100
C	-3.75080700	-1.08853400	3.32073100
F	-4.77050700	-0.23562400	3.27841900
F	-3.01370300	-0.74323200	4.39296200
F	-4.24223800	-2.31817500	3.53941400
H	-0.42719000	-0.76359100	-1.37183500
C	-2.57256900	3.85540800	-1.15274500
C	-2.44337300	4.90792400	-2.05584600
C	-3.58457900	3.90800800	-0.19021900
C	-3.30618000	6.00186800	-1.99905900
H	-1.64972500	4.87999400	-2.79914400
C	-4.44690700	4.99718500	-0.13106800
H	-3.66568300	3.10045300	0.53294700
C	-4.30912700	6.04988300	-1.03628800
H	-3.19358600	6.81507300	-2.70966800
H	-5.22503600	5.02945900	0.62605900
H	-4.98355800	6.89905700	-0.99258900
C	0.54589300	-3.94763600	4.42858800
F	1.33245300	-3.05396000	5.04965400
F	-0.40750500	-4.29601600	5.30774800
F	1.29600300	-5.03364900	4.19453500
C	-5.09110400	-0.86498300	0.62633200
C	-6.23230300	-1.65828500	0.72893900
C	-5.23265900	0.50220300	0.37573600
C	-7.49938200	-1.09898000	0.58292900
H	-6.13009900	-2.72256800	0.92618500
C	-6.49533000	1.06025600	0.22801600
H	-4.34726700	1.12255300	0.29417400
C	-7.63278200	0.26162000	0.33208800
H	-8.37919100	-1.72916700	0.66275600
H	-6.58854600	2.12251400	0.02384800
H	-8.61885800	0.69926800	0.21368600
H	-3.87356500	-2.58111500	0.91688900

#### IM7d

C	-5.17291600	-2.62109800	-2.20354500
C	-5.48953500	-1.31692800	-1.92680000
C	-4.48219100	-0.37686000	-1.59439300
C	-3.12160400	-0.78998100	-1.54026900
C	-2.82470100	-2.14413500	-1.85808100
C	-3.82042900	-3.03218600	-2.17458800
H	-5.82802800	1.29676800	-1.35523800

H	-5.94989000	-3.33447300	-2.45619200
H	-6.52183600	-0.97902700	-1.96018400
C	-4.78996800	0.97816800	-1.31611900
C	-2.11675200	0.14971900	-1.17738800
H	-1.78986200	-2.47173000	-1.88093900
H	-3.56730000	-4.05947100	-2.41706000
C	-2.44528100	1.48775400	-0.95339600
C	-3.81089500	1.88582300	-1.02311500
H	-4.07448800	2.92102300	-0.84050600
C	-0.71882600	-0.28897800	-0.91611500
C	-0.44143000	-1.31925500	0.19335500
H	-0.27563600	-2.29174000	-0.29095800
C	-1.60035300	-1.44821200	1.16112900
C	-2.13931900	-2.70233800	1.44606400
C	-2.14543600	-0.31775500	1.78161400
C	-3.19846000	-2.83190800	2.33774500
H	-1.72353200	-3.58376200	0.96452600
C	-3.20181300	-0.44879800	2.67778500
H	-1.76979300	0.67271700	1.52868800
C	-3.73012000	-1.70541200	2.95804900
H	-3.61076700	-3.81393800	2.54459100
H	-3.62104500	0.43589900	3.14580100
H	-4.55913900	-1.80537600	3.65077500
N	-1.46507600	2.38159900	-0.56544700
C	-1.73329600	3.77249900	-0.28311800
H	-2.51966600	3.82753000	0.48160100
H	-2.11061200	4.31957000	-1.16240700
H	0.14922000	0.14691400	2.28308100
N	0.21898200	0.25846800	-1.59364100
C	1.54929500	-0.13243500	-1.36585500
C	2.45622200	0.14662300	-2.38990400
C	1.97071500	-0.77931200	-0.19282000
C	3.78269800	-0.23427100	-2.27438700
H	2.08181400	0.65228300	-3.27273500
C	3.30928300	-1.14687900	-0.07936300
C	4.19879000	-0.88543300	-1.11778900
H	4.49014500	-0.03731800	-3.07251300
H	3.68244300	-1.65249700	0.79964500
C	0.91025400	-0.96297300	0.88689100
O	0.84008300	0.24454600	1.60969500
C	1.28207200	-2.06574900	1.89324500
F	0.38505700	-2.13312000	2.88626000
F	2.45915800	-1.83163200	2.48852500
F	1.34413200	-3.26676400	1.30544700

