

Supporting information

Chiral Phosphoric Acid Catalyzed Atroposelective C-H Amination of Arenes: Mechanisms, Origin and Influencing Factors of Enantioselectivity

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1. Study on the stability of the dimeric and trimeric complexes in paths I-IV.

Table S1 The relative Gibbs free energies (ΔG , in kcal/mol) and intermolecular interaction energies (ΔE , in kcal/mol) for the dimeric and trimeric complexes formed in the amination reaction.

Complex	ΔG^a	$\Delta E/(\text{kcal/mol})^b$
DI	4.2	-15.3
DI_{R2}	5.8	-9.5
COMI	6.3	-30.2
DII	4.2	-15.3
DII_{R2}	5.7	-10.2
COMII	9.0	-28.9
DIII	3.0	-13.3
DIII_{R2}	13.8	-2.1
COMIII	23.6	-13.8
DIV	4.1	-13.5
DIV_{R2}	6.4	-10.5
COMIV	16.4	-18.2

^a The ΔG is calculated as the difference between the Gibbs free energy of the dimeric (or trimeric) complex and the sum of the Gibbs free energy of [(S)-C6 + R1 (or R2)] (or [(S)-C6 + R1 + R2]).

^b The ΔE is calculated as the difference between the total energy of the dimeric (or trimeric) complex and the sum of the total energy of [(S)-C6 + R1 (or R2)] (or [(S)-C6 + R1 + R2]).

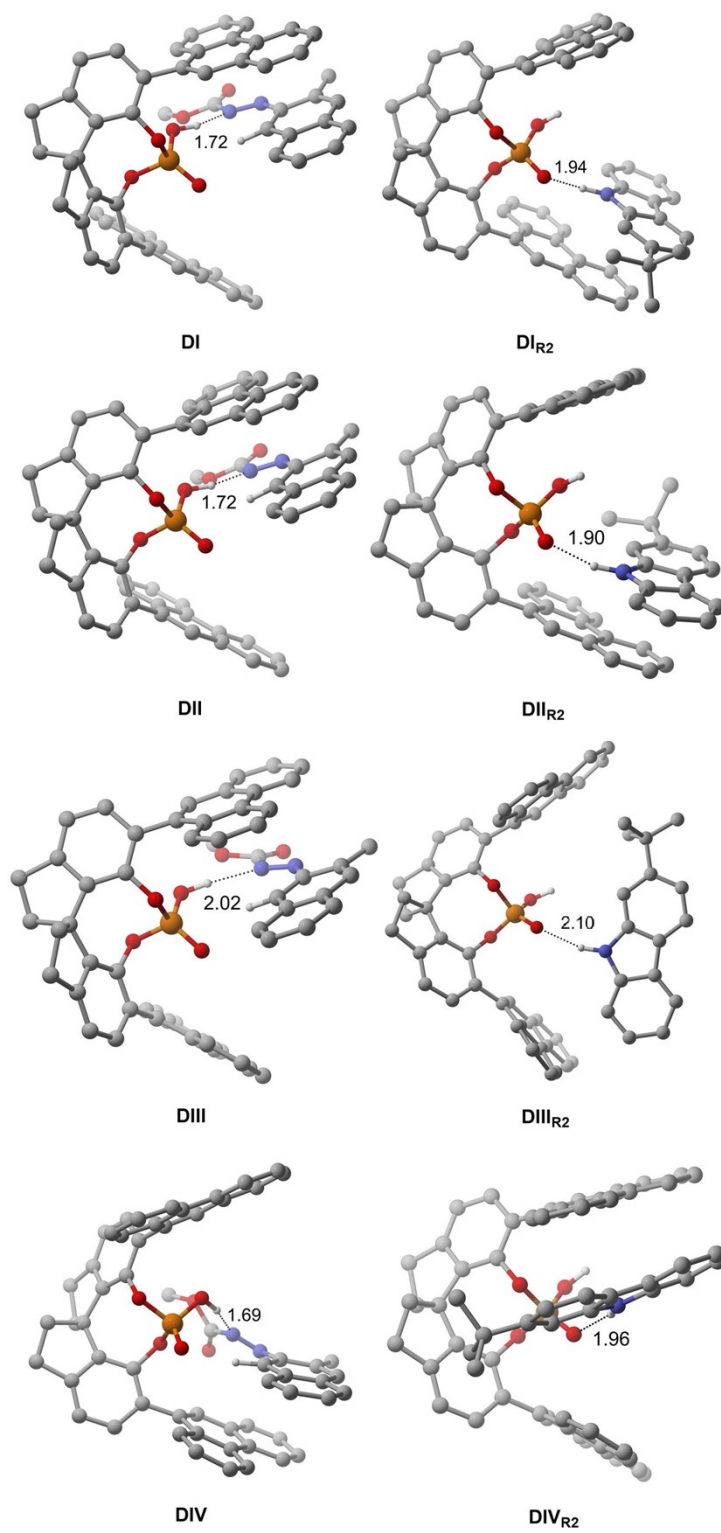


Fig. S1 The optimized geometries of the dimeric complexes in paths I-IV. The distances are in Å.

2. QTAIM Analyses

QTAIM analyses were carried out on the optimized complexes, transition states and intermediates of path **I** and path **II** to figure out the intermolecular interactions.

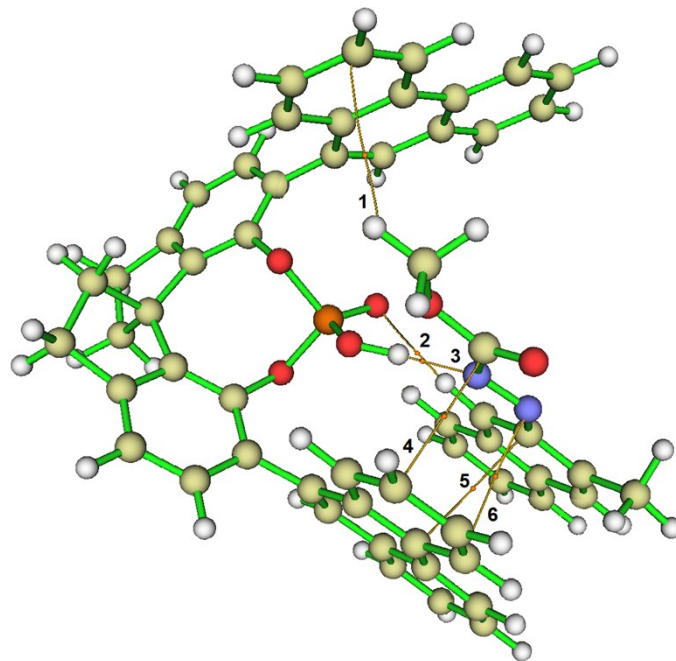


Fig. S2 Intermolecular interactions in **DI** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **DI**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
DI	1	C-H... π	3.81	0.0008	0.0031	-0.0003	0.0005	0.0002
	2	C-H...O	2.34	0.0135	0.0402	-0.0099	0.0100	0.0001
	3	O-H...N	1.72	0.0493	0.1049	-0.0358	0.0310	-0.0048
	4	π ... π	3.07	0.0082	0.0285	-0.0043	0.0057	0.0014
	5	π ... π	3.35	0.0064	0.0194	-0.0032	0.0040	0.0008
	6	π ... π	3.21	0.0072	0.0215	-0.0038	0.0046	0.0008

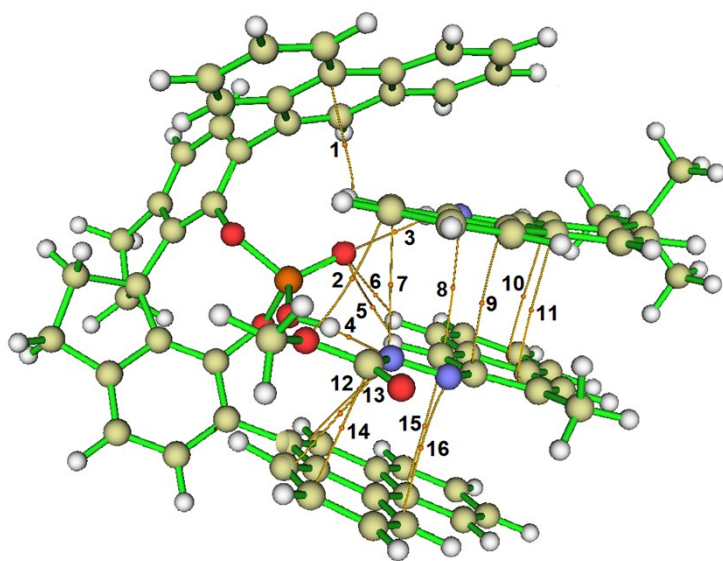


Fig. S3 Intermolecular interactions in **COMI** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **COMI**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
COMI	1	C-H... π	2.72	0.0083	0.0282	-0.0042	0.0056	0.0014
	2	lp... π	3.06	0.0091	0.0316	-0.0059	0.0069	0.0010
	3	N-H...O	2.07	0.0186	0.0634	-0.0156	0.0157	0.0001
	4	O-H...N	1.73	0.0476	0.1000	-0.0336	0.0293	-0.0043
	5	C-H... π	2.43	0.0123	0.0417	-0.0088	0.0096	0.0008
	6	C-H...O	2.49	0.0098	0.0335	-0.0069	0.0076	0.0007
	7	π ... π	3.09	0.0099	0.0289	-0.0056	0.0064	0.0008
	8	lp... π	3.12	0.0090	0.0260	-0.0053	0.0059	0.0006
	9	π ... π	3.35	0.0068	0.0206	-0.0036	0.0044	0.0008
	10	π ... π	3.43	0.0060	0.0166	-0.0028	0.0035	0.0007
	11	π ... π	3.39	0.0064	0.0182	-0.0031	0.0038	0.0007
	12	C-H... π	3.26	0.0038	0.0119	-0.0018	0.0024	0.0006
	13	π ... π	3.19	0.0082	0.0247	-0.0047	0.0054	0.0007
	14	π ... π	2.96	0.0100	0.0361	-0.0056	0.0073	0.0017
	15	π ... π	3.27	0.0073	0.0212	-0.0035	0.0044	0.0009
	16	π ... π	3.26	0.0068	0.0201	-0.0036	0.0043	0.0007

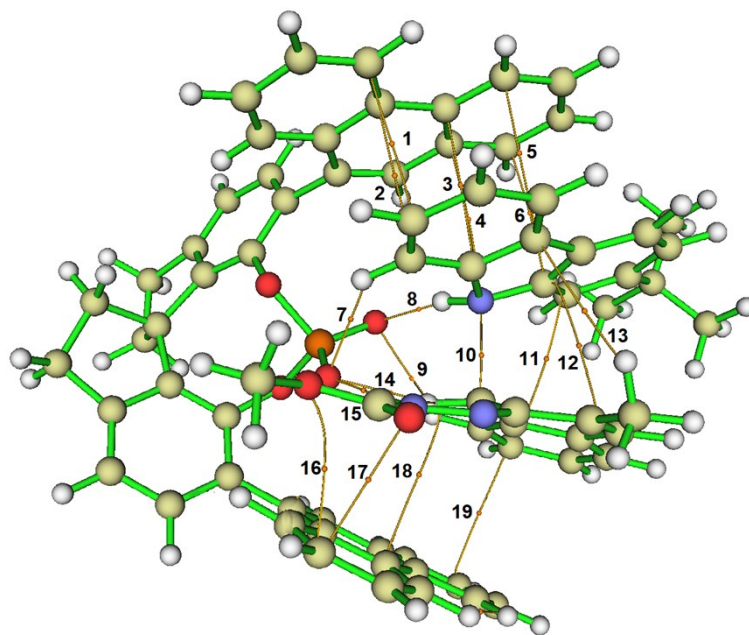


Fig. S4 Intermolecular interactions in **TSI-1** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TSI-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSI-1	1	$\pi\dots\pi$	3.35	0.0065	0.0183	-0.0031	0.0038	0.0007
	2	$\pi\dots\pi$	3.36	0.0064	0.0185	-0.0031	0.0039	0.0008
	3	$\pi\dots\pi$	3.45	0.0057	0.0159	-0.0027	0.0033	0.0006
	4	$lp\dots\pi$	3.57	0.0041	0.0137	-0.0025	0.0029	0.0004
	5	$\pi\dots\pi$	3.44	0.0059	0.0165	-0.0028	0.0035	0.0007
	6	$\pi\dots\pi$	3.37	0.0066	0.0182	-0.0031	0.0038	0.0007
	7	C-H...O	2.28	0.0158	0.0493	-0.0122	0.0123	0.0001
	8	N-H...O	1.73	0.0416	0.1255	-0.0331	0.0322	-0.0009
	9	C-H...O	2.48	0.0104	0.0347	-0.0073	0.0080	0.0007
	10	C...N	2.08	0.0687	0.0794	-0.0483	0.0341	-0.0142
	11	$\pi\dots\pi$	3.07	0.0108	0.0358	-0.0059	0.0074	0.0015
	12	$\pi\dots\pi$	3.48	0.0061	0.0174	-0.0030	0.0037	0.0007
	13	C-H... π	3.24	0.0030	0.0097	-0.0013	0.0019	0.0006
	14	C-H...O	2.13	0.0211	0.0594	-0.0172	0.0160	-0.0012
	15	N-H...O	1.76	0.0356	0.1225	-0.0281	0.0294	0.0013
	16	$lp\dots\pi$	3.13	0.0084	0.0314	-0.0053	0.0066	0.0013
	17	$lp\dots\pi$	3.17	0.0089	0.0279	-0.0052	0.0061	0.0009
	18	C-H... π	3.36	0.0027	0.0088	-0.0012	0.0017	0.0005
	19	$\pi\dots\pi$	3.38	0.0062	0.0174	-0.0029	0.0036	0.0007

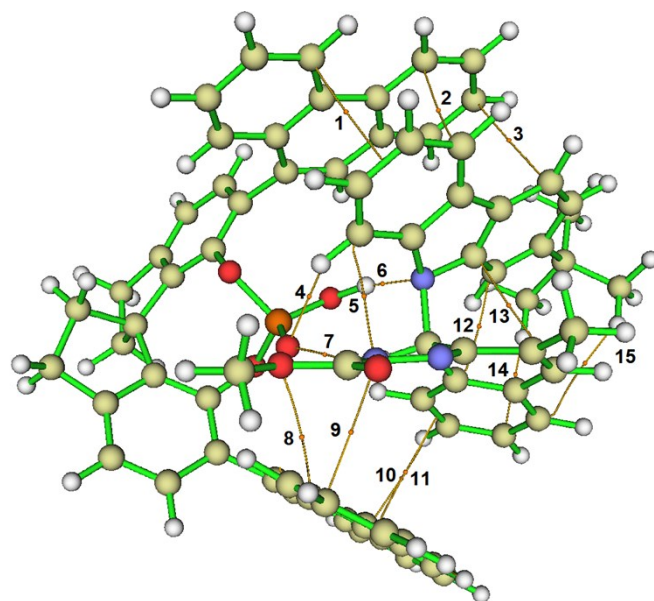


Fig. S5 Intermolecular interactions in **IMI-1** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMI-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMI-1	1	$\pi\dots\pi$	3.36	0.0066	0.0182	-0.0030	0.0038	0.0008
	2	$\pi\dots\pi$	3.38	0.0060	0.0166	-0.0028	0.0035	0.0007
	3	$\pi\dots\pi$	3.32	0.0069	0.0196	-0.0033	0.0041	0.0008
	4	C-H...O	2.22	0.0171	0.0516	-0.0135	0.0132	-0.0003
	5	lp... π	2.94	0.0122	0.0411	-0.0076	0.0089	0.0013
	6	O-H...N	1.61	0.0680	0.0928	-0.0567	0.0400	-0.0167
	7	N-H...O	2.02	0.0199	0.0640	-0.0163	0.0162	-0.0001
	8	C-H...O	2.63	0.0082	0.0322	-0.0054	0.0068	0.0014
	9	lp... π	3.13	0.0089	0.0259	-0.0052	0.0058	0.0006
	10	C-H... π	2.81	0.0070	0.0222	-0.0034	0.0045	0.0011
	11	$\pi\dots\pi$	3.45	0.0063	0.0177	-0.0029	0.0037	0.0008
	12	$\pi\dots\pi$	2.98	0.0123	0.0450	-0.0073	0.0093	0.0020
	13	$\pi\dots\pi$	3.34	0.0073	0.0222	-0.0040	0.0048	0.0008
	14	C-H... π	2.77	0.0069	0.0197	-0.0032	0.0041	0.0009
	15	C-H... π	3.24	0.0028	0.0084	-0.0011	0.0016	0.0005

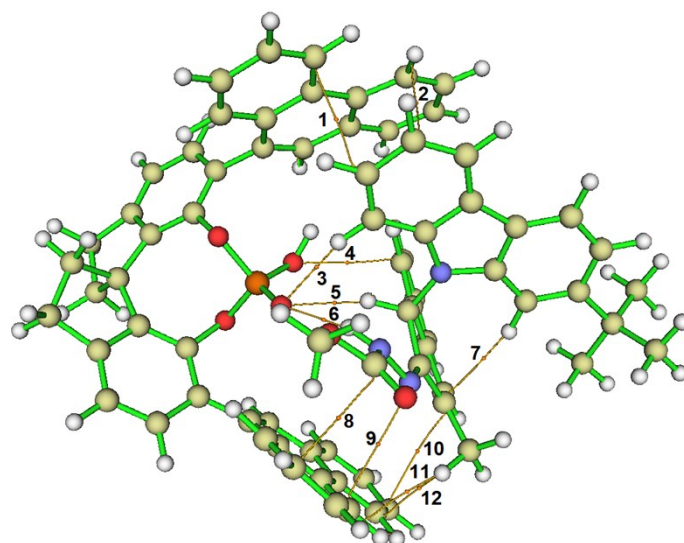


Fig. S6 Intermolecular interactions in **IMI-2** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMI-2**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMI-2	1	$\pi\dots\pi$	3.29	0.0074	0.0237	-0.0036	0.0048	0.0012
	2	C-H... π	3.16	0.0044	0.0130	-0.0020	0.0026	0.0006
	3	C-H...O	2.24	0.0163	0.0473	-0.0128	0.0123	-0.0005
	4	lp... π	3.07	0.0079	0.0280	-0.0051	0.0061	0.0010
	5	C-H...O	2.37	0.0130	0.0389	-0.0098	0.0097	-0.0001
	6	N-H...O	2.06	0.0183	0.0591	-0.0150	0.0149	-0.0001
	7	C-H... π	2.55	0.0118	0.0356	-0.0065	0.0077	0.0012
	8	$\pi\dots\pi$	3.11	0.0074	0.0269	-0.0039	0.0053	0.0014
	9	lp... π	3.49	0.0051	0.0153	-0.0027	0.0033	0.0006
	10	$\pi\dots\pi$	3.65	0.0044	0.0131	-0.0020	0.0027	0.0007
	11	C-H... π	2.66	0.0082	0.0280	-0.0042	0.0056	0.0014
	12	C-H... π	2.89	0.0068	0.0244	-0.0034	0.0048	0.0014

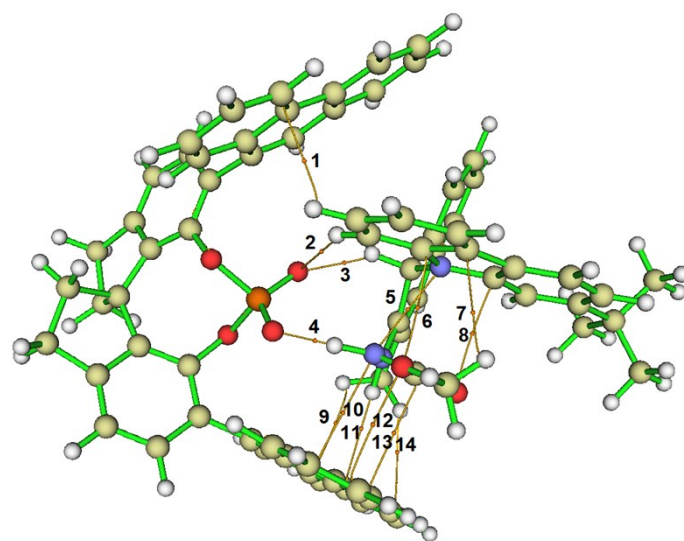


Fig. S7 Intermolecular interactions in **IMI-3** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMI-3**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMI-3	1	C-H... π	2.79	0.0073	0.0240	-0.0036	0.0048	0.0012
	2	C-H... π	2.60	0.0088	0.0282	-0.0056	0.0063	0.0007
	3	C-H...O	2.03	0.0234	0.0726	-0.0192	0.0187	-0.0005
	4	N-H...O	1.58	0.0601	0.1575	-0.0530	0.0462	-0.0068
	5	lp...lp	2.80	0.0168	0.0570	-0.0124	0.0133	0.0009
	6	lp... π	3.14	0.0083	0.0288	-0.0055	0.0063	0.0008
	7	C-H... π	2.84	0.0067	0.0227	-0.0035	0.0046	0.0011
	8	π ... π	3.11	0.0080	0.0278	-0.0052	0.0061	0.0009
	9	C-H... π	2.73	0.0083	0.0282	-0.0042	0.0056	0.0014
	10	lp... π	3.43	0.0061	0.0182	-0.0036	0.0041	0.0005
	11	N-H... π	2.65	0.0074	0.0238	-0.0041	0.0050	0.0009
	12	lp... π	3.15	0.0081	0.0264	-0.0051	0.0058	0.0007
	13	π ... π	3.28	0.0066	0.0223	-0.0032	0.0044	0.0012
	14	C-H... π	2.93	0.0058	0.0183	-0.0030	0.0038	0.0008