H	-0.55755000	2.19877300	-0.97442600
C	-0.48891100	4.46220500	0.23599300
C	-0.35404100	5.84281000	0.07861400
C	0.51894500	3.75267600	0.89273100
C	0.76112700	6.50790600	0.57511800
H	-1.12911900	6.39989800	-0.44192900
C	1.63993700	4.41903500	1.38179200
H	0.43619800	2.67637200	1.01778600
C	1.76401200	5.79572800	1.22825800
H	0.85190200	7.58142800	0.44350300
H	2.41821100	3.85295900	1.88371200
H	2.63914800	6.31178500	1.60967700
C	5.64540100	-1.25334700	-0.95697800
F	6.36225900	-0.24110100	-0.44374000
F	5.80682000	-2.30119300	-0.13620600
F	6.20772100	-1.56859300	-2.13344400

**P**

C	-0.77848500	4.81755000	1.37519800
C	-0.47331400	3.59339200	0.83708300
C	-1.44449100	2.85688400	0.10159200
C	-2.74041000	3.42525600	-0.05377000
C	-3.02100600	4.69549400	0.50933500
C	-2.06469000	5.38206800	1.21069600
H	-0.02213600	5.36197800	1.93171000
H	0.52315300	3.18252000	0.96211800
C	-1.17878300	1.56881700	-0.44275900
C	-3.72148000	2.69043300	-0.76584000
H	-4.01568200	5.11238900	0.37547800
H	-2.28839700	6.35264300	1.64034800
C	-3.44740000	1.46381600	-1.30140800
C	-2.15510400	0.88175200	-1.15223400
H	-4.71276300	3.11941800	-0.88313500
H	-4.22151600	0.92109200	-1.83089100
N	-1.88372600	-0.37110600	-1.67700700
H	-0.90469100	-0.57134400	-1.81119700
C	-2.77743100	-1.03520600	-2.60089300
H	-3.12326900	-0.34615800	-3.38736000
H	-2.19472200	-1.81026400	-3.10809300
C	-3.98198000	-1.68612900	-1.94271800
C	-4.95033400	-2.29096400	-2.74729500
C	-4.14430700	-1.69514700	-0.55939800
C	-6.05794000	-2.90793400	-2.17780200
H	-4.83277500	-2.28062100	-3.82882000