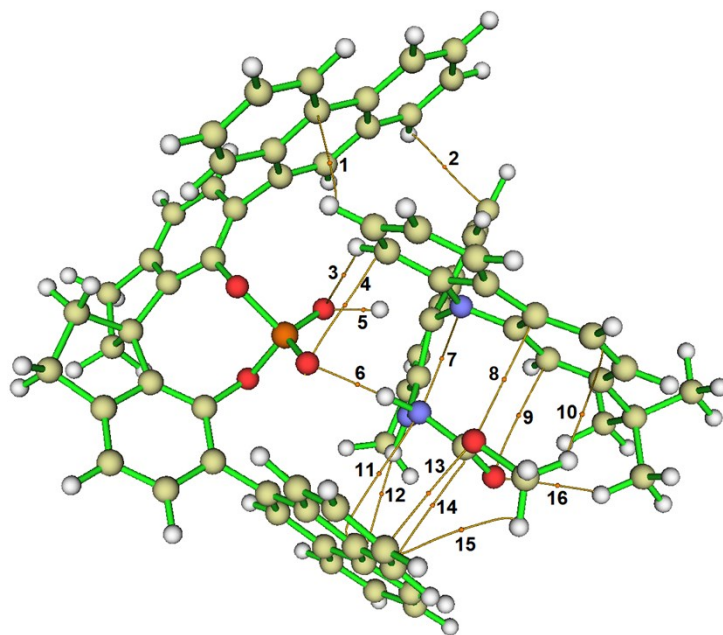


Fig. S8 Intermolecular interactions in **TSI-2** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TSI-2**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSI-2	1	C-H... π	2.74	0.0085	0.0307	-0.0045	0.0061	0.0016
	2	C-H... π	2.82	0.0068	0.0225	-0.0032	0.0044	0.0012
	3	C-H... π	2.78	0.0070	0.0211	-0.0035	0.0044	0.0009
	4	π ... π	3.15	0.0082	0.0272	-0.0048	0.0058	0.0010
	5	O...H	1.38	0.1071	0.0743	-0.1220	0.0703	-0.0517
	6	N-H...O	1.96	0.0245	0.0787	-0.0204	0.0200	-0.0004
	7	lp...lp	2.75	0.0183	0.0626	-0.0137	0.0147	0.0010
	8	lp... π	3.23	0.0068	0.0231	-0.0044	0.0051	0.0007
	9	π ... π	3.24	0.0071	0.0224	-0.0042	0.0049	0.0007
	10	C-H... π	2.84	0.0071	0.0205	-0.0033	0.0042	0.0009
	11	lp... π	3.39	0.0064	0.0191	-0.0038	0.0043	0.0005
	12	N-H... π	2.69	0.0068	0.0223	-0.0038	0.0047	0.0009
	13	lp... π	3.03	0.0095	0.0308	-0.0063	0.0070	0.0007
	14	π ... π	3.14	0.0077	0.0269	-0.0040	0.0054	0.0014
	15	C-H... π	2.91	0.0062	0.0234	-0.0031	0.0045	0.0014
	16	C-H...O	2.67	0.0060	0.0220	-0.0039	0.0047	0.0008

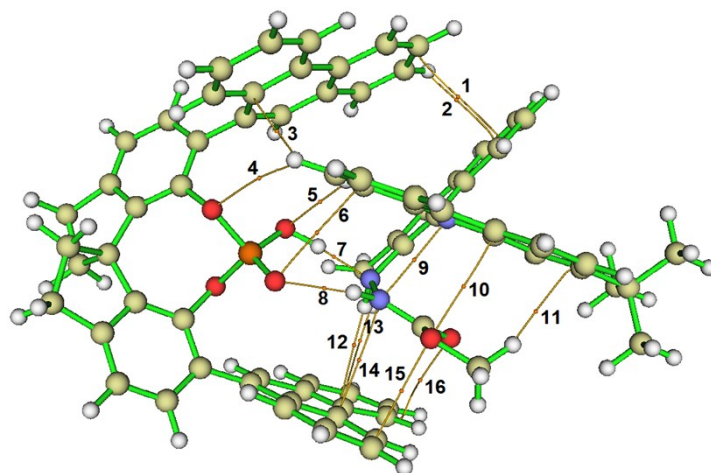


Fig. S9 Intermolecular interactions in **IMI-4** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMI-4**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMI-4	1	$\pi\dots\pi$	3.55	0.0050	0.0136	-0.0023	0.0028	0.0005
	2	C-H... π	2.92	0.0062	0.0189	-0.0029	0.0038	0.0009
	3	C-H... π	2.72	0.0080	0.0273	-0.0044	0.0056	0.0012
	4	C-H...O	3.15	0.0025	0.0108	-0.0013	0.0020	0.0007
	5	C-H...O	2.57	0.0085	0.0290	-0.0057	0.0065	0.0008
	6	$\pi\dots\pi$	3.38	0.0057	0.0181	-0.0031	0.0038	0.0007
	7	O-H...N	1.69	0.0561	0.1038	-0.0432	0.0346	-0.0086
	8	N-H...O	2.06	0.0204	0.0639	-0.0170	0.0165	-0.0005
	9	lp...lp	2.79	0.0171	0.0576	-0.0124	0.0134	0.0010
	10	lp... π	3.20	0.0074	0.0263	-0.0049	0.0058	0.0009
	11	C-H... π	2.74	0.0078	0.0247	-0.0042	0.0052	0.0010
	12	N-H... π	2.87	0.0050	0.0163	-0.0025	0.0033	0.0008
	13	C-H... π	2.77	0.0072	0.0216	-0.0035	0.0044	0.0009
	14	lp... π	3.36	0.0065	0.0186	-0.0036	0.0041	0.0005
	15	lp... π	3.14	0.0084	0.0272	-0.0053	0.0060	0.0007
	16	$\pi\dots\pi$	3.38	0.0047	0.0179	-0.0027	0.0036	0.0009

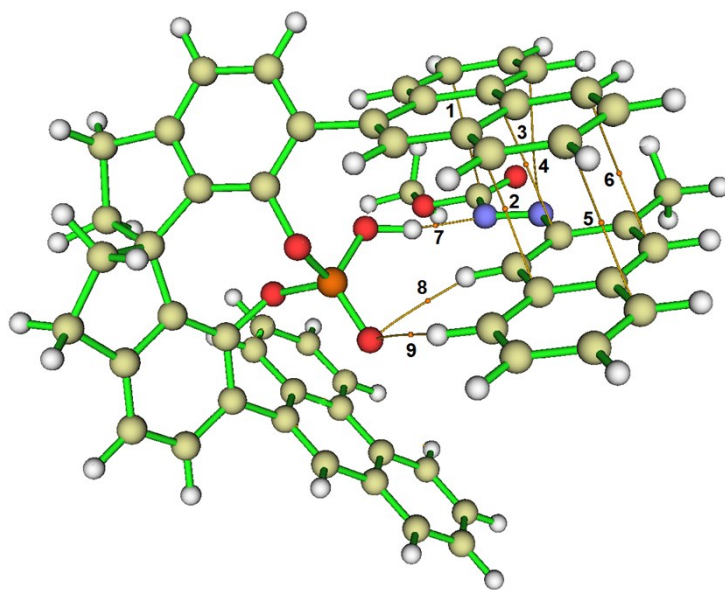


Fig. S10 Intermolecular interactions in **DII** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **DII**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
DII	1	$\pi\dots\pi$	3.07	0.0082	0.0285	-0.0043	0.0057	0.0014
	2	$\pi\dots\pi$	3.43	0.0058	0.0169	-0.0028	0.0035	0.0007
	3	$\pi\dots\pi$	3.35	0.0064	0.0194	-0.0032	0.0040	0.0008
	4	$\pi\dots\pi$	3.21	0.0072	0.0215	-0.0038	0.0046	0.0008
	5	$\pi\dots\pi$	3.43	0.0060	0.0163	-0.0027	0.0034	0.0007
	6	$\pi\dots\pi$	3.39	0.0066	0.0177	-0.0031	0.0038	0.0007
	7	O-H...N	1.72	0.0492	0.1048	-0.0358	0.0310	-0.0048
	8	C-H...O	2.34	0.0135	0.0402	-0.0099	0.0100	0.0001
	9	C-H...O	2.61	0.0073	0.0255	-0.0048	0.0056	0.0008

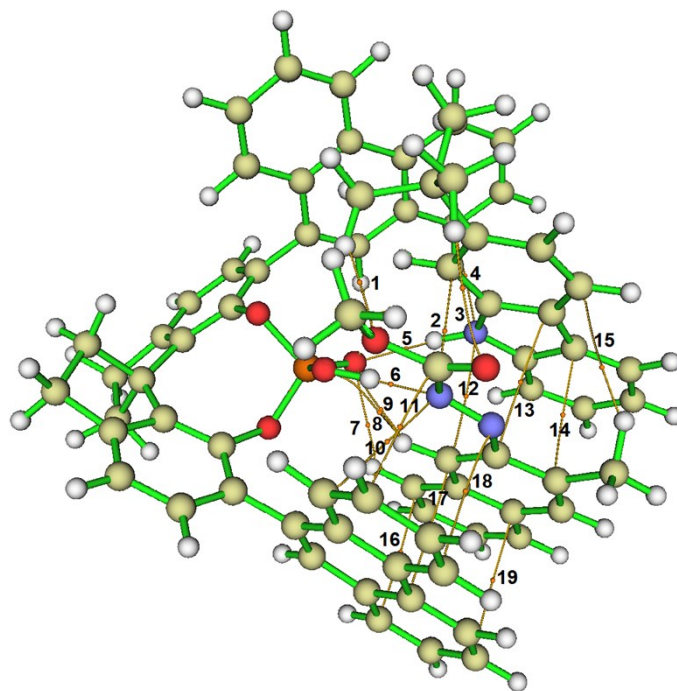


Fig. S11 Intermolecular interactions in **COMII** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **COMII**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
COMII	1	C-H...O	2.36	0.0126	0.0407	-0.0095	0.0099	0.0004
	2	π ... π	3.23	0.0079	0.0221	-0.0043	0.0049	0.0006
	3	C-H... π	2.63	0.0078	0.0275	-0.0051	0.0060	0.0009
	4	lp... π	3.29	0.0067	0.0190	-0.0038	0.0043	0.0005
	5	N-H...O	1.95	0.0235	0.0815	-0.0197	0.0200	0.0003
	6	O-H...N	1.68	0.0543	0.1034	-0.0406	0.0332	-0.0074
	7	C-H...O	2.58	0.0085	0.0301	-0.0057	0.0066	0.0009
	8	C-H...O	2.54	0.0101	0.0405	-0.0070	0.0086	0.0016
	9	C-H... π	2.54	0.0105	0.0383	-0.0070	0.0083	0.0013
	10	π ... π	3.26	0.0072	0.0219	-0.0041	0.0048	0.0007
	11	π ... π	3.00	0.0094	0.0349	-0.0054	0.0071	0.0017
	12	lp... π	3.21	0.0079	0.0225	-0.0046	0.0051	0.0005
	13	π ... π	3.38	0.0065	0.0189	-0.0033	0.0040	0.0007
	14	π ... π	3.33	0.0069	0.0198	-0.0034	0.0042	0.0008
	15	C-H... π	2.98	0.0045	0.0140	-0.0020	0.0028	0.0008
	16	π ... π	3.27	0.0074	0.0211	-0.0036	0.0044	0.0008
	17	π ... π	3.23	0.0078	0.0229	-0.0038	0.0048	0.0010
	18	π ... π	3.29	0.0063	0.0187	-0.0033	0.0040	0.0007
	19	π ... π	3.50	0.0052	0.0149	-0.0024	0.0031	0.0007

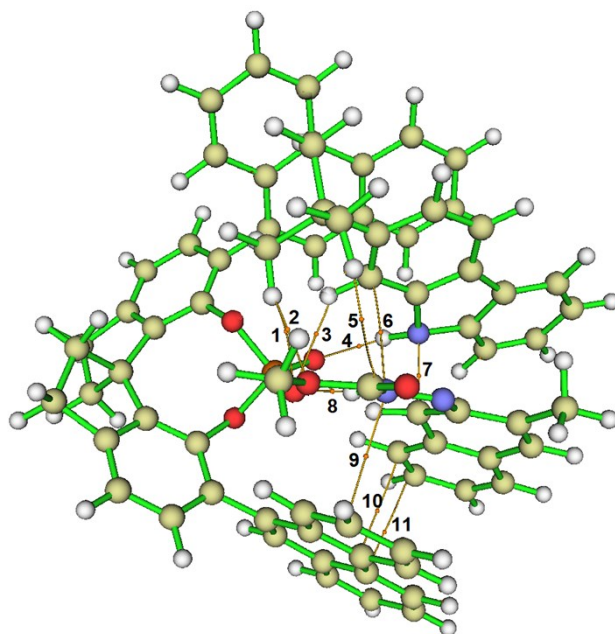


Fig. S12 Intermolecular interactions in **TSII-1** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TSII-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSII-1	1	C-H...O	2.91	0.0046	0.0175	-0.0026	0.0035	0.0009
	2	C-H...O	2.46	0.0104	0.0336	-0.0075	0.0080	0.0005
	3	C-H... π	2.40	0.0132	0.0442	-0.0096	0.0103	0.0007
	4	N-H...O	1.86	0.0313	0.0946	-0.0249	0.0243	-0.0006
	5	C-H... π	2.60	0.0075	0.0309	-0.0045	0.0061	0.0016
	6	lp... π	3.08	0.0094	0.0291	-0.0057	0.0065	0.0008
	7	C...N	2.05	0.0715	0.0790	-0.0514	0.0356	-0.0158
	8	N-H...O	1.76	0.0355	0.1210	-0.0279	0.0291	0.0012
	9	lp... π	3.09	0.0098	0.0289	-0.0057	0.0065	0.0008
	10	π ... π	3.37	0.0063	0.0180	-0.0029	0.0037	0.0008
	11	π ... π	3.46	0.0056	0.0166	-0.0027	0.0034	0.0007

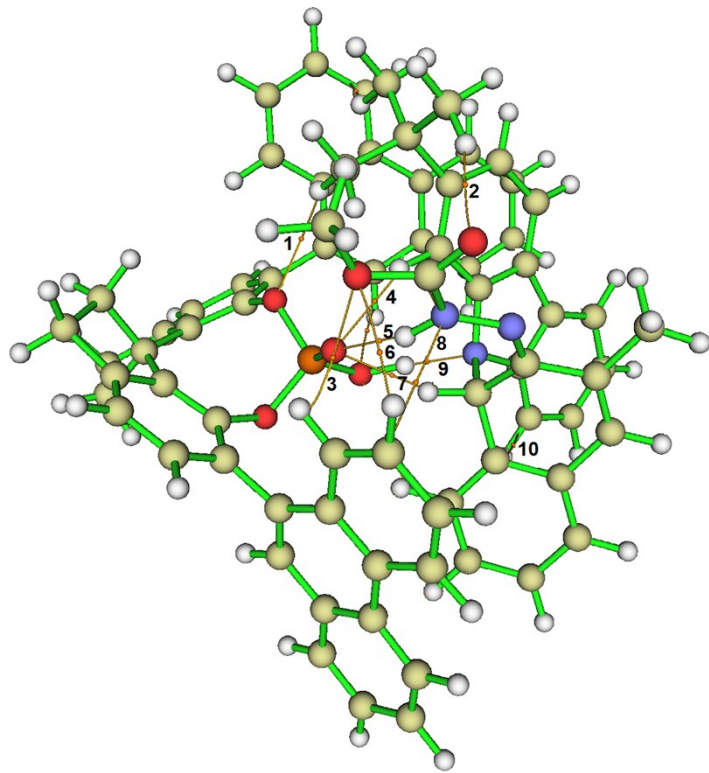


Fig. S13 Intermolecular interactions in **IMII-1** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMII-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMII-1	1	C-H...O	2.86	0.0043	0.0163	-0.0025	0.0033	0.0008
	2	C-H... π	2.70	0.0063	0.0213	-0.0037	0.0045	0.0008
	3	C-H...O	2.81	0.0054	0.0219	-0.0034	0.0044	0.0010
	4	C-H... π	2.21	0.0178	0.0525	-0.0142	0.0137	-0.0005
	5	N-H...O	1.97	0.0221	0.0740	-0.0182	0.0184	0.0002
	6	C-H...O	2.67	0.0073	0.0286	-0.0048	0.0060	0.0012
	7	C-H...O	2.14	0.0208	0.0607	-0.0170	0.0161	-0.0009
	8	lp... π	3.23	0.0076	0.0220	-0.0043	0.0049	0.0006
	9	O-H...N	1.64	0.0624	0.0964	-0.0498	0.0369	-0.0129
	10	π ... π	2.95	0.0132	0.0503	-0.0079	0.0102	0.0023

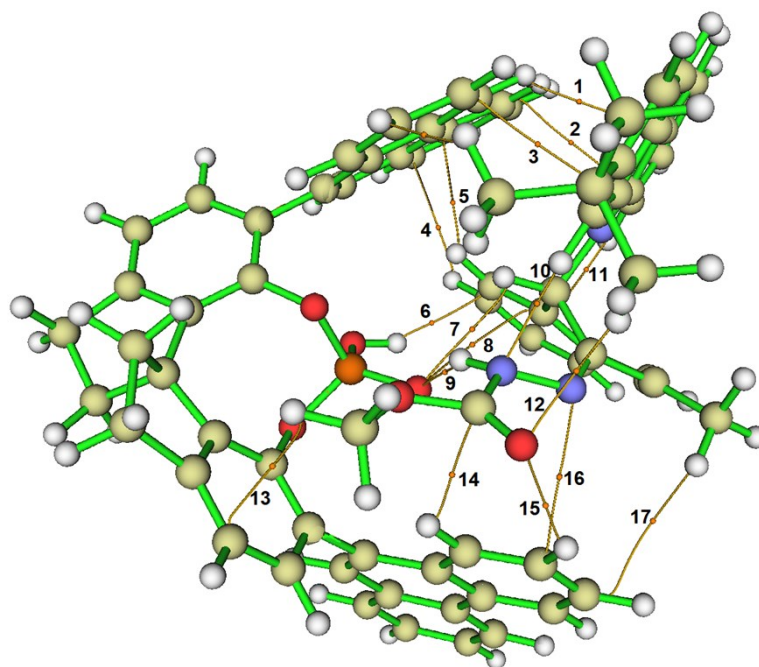


Fig. S14 Intermolecular interactions in **IMII-2** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMII-2**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMII-2	1	C-H... π	2.83	0.0064	0.0209	-0.0032	0.0042	0.0010
	2	π ... π	3.38	0.0064	0.0198	-0.0030	0.0040	0.0010
	3	π ... π	3.30	0.0072	0.0215	-0.0035	0.0044	0.0009
	4	C-H... π	2.94	0.0052	0.0161	-0.0024	0.0032	0.0008
	5	C-H... π	2.64	0.0090	0.0315	-0.0050	0.0065	0.0015
	6	O-H... π	2.33	0.0138	0.0431	-0.0084	0.0096	0.0012
	7	C-H...O	2.73	0.0074	0.0287	-0.0049	0.0060	0.0011
	8	lp... π	3.21	0.0072	0.0236	-0.0043	0.0051	0.0008
	9	N-H...O	1.91	0.0270	0.0893	-0.0224	0.0224	0.0000
	10	C-H...N	2.19	0.0196	0.0579	-0.0147	0.0146	-0.0001
	11	C-H... π	2.42	0.0148	0.0556	-0.0094	0.0117	0.0023
	12	C-H... π	2.55	0.0087	0.0290	-0.0059	0.0066	0.0007
	13	C-H... π	3.02	0.0054	0.0169	-0.0024	0.0033	0.0009
	14	C-H... π	2.57	0.0079	0.0335	-0.0046	0.0065	0.0019
	15	C-H...O	2.48	0.0097	0.0333	-0.0068	0.0076	0.0008
	16	π ... π	3.15	0.0081	0.0255	-0.0046	0.0055	0.0009
	17	C-H... π	3.17	0.0031	0.0102	-0.0013	0.0019	0.0006

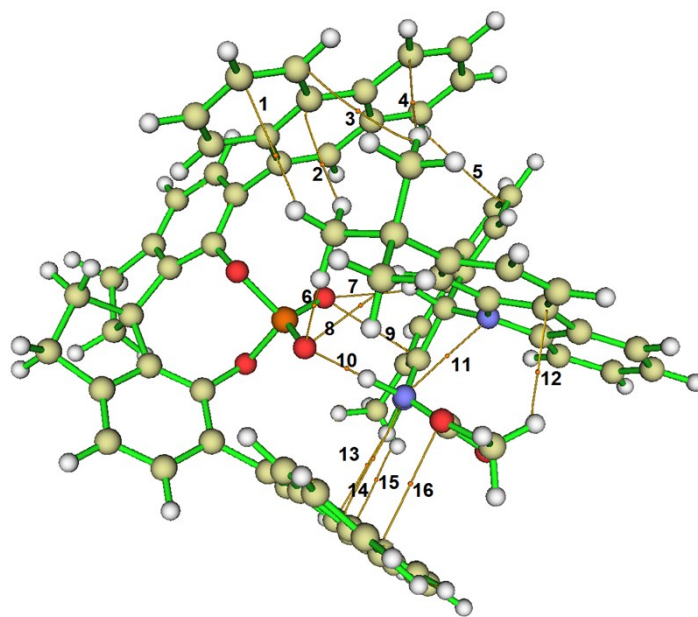


Fig. S15 Intermolecular interactions in **IMII-3** and numbers of bond critical points (BCPs No.).

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 (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMII-3**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMII-3	1	C-H... π	3.10	0.0044	0.0138	-0.0021	0.0028	0.0007
	2	C-H... π	2.66	0.0089	0.0289	-0.0047	0.0059	0.0012
	3	C-H... π	3.14	0.0041	0.0128	-0.0019	0.0026	0.0007
	4	C-H... π	3.04	0.0039	0.0119	-0.0017	0.0023	0.0006
	5	C-H... π	2.86	0.0063	0.0200	-0.0028	0.0039	0.0011
	6	C-H...O	2.31	0.0143	0.0427	-0.0109	0.0108	-0.0001
	7	C-H...O	2.15	0.0195	0.0620	-0.0157	0.0156	-0.0001
	8	C-H... π	2.71	0.0069	0.0248	-0.0044	0.0053	0.0009
	9	lp... π	2.83	0.0123	0.0455	-0.0093	0.0103	0.0010
	10	N-H...O	1.62	0.0552	0.1508	-0.0468	0.0422	-0.0046
	11	lp...lp	2.80	0.0166	0.0568	-0.0123	0.0132	0.0009
	12	C-H... π	2.84	0.0067	0.0207	-0.0032	0.0042	0.0010
	13	N-H... π	2.45	0.0105	0.0322	-0.0063	0.0072	0.0009
	14	lp... π	3.36	0.0069	0.0205	-0.0039	0.0045	0.0006
	15	C-H... π	2.83	0.0070	0.0235	-0.0035	0.0047	0.0012
	16	π ... π	3.17	0.0080	0.0272	-0.0053	0.0061	0.0008

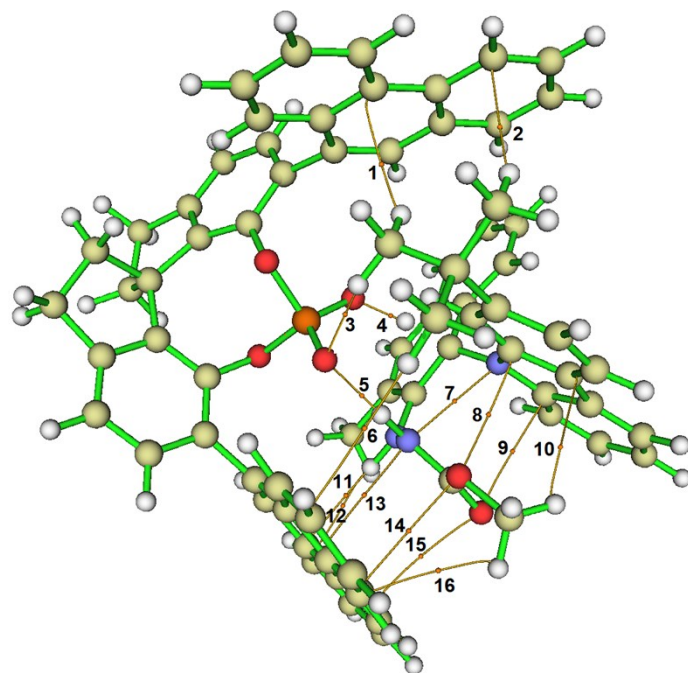


Fig. S16 Intermolecular interactions in TSII-2 and numbers of bond critical points (BCPs No.).

Table S16 Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms (d , in Å), classifications of the intermolecular interactions, electron density (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **TSII-2**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSII-2	1	C-H... π	2.68	0.0090	0.0311	-0.0048	0.0063	0.0015
	2	C-H... π	2.79	0.0065	0.0193	-0.0030	0.0039	0.0009
	3	C-H...O	2.28	0.0153	0.0454	-0.0118	0.0116	-0.0002
	4	O...H	1.33	0.1193	0.0122	-0.1481	0.0756	-0.0725
	5	N-H...O	1.81	0.0342	0.1046	-0.0268	0.0265	-0.0003
	6	C-H... π	3.63	0.0012	0.0038	-0.0004	0.0007	0.0003
	7	lp...lp	2.79	0.0170	0.0573	-0.0125	0.0134	0.0009
	8	lp... π	3.17	0.0078	0.0273	-0.0051	0.0060	0.0009
	9	π ... π	3.22	0.0067	0.0230	-0.0042	0.0050	0.0008
	10	C-H... π	2.90	0.0064	0.0205	-0.0031	0.0041	0.0010
	11	N-H... π	2.37	0.0125	0.0390	-0.0080	0.0089	0.0009
	12	C-H... π	2.80	0.0070	0.0233	-0.0034	0.0046	0.0012
	13	lp... π	3.27	0.0079	0.0237	-0.0046	0.0053	0.0007
	14	lp... π	3.18	0.0076	0.0253	-0.0050	0.0056	0.0006
	15	π ... π	3.36	0.0051	0.0169	-0.0029	0.0035	0.0006
	16	C-H... π	2.89	0.0059	0.0201	-0.0029	0.0040	0.0011

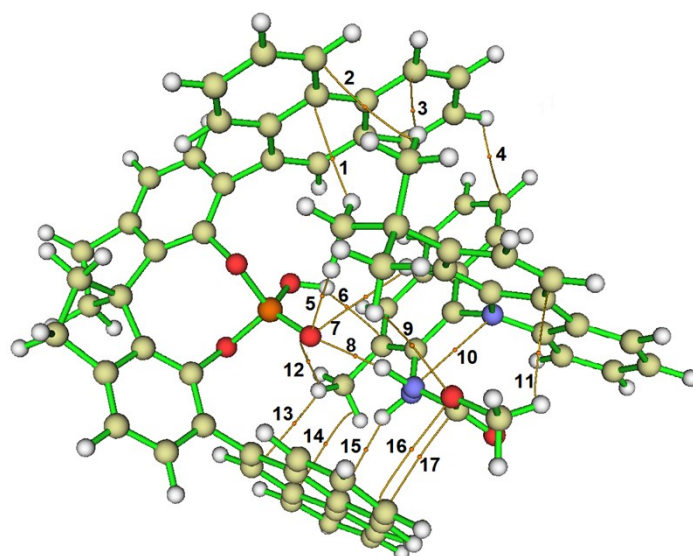


Fig. S17 Intermolecular interactions in **IMII-4** and numbers of bond critical points (BCPs No.).

Table S17 Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms (d , in Å), classifications of the intermolecular interactions, electron density (ρ , in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G , in a.u.), the electronic potential energy density (V , in a.u.) and the electronic energy density (H , in a.u.) at the BCPs of **IMII-4**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMII-4	1	C-H... π	2.73	0.0080	0.0272	-0.0042	0.0055	0.0013
	2	C-H... π	3.04	0.0049	0.0157	-0.0024	0.0031	0.0007
	3	C-H... π	2.87	0.0055	0.0165	-0.0025	0.0033	0.0008
	4	C-H... π	2.73	0.0072	0.0243	-0.0035	0.0048	0.0013
	5	C-H...O	2.49	0.0099	0.0316	-0.0069	0.0074	0.0005
	6	O-H... π	2.30	0.0154	0.0432	-0.0094	0.0101	0.0007
	7	C-H...O	2.96	0.0039	0.0153	-0.0022	0.0030	0.0008
	8	N-H...O	2.03	0.0196	0.0721	-0.0166	0.0173	0.0007
	9	C-H...O	3.14	0.0023	0.0102	-0.0013	0.0019	0.0006
	10	lp...lp	2.88	0.0143	0.0483	-0.0105	0.0113	0.0008
	11	C-H... π	2.89	0.0064	0.0204	-0.0030	0.0041	0.0011
	12	C-H... π	2.88	0.0058	0.0220	-0.0030	0.0043	0.0013
	13	C-H... π	2.68	0.0086	0.0277	-0.0046	0.0057	0.0011
	14	C-H... π	2.81	0.0080	0.0281	-0.0042	0.0056	0.0014
	15	N-H... π	2.58	0.0087	0.0295	-0.0051	0.0062	0.0011
	16	lp... π	3.16	0.0081	0.0279	-0.0051	0.0060	0.0009
	17	π ... π	3.08	0.0081	0.0301	-0.0045	0.0060	0.0015

3. Mechanisms of Paths III and IV of the enantioselective (*S*)-C6-catalyzed Atroposelective C-H Amination Reaction.

Compared to paths I and II, paths III and IV are less favorable to generate experimental desired product **P** and undesired product *ent*-**P**, respectively. The Gibbs free energy profiles for paths III and IV are shown in Fig. S18 and Fig. S19, respectively. The optimized geometries of complexes, intermediates, transition states for paths III and IV are displayed in Fig. S20 and Fig. S21, respectively.

Similar to the cases in paths I and II, in path III (or IV), the interaction between the N1=N2R group of **R1** and O2-H2 group of (*S*)-C6 firstly occurs which needs an energy of 3.0 kcal/mol (or 4.1 kcal/mol), forming the dimeric complex **DIII** (or **DIV**), as shown in Fig. S18 (or Fig. S19). Then **DIII** (or **DIV**) interacts with **R2** via the O1...H3-N3 HB between the P=O1 group of (*S*)-C6 and N3-H3 group of **R2**, leading to the trimeric complex **COMIII** (or **COMIV**). Note that the process in forming **COMIII** (or **COMIV**) is endothermic which needs an energy of 20.6 (or 12.3) kcal/mol. It is even higher than that for the formation of **COMI** (or **COMII**), suggesting that the trimeric complex **COMIII** (or **COMIV**) formed in path III (or IV) is less favorable than that in path I (or II). In **COMIII** or **COMIV**, both **R1** and **R2** interact with (*S*)-C6 via O2-H2...N2 and O1...H3-N3 HBs, respectively. Then the proton transfer occurs in which the H2 atom is shifted to N2 atom, causing the conversion of O2-H2...N2 HB into O2...H2-N2 HB and the approaching of C1 and N3 atom with a distance of 2.12 Å in **TSIII** (or 2.11 Å **TSIV**). It needs to overcome an energy barrier of 15.9 kcal/mol (or 22.1 kcal/mol) from **COMIII** (or **COMIV**) to **TSIII** (or **TSIV**). The C1-N3 bond forms in **IMIII-1** (or **IMIV-1**) with a bond length of 1.51 Å (or 1.52 Å), and an energy of 10.4 kcal/mol (or 11.8 kcal/mol) is released. The O1...H3-

N3 HB is converted into O1–H3···N3 HB in **IMIII-1** (or **IMIV-1**) due to the proton transfer of H3 atom to O1 atom. The breakage of O1–H3···N3 HB results in **IMIII-2** (or **IMIV-2**) in which the N3 atom is recovered to sp³ hybridization state, and (*S*)-**C6** is converted into its tautomer. The strong acidity of the tautomer (*S*)-**C6** enables the N1 atom to be protonation as N1–H3 bond in **IMIII-3** (or **IMIV-3**). Because of the steric repulsion existing between the *t*-Bu group and (*S*)-**C6** in **IMIII-3**, the O1···H1 interaction is not found. From **IMIV-2** to **IMIV-3**, the O2···H2–N2 HB is broken and the O2 atom further interacts with the newly formed N1–H3 bond as O2···H3–N1 HB. In addition, the O1···H1 interaction is found in **IMIV-3**. After absorbing an energy of 5.3 kcal/mol (or 6.1 kcal/mol), the transition state **TSIII-2** (or **TSIV-2**) forms in which the hydrogen abstraction occurs, and the H1 atom is located between O1 anion and C1 atom. The distance is 1.35 Å (or 1.37 Å) for O1···H1 interaction and 1.30 Å (or 1.30 Å) for C1···H1 interaction in **TSIII-2** (or **TSIV-2**). The H1 atom is finally transferred to O1 anion as O1–H1 bond, and the catalyst (*S*)-**C6** is recovered which interacts with the product **P** (or *ent*-**P**) via intermolecular interactions in **IMIII-4** (or **IMIV-4**). The broken of intermolecular interactions in **IMIII-4** (or **IMIV-4**) generates the catalyst (*S*)-**C6** and product **P** (or *ent*-**P**).

After comparison, it can be seen that paths **I** and **II** are considered to be the real reaction processes in leading to the product **P** and *ent*-**P**, respectively. The corresponding activation Gibbs free energies for paths **I** and **II** can be calculated as follows:

$$\Delta G_{\text{act}}(\mathbf{TSI-1}) = G(\mathbf{TSI-1}) - (G(\mathbf{R1}) + G(\mathbf{R2}) + G((S)\text{-C6}))$$

$$\Delta G_{\text{act}}(\mathbf{TSII-1}) = G(\mathbf{TSII-1}) - (G(\mathbf{R1}) + G(\mathbf{R2}) + G((S)\text{-C6}))$$

Therefore, the relative ratios for path **I** leading to the product **P** and path **II** leading to the product *ent*-**P** can be obtained:

$$\begin{aligned}
 & \mathbf{P}(\mathbf{TSI-1}) : \mathit{ent}\text{-}\mathbf{P}(\mathbf{TSII-1}) \\
 & = \exp\left(-\frac{\Delta G_{\text{act}}(\mathbf{TSI-1})}{RT}\right) : \exp\left(-\frac{\Delta G_{\text{act}}(\mathbf{TSII-1})}{RT}\right) \\
 & = 19.33 : 1.00
 \end{aligned}$$

where $R = 1.986 \times 10^{-3} \text{ kcal (mol}\cdot\text{K)}^{-1}$ and $T = 323.0 \text{ K}$.

Accordingly, the ee value is calculated as:

$$\text{ee} = \frac{[\mathbf{P}] - [\mathit{ent}\text{-}\mathbf{P}]}{[\mathbf{P}] + [\mathit{ent}\text{-}\mathbf{P}]} \times 100\% = \frac{19.33 - 1.00}{19.33 + 1.00} \times 100\% = 90\%$$

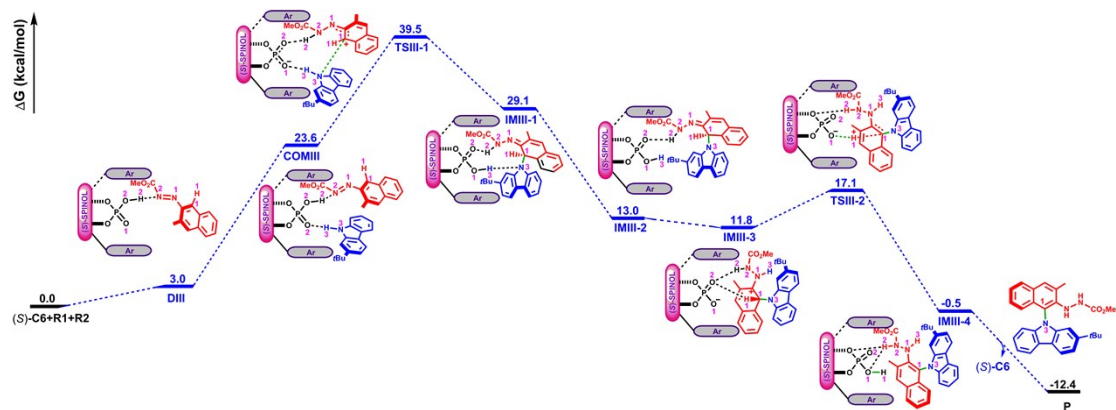


Fig. S18 The path III for the reaction between **R1** and **R2** catalyzed by **(S)-C6** and the free energy profile of the whole processes. The Gibbs free energies of **[R1+R2+(S)-C6]** were set to 0.0 kcal/mol as a reference.

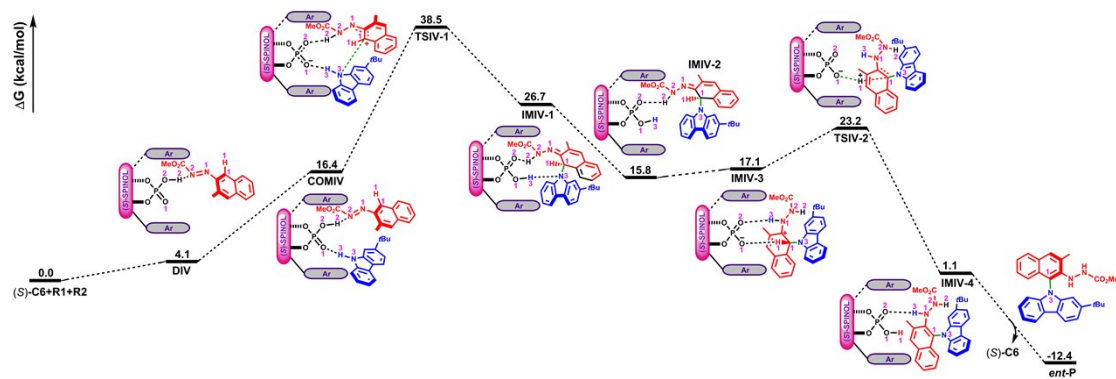


Fig. S19 The path IV for the reaction between **R1** and **R2** catalyzed by **(S)-C6** and the free energy profile of the whole processes. The Gibbs free energies of **[R1+R2+(S)-C6]** were set to 0.0 kcal/mol as a reference.

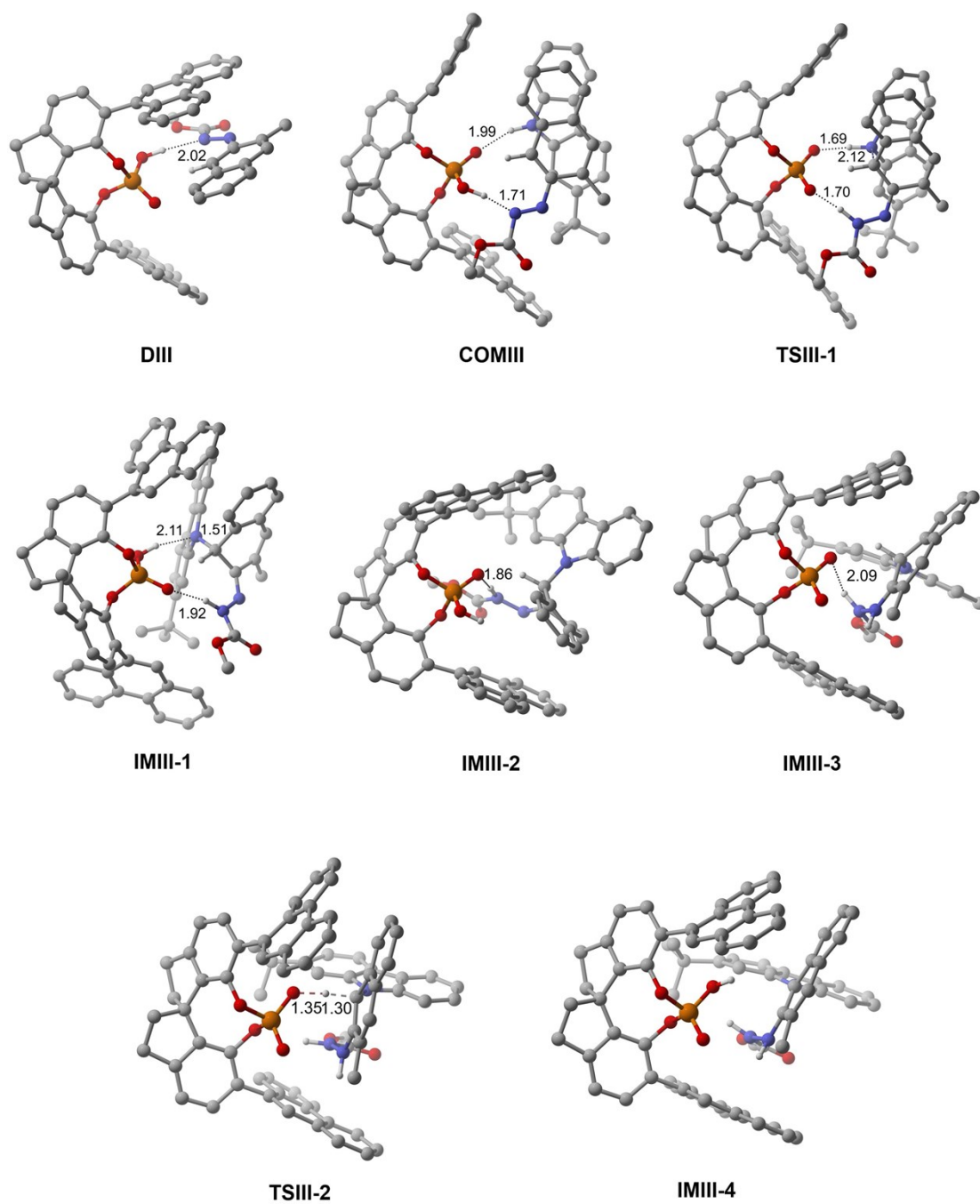


Fig. S20 The optimized geometries of the complexes, transition states and intermediates in path **III**. The distances are in Å.

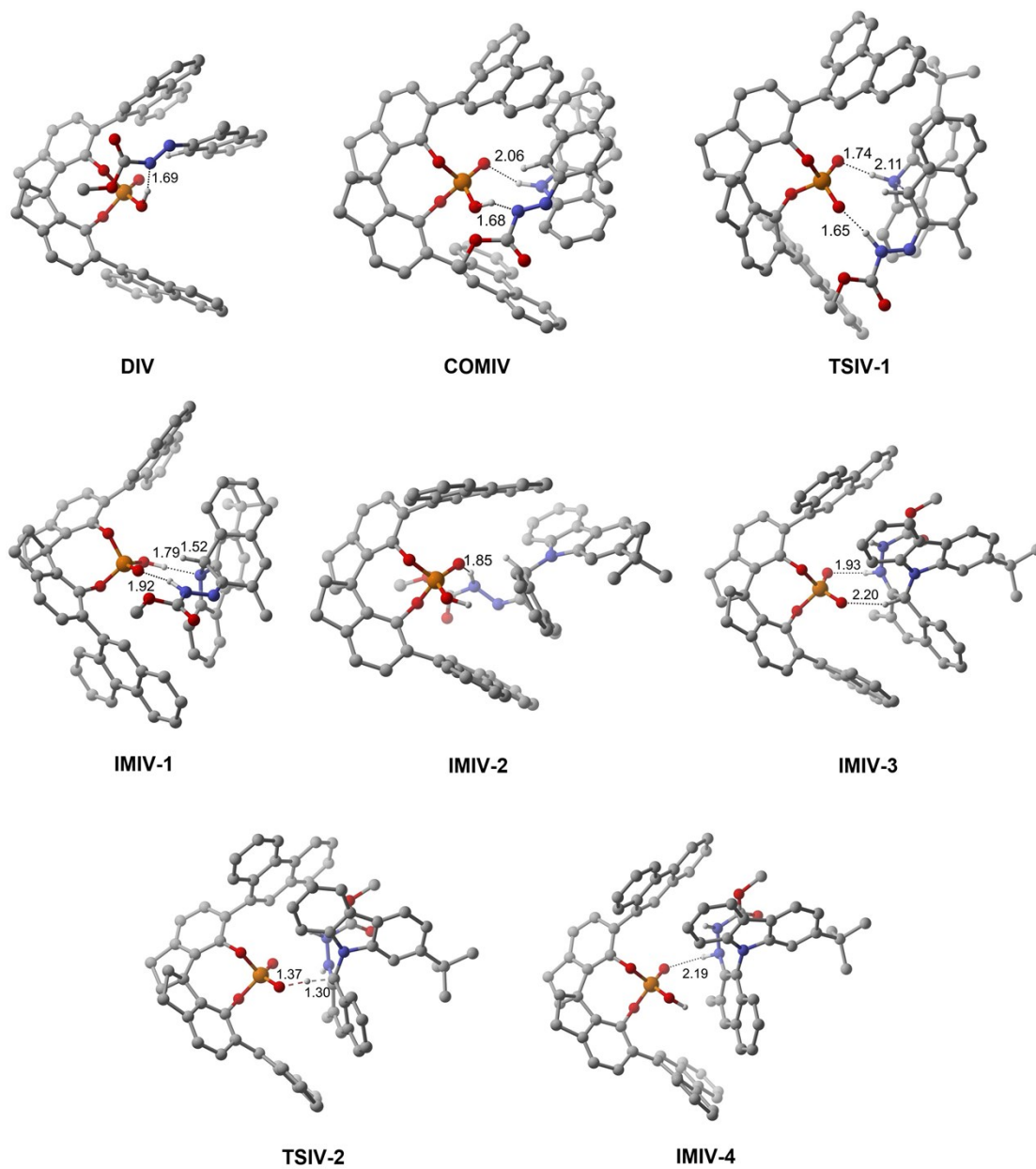


Fig. S21 The optimized geometries of the complexes, transition states and intermediates in path IV. The distances are in Å.