C	-5.25632900	-2.31090100	0.01088400
H	-3.39952200	-1.21760300	0.06977500
C	-6.21371000	-2.91974900	-0.79295900
H	-6.80123100	-3.37797000	-2.81394300
H	-5.36926100	-2.30833900	1.09087400
H	-7.07929100	-3.39836100	-0.34635000
C	4.62551500	0.98712900	-1.85123900
C	3.35088500	1.47768400	-1.84981000
C	2.38024000	0.94998900	-0.95825100
C	2.73351700	-0.07144500	-0.04235800
C	4.06346600	-0.57514300	-0.07153400
C	4.96929100	-0.05538500	-0.95659000
H	5.37518000	1.37599900	-2.53255000
H	3.03062100	2.26592500	-2.52157200
C	1.70261700	-0.54778000	0.82720900
H	4.36780400	-1.37810400	0.58599900
C	0.40502700	-0.09918500	0.67848400
C	0.17695100	0.96251600	-0.27742500
N	1.12342000	1.46256300	-1.03495500
C	-0.75111500	-0.69243000	1.40864500
C	-1.00618500	-2.06269900	1.28432900
C	-1.58967500	0.08874800	2.20748000
C	-2.06113600	-2.64932600	1.97217700
H	-0.36086100	-2.66982800	0.65480000
C	-2.64898100	-0.49990500	2.89214800
H	-1.40227600	1.15355300	2.30626400
C	-2.88146300	-1.86831200	2.78329900
H	-2.24831500	-3.71277500	1.86774800
H	-3.28804800	0.11396000	3.51803100
H	-3.70221600	-2.32546500	3.32702600
C	2.12482000	-1.52577200	1.90953600
F	2.40026600	-2.73160900	1.38165300
F	3.24789600	-1.09553400	2.51103400
F	1.23262400	-1.70015400	2.87948200
C	6.37544500	-0.58018900	-1.00859600
F	6.57589400	-1.59275600	-0.15747700
F	7.26248600	0.38144300	-0.71031300
F	6.68308000	-1.01810300	-2.23924700
<b>mP</b>			
C	1.92133700	-2.83907300	3.18370600
C	1.39992600	-1.99061400	2.24113400
C	2.24508900	-1.30973600	1.32245700
C	3.64856000	-1.51534600	1.42534400

C	4.15772400	-2.39845800	2.41002500
C	3.31617500	-3.05384900	3.27040900
H	1.25677200	-3.34774800	3.87492200
H	0.32735300	-1.82460100	2.20101800
C	1.74002000	-0.42936800	0.32380500
C	4.50258300	-0.80927300	0.54112700
H	5.23319900	-2.54241700	2.47010300
H	3.71366100	-3.72863800	4.02098500
C	4.00604700	0.05691200	-0.39118800
C	2.60246000	0.25837500	-0.52010900
H	5.57607600	-0.95464600	0.62410400
H	4.68745000	0.60367500	-1.03210300
N	2.09445100	1.07156000	-1.53164100
H	1.16094000	1.40511200	-1.33240500
C	2.92576500	2.07323800	-2.16806300
H	3.74492400	1.58082200	-2.70365100
H	2.31007500	2.54463400	-2.94134400
C	3.48640200	3.14594600	-1.24687600
C	4.58633800	3.89951600	-1.66023000
C	2.90656300	3.41476000	-0.00662600
C	5.09475700	4.91317200	-0.85556000
H	5.04884900	3.68875200	-2.62199000
C	3.41791900	4.42792200	0.80063800
H	2.06047600	2.82406800	0.33772200
C	4.50970500	5.18018400	0.37958500
H	5.95130500	5.49027300	-1.18929000
H	2.96238500	4.62518200	1.76590800
H	4.90736600	5.96696600	1.01237500
C	-3.31143900	2.75843700	0.92237500
C	-1.97658300	2.46840500	0.90412000
C	-1.52632200	1.19395000	0.47219100
C	-2.45611100	0.22097900	0.03046300
C	-3.84055200	0.54103100	0.07185900
C	-4.24203000	1.77498600	0.50910000
H	-3.66945600	3.72679600	1.25631100
H	-1.22454300	3.18076800	1.22457300
C	-1.92495100	-1.02267900	-0.43955700
H	-4.58612200	-0.18186700	-0.23095400
C	-0.57388200	-1.27779600	-0.34968300
C	0.26792500	-0.22640300	0.17885500
N	-0.18723100	0.95580300	0.52064700
C	0.08919300	-2.54581100	-0.76727700
C	-0.18452400	-3.74547400	-0.10746000
C	1.04623300	-2.52078100	-1.78416800