4. Cartesian Coordinates

R1

C	-4.81723200	-0.80844700	-0.02096300
C	-4.16985300	0.40106700	0.00207400
C	-2.75162600	0.45975600	0.01353300
C	-2.01474500	-0.75992100	0.00016000
C	-2.71321000	-1.99849600	-0.02098300
C	-4.08324100	-2.02175100	-0.03277600
H	-2.62490500	2.61650800	0.05908700
H	-5.90233400	-0.84206000	-0.03007500
H	-4.73222200	1.33056900	0.01207900
C	-2.04958300	1.69399300	0.04386100
C	-0.60478000	-0.70052900	0.00665000
H	-2.13912700	-2.92081300	-0.03085300
H	-4.61394700	-2.96819300	-0.05153200
C	0.04340000	0.51633400	0.02879600
C	-0.67774000	1.75069800	0.05975600
H	-0.02253700	-1.61682500	0.00279800
N	1.45751600	0.63793300	0.04561500
N	2.08152400	-0.41949400	-0.15781100
C	3.51088200	-0.18805400	-0.12378200
O	4.07420000	0.85340100	-0.33241700
O	4.09416200	-1.35093700	0.13458500
C	5.52507300	-1.30915600	0.18979300
H	5.85404600	-0.63473000	0.98333500
H	5.84191600	-2.32885300	0.40067600
H	5.92930300	-0.97173700	-0.76678800
C	0.05803400	3.06236400	0.09804500
H	0.70872100	3.12428200	0.97481600
H	0.69907300	3.18347100	-0.77988400
H	-0.65043800	3.89245200	0.12939400

R2

C	-1.48280000	-1.42288300	-0.00018200
C	-1.99126000	-0.10212100	-0.00024800
C	-1.09927400	0.96564100	-0.00033100
C	0.27241100	0.69385600	-0.00015500
C	0.77939100	-0.62244000	-0.00014600
C	-0.12427000	-1.69035600	-0.00015400
H	-2.18007800	-2.25513100	0.00019600
H	-1.44356600	1.99368600	-0.00034300
H	0.23351600	-2.71611400	0.00004100
C	2.51915700	0.87372400	-0.00000100

C	3.83351900	1.34572700	0.00010100
C	4.85348200	0.40424600	0.00007500
C	4.57975700	-0.97413900	0.00000400
C	3.27153000	-1.43741200	-0.00005000
C	2.22434300	-0.51110400	-0.00004300
H	4.04696600	2.40998200	0.00026700
H	5.88538100	0.74187000	0.00017700
H	5.40259900	-1.68158100	-0.00001300
H	3.06169600	-2.50321400	-0.00006500
N	1.33236800	1.57806600	0.00009600
H	1.25137600	2.58367000	0.00040100
C	-3.50944500	0.10634400	0.00009700
C	-3.89139800	1.58950900	-0.00037400
C	-4.11377900	-0.54763600	-1.25352300
C	-4.11293800	-0.54711100	1.25445700
H	-3.51215000	2.10615000	0.88744200
H	-3.51291900	2.10519500	-0.88909400
H	-4.98170200	1.68495500	-0.00001500
H	-3.91943100	-1.62381700	-1.28201200
H	-5.19954400	-0.40201700	-1.26823500
H	-3.69680500	-0.10456400	-2.16381800
H	-5.19872200	-0.40179300	1.26976300
H	-3.91822700	-1.62322300	1.28311300
H	-3.69551400	-0.10359800	2.16435400

(S)-C6

C	-1.07838700	2.99868700	0.25264000
C	-1.64966400	3.82025800	1.23006800
C	-2.84766400	3.47074000	1.84008300
C	-3.46753000	2.27584400	1.48246100
C	-2.89440600	1.40727500	0.54565300
C	-1.68827400	1.79156900	-0.05477900
C	0.57337100	4.56659900	0.87178500
C	-0.76200900	5.01381900	1.49125400
H	-3.29159300	4.11159500	2.59618800
H	-4.40448800	1.98745300	1.95064400
H	1.12951800	3.96215800	1.59701600
H	-1.15521500	5.90677900	0.98999500
C	0.16299700	3.65591900	-0.32217100
C	1.34709000	2.86122100	-0.84049800
C	-0.15331800	4.53126500	-1.56792900
C	2.01573200	3.59121200	-1.83078100
C	1.84774500	1.62607000	-0.46211700
C	1.22623700	4.83128000	-2.18338100

H	-0.72075300	5.42909700	-1.30759900
C	3.21055800	3.12859500	-2.36556700
C	3.06386900	1.14080000	-0.96312800
H	1.18205600	5.00197500	-3.26231100
C	3.73727500	1.92116800	-1.90829700
H	3.72955800	3.69346600	-3.13437000
H	4.68037400	1.55397400	-2.30166100
H	-0.68015600	5.24768300	2.55597500
H	1.21084300	5.39690800	0.55593900
H	-0.74976200	3.93876100	-2.27003600
H	1.67872600	5.72196300	-1.73070300
O	1.10097600	0.81875600	0.40105100
O	-1.05811400	0.91991900	-0.94217900
P	0.01716600	-0.12119300	-0.33327200
O	-0.62324200	-0.73465900	0.98239800
O	0.48526100	-1.03756900	-1.37859400
H	-1.17893000	-1.51434300	0.81478400
C	3.60612300	-0.18253400	-0.54917300
C	3.82068000	-1.13134600	-1.49834800
C	3.92611400	-0.46566000	0.83930000
C	4.32945200	-2.43230100	-1.17572000
H	3.56579600	-0.92260000	-2.53428100
C	4.42496600	-1.74558800	1.19809500
C	3.77167000	0.51609800	1.84476600
C	4.51876400	-3.39445700	-2.19228600
C	4.62530700	-2.75849700	0.16922600
C	4.72443300	-1.99395900	2.55632100
H	3.41397600	1.50295300	1.56971000
C	4.07607900	0.24687200	3.16039700
C	4.99218900	-4.65209400	-1.89298700
H	4.27830600	-3.12231200	-3.21644800
C	5.10702800	-4.05635700	0.44844900
C	4.55168800	-1.02426200	3.52008200
H	5.10171500	-2.96408000	2.85844500
H	3.94963600	1.01588100	3.91581100
C	5.28728700	-4.98217400	-0.55829100
H	5.13393700	-5.38689600	-2.67906200
H	5.34232000	-4.34419300	1.46663000
H	4.78968100	-1.24387700	4.55619500
H	5.65798900	-5.97332500	-0.31584300
C	-3.56240500	0.12487300	0.18258600
C	-3.95596500	-0.08021400	-1.10282700
C	-3.82312500	-0.89569500	1.18432400
C	-4.67274800	-1.25488700	-1.50651200

H	-3.74998400	0.67611700	-1.85620600
C	-4.53714600	-2.07075700	0.82340400
C	-3.34525900	-0.76268000	2.50972400
C	-5.08250400	-1.41028800	-2.84915500
C	-4.98707400	-2.25075200	-0.55178200
C	-4.76854700	-3.04795200	1.81738600
H	-2.76511300	0.11434000	2.77462000
C	-3.58062900	-1.73727800	3.45460200
C	-5.79181300	-2.52189900	-3.24454000
H	-4.82649100	-0.63278400	-3.56388300
C	-5.71925700	-3.37911700	-0.98384700
C	-4.30814300	-2.88681200	3.10638600
H	-5.31219000	-3.95180700	1.56900600
H	-3.19724400	-1.61847100	4.46287800
C	-6.11241400	-3.51223300	-2.29930600
H	-6.10296800	-2.63481400	-4.27820600
H	-5.98536600	-4.16139400	-0.28227800
H	-4.49622400	-3.65696700	3.84766000
H	-6.67477300	-4.38917100	-2.60435200

DI

C	-1.61088500	-3.69639100	0.22777300
C	-1.65817500	-4.65036400	1.24941000
C	-0.53446600	-4.91895600	2.02053900
C	0.63787200	-4.20481700	1.78267900
C	0.70087600	-3.20439200	0.80526200
C	-0.44712100	-2.96716100	0.03685200
C	-3.88992200	-4.19448500	0.58615300
C	-3.05015600	-5.22668200	1.35890700
H	-0.56976600	-5.66313600	2.81097300
H	1.52384600	-4.40220400	2.37973400
H	-4.15160000	-3.36312700	1.25036500
H	-3.10068700	-6.21489600	0.88554600
C	-2.93196300	-3.66029800	-0.51938400
C	-3.47628700	-2.39406800	-1.15553300
C	-2.94899200	-4.61830900	-1.74374100
C	-4.28594500	-2.71602500	-2.25085800
C	-3.32951300	-1.06389000	-0.79509700
C	-4.19372800	-4.19559300	-2.54714800
H	-2.95945400	-5.67006100	-1.44417200
C	-5.00211000	-1.72921700	-2.91586800
C	-4.06354100	-0.04761700	-1.42270300
H	-4.09670000	-4.39955200	-3.61685900
C	-4.90566100	-0.40785800	-2.47995700
H	-5.62750700	-1.97905000	-3.76795100
H	-5.47495200	0.37339800	-2.97483600
H	-3.37176500	-5.34591700	2.39694100
H	-4.81429500	-4.60446700	0.16971600
H	-2.04718800	-4.43899000	-2.33908800
H	-5.09125300	-4.71943000	-2.19673400
O	-2.40357500	-0.72037300	0.18694500
O	-0.44918200	-1.92937900	-0.89187500
P	-0.89107700	-0.47352200	-0.33348400
O	-0.18402400	-0.30198100	1.04685500
O	-0.69759300	0.54163000	-1.38283900
H	0.48722300	0.43518900	1.18287500
C	-3.91920800	1.37515700	-1.00768300
C	-3.51511700	2.29529000	-1.92264400
C	-4.20975600	1.79429200	0.35357300
C	-3.32921800	3.67733200	-1.58736300
H	-3.28050500	1.97873300	-2.93587100
C	-4.02312800	3.15123800	0.72670200
C	-4.69431300	0.88050500	1.31711800
C	-2.89066100	4.59488300	-2.56736300

C	-3.56638400	4.11797800	-0.26403200
C	-4.29946400	3.52705300	2.06050500
H	-4.86681400	-0.15135900	1.02932400
C	-4.95980100	1.27599500	2.60911000
C	-2.69127300	5.92053400	-2.25288000
H	-2.70833000	4.23089200	-3.57499100
C	-3.35141000	5.48226800	0.03171300
C	-4.75192100	2.61248100	2.98649900
H	-4.15976300	4.55570000	2.37225900
H	-5.33271700	0.55651900	3.33129200
C	-2.92497900	6.36405300	-0.93951700
H	-2.35122700	6.61903100	-3.01090600
H	-3.51784000	5.85792400	1.03473000
H	-4.95761900	2.92923700	4.00440500
H	-2.76582400	7.40737200	-0.68523400
C	1.96316000	-2.44506600	0.57580400
C	2.55363900	-2.49311600	-0.64912800
C	2.60232900	-1.70143200	1.64872600
C	3.83885200	-1.91128900	-0.90262100
H	2.06525000	-3.02672000	-1.46088500
C	3.88195100	-1.12288500	1.43896200
C	1.95529500	-1.50127200	2.89198400
C	4.42867400	-2.01971300	-2.18119100
C	4.53284200	-1.25693900	0.14268800
C	4.47233000	-0.39229300	2.49562500
H	0.95803800	-1.90387900	3.03434400
C	2.55682100	-0.78303200	3.90355400
C	5.68537800	-1.51073400	-2.42080600
H	3.87263800	-2.51724300	-2.97117000
C	5.82320700	-0.75090800	-0.12890900
C	3.82974600	-0.22397800	3.70366400
H	5.44815600	0.06023800	2.35938400
H	2.03951800	-0.63566800	4.84719100
C	6.38899200	-0.87842600	-1.38034100
H	6.13278600	-1.59707600	-3.40604200
H	6.38835600	-0.24948300	0.64892500
H	4.30060200	0.35490600	4.49183800
H	7.38086300	-0.47631900	-1.56439600
C	4.25034100	1.01998600	-4.59804600
C	4.94647500	1.62969400	-3.58371000
C	4.37614300	1.74610000	-2.28970600
C	3.07125500	1.22061100	-2.06951500
C	2.37141100	0.59211000	-3.13620000
C	2.95295700	0.49322500	-4.37405700

H	6.06071400	2.76218000	-1.39347100
H	4.69576100	0.93544900	-5.58476500
H	5.94215300	2.03002200	-3.75530000
C	5.06351000	2.36744500	-1.21305800
C	2.49826900	1.33469000	-0.78663900
H	1.37404000	0.20435000	-2.94080900
H	2.42248700	0.01350300	-5.19039900
C	3.19875100	1.93519000	0.24134700
C	4.51033900	2.47348000	0.03823400
H	1.48257700	0.98194800	-0.64553200
N	2.69338500	2.10601600	1.54224100
N	1.60969700	1.56234100	1.82681200
C	1.20989500	1.88058900	3.18926200
O	1.85336400	2.48600200	4.00210400
O	-0.00588200	1.38648000	3.35647400
C	-0.60071800	1.63845700	4.63373100
H	-0.66057600	2.71375800	4.81470900
H	-1.59735900	1.20445300	4.58283000
H	-0.01305300	1.16676400	5.42468600
C	5.24979100	3.12509000	1.17439000
H	4.70653100	3.99671400	1.55073600
H	5.36286000	2.43831700	2.01840300
H	6.24038300	3.44616900	0.84537200

DI_{R2}

C	4.35265500	-1.61785600	-0.53336100
C	5.55546000	-1.82420200	0.15126000
C	6.22408500	-0.76262200	0.74772500
C	5.66955900	0.51301600	0.68055100
C	4.44045400	0.74344100	0.05090100
C	3.79925000	-0.34705400	-0.55103700
C	4.57190800	-3.94863100	-0.23431100
C	5.90872200	-3.29281000	0.15365100
H	7.15991200	-0.92422200	1.27452400
H	6.17721900	1.35219000	1.14738300
H	3.95056200	-4.07111300	0.65989000
H	6.68757200	-3.50636700	-0.58841100
C	3.89087300	-2.91286000	-1.17571300
C	2.42694400	-3.24915700	-1.39900300
C	4.44034900	-3.07699200	-2.62063200
C	2.30095800	-4.10347900	-2.50053400
C	1.29045400	-2.89237600	-0.68923800
C	3.62936900	-4.24746100	-3.20538100
H	5.52096000	-3.24293800	-2.63213400
C	1.06999200	-4.65389700	-2.82879800
C	0.03178800	-3.43435100	-0.98594500
H	3.52839400	-4.19329600	-4.29260600
C	-0.04472600	-4.33409000	-2.05691100
H	0.97057100	-5.32132300	-3.67979200
H	-1.01066300	-4.77030800	-2.29256400
H	6.28218600	-3.62939800	1.12432300
H	4.68398400	-4.92618900	-0.71096400
H	4.22678600	-2.16183000	-3.18322400
H	4.09379000	-5.21211000	-2.96816000
O	1.39908700	-1.92031100	0.31506000
O	2.54035100	-0.16102900	-1.13157700
P	1.25625500	-0.40645600	-0.19616700
O	1.52331900	0.29939200	1.19794700
O	0.02392300	-0.04528500	-0.91924600
H	1.33737800	1.25438800	1.20162800
C	-1.21094900	-3.04767700	-0.26123800
C	-2.27896400	-2.62087300	-0.99005200
C	-1.33153100	-3.16496300	1.18225200
C	-3.52580700	-2.25452500	-0.38633300
H	-2.18866600	-2.52717300	-2.07000700
C	-2.53946400	-2.77288100	1.81910000
C	-0.28452900	-3.69751400	1.96935200
C	-4.60944700	-1.83385500	-1.18820600

C	-3.65905700	-2.28885900	1.02166700
C	-2.62890300	-2.89628600	3.22431900
H	0.62413000	-4.03586000	1.48275900
C	-0.40278400	-3.81070900	3.33641000
C	-5.79769800	-1.43814000	-0.61609700
H	-4.48128100	-1.82130300	-2.26780000
C	-4.87901300	-1.85451200	1.58483100
C	-1.58525900	-3.39663700	3.97135000
H	-3.53591000	-2.59396200	3.73505200
H	0.41412600	-4.22438900	3.91938800
C	-5.92433000	-1.44115300	0.78422000
H	-6.62334200	-1.10519800	-1.23789000
H	-5.00574900	-1.82662400	2.66111700
H	-1.68306900	-3.47889000	5.04944300
H	-6.84844100	-1.10150400	1.24237100
C	3.84342100	2.10843300	0.01222700
C	3.60554000	2.70005300	-1.18901400
C	3.53598400	2.82511300	1.23978100
C	3.10629800	4.03976100	-1.29784700
H	3.82325300	2.15962600	-2.10691800
C	3.04430100	4.15679400	1.17129500
C	3.67476800	2.20859300	2.50649400
C	2.90356700	4.62220900	-2.56852000
C	2.83811700	4.78738900	-0.12655900
C	2.74966700	4.82687800	2.37965600
H	4.00846000	1.17788800	2.55717300
C	3.37217800	2.88676200	3.66712400
C	2.45077800	5.91711200	-2.68468300
H	3.11778000	4.02870300	-3.45316100
C	2.37745900	6.11428700	-0.27493400
C	2.91454300	4.21237700	3.60211900
H	2.37470500	5.84326700	2.35500300
H	3.48114800	2.39332200	4.62761200
C	2.18730500	6.66652000	-1.52437800
H	2.29929500	6.35959900	-3.66404300
H	2.16638600	6.72062200	0.59834100
H	2.67625600	4.75154700	4.51339600
H	1.83217500	7.68858000	-1.61052700
C	-5.63889700	2.19600000	-1.13169700
C	-4.59920600	1.77216000	-1.99550800
C	-3.42570700	1.27124200	-1.44330500
C	-3.32202500	1.19294400	-0.05027200
C	-4.35265300	1.62391200	0.81201900
C	-5.52728300	2.13324900	0.24765600

H	-6.55605300	2.58647700	-1.56297800
H	-2.59931400	0.92476000	-2.05457700
H	-6.34558000	2.46735200	0.87991600
C	-2.60417600	0.78577200	2.03625600
C	-1.86761800	0.38599600	3.15451700
C	-2.44618400	0.56793700	4.40332500
C	-3.72477500	1.13561200	4.54543900
C	-4.45173400	1.53512500	3.43153700
C	-3.89319100	1.36444400	2.16079500
H	-0.88630800	-0.06671100	3.04461200
H	-1.89903200	0.25821300	5.28890700
H	-4.14605000	1.26070200	5.53793000
H	-5.44049800	1.97154300	3.54366500
N	-2.27778500	0.70471100	0.70176500
H	-1.44055200	0.29190900	0.30000600
C	-4.81421200	1.86537800	-3.50968900
C	-3.59508500	1.37841600	-4.29843600
C	-6.02088300	0.99633700	-3.90204800
C	-5.09094800	3.32573600	-3.90391900
H	-2.70469400	1.97528400	-4.07610100
H	-3.36598800	0.32922500	-4.08336200
H	-3.79543100	1.46265900	-5.37143300
H	-6.93417600	1.31679900	-3.39174300
H	-6.19924200	1.05789700	-4.98155300
H	-5.84061000	-0.05356500	-3.64673500
H	-5.24647200	3.40129500	-4.98591800
H	-5.98456400	3.71859300	-3.40983600
H	-4.24634100	3.96810800	-3.63469400

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C	-4.86167000	-1.15402800	-1.03049000
C	-5.88282500	-1.89664000	-0.42775400
C	-5.62398400	-3.15125800	0.10817400
C	-4.32466800	-3.65149900	0.06534400
C	-3.26657400	-2.89964200	-0.45942100
C	-3.56326200	-1.64086500	-1.00005400
C	-6.69623300	0.30846400	-0.77892300
C	-7.17624700	-1.11607000	-0.44425200
H	-6.41829000	-3.73321500	0.56645600
H	-4.10918000	-4.63395600	0.47545500
H	-6.38548000	0.81861300	0.13943100
H	-7.85524000	-1.50070200	-1.21482200
C	-5.44454600	0.09062300	-1.67515200
C	-4.64703400	1.36652600	-1.87500400
C	-5.89252900	-0.19248000	-3.13846500
C	-5.09929600	2.03892800	-3.01742400
C	-3.62119000	1.92414400	-1.12565900
C	-6.12297600	1.20116100	-3.74648400
H	-6.77189200	-0.84069200	-3.18018700
C	-4.58114100	3.27833600	-3.36514600
C	-3.07416700	3.17362900	-1.45298700
H	-5.98261900	1.22190900	-4.83039000
C	-3.58356700	3.84078900	-2.57222500
H	-4.93363500	3.79772900	-4.25145200
H	-3.16327400	4.80873700	-2.82863900
H	-7.70438800	-1.17267000	0.51129800
H	-7.45521100	0.92159000	-1.27301700
H	-5.07237200	-0.69190900	-3.66507400
H	-7.13823800	1.56166600	-3.54135900
O	-3.09912600	1.20673100	-0.04656700
O	-2.52162100	-0.82965900	-1.45373800
P	-1.88360000	0.19326000	-0.37406600
O	-1.80576500	-0.57408600	0.98308500
O	-0.65927500	0.79961900	-0.93152300
H	-0.91616800	-0.81789900	1.39648500
C	-1.92195900	3.74699300	-0.70460000
C	-0.75602300	3.95324100	-1.37309600
C	-2.01496000	4.08521800	0.70235400
C	0.42895900	4.41710400	-0.71444800
H	-0.68796100	3.69400300	-2.42691500
C	-0.87004600	4.57707500	1.38233500
C	-3.22908900	3.94254300	1.41147400
C	1.64385400	4.52585100	-1.42781200

C	0.39635300	4.69488600	0.67256500
C	-0.99172000	4.90993600	2.74972700
H	-4.10603300	3.57494000	0.88757000
C	-3.31669800	4.26873300	2.74672300
C	2.80890700	4.87530400	-0.78299000
H	1.64340300	4.30869800	-2.49315800
C	1.60885600	5.03552000	1.31167800
C	-2.18608600	4.75966400	3.42107600
H	-0.13303400	5.29362300	3.28884100
H	-4.25860400	4.15228200	3.27349600
C	2.78917100	5.11881000	0.60247600
H	3.74244600	4.94270500	-1.33312700
H	1.62968700	5.21221900	2.38115600
H	-2.25137500	5.02388900	4.47206300
H	3.71084100	5.36373200	1.12078300
C	-1.87701600	-3.43808400	-0.46694700
C	-1.21914400	-3.56667700	-1.65146700
C	-1.23388000	-3.87963800	0.75896800
C	0.08315300	-4.15722700	-1.74515800
H	-1.69533500	-3.23268400	-2.57038200
C	0.04833000	-4.48901800	0.70320300
C	-1.84962900	-3.69671400	2.02039800
C	0.72694600	-4.26067400	-2.99794100
C	0.72915600	-4.62713300	-0.57738700
C	0.64224100	-4.92220200	1.91029600
H	-2.79760400	-3.17266000	2.07339800
C	-1.25542700	-4.15206300	3.17752000
C	1.99029800	-4.79804300	-3.09770700
H	0.21139300	-3.88980700	-3.87993300
C	2.02425800	-5.17721500	-0.70810100
C	0.00244800	-4.77233600	3.12215800
H	1.62242900	-5.38486300	1.89324400
H	-1.74812000	-4.00681800	4.13493900
C	2.64218200	-5.25651400	-1.93851100
H	2.48572600	-4.86108700	-4.06152700
H	2.55684900	-5.53604800	0.16514400
H	0.48205600	-5.11227100	4.03435200
H	3.64259400	-5.67236400	-2.01122800
C	3.53184700	-1.56653000	-3.82554000
C	4.17838100	-1.96229500	-2.67971700
C	3.52117800	-1.90414700	-1.42368300
C	2.16136600	-1.48543800	-1.38693400
C	1.51525500	-1.07513600	-2.58524400
C	2.19335600	-1.10026400	-3.77731000

H	5.22808600	-2.51895000	-0.24785700
H	4.04954700	-1.60737500	-4.77972900
H	5.20127000	-2.32614100	-2.71740000
C	4.17777900	-2.23895400	-0.20939600
C	1.48811600	-1.47873700	-0.14913100
H	0.48399600	-0.73605400	-2.52373300
H	1.70410100	-0.77978300	-4.69185700
C	2.14914900	-1.81274500	1.01444800
C	3.53263100	-2.18382200	1.00114400
H	0.44045200	-1.20936600	-0.13149200
N	1.54819000	-1.81809200	2.28855400
N	0.36594000	-1.43650100	2.38213000
C	-0.08812100	-1.50056000	3.76263200
O	0.53388900	-1.90698100	4.70543600
O	-1.32768900	-1.03024600	3.78753100
C	-1.92078700	-0.96388100	5.08536700
H	-1.31158900	-0.34395900	5.74783400
H	-2.90293000	-0.51748700	4.94065200
H	-2.01438600	-1.96465200	5.51378500
C	4.25039300	-2.45836500	2.29193600
H	4.21796300	-1.57529800	2.93929200
H	3.77935500	-3.27336800	2.84880000
H	5.29471400	-2.71342600	2.10026900
C	5.97079600	1.06845800	0.21706200
C	5.37285000	1.33428600	-1.03920200
C	3.99047000	1.47812100	-1.11341300
C	3.24218200	1.40694600	0.06753200
C	3.84413000	1.17142800	1.32436500
C	5.22919200	0.98524900	1.38393900
H	7.04934900	0.95413500	0.27504900
H	3.48415000	1.66675800	-2.05421900
H	5.72127500	0.79780500	2.33488200
C	1.59146900	1.49149700	1.58492700
C	0.36238000	1.65057500	2.22966700
C	0.34212000	1.53088500	3.61372800
C	1.50616400	1.22944600	4.34251100
C	2.72466400	1.06598200	3.69577500
C	2.78045000	1.21743600	2.30542100
H	-0.53721400	1.89236400	1.67280500
H	-0.59950600	1.67091000	4.13724100
H	1.45018200	1.12215700	5.42126100
H	3.62462100	0.84255200	4.26239500
N	1.88911400	1.58906700	0.24553800
H	1.18101700	1.64073900	-0.47857700

C	6.27833200	1.53789000	-2.25970800
C	5.47345200	1.77156600	-3.54099000
C	7.16215200	2.77280800	-2.01232800
C	7.18217200	0.31465000	-2.47191100
H	4.80979400	0.92750700	-3.75659400
H	4.86522900	2.68008800	-3.47368700
H	6.15728700	1.89150700	-4.38763100
H	7.80125000	2.63869900	-1.13431800
H	7.80965500	2.95603700	-2.87733300
H	6.54842700	3.66505400	-1.84931500
H	7.84443100	0.48135000	-3.32882800
H	7.81106400	0.11345100	-1.59988100
H	6.58276300	-0.57803000	-2.67194700

TSI-1Value of imaginary frequency = -295.7 cm⁻¹

C	4.98977400	0.11592000	-1.04255000
C	6.15983100	0.43658800	-0.34838900
C	6.28070300	1.65747000	0.30428900
C	5.20606000	2.54567500	0.28454000
C	3.99868700	2.22123700	-0.34499200
C	3.91228900	0.98804500	-1.01044100
C	6.23128800	-1.88068200	-0.86983800
C	7.13392700	-0.71729900	-0.41544300
H	7.19127100	1.91500100	0.83745500
H	5.28857700	3.50434000	0.78924700
H	5.73782200	-2.32419300	0.00225300
H	7.92390600	-0.51864900	-1.15025900
C	5.15001200	-1.20797600	-1.76425000
C	3.98020400	-2.13880600	-2.04250500
C	5.70604000	-1.01600500	-3.20409100
C	4.22160300	-2.86943000	-3.21165100
C	2.81125600	-2.36999000	-1.32686100
C	5.47788300	-2.37478300	-3.88940500
H	6.75188500	-0.69571500	-3.20230400
C	3.34808300	-3.86744300	-3.62113500
C	1.92729100	-3.39351900	-1.69991200
H	5.36214200	-2.29090300	-4.97345400
C	2.21916300	-4.13653500	-2.84891800
H	3.53645500	-4.42926200	-4.53154200
H	1.53400200	-4.92642900	-3.14281600
H	7.62316100	-0.90767900	0.54369200
H	6.77199200	-2.67182700	-1.39724400
H	5.11169900	-0.24600900	-3.70789500
H	6.31379800	-3.06017500	-3.70296800
O	2.49533900	-1.56010600	-0.25170700
O	2.72266100	0.59419800	-1.59736600
P	1.67522100	-0.17462500	-0.59706500
O	1.57322300	0.53925700	0.71528400
O	0.45280600	-0.44317200	-1.42353600
H	0.55731200	1.12685600	2.02707700
C	0.69280900	-3.69352800	-0.91768700
C	-0.52324900	-3.52803500	-1.50196500
C	0.77328200	-4.24617700	0.42372600
C	-1.74704000	-3.87183900	-0.83647200
H	-0.58408200	-3.10881300	-2.50312500
C	-0.41508600	-4.62491100	1.10363500
C	2.01952500	-4.43553000	1.06385700

C	-2.98823700	-3.68218300	-1.48604600
C	-1.71000500	-4.41408500	0.46991700
C	-0.30080500	-5.20055400	2.38841700
H	2.92788300	-4.14868000	0.54412500
C	2.09867700	-4.98405400	2.32498800
C	-4.16935800	-4.01015400	-0.86035400
H	-2.98953700	-3.26620700	-2.49082100
C	-2.93822100	-4.72694100	1.09533000
C	0.92593900	-5.37640800	2.99122800
H	-1.19195400	-5.50921500	2.92299800
H	3.06619100	-5.11977100	2.79824400
C	-4.13929900	-4.52914500	0.44661600
H	-5.11969200	-3.85095600	-1.36103600
H	-2.95240700	-5.11866300	2.10601200
H	0.98480000	-5.81987500	3.98050700
H	-5.06896400	-4.77203700	0.95281400
C	2.83168100	3.14768300	-0.34159100
C	2.34267800	3.58488200	-1.53217300
C	2.21067800	3.59399400	0.89488900
C	1.21273200	4.46178200	-1.62462000
H	2.81245800	3.25918100	-2.45695900
C	1.07150300	4.44295600	0.84334500
C	2.70855700	3.19509800	2.15654700
C	0.76031800	4.90902000	-2.88556400
C	0.54150200	4.86851100	-0.44724300
C	0.49503200	4.87316500	2.06077700
H	3.53754500	2.49804800	2.19850100
C	2.14756100	3.66141100	3.32531000
C	-0.34736800	5.71969100	-2.98939900
H	1.30253800	4.59398400	-3.77347200
C	-0.61093700	5.67415400	-0.58495100
C	1.02644600	4.50556500	3.27830900
H	-0.37568500	5.51861700	2.04709700
H	2.55442600	3.35147900	4.28414500
C	-1.04704100	6.08911400	-1.82654100
H	-0.69128000	6.05857700	-3.96187200
H	-1.17458700	5.97559900	0.29078200
H	0.56985200	4.85672400	4.19847600
H	-1.93742600	6.70564600	-1.90301500
C	-3.34463000	3.35879900	-2.86879000
C	-3.98492400	3.30332100	-1.64029800
C	-3.35661400	2.70575300	-0.53776700
C	-2.05300400	2.18036200	-0.70692900
C	-1.41835000	2.22830400	-1.96233300

C	-2.06351800	2.81135600	-3.03868500
H	-5.03849400	2.95999600	0.82602200
H	-3.84352800	3.82789000	-3.71213500
H	-4.97633200	3.73015400	-1.51721200
C	-4.00143800	2.64150300	0.75978000
C	-1.39200200	1.57654800	0.42063900
H	-0.43069000	1.78525800	-2.06748900
H	-1.57605400	2.85830200	-4.00670400
C	-1.94128200	1.83172200	1.74334000
C	-3.34410600	2.23852100	1.86907900
H	-0.31969900	1.42410500	0.32616100
N	-1.26862600	1.71046300	2.85935200
N	-0.00301600	1.37714600	2.86414500
C	0.59191400	1.16918800	4.10799000
O	0.10579700	1.44321400	5.17546200
O	1.78387300	0.60667800	3.90838600
C	2.53623500	0.35970800	5.09831200
H	2.00688200	-0.34334500	5.74521100
H	3.48054800	-0.06649100	4.76443600
H	2.70850600	1.29135400	5.64270300
C	-3.97959200	2.20009100	3.22519000
H	-3.92925800	1.18717600	3.63944600
H	-3.44982300	2.85260200	3.92517500
H	-5.02431700	2.51171300	3.16885900
C	-5.83576200	-0.90274600	-0.37610200
C	-5.09850700	-0.49397500	-1.50265800
C	-3.71561400	-0.31139700	-1.37415700
C	-3.12672900	-0.58968600	-0.14774100
C	-3.85390500	-1.06443500	0.95158900
C	-5.23292200	-1.19857000	0.84231400
H	-6.91154400	-1.02427300	-0.46585100
H	-3.10194600	0.00851200	-2.20933500
H	-5.82654400	-1.55448300	1.67929300
C	-1.61532200	-1.11077900	1.46961000
C	-0.44898600	-1.43127900	2.15320700
C	-0.58507100	-2.02575800	3.40513500
C	-1.84573500	-2.29734300	3.94992400
C	-3.00735100	-1.99558800	3.24561500
C	-2.88624800	-1.40198700	1.99020500
H	0.53310900	-1.21282200	1.74767300
H	0.30974100	-2.29539300	3.95730100
H	-1.91674700	-2.76131200	4.92882400
H	-3.98554900	-2.23090200	3.65449400
N	-1.75631700	-0.45559000	0.20884400

H	-1.00920000	-0.60385700	-0.50754000
C	-5.82910500	-0.28023400	-2.83249000
C	-4.86728800	0.08238200	-3.96704500
C	-6.56170500	-1.57351300	-3.22708300
C	-6.85093100	0.85620100	-2.67212500
H	-4.34279500	1.02262300	-3.77045400
H	-4.11910500	-0.70145400	-4.12728400
H	-5.43021200	0.19987800	-4.89854900
H	-7.29153200	-1.87992900	-2.47198400
H	-7.09861400	-1.42530100	-4.17040900
H	-5.85108700	-2.39487000	-3.36946100
H	-7.38206500	1.02349500	-3.61551900
H	-7.59475700	0.62530400	-1.90332100
H	-6.34842800	1.78726000	-2.39038400

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C	4.77729200	-1.08974900	-0.82253300
C	5.97213100	-1.05106000	-0.09746600
C	6.36181800	0.10985900	0.55900700
C	5.55038700	1.24064400	0.47987100
C	4.32412500	1.21427400	-0.19408000
C	3.94398800	0.01802600	-0.81370300
C	5.52772500	-3.32102900	-0.66618000
C	6.64910900	-2.40246200	-0.14113400
H	7.28762600	0.14137900	1.12587500
H	5.85433500	2.16330400	0.96634800
H	4.90701600	-3.66040200	0.17023800
H	7.50532400	-2.38695100	-0.82608800
C	4.67136300	-2.39980000	-1.57851800
C	3.33759000	-3.01724100	-1.95778200
C	5.33505000	-2.27690900	-2.98190600
C	3.45066300	-3.70254300	-3.17274700
C	2.11567400	-3.00303700	-1.30087700
C	4.82704600	-3.50103300	-3.76065800
H	6.42486500	-2.21743200	-2.91501200
C	2.37318100	-4.40538100	-3.69323600
C	1.01180400	-3.71045100	-1.79197700
H	4.80048900	-3.33852600	-4.84129600
C	1.16938600	-4.41359500	-2.99272200
H	2.45964300	-4.93317200	-4.63848200
H	0.31803700	-4.96521000	-3.38014100
H	7.02328200	-2.71001000	0.83896800
H	5.89756400	-4.20137600	-1.19954100
H	4.97057900	-1.36146500	-3.46032000
H	5.45709500	-4.37978600	-3.57700300
O	1.98051300	-2.24423800	-0.13779500
O	2.65591500	-0.09807100	-1.35366800
P	1.58966600	-0.68569800	-0.29052700
O	1.63529600	-0.05232200	1.04673500
O	0.26954800	-0.58841500	-1.11487700
H	0.65898400	0.86081000	2.56648500
C	-0.31794700	-3.72850900	-1.11692300
C	-1.39394600	-3.23358300	-1.78574300
C	-0.50608900	-4.37297100	0.16974300
C	-2.73018500	-3.35089900	-1.28131200
H	-1.25100600	-2.74691400	-2.74753100
C	-1.81910700	-4.52651200	0.69254700
C	0.58843100	-4.89182400	0.89793400
C	-3.81885200	-2.85209700	-2.03343100

C	-2.96103800	-4.01177200	-0.05248300
C	-1.97600500	-5.20264400	1.92269700
H	1.59012000	-4.78758600	0.49422200
C	0.40393600	-5.53690800	2.10100800
C	-5.11122700	-3.02236400	-1.59499300
H	-3.61206800	-2.34029300	-2.96992500
C	-4.29862700	-4.15767200	0.38183300
C	-0.89265200	-5.69723200	2.61618200
H	-2.96651800	-5.33360400	2.34298300
H	1.25900200	-5.92756000	2.64393900
C	-5.34863500	-3.68085500	-0.37367000
H	-5.94390900	-2.63995300	-2.17748500
H	-4.51632200	-4.65742100	1.31914600
H	-1.04368000	-6.20919100	3.56153700
H	-6.36723000	-3.81213600	-0.02077000
C	3.48748100	2.44200100	-0.32293000
C	3.33568500	2.98806100	-1.55935900
C	2.89370600	3.09250900	0.82982000
C	2.62502100	4.21428200	-1.77303900
H	3.78959800	2.50340300	-2.42064800
C	2.15526000	4.29404800	0.65302700
C	3.03077500	2.55015700	2.12828700
C	2.53652800	4.76931600	-3.06885200
C	2.02155900	4.87560500	-0.67693500
C	1.57413000	4.89752700	1.79068300
H	3.55419100	1.60821200	2.25342300
C	2.48364400	3.18483200	3.22187400
C	1.85613100	5.94713900	-3.28556800
H	3.01734900	4.24730300	-3.89216500
C	1.32206000	6.07625100	-0.92892400
C	1.73971700	4.36325100	3.05028000
H	0.98813300	5.80298400	1.68257800
H	2.61194800	2.76170900	4.21367900
C	1.24058300	6.60062400	-2.20261500
H	1.79313900	6.36960400	-4.28355700
H	0.83737700	6.60603300	-0.11700800
H	1.28564100	4.84857700	3.90843500
H	0.69864100	7.52669500	-2.36832200
C	-1.73468100	4.40858400	-2.26984900
C	-2.58052500	4.36160400	-1.16503300
C	-2.37362800	3.42259300	-0.14952400
C	-1.29365400	2.52784100	-0.25723800
C	-0.43942300	2.59188300	-1.35422900
C	-0.66588200	3.52069600	-2.36885800

H	-4.17526400	3.94204000	0.98425600
H	-1.90425500	5.14307000	-3.05168700
H	-3.40826100	5.06082900	-1.07916200
C	-3.25407500	3.36470400	1.01865600
C	-1.10911900	1.47119100	0.80425900
H	0.40370600	1.90846300	-1.42464600
H	0.00264000	3.56287400	-3.22194200
C	-1.64930800	1.94358300	2.14026900
C	-2.92914200	2.67930300	2.13062400
H	-0.04537800	1.25000300	0.87857500
N	-1.09174500	1.76630300	3.28482700
N	0.10372700	1.15628200	3.37164900
C	0.63142800	0.93446000	4.61769800
O	0.15149000	1.26855400	5.67553400
O	1.79361800	0.27073500	4.47452000
C	2.46878400	-0.01573600	5.69945500
H	1.85340500	-0.65400400	6.33733900
H	3.38326600	-0.53521000	5.41661800
H	2.70731900	0.90542700	6.23678200
C	-3.76549100	2.66997100	3.37378300
H	-4.02583200	1.64298100	3.65154000
H	-3.20980300	3.09271500	4.21596500
H	-4.68342700	3.24339900	3.22821700
C	-5.75357100	0.31006700	-0.87824000
C	-4.79777600	0.84344200	-1.76253600
C	-3.44668300	0.80859100	-1.39993300
C	-3.09383700	0.24680700	-0.17709000
C	-4.04199700	-0.36836900	0.64642200
C	-5.39098900	-0.31563900	0.30619400
H	-6.80619900	0.35507700	-1.14261300
H	-2.68385900	1.21118400	-2.05487700
H	-6.14158900	-0.77291800	0.94434600
C	-1.95406800	-0.76766500	1.51667700
C	-0.97969900	-1.36351900	2.30814500
C	-1.40368300	-2.17279700	3.36091800
C	-2.76128000	-2.40020500	3.60235200
C	-3.72978400	-1.84323200	2.77347400
C	-3.31595100	-1.02473000	1.72468700
H	0.07831800	-1.21601800	2.12727000
H	-0.65711800	-2.64922700	3.98867000
H	-3.05912600	-3.03877200	4.42832000
H	-4.78500000	-2.04818900	2.92907600
N	-1.76643900	0.13265100	0.39154000
H	-0.59454400	-0.40927600	-0.56811200

C	-5.26642200	1.46391200	-3.08318200
C	-4.09249300	1.87351000	-3.97664400
C	-6.12901400	0.45576300	-3.85985100
C	-6.10255400	2.71595500	-2.77011700
H	-3.47085200	2.63890300	-3.50181800
H	-3.45522900	1.01698600	-4.22241700
H	-4.47456200	2.28715900	-4.91535000
H	-7.01368500	0.14874900	-3.29476100
H	-6.47458500	0.90362400	-4.79799000
H	-5.55284500	-0.44241700	-4.10668600
H	-6.44770600	3.18514000	-3.69818900
H	-6.98312300	2.47172000	-2.16752000
H	-5.50539200	3.44846100	-2.21628000

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C	-4.93552400	-1.77324400	-0.10859800
C	-5.69718000	-2.52154300	0.79309200
C	-5.17273300	-3.67261300	1.36749500
C	-3.87009700	-4.05482100	1.05807400
C	-3.05218700	-3.28409300	0.21855900
C	-3.62225500	-2.14127100	-0.35370500
C	-6.81814000	-0.45624400	0.42824200
C	-7.04089300	-1.86502600	1.01029700
H	-5.76431400	-4.26670200	2.05780100
H	-3.45527400	-4.95700800	1.49704700
H	-6.37100600	0.19189600	1.18993400
H	-7.82887000	-2.40059500	0.46740500
C	-5.78407900	-0.67175900	-0.71333200
C	-5.20058800	0.63703900	-1.21875100
C	-6.51416200	-1.16925500	-1.99466000
C	-5.96934700	1.11921400	-2.28631800
C	-4.11051200	1.38023300	-0.79098900
C	-7.02968700	0.11380600	-2.66531100
H	-7.30160000	-1.89125100	-1.76232400
C	-5.68773600	2.34437800	-2.87321300
C	-3.80248400	2.62363200	-1.35912600
H	-7.14137200	0.01459200	-3.74816300
C	-4.61532400	3.09386600	-2.39567900
H	-6.28485900	2.71027200	-3.70320100
H	-4.38080900	4.05684500	-2.83919600
H	-7.32745400	-1.84766400	2.06511700
H	-7.73558500	0.01749300	0.06815400
H	-5.78290700	-1.65706900	-2.64819200
H	-8.00487800	0.41187300	-2.26146600
O	-3.26438700	0.86112900	0.19729100
O	-2.83061500	-1.28612300	-1.13453500
P	-2.09857200	-0.14816200	-0.27734900
O	-1.31603000	-0.60348500	0.88664000
O	-1.32834700	0.55722300	-1.46577000
H	0.46875300	-0.82441100	1.89100200
C	-2.62367000	3.42940600	-0.92677100
C	-1.61773900	3.65802700	-1.81826100
C	-2.58177400	4.05866500	0.38204400
C	-0.46752000	4.45246500	-1.48722200
H	-1.66919800	3.21494800	-2.81189000
C	-1.49486100	4.90897700	0.71432000
C	-3.62815700	3.88045400	1.31477700
C	0.58455600	4.60774700	-2.41591100

C	-0.38090400	5.05956200	-0.21231300
C	-1.52704300	5.58835200	1.95135800
H	-4.45893700	3.22976200	1.06133900
C	-3.61885900	4.53572400	2.52693100
C	1.71884800	5.31390100	-2.08165100
H	0.48335000	4.15540700	-3.39900500
C	0.79484000	5.77319900	0.10656800
C	-2.56443500	5.40956800	2.84095200
H	-0.72294300	6.26633900	2.21339200
H	-4.43202500	4.38903800	3.23050500
C	1.82438400	5.89170000	-0.80441000
H	2.52921500	5.41835800	-2.79570400
H	0.91185500	6.22062900	1.08679500
H	-2.56518300	5.94554800	3.78487700
H	2.72402000	6.43307300	-0.52960200
C	-1.65647700	-3.70932700	-0.07769400
C	-1.23701600	-3.81072100	-1.36836800
C	-0.76460600	-4.11363300	0.99632700
C	0.02760700	-4.39234100	-1.71517800
H	-1.88920300	-3.49361400	-2.17790300
C	0.44033400	-4.79715500	0.68754600
C	-1.06027400	-3.82140600	2.34824700
C	0.43612500	-4.45928800	-3.06562500
C	0.84100000	-4.95794500	-0.70411700
C	1.23956500	-5.26417000	1.75514500
H	-1.93695900	-3.22654500	2.58072600
C	-0.23882200	-4.25405800	3.36558900
C	1.61201500	-5.08536600	-3.41600400
H	-0.19746800	-4.00696000	-3.82388800
C	2.02317500	-5.62458700	-1.09488800
C	0.90961400	-5.00499200	3.06715700
H	2.14613100	-5.82124600	1.54712800
H	-0.47600500	-4.00783000	4.39630400
C	2.40279000	-5.68586900	-2.41973000
H	1.92086600	-5.12854600	-4.45595100
H	2.65601800	-6.09350900	-0.34994500
H	1.55442200	-5.35315000	3.86736000
H	3.31914100	-6.20062600	-2.69269700
C	2.18795100	0.17670000	-4.47772500
C	2.69509000	-0.95133800	-3.84727100
C	2.63935800	-1.08013500	-2.45241100
C	2.04629900	-0.05829000	-1.69687900
C	1.57325300	1.08691700	-2.33265900
C	1.63710100	1.20804000	-3.71676800