C	0.48911400	-4.90824500	-0.46175300
H	-0.92661700	-3.76251500	0.68649500
C	1.71413400	-3.68696300	-2.14065300
H	1.26907700	-1.58259500	-2.28658200
C	1.43949800	-4.88011700	-1.47834700
H	0.27477900	-5.83496600	0.05993400
H	2.45505400	-3.66085700	-2.93273000
H	1.96806000	-5.78738500	-1.75215900
C	-2.91905900	-1.98299500	-1.06493600
F	-3.76420300	-2.45699400	-0.13226400
F	-3.66632800	-1.34543400	-1.98273100
F	-2.37504800	-3.02651000	-1.68106500
C	-5.70033000	2.12873100	0.56950400
F	-6.48630700	1.13386000	0.14285500
F	-5.96711600	3.20779400	-0.18222500
F	-6.07407300	2.43153600	1.82214700

### TSX

Value of imaginary frequency = -29.33 cm<sup>-1</sup>

C	-0.10987800	4.73032500	0.62729800
C	-0.11213900	3.35901700	0.53650000
C	-1.10486200	2.65114400	-0.19772100
C	-2.14239300	3.44634200	-0.75150400
C	-2.09729500	4.85999400	-0.69053500
C	-1.08883800	5.50544300	-0.02496500
H	0.65538100	5.21840500	1.22296800
H	0.64572300	2.80804400	1.07565600
C	-1.14915200	1.18754000	-0.30373700
C	-3.27571800	2.79585800	-1.31020300
H	-2.90303000	5.41908700	-1.15869600
H	-1.06326700	6.58834900	0.03268700
C	-3.45077400	1.46431400	-1.13157700
C	-2.44525000	0.64961100	-0.50625000
H	-4.04216000	3.38835600	-1.80176300
H	-4.37538000	0.99689500	-1.44629800
N	-2.83269900	-0.59982000	-0.13375500
H	-2.20896300	-1.13734900	0.43940500
C	-4.09149500	-1.23022400	-0.46370800
H	-4.26302400	-1.19345600	-1.54786600
H	-3.97500300	-2.28886900	-0.21384300
C	-5.30784200	-0.68187600	0.26629900
C	-6.58210300	-0.98691000	-0.21509700
C	-5.18511400	0.09159200	1.41859300
C	-7.71673800	-0.53506000	0.44974600

H	-6.68556300	-1.58275200	-1.11923000
C	-6.32038000	0.54764700	2.08323800
H	-4.19563800	0.34525100	1.78656100
C	-7.58798100	0.23469600	1.60309800
H	-8.70159500	-0.77881000	0.06426900
H	-6.21206700	1.15359700	2.97713900
H	-8.47177600	0.59275900	2.12085200
C	4.70897700	1.92804200	-0.32816300
C	3.38683500	2.11441000	-0.60761800
C	2.46100000	1.04595500	-0.43399300
C	2.91473100	-0.24186000	-0.05986600
C	4.29084900	-0.39840900	0.26514600
C	5.14709900	0.66312900	0.13746800
H	5.42477800	2.73713500	-0.43193500
H	2.98442300	3.06992100	-0.92568800
C	1.90129700	-1.24980700	-0.07882600
H	4.67722200	-1.33689000	0.63307800
C	0.55693200	-0.92251300	-0.19378700
C	0.18317300	0.48915200	-0.32684900
N	1.16070900	1.34225100	-0.58177500
C	-0.40651100	-2.05820200	-0.28567200
C	-0.93384300	-2.41418900	-1.53091600
C	-0.72225200	-2.82293500	0.83931900
C	-1.75442000	-3.52753400	-1.65032400
H	-0.68685200	-1.81578100	-2.40279300
C	-1.56433600	-3.92900200	0.72008200
H	-0.29990800	-2.55769300	1.80363100
C	-2.07015500	-4.28946000	-0.52438100
H	-2.14877100	-3.80556400	-2.62233700
H	-1.80724500	-4.51703300	1.59891700
H	-2.71101400	-5.15993300	-0.61916100
C	2.33456300	-2.71119700	0.03088800
F	3.61357800	-2.88589300	-0.33611100
F	2.23051200	-3.14472200	1.29831000
F	1.63812600	-3.54742900	-0.74213200
C	6.59724500	0.52038100	0.49404500
F	6.90106400	-0.70636900	0.93544500
F	6.95176100	1.39212300	1.45240000
F	7.38587800	0.77527100	-0.56269100