H	3.86735900	-2.88643400	-2.40758400
H	2.23654500	0.26280700	-5.55874800
H	3.15459700	-1.74714100	-4.42798500
C	3.28885000	-2.20714500	-1.78481900
C	1.90580500	-0.18053400	-0.18805700
H	1.17506500	1.90275000	-1.73019800
H	1.26248600	2.10367300	-4.20196300
C	2.42577100	-1.50647500	0.37799100
C	3.26976600	-2.38297000	-0.44987000
H	0.83489100	-0.10178400	0.02835800
N	2.20168700	-1.91003500	1.57814700
N	1.30775600	-1.20763600	2.32907700
C	1.21308900	-1.51994500	3.66348900
O	2.03828200	-2.11015200	4.32113700
O	0.06748000	-1.00556000	4.14632700
C	-0.08305000	-1.11916200	5.55993100
H	0.71661200	-0.58218500	6.07566500
H	-1.04827200	-0.67038900	5.79132400
H	-0.06803600	-2.16665200	5.86982100
C	4.07409500	-3.43790900	0.24588100
H	4.80528700	-2.96351700	0.91110400
H	3.43880200	-4.06327400	0.87692000
H	4.60342800	-4.06182200	-0.47801400
C	6.46841700	2.23415500	0.57931000
C	6.20480200	1.09933300	-0.22089800
C	4.90453500	0.61025300	-0.29614100
C	3.89678200	1.25472000	0.42612400
C	4.16063400	2.38395400	1.22514200
C	5.46885600	2.87321200	1.29473200
H	7.48346700	2.61514600	0.64226800
H	4.67179700	-0.25837000	-0.89525600
H	5.70089100	3.74090600	1.90593100
C	1.93277600	1.84961900	1.35977200
C	0.60076400	1.93029000	1.77748200
C	0.26406100	2.93016800	2.67922900
C	1.21419500	3.85060700	3.14870100
C	2.53394300	3.77548300	2.72385400
C	2.90318500	2.76727500	1.82938100
H	-0.15422000	1.22652700	1.44483200
H	-0.76440900	2.99940900	3.02125400
H	0.91039900	4.62150200	3.85051600
H	3.27558600	4.48076000	3.08881000
N	2.54473100	0.94032900	0.50492400
H	-0.99772900	1.44898200	-1.25061900

C	7.35520500	0.42858700	-0.97837900
C	6.87759500	-0.77057900	-1.80489900
C	8.00509400	1.44497600	-1.93130000
C	8.40590300	-0.06539400	0.02965300
H	6.43049500	-1.54584900	-1.17243000
H	6.13778200	-0.47406500	-2.55695100
H	7.72956900	-1.21599400	-2.32852900
H	8.41765900	2.30134800	-1.38955700
H	8.82464700	0.97203200	-2.48379800
H	7.27550100	1.82188700	-2.65532400
H	9.23581300	-0.55035500	-0.49631300
H	8.81750400	0.75951400	0.61891500
H	7.96850100	-0.79083700	0.72333800

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C	5.18058900	1.37089800	-0.11813300
C	6.11928100	1.94892400	0.74137500
C	5.81756200	3.10762700	1.44603900
C	4.56050700	3.68646700	1.28330700
C	3.58816700	3.10364300	0.46275900
C	3.90759400	1.91903200	-0.21694900
C	6.90661000	-0.21475300	0.15867500
C	7.37956600	1.11510300	0.77320900
H	6.54397200	3.55420200	2.11876600
H	4.30963200	4.59945500	1.81673200
H	6.45387900	-0.83738000	0.93837100
H	8.16680500	1.57717400	0.16455700
C	5.79688300	0.19490300	-0.85253100
C	4.98863500	-1.00630600	-1.30881300
C	6.44499800	0.62686400	-2.19894100
C	5.56979300	-1.56948900	-2.44910400
C	3.86655700	-1.59808600	-0.74273100
C	6.69635700	-0.69444000	-2.94847700
H	7.34996900	1.22280600	-2.04839900
C	5.08485600	-2.75978100	-2.97456000
C	3.38403300	-2.82562800	-1.22447600
H	6.68261500	-0.57598900	-4.03545400
C	4.01502800	-3.38886700	-2.34101900
H	5.53275300	-3.20094500	-3.86032900
H	3.64661200	-4.33892400	-2.71674500
H	7.77847600	0.99846700	1.78451800
H	7.70797700	-0.78823900	-0.31622600
H	5.72245600	1.23350400	-2.75546600
H	7.66910300	-1.12492100	-2.68064000
O	3.22061200	-0.96205500	0.29655200
O	2.94553400	1.25393900	-0.95116900
P	2.06263600	0.13750700	-0.11069100
O	1.62791100	0.71854200	1.20350500
O	1.08331800	-0.42189700	-1.08583100
H	0.08643900	1.06874500	1.27730800
C	2.23782900	-3.54812100	-0.60317300
C	1.19149700	-3.91976400	-1.38976700
C	2.27301800	-3.97956600	0.78637200
C	0.10892900	-4.72395300	-0.90278100
H	1.16293400	-3.60057900	-2.42885700
C	1.21353300	-4.77012500	1.30697600
C	3.36560300	-3.66711800	1.62810700
C	-0.92928200	-5.12647900	-1.77211800

C	0.09282600	-5.13668800	0.45092900
C	1.29375700	-5.21023100	2.64761400
H	4.18813500	-3.08167200	1.23411900
C	3.41294400	-4.10279700	2.93379700
C	-1.96945600	-5.90559200	-1.31528500
H	-0.88953900	-4.80896400	-2.81097500
C	-1.00438100	-5.90347600	0.90137000
C	2.36589600	-4.88385800	3.44913600
H	0.49982900	-5.81928300	3.06419700
H	4.26347200	-3.84805200	3.55811200
C	-2.01223100	-6.28210200	0.03884100
H	-2.75558300	-6.22482400	-1.99284600
H	-1.06758000	-6.20837200	1.93948200
H	2.40144400	-5.23482000	4.47579500
H	-2.84027600	-6.87883300	0.40862400
C	2.26837000	3.77562600	0.27785700
C	1.98831800	4.35196900	-0.92230000
C	1.32059300	3.89717900	1.36896600
C	0.78396100	5.09592000	-1.15075300
H	2.70340900	4.27323100	-1.73773900
C	0.10555600	4.60795200	1.17729900
C	1.57985800	3.29834100	2.62359100
C	0.55006900	5.70474100	-2.40497600
C	-0.17588300	5.22086500	-0.11618000
C	-0.79663600	4.70461300	2.26288600
H	2.48258400	2.71084100	2.74257900
C	0.69025000	3.42177500	3.66571400
C	-0.60975400	6.40614600	-2.64391400
H	1.30511000	5.60038200	-3.17990100
C	-1.36413800	5.93833600	-0.39263000
C	-0.50502500	4.13889200	3.48439600
H	-1.73477400	5.23397400	2.14453400
H	0.90100200	2.94879900	4.61965900
C	-1.57660700	6.51763300	-1.62641900
H	-0.78025500	6.87110800	-3.60989700
H	-2.12663300	6.04599000	0.37035800
H	-1.20819300	4.23911200	4.30566100
H	-2.49537700	7.06535000	-1.81159000
C	-3.76118500	-2.59715100	-4.21774600
C	-3.25490200	-1.32115400	-4.41161100
C	-2.65181700	-0.63596300	-3.34712300
C	-2.55364500	-1.24066600	-2.08730200
C	-3.05856100	-2.52301900	-1.89934900
C	-3.66146900	-3.19439300	-2.95990800

H	-2.22727900	1.13272800	-4.52501100
H	-4.23620800	-3.12564600	-5.03745000
H	-3.32571900	-0.83608700	-5.38099900
C	-2.16708500	0.71381800	-3.52224400
C	-1.89306100	-0.51645900	-0.92959800
H	-2.98831800	-2.99403300	-0.92286800
H	-4.06001500	-4.19122500	-2.80023000
C	-1.58235700	0.94691300	-1.19906700
C	-1.66022900	1.49366400	-2.53496400
H	-0.86703800	-0.92492000	-0.83853700
N	-1.12762700	1.72810100	-0.25224800
N	-0.91315000	1.33709200	1.04601900
C	-1.90289100	1.63266400	1.94716200
O	-2.95156800	2.17813100	1.67431500
O	-1.55163700	1.18438500	3.15538400
C	-2.53660700	1.38216000	4.16824700
H	-3.45147300	0.83620900	3.92251500
H	-2.09775500	0.99191600	5.08579000
H	-2.76957400	2.44401300	4.27828800
C	-1.15566800	2.88157500	-2.79665400
H	-1.66771900	3.63487900	-2.18475500
H	-0.08342800	2.94155100	-2.57982600
H	-1.30567000	3.14580800	-3.84443800
C	-6.53767000	-0.21364800	1.34872500
C	-6.17523800	0.23044100	0.05648900
C	-4.85719700	0.07657900	-0.36326400
C	-3.94595400	-0.52418100	0.50527400
C	-4.30401300	-0.97647100	1.78914200
C	-5.62616900	-0.80534000	2.20975400
H	-7.56444000	-0.09145200	1.68038000
H	-4.53105200	0.41331400	-1.34144900
H	-5.93879200	-1.13518000	3.19670000
C	-2.07266000	-1.38984100	1.43031200
C	-0.75751800	-1.77646000	1.68549200
C	-0.48212100	-2.28791600	2.94601400
C	-1.48857400	-2.43316600	3.91604800
C	-2.79875100	-2.06121800	3.64437500
C	-3.10093900	-1.52541900	2.38869900
H	0.02636400	-1.66719600	0.94000800
H	0.53836700	-2.57359100	3.18177400
H	-1.23327600	-2.83753400	4.89066100
H	-3.57484100	-2.17106600	4.39692400
N	-2.59678300	-0.77325800	0.29926300
C	-7.24322700	0.85176700	-0.84927400

C	-6.66897300	1.28938400	-2.20023000
C	-8.34851200	-0.18539700	-1.10879400
C	-7.85417800	2.08264700	-0.16037500
H	-5.89025200	2.05059100	-2.08221700
H	-6.24314200	0.44392900	-2.75178200
H	-7.46653300	1.72112800	-2.81322200
H	-8.83221100	-0.50083900	-0.17958500
H	-9.11929100	0.23873100	-1.76201800
H	-7.93883500	-1.07642700	-1.59580600
H	-8.61758700	2.53313000	-0.80432200
H	-8.32969700	1.82071600	0.78938800
H	-7.08795600	2.83757300	0.04260900
H	-0.87857200	2.69323800	-0.48025300

TSI-2Value of imaginary frequency = -1098.8 cm⁻¹

C	3.77763500	-3.34278400	-0.11099400
C	4.30174300	-4.28034000	-1.00502200
C	3.46498900	-5.16297300	-1.67563500
C	2.09619100	-5.10186800	-1.43250400
C	1.54294800	-4.14741900	-0.56864400
C	2.40328400	-3.24323300	0.06753800
C	6.03760200	-2.75339000	-0.45949500
C	5.80273300	-4.13420800	-1.09678400
H	3.86678600	-5.89044500	-2.37475500
H	1.42444800	-5.79828100	-1.92716300
H	5.91274600	-1.97416600	-1.21938100
H	6.30425300	-4.92699200	-0.52814100
C	4.89884100	-2.60756900	0.59114200
C	4.76872500	-1.17360600	1.06468800
C	5.30722000	-3.31200800	1.91550400
C	5.59790700	-0.96655100	2.17252300
C	4.04356200	-0.11366800	0.53447500
C	6.18045800	-2.27763400	2.64727400
H	5.81272800	-4.26540000	1.73608200
C	5.77589300	0.30650300	2.69405100
C	4.25272300	1.19303300	1.00312000
H	6.13864000	-2.37970700	3.73519200
C	5.12755300	1.37602500	2.08196700
H	6.41689700	0.47352200	3.55490000
H	5.28837900	2.38694700	2.44437800
H	6.16651100	-4.19430600	-2.12611400
H	7.02897500	-2.63911500	-0.01194000
H	4.40112800	-3.50872000	2.49894800
H	7.23353300	-2.36434900	2.35380000
O	3.10078900	-0.36011500	-0.45399100
O	1.90374500	-2.21424900	0.85461400
P	1.60393800	-0.80884200	0.05415600
O	0.75960000	-1.04556000	-1.14497200
O	1.17398800	0.15936100	1.14493100
H	-1.15906100	-0.79274500	-1.46356300
C	3.62198300	2.40250800	0.40405400
C	2.91500700	3.24389300	1.20667000
C	3.88385900	2.78352100	-0.97540100
C	2.42652900	4.51210100	0.74891700
H	2.71654600	2.96205500	2.23818400
C	3.41312600	4.03244800	-1.46343100
C	4.62408900	1.94896900	-1.84403400

C	1.74433800	5.37426700	1.63538000
C	2.65744100	4.91598300	-0.58653000
C	3.70023100	4.38815900	-2.80021900
H	5.00131200	1.00223700	-1.47501100
C	4.88102000	2.31756100	-3.14645300
C	1.27879500	6.59894800	1.21100800
H	1.59730700	5.04946100	2.66162800
C	2.15701800	6.17059400	-1.00036000
C	4.41388800	3.55083300	-3.62973200
H	3.34915000	5.33517900	-3.19299600
H	5.44853700	1.65715600	-3.79442800
C	1.48105500	6.99301600	-0.12365200
H	0.76123000	7.25948500	1.90029000
H	2.30145700	6.50679300	-2.02045700
H	4.61703800	3.84639200	-4.65438000
H	1.10876300	7.95311300	-0.46712600
C	0.07812400	-4.19894400	-0.29462500
C	-0.34680000	-4.67044100	0.90835600
C	-0.88812400	-3.91115800	-1.33644600
C	-1.73768000	-4.86180500	1.20423400
H	0.38053100	-4.92530100	1.67596100
C	-2.27039400	-4.12360600	-1.09526800
C	-0.47110200	-3.43465300	-2.60110600
C	-2.13962300	-5.32848000	2.47607700
C	-2.71335300	-4.55427500	0.22547200
C	-3.17792300	-3.92491500	-2.16185900
H	0.57856600	-3.21136200	-2.75234100
C	-1.37857500	-3.23522200	-3.61634200
C	-3.47397500	-5.45378700	2.79075000
H	-1.37179500	-5.56972500	3.20695700
C	-4.07690900	-4.66573600	0.58374300
C	-2.74092800	-3.50675100	-3.39983200
H	-4.23482700	-4.11594300	-2.01399900
H	-1.04278500	-2.86916400	-4.58114400
C	-4.44882800	-5.10302500	1.83811200
H	-3.77608500	-5.80641200	3.77185400
H	-4.84957100	-4.39014100	-0.12511900
H	-3.45518600	-3.37175700	-4.20660300
H	-5.50196200	-5.17544700	2.09092900
C	-1.15930100	3.93900300	4.43829400
C	-1.24024000	2.57500000	4.64594900
C	-1.29068300	1.69692800	3.54920900
C	-1.23518000	2.19770600	2.23634500
C	-1.14193800	3.57965100	2.03789700

C	-1.11864700	4.43625400	3.12898000
H	-1.46993200	-0.09093900	4.75809600
H	-1.13399500	4.62117500	5.28153000
H	-1.28121700	2.16518200	5.65129900
C	-1.46246300	0.28328200	3.73646800
C	-1.23741200	1.25422900	1.08698600
H	-1.09505000	3.97550900	1.02830500
H	-1.06223700	5.50720900	2.95948300
C	-1.67160600	-0.11793600	1.36299600
C	-1.64767500	-0.60638300	2.72775800
H	-0.02309500	0.83245800	1.02396300
N	-1.89129400	-1.02371000	0.41703700
N	-2.02540200	-0.74659500	-0.91972200
C	-3.29157200	-0.87686800	-1.43599700
O	-4.26611900	-1.18415800	-0.78134600
O	-3.28826100	-0.59719300	-2.73998800
C	-4.57108100	-0.68054900	-3.36093300
H	-5.24825000	0.06339200	-2.93440500
H	-4.39946300	-0.47643700	-4.41729500
H	-4.99957700	-1.67721700	-3.23107800
C	-1.83608700	-2.07008000	2.99605100
H	-2.78132700	-2.45269100	2.59008300
H	-1.01754200	-2.64387600	2.54736100
H	-1.83455900	-2.26058900	4.07051200
C	-5.53185800	2.46801400	-1.43425100
C	-5.38943300	2.00836200	-0.10520200
C	-4.10989400	1.82088400	0.40976400
C	-3.01457300	2.05509100	-0.42207100
C	-3.15385100	2.47417900	-1.75757900
C	-4.43974800	2.69677200	-2.25792800
H	-6.52911300	2.62519900	-1.83519000
H	-3.95603200	1.46957100	1.42478200
H	-4.58482500	3.02751200	-3.28285400
C	-0.93105700	2.13333900	-1.28603400
C	0.44737900	2.07289800	-1.49380200
C	0.91380500	2.33815600	-2.77480400
C	0.04585600	2.70947000	-3.81309900
C	-1.31941700	2.81604100	-3.58870900
C	-1.81854000	2.51890800	-2.31777700
H	1.13429700	1.82710000	-0.69016800
H	1.97797000	2.25319100	-2.97038200
H	0.45187400	2.91646600	-4.79834400
H	-1.99331600	3.11338900	-4.38724200
N	-1.66937400	1.86136100	-0.13754300

C	-6.64323300	1.65883800	0.70081600
C	-6.30099900	1.16812400	2.11046800
C	-7.55808000	2.88738100	0.81888200
C	-7.38751500	0.53047000	-0.03509600
H	-5.69387000	0.25696600	2.08189400
H	-5.75895800	1.92787800	2.68353500
H	-7.22407400	0.93748900	2.65169000
H	-7.87426900	3.25214900	-0.16289700
H	-8.46022000	2.63289500	1.38626100
H	-7.04947000	3.70687900	1.33694500
H	-8.25574300	0.20377500	0.54849400
H	-7.74865900	0.86141700	-1.01399900
H	-6.72284500	-0.32555600	-0.19080900
H	-2.04072900	-1.99468200	0.68565900

IMI-4

C	5.36486300	-1.49064000	-0.46549200
C	6.06503300	-2.24424500	-1.41078100
C	5.61457000	-3.50858500	-1.77143400
C	4.44094600	-4.00530600	-1.20251000
C	3.67646400	-3.23707700	-0.31619600
C	4.16661900	-1.97134900	0.03022200
C	6.93379900	-0.02404800	-1.43228900
C	7.24715900	-1.45285600	-1.92501300
H	6.15928300	-4.10357000	-2.49861300
H	4.08537400	-4.99451500	-1.47607700
H	6.28401700	0.48243500	-2.15426200
H	8.18469200	-1.82551100	-1.49531900
C	6.14332400	-0.23985600	-0.11106000
C	5.47926600	1.02564000	0.41537600
C	7.13858000	-0.53740000	1.04971600
C	6.33902000	1.67430000	1.31291300
C	4.23801000	1.59461200	0.15559900
C	7.57991300	0.84727600	1.54542800
H	7.96571900	-1.17505800	0.72605500
C	5.99067800	2.88480500	1.89457100
C	3.86351100	2.82350400	0.71584800
H	7.89091100	0.84730900	2.59340100
C	4.76047600	3.45704000	1.58118700
H	6.66213100	3.37511600	2.59333500
H	4.47099000	4.40816000	2.01774900
H	7.34297600	-1.51293500	-3.01241400
H	7.82687100	0.58936500	-1.28305400
H	6.59717600	-1.05603000	1.84823900
H	8.41952700	1.23323800	0.95449200
O	3.32638300	0.93931400	-0.67456100
O	3.38436100	-1.11994100	0.80995700
P	2.37498300	-0.21002700	-0.06899500
O	1.65273100	-0.91892500	-1.14135000
O	1.50243800	0.45002700	1.05777400
H	-0.37535400	-1.22074700	-0.96102000
C	2.54213500	3.45233700	0.43188800
C	1.64161300	3.59153900	1.43949600
C	2.23204500	3.96827100	-0.88785600
C	0.36823700	4.22228500	1.24422800
H	1.87148200	3.19469400	2.42530700
C	0.98927300	4.61601200	-1.11629500
C	3.15195700	3.84613800	-1.95431000
C	-0.54943800	4.31766900	2.31353100

C	0.02747100	4.73946100	-0.02864500
C	0.71756800	5.10660100	-2.41253800
H	4.10782700	3.36424600	-1.77598000
C	2.85540300	4.32788200	-3.21062200
C	-1.77519700	4.91830600	2.13642100
H	-0.26890900	3.90281000	3.27831800
C	-1.24049900	5.34276100	-0.18444300
C	1.62454300	4.96415800	-3.44081400
H	-0.22613900	5.59849600	-2.61695200
H	3.57368000	4.21879500	-4.01708300
C	-2.11986100	5.43274400	0.87389000
H	-2.48013600	4.98338700	2.95911300
H	-1.54299800	5.74022100	-1.14633200
H	1.38456800	5.34405400	-4.42902800
H	-3.09087200	5.89636800	0.72859700
C	2.39042700	-3.70771300	0.27092400
C	2.25808600	-3.71803300	1.62561700
C	1.27998800	-4.13646600	-0.56056000
C	1.04292700	-4.10946500	2.27668400
H	3.09081400	-3.40481000	2.25035100
C	0.07919400	-4.58714300	0.05086900
C	1.35338200	-4.09425900	-1.97096800
C	0.94305500	-4.07937400	3.68611200
C	-0.06753400	-4.51765500	1.49881900
C	-0.95392800	-5.08251800	-0.77458400
H	2.23406500	-3.67020000	-2.43921800
C	0.31855100	-4.55896300	-2.75271400
C	-0.23342700	-4.42124200	4.31575800
H	1.81322800	-3.77704300	4.26296400
C	-1.27454300	-4.82368700	2.16801200
C	-0.83324000	-5.08574200	-2.14772800
H	-1.85821500	-5.47779700	-0.32521700
H	0.39508800	-4.51601400	-3.83449600
C	-1.35537400	-4.77952100	3.54508900
H	-0.30315700	-4.39593400	5.39878200
H	-2.16153200	-5.07726100	1.59950700
H	-1.64053900	-5.47462900	-2.76128400
H	-2.29387100	-5.01737700	4.03582800
C	-5.05583000	3.56158200	3.05631000
C	-4.18200900	2.74490200	3.72921500
C	-3.34877100	1.83957900	3.02289900
C	-3.42962000	1.76673000	1.60913800
C	-4.31657000	2.64820600	0.93536800
C	-5.10991800	3.51829500	1.64369100