### TSad

Value of imaginary frequency = -16.28 cm<sup>-1</sup>

C	0.71997000	-4.84793200	1.42564400
C	-0.64230800	-4.72464200	1.35375700

C	-1.25793600	-3.46564200	1.15709000
C	-0.48271300	-2.28556100	0.94081900
C	0.92244600	-2.44857400	1.12862000
C	1.49667900	-3.67765000	1.35483900
H	-3.25392400	-4.27132500	1.39209600
H	1.18672300	-5.81389100	1.58358700
H	-1.28562900	-5.59176900	1.47663300
C	-2.67021800	-3.36604400	1.25184300
C	-1.16407600	-1.02676700	0.64256600
H	1.57116200	-1.58860800	1.16842700
H	2.57070600	-3.73237200	1.50349900
C	-2.52924700	-0.96041100	0.99811700
C	-3.27777900	-2.15300400	1.24960600
H	-4.34978300	-2.08099500	1.38880000
C	-0.48342700	0.08554400	-0.08336800
C	-0.86265900	1.28828900	-0.60045700
H	-0.03847400	1.77445100	-1.12068000
C	-2.09042800	2.11871300	-0.68447800
C	-3.18899000	1.72899600	-1.45543200
C	-2.12593800	3.36293200	-0.04240300
C	-4.31361200	2.54160700	-1.55031400
H	-3.16266100	0.76991600	-1.96216000
C	-3.25356600	4.17490800	-0.13217000
H	-1.26788300	3.68644100	0.54090800
C	-4.35174200	3.76337200	-0.88295400
H	-5.17065700	2.20407400	-2.12540000
H	-3.27265200	5.12870200	0.38518100
H	-5.23359500	4.39206900	-0.94861500
N	-3.18830300	0.22838700	1.07787200
C	-4.55985800	0.41640200	1.50024700
H	-4.63963900	1.45724100	1.82648200
H	-4.77392600	-0.20001300	2.38532300
H	-2.62107200	1.05742000	1.09857600
N	0.86938400	-0.22388600	-0.46688500
C	1.98778900	0.42724900	-0.08366500
C	1.93265000	1.49978800	0.84888500
C	3.27631600	0.02183400	-0.56185300
C	3.07289200	2.14871400	1.24604300
H	0.97112100	1.79164800	1.24992100
C	4.42322100	0.72339700	-0.13803800
C	4.33152200	1.77329200	0.74344200
H	3.00574100	2.95982900	1.96524200
H	5.40183400	0.43621500	-0.50050700
C	3.39842500	-1.11019500	-1.47626800

O	2.47970400	-1.79819600	-1.88722400
C	4.80947600	-1.49880600	-1.98321700
F	4.73937700	-2.53114100	-2.80872900
F	5.61079200	-1.83394000	-0.96103600
F	5.38616600	-0.47924300	-2.63589900
H	1.00993700	-1.04728100	-1.04428400
C	-5.62591700	0.17388800	0.44275200
C	-5.39547900	-0.58708400	-0.70302700
C	-6.88622800	0.74497400	0.62886600
C	-6.40516600	-0.76883300	-1.64543600
H	-4.41794700	-1.02806900	-0.87035000
C	-7.89576100	0.56558000	-0.31039800
H	-7.07416400	1.34875100	1.51370000
C	-7.65698600	-0.19233300	-1.45397300
H	-6.20911700	-1.36139600	-2.53345500
H	-8.86652100	1.02474100	-0.15354000
H	-8.44109500	-0.33072200	-2.19104800
C	5.54192600	2.52497300	1.19515100
F	5.67492200	2.49128000	2.53232300
F	6.67079900	2.03344800	0.66655900
F	5.47312800	3.82439200	0.85872900