H	-2.34669000	1.08080500	4.77978000
H	-5.69613700	4.24786400	3.60162800
H	-4.11226200	2.77541300	4.81337200
C	-2.42030900	1.00874500	3.69728500
C	-2.62542900	0.80754600	0.90576900
H	-4.35776800	2.63932900	-0.14816400
H	-5.78220900	4.18416700	1.11117400
C	-1.73936700	0.00414200	1.60330700
C	-1.61681500	0.12576900	3.02879200
H	0.60997400	-0.03190100	1.07585100
N	-0.81709200	-0.93213200	1.02618500
N	-1.06069100	-1.43708800	-0.24202200
C	-2.19999800	-2.14527200	-0.47319000
O	-2.97191600	-2.50678400	0.39439000
O	-2.34646700	-2.35945700	-1.78503100
C	-3.52762500	-3.07370800	-2.14580100
H	-4.41759300	-2.51179800	-1.85220100
H	-3.48924700	-3.18030900	-3.22960900
H	-3.54616900	-4.05717200	-1.66901000
C	-0.64394300	-0.74526700	3.78039300
H	-0.91805400	-1.80593700	3.71191200
H	0.38030400	-0.64242000	3.40398100
H	-0.64041200	-0.47736000	4.83843200
C	-6.14730400	-0.45266300	-2.66914300
C	-6.25865600	-0.56426600	-1.26307700
C	-5.17431200	-0.20178300	-0.46770800
C	-4.01791700	0.27447800	-1.08915000
C	-3.90317000	0.38164900	-2.48778100
C	-4.99144800	0.00539700	-3.28173200
H	-6.99018700	-0.73957300	-3.29095100
H	-5.20603300	-0.28593400	0.61207000
H	-4.93300300	0.07425000	-4.36448900
C	-1.95084000	1.08604600	-1.50690700
C	-0.64044700	1.55118000	-1.39941100
C	0.04758500	1.79703200	-2.58187100
C	-0.55579600	1.61137300	-3.83552300
C	-1.86579400	1.16256300	-3.93339200
C	-2.57284700	0.88685000	-2.76029100
H	-0.17383800	1.71154900	-0.43019300
H	1.07705700	2.14004900	-2.53212400
H	0.01453200	1.82126500	-4.73486300
H	-2.33322900	1.01682700	-4.90316200
N	-2.83115500	0.70688400	-0.49808500
C	-7.56025400	-1.09955000	-0.65787900

C	-7.51487800	-1.12628800	0.87251400
C	-8.73447700	-0.20675000	-1.09186900
C	-7.79786300	-2.53319400	-1.16039600
H	-6.72174000	-1.78474700	1.24135800
H	-7.35420400	-0.12651600	1.28987400
H	-8.46752000	-1.50140500	1.25987200
H	-8.85102800	-0.18817100	-2.17946500
H	-9.67072100	-0.58036600	-0.66256900
H	-8.58877100	0.82279700	-0.74911200
H	-8.72918400	-2.93275900	-0.74354300
H	-7.87562700	-2.57107200	-2.25127200
H	-6.97763800	-3.19169600	-0.85492200
H	-0.66624700	-1.71268600	1.66814900

DII

C	-1.60931000	-3.69677200	0.22930200
C	-1.65631300	-4.65031500	1.25135300
C	-0.53258100	-4.91813600	2.02271100
C	0.63950200	-4.20364400	1.78466100
C	0.70220900	-3.20362700	0.80682000
C	-0.44581700	-2.96714900	0.03821000
C	-3.88819600	-4.19571900	0.58761800
C	-3.04806000	-5.22719000	1.36095000
H	-0.56768900	-5.66198400	2.81346700
H	1.52550400	-4.40042200	2.38188000
H	-4.15036700	-3.36420100	1.25143200
H	-3.09809100	-6.21563500	0.88801700
C	-2.93033700	-3.66154700	-0.51800900
C	-3.47513900	-2.39580100	-1.15473500
C	-2.94678100	-4.62002800	-1.74199700
C	-4.28444900	-2.71851500	-2.25008900
C	-3.32899700	-1.06543400	-0.79474000
C	-4.19155100	-4.19815000	-2.54579600
H	-2.95687200	-5.67167000	-1.44203500
C	-5.00090300	-1.73223500	-2.91558100
C	-4.06330100	-0.04968800	-1.42285900
H	-4.09424700	-4.40248100	-3.61541100
C	-4.90507200	-0.41068100	-2.48013600
H	-5.62606100	-1.98261100	-3.76768000
H	-5.47459700	0.37016600	-2.97539500
H	-3.36974100	-5.34609700	2.39899600
H	-4.81231500	-4.60631500	0.17121600
H	-2.04495000	-4.44058400	-2.33726700
H	-5.08892100	-4.72222100	-2.19533800
O	-2.40338500	-0.72128100	0.18740900
O	-0.44820800	-1.92964900	-0.89082000
P	-0.89095400	-0.47385900	-0.33292700
O	-0.18416900	-0.30154300	1.04749900
O	-0.69776100	0.54107100	-1.38254900
H	0.48686700	0.43584300	1.18292900
C	-3.91968700	1.37330900	-1.00835700
C	-3.51571500	2.29326000	-1.92355500
C	-4.21091100	1.79286300	0.35261800
C	-3.33054100	3.67551300	-1.58875500
H	-3.28064700	1.97639800	-2.93657900
C	-4.02504200	3.15004700	0.72527300
C	-4.69544600	0.87924400	1.31633300
C	-2.89202300	4.59285600	-2.56896800

C	-3.56837800	4.11659600	-0.26568400
C	-4.30209800	3.52627200	2.05880700
H	-4.86735300	-0.15281300	1.02888400
C	-4.96167300	1.27514500	2.60805000
C	-2.69330400	5.91871700	-2.25494800
H	-2.70916200	4.22853300	-3.57637800
C	-3.35413100	5.48110400	0.02957500
C	-4.75456900	2.61188000	2.98497700
H	-4.16297500	4.55510900	2.37019600
H	-5.33458100	0.55579400	3.33036000
C	-2.92771100	6.36267300	-0.94186000
H	-2.35326000	6.61705600	-3.01311900
H	-3.52114000	5.85711200	1.03236500
H	-4.96087400	2.92897100	4.00265400
H	-2.76912200	7.40616800	-0.68794300
C	1.96425700	-2.44393400	0.57721200
C	2.55521400	-2.49260700	-0.64746900
C	2.60279900	-1.69940500	1.64987900
C	3.84034500	-1.91053600	-0.90086100
H	2.06732700	-3.02694400	-1.45904800
C	3.88232300	-1.12060500	1.44023800
C	1.95523500	-1.49868500	2.89278600
C	4.43071100	-2.01961900	-2.17913200
C	4.53373900	-1.25529800	0.14429200
C	4.47209300	-0.38919700	2.49669200
H	0.95808400	-1.90159300	3.03504700
C	2.55610800	-0.77953600	3.90408800
C	5.68739000	-1.51048600	-2.41856700
H	3.87509000	-2.51775400	-2.96902200
C	5.82405500	-0.74903300	-0.12714900
C	3.82896300	-0.22025500	3.70434200
H	5.44788500	0.06344500	2.36059200
H	2.03839200	-0.63168200	4.84741800
C	6.39040400	-0.87726900	-1.37825100
H	6.13522100	-1.59735800	-3.40356400
H	6.38870000	-0.24682800	0.65054600
H	4.29934000	0.35927500	4.49232600
H	7.38225100	-0.47503800	-1.56216500
C	4.24960100	1.01690900	-4.59874400
C	4.94575400	1.62754000	-3.58497700
C	4.37552300	1.74495800	-2.29101300
C	3.07068900	1.21955900	-2.07030800
C	2.37080600	0.59012000	-3.13641400
C	2.95229200	0.49019700	-4.37421700

H	6.06009600	2.76187700	-1.39570600
H	4.69495100	0.93161000	-5.58542600
H	5.94139200	2.02779400	-3.75699400
C	5.06291900	2.36724700	-1.21492800
C	2.49777500	1.33469800	-0.78749300
H	1.37346300	0.20249400	-2.94062600
H	2.42181300	0.00974300	-5.19012100
C	3.19831200	1.93604000	0.23995300
C	4.50983800	2.47423700	0.03632000
H	1.48205300	0.98218600	-0.64605700
N	2.69292700	2.10798600	1.54070400
N	1.60936300	1.56431700	1.82573600
C	1.20928700	1.88391000	3.18775500
O	1.85313900	2.48883000	4.00066300
O	-0.00727000	1.39157800	3.35451600
C	-0.60247100	1.64489400	4.63134700
H	-0.65845700	2.72026100	4.81310500
H	-1.60062800	1.21454300	4.57918500
H	-0.01735200	1.17043900	5.42254500
C	5.24935900	3.12671000	1.17193600
H	4.70625900	3.99878200	1.54748300
H	5.36221700	2.44067000	2.01657200
H	6.24003400	3.44730600	0.84270300

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C	4.22773700	-1.51392200	-0.11015900
C	5.23610000	-1.69978700	0.84125100
C	5.73347500	-0.62448300	1.56669000
C	5.19671300	0.64356800	1.35588000
C	4.14981900	0.85392900	0.45020100
C	3.68412500	-0.24965000	-0.27598800
C	4.38388700	-3.83827000	0.26698800
C	5.59149600	-3.16427200	0.94199500
H	6.51796500	-0.76858700	2.30354700
H	5.57004900	1.49259500	1.92172200
H	3.57603300	-3.95879300	0.99707900
H	6.52051900	-3.37572200	0.39896100
C	3.92510700	-2.82151600	-0.81926700
C	2.54294700	-3.16763600	-1.34480400
C	4.77173700	-3.01199400	-2.10900900
C	2.65131900	-4.04110900	-2.43415200
C	1.28061200	-2.81072700	-0.89845800
C	4.10044700	-4.19269100	-2.83580900
H	5.82824200	-3.18209800	-1.88414800
C	1.51840500	-4.60160300	-3.00811900
C	0.11811300	-3.37877900	-1.43444700
H	4.23694900	-4.15668300	-3.91978200
C	0.26329100	-4.28729200	-2.48711900
H	1.60295900	-5.27603200	-3.85515700
H	-0.63140500	-4.73369100	-2.91052600
H	5.73704000	-3.48790200	1.97577100
H	4.61048400	-4.81961500	-0.15864000
H	4.69084500	-2.10743400	-2.72126700
H	4.50077600	-5.15265300	-2.48839300
O	1.15156800	-1.80027700	0.06594500
O	2.60534200	-0.09063400	-1.15010000
P	1.12808600	-0.31931600	-0.55885300
O	1.03066400	0.47319200	0.80825400
O	0.12758100	-0.03313200	-1.60042200
H	0.75379800	1.40114200	0.71395100
C	-1.23273100	-3.02569200	-0.91349900
C	-2.12773800	-2.40474900	-1.72665100
C	-1.62342200	-3.40131600	0.43496800
C	-3.44310300	-2.04321000	-1.28090200
H	-1.83487900	-2.13177900	-2.73795600
C	-2.93328900	-3.10006500	0.89223300
C	-0.74143700	-4.09874800	1.29136400
C	-4.31511200	-1.33280300	-2.13395000

C	-3.84473700	-2.34885100	0.03971400
C	-3.31894800	-3.55704900	2.17142800
H	0.25910000	-4.33572100	0.94324600
C	-1.13502100	-4.50077800	2.55003300
C	-5.54261300	-0.90043600	-1.68526200
H	-3.98580900	-1.10225600	-3.14400400
C	-5.10028200	-1.87706400	0.48390200
C	-2.44139200	-4.23664100	2.98989700
H	-4.33099800	-3.38462100	2.51984100
H	-0.44088800	-5.03491000	3.19123100
C	-5.92927900	-1.16626200	-0.35861400
H	-6.19468100	-0.33114700	-2.34080700
H	-5.41555500	-2.04540000	1.50784100
H	-2.76601000	-4.57146500	3.97021600
H	-6.88097500	-0.79671600	0.01078600
C	3.55237500	2.20693000	0.26342800
C	3.60078100	2.79696300	-0.96090000
C	2.91877300	2.90268300	1.37274300
C	3.07436700	4.10931100	-1.19995100
H	4.06192300	2.27249300	-1.79418100
C	2.39099100	4.20717100	1.17484300
C	2.76817300	2.28668000	2.63805900
C	3.15697200	4.68557200	-2.48672700
C	2.47517000	4.83062300	-0.14017200
C	1.77197300	4.85536400	2.26754900
H	3.12984100	1.27403300	2.77726000
C	2.14951200	2.94003300	3.68129500
C	2.65880600	5.94621900	-2.72673900
H	3.62240900	4.11284200	-3.28428100
C	1.97145700	6.12103500	-0.41430100
C	1.65573200	4.24179200	3.49588700
H	1.36845100	5.85364000	2.14442500
H	2.03665900	2.44553900	4.64099300
C	2.05992600	6.66671600	-1.67800900
H	2.72540100	6.38266200	-3.71815900
H	1.50052900	6.70151100	0.37056000
H	1.16938600	4.76106600	4.31555900
H	1.66243800	7.65986400	-1.86210400
C	-5.44673200	3.26340600	-3.34172600
C	-4.39052600	2.77270400	-4.12870100
C	-3.34730800	2.04588300	-3.57118800
C	-3.38114700	1.81513900	-2.19281400
C	-4.43920700	2.30226100	-1.38518400
C	-5.47617500	3.03327900	-1.97271500

H	-6.24631400	3.82619100	-3.81280400
H	-2.53255200	1.66718800	-4.18073000
H	-6.29507500	3.41019000	-1.36602400
C	-2.95319800	1.12210400	-0.10075800
C	-2.38100100	0.53243100	1.03282400
C	-2.99962100	0.71564900	2.26658200
C	-4.20643800	1.45326200	2.32791800
C	-4.78769700	2.01180100	1.20156800
C	-4.15550700	1.85994300	-0.03632300
H	-1.47648300	-0.05970500	0.93858000
H	-4.68910300	1.59860900	3.28984600
H	-5.71712200	2.56919600	1.28292200
N	-2.50039300	1.11440800	-1.40219100
H	-1.63894000	0.66595900	-1.70128200
H	-4.38946800	2.96594900	-5.19726400
C	-2.37977500	0.19040500	3.56673800
C	-1.16278200	-0.70238100	3.30351400
C	-1.92593900	1.39447400	4.41095500
C	-3.41370900	-0.61725700	4.36643500
H	-1.41160700	-1.54403200	2.64850400
H	-0.34203700	-0.14410400	2.84166000
H	-0.79576500	-1.11177300	4.25069700
H	-2.76865500	2.04352500	4.67004900
H	-1.46390700	1.05115800	5.34389500
H	-1.19042700	1.99591900	3.86615200
H	-2.95971600	-0.99950200	5.28768700
H	-4.27971000	-0.01283400	4.65127700
H	-3.77032000	-1.47218500	3.78519100

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C	2.09889000	4.24099800	0.07847800
C	2.36745900	5.18591500	1.07370200
C	1.36574800	5.59766300	1.94378100
C	0.09052200	5.04973500	1.81826500
C	-0.19244200	4.05541500	0.87308900
C	0.84637800	3.64841500	0.02335400
C	4.44381500	4.50002200	0.13680900
C	3.82170400	5.59614900	1.02294300
H	1.56786300	6.33731400	2.71275100
H	-0.70826100	5.38267800	2.47468000
H	4.70353200	3.63132100	0.75183000
H	3.92999000	6.58678800	0.56531300
C	3.30062700	4.09609200	-0.83649000
C	3.61206000	2.81371000	-1.58456300
C	3.23489500	5.10334400	-2.02181600
C	4.25588100	3.10261900	-2.79380900
C	3.39285600	1.48998500	-1.23757700
C	4.28993500	4.59593200	-3.02074600
H	3.39990400	6.13362400	-1.69490900
C	4.72325600	2.08166600	-3.60999800
C	3.87534500	0.43720500	-2.02490500
H	4.06089200	4.86583000	-4.05498000
C	4.54868400	0.75777300	-3.20784400
H	5.21643500	2.30630300	-4.55110400
H	4.92540500	-0.05361400	-3.82315100
H	4.27444300	5.64595700	2.01679100
H	5.34171800	4.82468000	-0.39609300
H	2.24030500	5.04315200	-2.47629400
H	5.28314300	4.99960400	-2.79007200
O	2.63229000	1.19975200	-0.10229700
O	0.63668600	2.59862700	-0.87024800
P	1.04176300	1.11091500	-0.37228800
O	0.53123300	0.96986900	1.09250800
O	0.61624300	0.14307700	-1.40138600
H	-0.26822400	0.38535100	1.32383600
C	3.70962400	-0.98965000	-1.62469900
C	2.89463400	-1.80696400	-2.34114400
C	4.48292300	-1.52872300	-0.52111600
C	2.75794000	-3.20307400	-2.03900500
H	2.31101500	-1.39826600	-3.16196400
C	4.41696300	-2.91710500	-0.22818000
C	5.31868300	-0.69899000	0.26169400
C	1.86173100	-4.00665800	-2.77775900

C	3.52149300	-3.77505300	-0.99313700
C	5.22177200	-3.41942300	0.81963400
H	5.36975600	0.36155700	0.03789700
C	6.06984900	-1.21383000	1.29507400
C	1.71336300	-5.34462700	-2.49066300
H	1.27919600	-3.54356700	-3.56993100
C	3.35979000	-5.15394900	-0.72863700
C	6.02701900	-2.59046300	1.57059800
H	5.20722800	-4.47852700	1.05014900
H	6.70044200	-0.55849000	1.88738900
C	2.47386000	-5.91998700	-1.45714300
H	1.01167600	-5.95119000	-3.05388700
H	3.92838400	-5.62911600	0.06295900
H	6.62828000	-3.00440300	2.37400900
H	2.36132000	-6.97459000	-1.22648700
C	-1.57158500	3.51006700	0.71932600
C	-2.20169600	3.66552600	-0.47755000
C	-2.27996800	2.88440100	1.82275500
C	-3.55251000	3.24154100	-0.69707700
H	-1.67734100	4.14206400	-1.30263400
C	-3.62215200	2.45125800	1.64171200
C	-1.66396800	2.68928800	3.08146800
C	-4.15748900	3.41944700	-1.96085400
C	-4.27058500	2.61583700	0.34840100
C	-4.29134000	1.85130800	2.73167000
H	-0.62651400	2.97940000	3.21043200
C	-2.35684800	2.13400100	4.13644200
C	-5.43671600	2.96988300	-2.19752500
H	-3.58476100	3.90069900	-2.74888600
C	-5.58022200	2.15879400	0.07798700
C	-3.68026200	1.70260800	3.95800000
H	-5.31208700	1.50655300	2.61427800
H	-1.87328500	2.00830300	5.10058400
C	-6.14880400	2.32945900	-1.16668400
H	-5.89164900	3.09688300	-3.17472800
H	-6.15377300	1.65344400	0.84639700
H	-4.21749500	1.24128800	4.78021100
H	-7.15235800	1.95961300	-1.35331200
C	-4.10990700	0.30760900	-4.35807700
C	-4.80333800	-0.36265400	-3.38131800
C	-4.27024500	-0.47853300	-2.07053800
C	-3.02556300	0.14858800	-1.78349900
C	-2.32915100	0.84315000	-2.81127300
C	-2.85554700	0.90833500	-4.07552100

H	-5.86054900	-1.71745400	-1.29121600
H	-4.51971100	0.37737300	-5.36120800
H	-5.75691100	-0.83508200	-3.60171900
C	-4.92234100	-1.22295800	-1.05226800
C	-2.49988700	0.04548200	-0.48088000
H	-1.37232500	1.29903300	-2.56833700
H	-2.32070100	1.42724800	-4.86473600
C	-3.14011600	-0.70984800	0.48173000
C	-4.37925100	-1.37031500	0.20009300
H	-1.59929700	0.59483400	-0.24078400
N	-2.67385500	-0.85740200	1.80081500
N	-1.54391200	-0.40879000	2.07558200
C	-1.24242600	-0.57011500	3.49077700
O	-1.92219700	-1.12994900	4.30573600
O	-0.08566800	0.04738700	3.69552100
C	0.35791600	0.24798800	5.04081200
H	-0.31007200	-0.24267800	5.74884600
H	1.36650300	-0.15875700	5.12297400
H	0.38413800	1.32498500	5.21956600
C	-5.02814500	-2.23232200	1.24501200
H	-4.35525600	-3.04506000	1.53901400
H	-5.24967600	-1.66346200	2.15261300
H	-5.95440200	-2.66474200	0.86073100
C	-4.09305700	-4.38614400	-2.44518800
C	-3.47936000	-3.57334500	-3.41420900
C	-2.31665800	-2.86643200	-3.13900700
C	-1.77214000	-2.98877900	-1.85810700
C	-2.37847000	-3.80400700	-0.86905300
C	-3.54833900	-4.50655600	-1.17285200
H	-4.99953900	-4.92711400	-2.69781700
H	-1.85474200	-2.22386900	-3.88293100
H	-4.02151800	-5.13723300	-0.42487700
C	-0.48022800	-2.82984900	-0.02828800
C	0.55710000	-2.54132700	0.86562800
C	0.51346500	-3.10690200	2.14167200
C	-0.59501500	-3.90866000	2.50238700
C	-1.61267300	-4.20548100	1.60971700
C	-1.55203100	-3.68562900	0.31328800
H	1.39006100	-1.92360700	0.53925100
H	-0.64344700	-4.32983000	3.50036000
H	-2.43549000	-4.84825600	1.91116800
N	-0.63374000	-2.41724700	-1.33472000
H	-0.11618700	-1.63727200	-1.72802300
H	-3.92796300	-3.48827800	-4.39962700