### TSbc

Value of imaginary frequency = -19.42 cm<sup>-1</sup>

C	6.07628300	-2.58561300	0.82364500
C	6.23777000	-1.25839400	0.50933600
C	5.13754100	-0.46126500	0.12148100
C	3.81974800	-0.99735600	0.12850000
C	3.70848600	-2.39266800	0.35996600
C	4.79935900	-3.16139400	0.69944400
H	6.34289700	1.28018000	-0.35461000
H	6.92731200	-3.19409500	1.10978900
H	7.22475300	-0.80363300	0.52041400
C	5.34120400	0.86015700	-0.36960200
C	2.69278300	-0.13631500	-0.18702900
H	2.76561500	-2.88827500	0.17067100
H	4.67305900	-4.22988700	0.84271800
C	2.98291800	1.01675600	-0.94458500
C	4.31904800	1.53557300	-0.95545300
H	4.51400900	2.47859000	-1.45300300
C	1.35025300	-0.34476700	0.41664300
C	0.98658300	-1.34124400	1.25865500
H	1.65356200	-2.17611800	1.40316600
C	-0.24931600	-1.42703000	2.06286700

C	-0.91910400	-2.65543700	2.13600600
C	-0.76082000	-0.34916800	2.79723600
C	-2.08529100	-2.79218400	2.87991800
H	-0.52753200	-3.50435700	1.58304700
C	-1.92252700	-0.48694000	3.54723600
H	-0.23533100	0.60107500	2.78283100
C	-2.59574300	-1.70524000	3.58337000
H	-2.59667600	-3.74898400	2.90848000
H	-2.30340900	0.36155600	4.10697500
H	-3.50779600	-1.80781000	4.16206300
N	2.03713200	1.63948900	-1.73100200
C	1.89838000	3.07577200	-1.89394900
H	1.34558900	3.25122300	-2.82110200
H	2.88515700	3.52368100	-2.03491100
H	1.18220900	1.10878400	-1.82741400
N	0.41202100	0.72210000	0.22935400
C	-0.91799100	0.60079000	-0.06333400
C	-1.80837800	1.58290600	0.41817000
C	-1.44740800	-0.47598700	-0.81509000
C	-3.16781100	1.44575600	0.24677100
H	-1.40225300	2.42945900	0.96555600
C	-2.83595100	-0.62751000	-0.92780100
C	-3.69246300	0.31911900	-0.39967000
H	-3.84158300	2.20206200	0.63774300
H	-3.24723700	-1.46771700	-1.47610500
C	-0.56197800	-1.32814600	-1.62761500
O	0.47402700	-0.96441600	-2.13922700
C	-1.01786000	-2.77597800	-1.91645600
F	0.00942200	-3.52120500	-2.30037700
F	-1.93645200	-2.79024800	-2.89612400
F	-1.57016400	-3.33880000	-0.83599900
H	0.69493900	1.62593200	0.59216900
C	1.18499400	3.76439800	-0.74304200
C	1.75313600	3.76687000	0.53852000
C	-0.05448600	4.37492500	-0.92903900
C	1.08479900	4.35602900	1.60770300
H	2.72334700	3.29996800	0.69590700
C	-0.71477200	4.98748100	0.13567700
H	-0.50792400	4.37370400	-1.91671500
C	-0.15039500	4.97378900	1.40698700
H	1.53478000	4.34827200	2.59532000
H	-1.67557800	5.46478800	-0.02897400
H	-0.66457200	5.44466400	2.23833400
C	-5.17618400	0.15731100	-0.49180900

F	-5.77221900	1.29539300	-0.88758400
F	-5.52629500	-0.80445400	-1.35796200
F	-5.72234400	-0.16055700	0.69372000