C	1.69966200	-2.98773500	3.10517600
C	2.53930200	-1.73359600	2.82268300
C	1.23333600	-2.98434700	4.57107700
C	2.58638700	-4.22801000	2.89319900
H	3.03271400	-1.79023600	1.84763800
H	1.92998900	-0.82467800	2.83705500
H	3.32965800	-1.64142900	3.57555300
H	0.91449700	-3.97999400	4.89369900
H	2.05883200	-2.68561100	5.22594900
H	0.39274200	-2.30598800	4.73599500
H	3.47578700	-4.17958200	3.53333400
H	2.03657100	-5.14428600	3.13290900
H	2.91016800	-4.29038900	1.85083600

TSII-1Value of imaginary frequency = -296.4 cm⁻¹

C	0.97752700	4.59850600	0.03374200
C	0.98068600	5.50813700	1.09514500
C	-0.17622200	5.73891700	1.82877300
C	-1.33436000	5.03188100	1.50681700
C	-1.34399200	4.06320600	0.49677300
C	-0.16051200	3.85137900	-0.22625600
C	3.23642300	5.12994000	0.44335000
C	2.36416100	6.09150400	1.27392600
H	-0.18200100	6.45122100	2.64885700
H	-2.24889100	5.20771300	2.06667300
H	3.51265100	4.26237500	1.05245100
H	2.41111400	7.11380700	0.87874900
C	2.30051200	4.65158400	-0.70366200
C	2.88680200	3.47245600	-1.46604800
C	2.26443500	5.72456000	-1.82940100
C	3.66805400	3.94325700	-2.52667100
C	2.80983600	2.10117900	-1.22628300
C	3.51675300	5.43911300	-2.67397800
H	2.22639700	6.74114900	-1.42782300
C	4.43646600	3.07279000	-3.28893100
C	3.59582700	1.20617500	-1.96597000
H	3.40597800	5.74514700	-3.71798600
C	4.41271900	1.71583800	-2.98286700
H	5.04436500	3.44036000	-4.11063100
H	5.02055700	1.01883100	-3.55300200
H	2.66344800	6.13566000	2.32469000
H	4.15391700	5.58883000	0.06372700
H	1.36683400	5.56156200	-2.43600400
H	4.39560500	5.95998600	-2.27461000
O	1.97340200	1.63174300	-0.23146300
O	-0.08920300	2.83323800	-1.16183100
P	0.37872500	1.38267900	-0.55251100
O	-0.23535100	1.15738200	0.79638400
O	0.17438900	0.39115800	-1.65761600
H	-0.89881100	-0.01329800	1.93442200
C	3.61999000	-0.26794700	-1.71511100
C	2.69988500	-1.07756400	-2.29848400
C	4.72402000	-0.85282300	-0.97319100
C	2.75357900	-2.50598300	-2.16970400
H	1.88868500	-0.64212500	-2.87218600
C	4.84951900	-2.26553400	-0.88508000
C	5.70300700	-0.03720500	-0.36061900

C	1.75020900	-3.30522500	-2.75602600
C	3.81270500	-3.11577200	-1.45587900
C	5.99200300	-2.80065900	-0.25043300
H	5.58893800	1.04135700	-0.40700800
C	6.79386400	-0.58870100	0.27740600
C	1.76515200	-4.67593400	-2.61652000
H	0.95290800	-2.81454300	-3.30955400
C	3.80513700	-4.52131300	-1.32512100
C	6.94929000	-1.98395700	0.31467400
H	6.12969700	-3.87510200	-0.20382800
H	7.53601600	0.05539700	0.73867000
C	2.80116200	-5.28460800	-1.88709000
H	0.97237500	-5.27886000	-3.05121100
H	4.58576100	-5.02012300	-0.76169200
H	7.81844000	-2.42291400	0.79454500
H	2.81231400	-6.36296200	-1.76137300
C	-2.57753400	3.29120800	0.17244300
C	-3.11978500	3.40877700	-1.06920900
C	-3.22252200	2.43800300	1.15736400
C	-4.32603400	2.73206800	-1.44894900
H	-2.64050800	4.04828400	-1.80657700
C	-4.40133400	1.72460400	0.80760900
C	-2.69140900	2.28724600	2.45888500
C	-4.87237300	2.91813100	-2.73802400
C	-4.97181400	1.87576400	-0.52550000
C	-4.99072000	0.87980200	1.77532800
H	-1.76455500	2.78989400	2.71123200
C	-3.31338300	1.48779800	3.39299600
C	-6.02563100	2.26650900	-3.11588100
H	-4.36277300	3.58610100	-3.42763000
C	-6.14328400	1.20761600	-0.94411300
C	-4.46660600	0.76637800	3.04554200
H	-5.87627800	0.30653800	1.52632700
H	-2.89674600	1.39294200	4.39227400
C	-6.65920200	1.39850200	-2.20960500
H	-6.44129400	2.41533300	-4.10770400
H	-6.65675600	0.52942200	-0.27216400
H	-4.93882800	0.11195400	3.77168100
H	-7.56093800	0.87073000	-2.50503900
C	-4.80169900	-1.33735100	-3.26689800
C	-4.97228700	-2.22083900	-2.21196900
C	-4.12023200	-2.17110200	-1.09831500
C	-3.10397000	-1.18723800	-1.07028200
C	-2.94852600	-0.28719500	-2.14144300

C	-3.78611100	-0.37006800	-3.23917000
H	-4.98382400	-3.90629600	-0.09925300
H	-5.46509600	-1.39208200	-4.12529700
H	-5.75827200	-2.97004600	-2.24549000
C	-4.24540000	-3.11450500	-0.00172300
C	-2.18421500	-1.15828700	0.03796800
H	-2.14622800	0.44596400	-2.09953900
H	-3.66717700	0.31891700	-4.06812700
C	-2.52069700	-1.93228800	1.22528500
C	-3.48983500	-3.02909100	1.11514500
H	-1.61506700	-0.24075000	0.16583000
N	-2.05093500	-1.68972500	2.42103600
N	-1.24051500	-0.68423200	2.65024300
C	-0.93043400	-0.40468000	3.97776600
O	-1.27413500	-1.04669400	4.93850400
O	-0.19311600	0.70810700	4.00270000
C	0.17581400	1.17131900	5.30397700
H	0.68767200	0.38809200	5.86603200
H	0.84143800	2.01602800	5.13423500
H	-0.71140000	1.49242400	5.85585200
C	-3.61224300	-3.99192500	2.25674300
H	-2.64794600	-4.47343800	2.45210000
H	-3.90021400	-3.47583300	3.17717200
H	-4.35397700	-4.76074000	2.03214600
C	-1.95423100	-5.91657400	-1.78279800
C	-2.22955600	-4.85829100	-2.65186700
C	-1.77532900	-3.56406600	-2.38450300
C	-1.04530600	-3.37811800	-1.22153300
C	-0.72070400	-4.44033700	-0.35981600
C	-1.18586700	-5.72024000	-0.63440900
H	-2.32505400	-6.90960200	-2.01616100
H	-1.98598400	-2.74294700	-3.06264600
H	-0.94290300	-6.55153100	0.02026200
C	0.33230700	-2.53780200	0.38715900
C	1.20693000	-1.72834700	1.10318100
C	1.92589800	-2.29631500	2.15577200
C	1.75264300	-3.66646500	2.43998000
C	0.89323400	-4.47311900	1.70818300
C	0.17232500	-3.90020100	0.66077300
H	1.30960900	-0.67713300	0.86860200
H	2.31396400	-4.11186500	3.25645900
H	0.79382600	-5.52939700	1.93909100
N	-0.54093900	-2.16090000	-0.67933300
H	-0.22165000	-1.38547800	-1.28937200

H	-2.80762000	-5.03935500	-3.55254000
C	2.87881800	-1.46306000	3.01798700
C	2.86585600	0.01433700	2.61316800
C	2.46208700	-1.58901300	4.49264300
C	4.31079000	-1.99002000	2.85031000
H	3.22251500	0.14704700	1.58565300
H	1.86600400	0.45597600	2.68441900
H	3.53491800	0.57694200	3.27328200
H	2.59804500	-2.60850300	4.86644300
H	3.07269600	-0.92394400	5.11353000
H	1.40933100	-1.32715100	4.63357900
H	4.99794900	-1.43213300	3.49706200
H	4.38807500	-3.05148500	3.10829800
H	4.63832100	-1.86431300	1.81581700

IMII-1

C	-0.95746100	4.49290300	0.03243900
C	-1.33915100	5.33573800	1.08017000
C	-2.49969300	5.07991900	1.79974600
C	-3.28410600	3.98059800	1.45345100
C	-2.89805500	3.09370500	0.44165200
C	-1.69988800	3.35526700	-0.23196400
C	0.88162300	5.90997700	0.43684800
C	-0.31320000	6.43216700	1.25982600
H	-2.79965900	5.72665000	2.61895500
H	-4.21102900	3.78626900	1.98565300
H	1.49229200	5.24296200	1.05506900
H	-0.68693100	7.38274400	0.86029800
C	0.23073600	5.07440100	-0.70144700
C	1.24080100	4.21848500	-1.44542800
C	-0.24592400	6.01425100	-1.84683600
C	1.74068900	4.92387300	-2.54542800
C	1.74364800	2.95225800	-1.16501500
C	1.00106700	6.22890900	-2.71761200
H	-0.67992500	6.94079600	-1.46128000
C	2.77153100	4.40408400	-3.31618900
C	2.81195900	2.42190000	-1.89527200
H	0.76021600	6.43749000	-3.76343500
C	3.31320100	3.17139400	-2.96741400
H	3.15480200	4.94981500	-4.17344500
H	4.14219500	2.75893300	-3.53496900
H	-0.06304500	6.59852600	2.31100300
H	1.52519700	6.70492600	0.04943700
H	-1.01364400	5.49197600	-2.42782800
H	1.60777500	7.06523500	-2.34964700
O	1.18413200	2.21204700	-0.12263600
O	-1.17623500	2.39860300	-1.11346400
P	-0.17427200	1.37592400	-0.36429200
O	-0.67122000	0.89256300	0.94380400
O	0.08081400	0.32831200	-1.49521400
H	-1.07720700	-0.53726800	2.23997000
C	3.51912500	1.14667300	-1.56324300
C	3.22855300	-0.00256800	-2.22444100
C	4.67671100	1.20205500	-0.68508500
C	4.05479000	-1.17340900	-2.11200800
H	2.37635500	-0.03815400	-2.89843500
C	5.53896100	0.07890800	-0.57960200
C	4.99073800	2.38046800	0.03047600
C	3.74369900	-2.33366100	-2.85197500

C	5.21905200	-1.14419500	-1.30543800
C	6.70405300	0.19916500	0.20992600
H	4.32500800	3.23490800	-0.04407700
C	6.12740000	2.46287500	0.80644400
C	4.56081500	-3.44185200	-2.80324300
H	2.84457500	-2.33931400	-3.46341500
C	6.02616200	-2.30098100	-1.25587200
C	6.99867600	1.36493400	0.88536800
H	7.39051300	-0.63560300	0.29298700
H	6.35097500	3.37659300	1.34802300
C	5.70762800	-3.42485600	-1.99137500
H	4.31359000	-4.32573500	-3.38258400
H	6.91579700	-2.32045700	-0.63688300
H	7.90229600	1.42809500	1.48355900
H	6.35001300	-4.29897200	-1.94408600
C	-3.79601100	1.97722500	0.03226900
C	-4.31472700	1.99990000	-1.22571200
C	-4.20923300	0.94239000	0.96209600
C	-5.32019600	1.07273800	-1.65508100
H	-4.00182000	2.77300500	-1.92373000
C	-5.21522000	0.01545200	0.57686600
C	-3.61443000	0.82683800	2.23983900
C	-5.85125600	1.15205800	-2.96199600
C	-5.80589800	0.09652800	-0.75287200
C	-5.60130500	-0.97888600	1.50234900
H	-2.81292100	1.50595700	2.51256800
C	-4.01750700	-0.15303800	3.12191900
C	-6.84173500	0.28768700	-3.37346800
H	-5.46434700	1.91174700	-3.63590600
C	-6.82535700	-0.77303900	-1.19891800
C	-5.02253100	-1.06035300	2.75059800
H	-6.36039700	-1.70354800	1.23184700
H	-3.55223900	-0.22686900	4.10048600
C	-7.33123500	-0.68194300	-2.47922100
H	-7.24618100	0.35543200	-4.37848500
H	-7.22164200	-1.53420100	-0.53667000
H	-5.33635100	-1.83645700	3.44150200
H	-8.11387600	-1.36359400	-2.79762400
C	-4.30589300	-3.32915000	-2.56588600
C	-3.72926600	-4.25815700	-1.70417000
C	-2.76634000	-3.86014200	-0.77307000
C	-2.38524700	-2.50752400	-0.72784000
C	-2.97923500	-1.57707500	-1.57313000
C	-3.93820000	-1.98660600	-2.49911900

H	-2.33677200	-5.87849100	-0.03560600
H	-5.05392700	-3.65071400	-3.28442800
H	-4.02250200	-5.30365400	-1.75014100
C	-2.14250100	-4.82247600	0.13822300
C	-1.25150300	-2.10686700	0.17814700
H	-2.67959200	-0.53091200	-1.51856800
H	-4.40460900	-1.25732000	-3.15482100
C	-1.22131800	-2.98737500	1.41341800
C	-1.40916800	-4.43718900	1.19939700
H	-1.38189100	-1.06016400	0.45066100
N	-1.08061400	-2.60027400	2.63027000
N	-0.99588600	-1.28885600	2.92792000
C	-0.90692600	-0.93201800	4.24880900
O	-0.78376900	-1.67740500	5.19299900
O	-0.96934100	0.41114300	4.33187800
C	-0.72442100	0.93919900	5.63601000
H	0.25939000	0.62778600	5.99638900
H	-0.76101900	2.02192200	5.52604100
H	-1.49004100	0.60271400	6.33859500
C	-0.84873800	-5.38761600	2.21333500
H	0.23091100	-5.24227400	2.32366900
H	-1.29386200	-5.20519500	3.19594800
H	-1.04257000	-6.42271100	1.92418900
C	1.07974400	-5.41394500	-3.06395300
C	-0.01776400	-4.63005800	-3.43492100
C	-0.41868300	-3.53463400	-2.67261700
C	0.29387700	-3.25200800	-1.50972600
C	1.43543000	-3.99412500	-1.16846200
C	1.82494600	-5.09017900	-1.93563000
H	1.36433100	-6.26494200	-3.67474000
H	-1.26186700	-2.93110700	-2.98634800
H	2.70586100	-5.66397500	-1.66367100
C	1.24707900	-2.23512100	0.29291800
C	1.59557300	-1.33674400	1.29084000
C	2.76062000	-1.55928100	2.02933300
C	3.55398300	-2.67997800	1.71942800
C	3.22065200	-3.55704000	0.69472900
C	2.04888000	-3.33385300	-0.02573800
H	0.97554000	-0.47465000	1.49021400
H	4.46097900	-2.86791700	2.28621700
H	3.86772100	-4.39521100	0.45334000
N	0.09100200	-2.17152900	-0.57124900
H	0.13829000	-0.65679700	-1.20313300
H	-0.57085100	-4.87145400	-4.33707200

C	3.14272000	-0.63204900	3.18759400
C	2.30907000	0.65431500	3.18907000
C	2.90091300	-1.38502700	4.50649900
C	4.61733700	-0.22078800	3.08103900
H	2.42663100	1.20577200	2.24943700
H	1.24210400	0.46350400	3.33702700
H	2.64412000	1.30226700	4.00612500
H	3.51906400	-2.28705600	4.56690100
H	3.15036900	-0.74469400	5.36071500
H	1.85216700	-1.68986200	4.59900300
H	4.88413900	0.43158100	3.92032100
H	5.29830700	-1.07672500	3.10074500
H	4.78797200	0.33145900	2.15310000

IMII-2

C	-4.10713200	1.88388600	1.30134800
C	-4.57067500	1.69873800	2.60693300
C	-4.97668400	0.44221300	3.04035900
C	-4.89144000	-0.63915900	2.16642000
C	-4.36945000	-0.49856500	0.87362200
C	-3.97625700	0.78321600	0.46986700
C	-3.58196800	3.85468200	2.48171200
C	-4.50350700	3.00010300	3.37197700
H	-5.34813100	0.29864700	4.05109900
H	-5.21059000	-1.62500400	2.49200100
H	-2.53452800	3.63478500	2.71801100
H	-5.49893900	3.45050900	3.46513000
C	-3.87721700	3.35943900	1.03623600
C	-2.85044200	3.87482600	0.04247900
C	-5.16205900	4.04990300	0.49464900
C	-3.27154900	5.10362300	-0.48126200
C	-1.62471300	3.36309800	-0.35319400
C	-4.67534500	5.41554200	-0.01986500
H	-5.94302500	4.12154000	1.25641800
C	-2.44542500	5.83776100	-1.32077300
C	-0.75253600	4.09006900	-1.17637600
H	-5.29883400	5.81384600	-0.82466500
C	-1.18540500	5.33725400	-1.64155100
H	-2.77411600	6.79100600	-1.72413300
H	-0.51741600	5.91087300	-2.27702900
H	-4.11274300	2.86876300	4.38500300
H	-3.74103300	4.93092600	2.59193800
H	-5.55072900	3.45846200	-0.34143200
H	-4.66245700	6.16273500	0.78292300
O	-1.25322500	2.07961000	0.05668200
O	-3.37851600	0.95956500	-0.78332700
P	-1.77832400	0.81817600	-0.78981700
O	-1.20755800	-0.42586100	-0.24151700
O	-1.49915800	1.13588900	-2.31374100
H	-0.18840000	-0.62753700	1.36071000
C	0.57641500	3.55873000	-1.58747600
C	0.86632100	3.46495400	-2.91384500
C	1.57905600	3.18103000	-0.60489600
C	2.12708500	2.97307800	-3.39042600
H	0.11468200	3.74604400	-3.64827500
C	2.82990600	2.66445200	-1.03901700
C	1.34767700	3.33851900	0.78043500
C	2.37650700	2.87930300	-4.77744700

C	3.10872000	2.54264900	-2.46513800
C	3.77725200	2.28513400	-0.06229500
H	0.40752400	3.76306400	1.11616900
C	2.29548200	2.97172900	1.70966100
C	3.56338500	2.35893300	-5.24449600
H	1.61061400	3.22192800	-5.46863700
C	4.30816700	1.99580600	-2.97041000
C	3.51919100	2.42966800	1.28422200
H	4.73151300	1.86908400	-0.36698300
H	2.09430300	3.10154600	2.76820100
C	4.53072800	1.90791800	-4.32950500
H	3.74984000	2.28940800	-6.31158200
H	5.06737000	1.61727600	-2.29334100
H	4.26305400	2.11565700	2.01168200
H	5.46077600	1.48007900	-4.69120000
C	-4.27129500	-1.66183100	-0.05242300
C	-4.92703900	-1.61730600	-1.24302200
C	-3.50934900	-2.84446200	0.30680700
C	-4.92930700	-2.72305700	-2.15539400
H	-5.49047800	-0.72865900	-1.51693300
C	-3.49542500	-3.96307600	-0.56764500
C	-2.75665600	-2.89760200	1.50091400
C	-5.63717500	-2.63910000	-3.37488200
C	-4.22750900	-3.90729900	-1.82640800
C	-2.74404600	-5.09889200	-0.19225100
H	-2.74501500	-2.02526200	2.14588200
C	-2.03181100	-4.01821200	1.84321300
C	-5.65864500	-3.69971800	-4.25242200
H	-6.16795200	-1.71922800	-3.60571100
C	-4.27141700	-4.98186900	-2.74213800
C	-2.03430700	-5.13271300	0.98848800
H	-2.71508200	-5.96623000	-0.84140000
H	-1.44425800	-4.01974200	2.75549400
C	-4.96776000	-4.88100900	-3.92863500
H	-6.20434400	-3.62739500	-5.18793200
H	-3.75082300	-5.90702000	-2.52314400
H	-1.46565700	-6.01953700	1.25108500
H	-4.98259200	-5.72169400	-4.61529300
C	0.98490600	-1.74344600	-4.35266600
C	1.23724300	-2.85089800	-3.54895800
C	1.50545600	-2.69666000	-2.18376200
C	1.51294600	-1.40189300	-1.64226100
C	1.25579500	-0.29648300	-2.44322300
C	0.99403600	-0.45937500	-3.80421900

H	2.00378600	-4.80089800	-1.80497200
H	0.78616500	-1.87962300	-5.41100600
H	1.23494200	-3.84856300	-3.97936700
C	1.81279500	-3.84508900	-1.32292200
C	1.91038800	-1.22862000	-0.19844800
H	1.28273200	0.69537400	-1.99713100
H	0.81958600	0.41038500	-4.43246100
C	1.41950000	-2.44110600	0.59052900
C	1.79125800	-3.75556800	0.01955300
H	1.48259500	-0.29793100	0.19081700
N	0.69603700	-2.45907500	1.64878800
N	0.15365900	-1.27831300	2.07149800
C	-0.54436600	-1.29447500	3.25510000
O	-0.50749700	-2.15854100	4.10239000
O	-1.25031100	-0.15347700	3.35405600
C	-1.91714500	0.02504000	4.60496800
H	-1.19405300	0.01875500	5.42442900
H	-2.40906300	0.99496800	4.54049500
H	-2.65496500	-0.76393500	4.76791400
C	1.98937800	-4.91325000	0.94791900
H	2.80666800	-4.70761300	1.64730500
H	1.08835700	-5.07282500	1.54802200
H	2.21569100	-5.82563400	0.39220200
C	6.84315600	-0.94222000	-2.40018500
C	5.64413600	-1.24892300	-3.05541200
C	4.42916400	-1.33157500	-2.38520500
C	4.41018000	-1.10909200	-0.99823600
C	5.63155300	-0.81738900	-0.33223600
C	6.83701300	-0.72547200	-1.03070100
H	7.77039100	-0.88244800	-2.96081700
H	3.54267800	-1.55331800	-2.95801300
H	7.75432600	-0.49398300	-0.49656500
C	3.94022900	-0.84571100	1.20164400
C	3.31309300	-0.72076000	2.43853700
C	4.07784200	-0.42966200	3.56978700
C	5.46594600	-0.23927300	3.43319500
C	6.09047400	-0.33982600	2.19463600
C	5.32848600	-0.65197500	1.06889900
H	2.24253000	-0.83074500	2.53530200
H	6.07024800	-0.00834700	4.30297200
H	7.16188400	-0.18112100	2.10702400
N	3.37989000	-1.12580400	-0.04340200
H	-0.92842500	0.45956800	-2.72373500
H	5.64980700	-1.42189500	-4.12764900

C	3.35637000	-0.35634000	4.92033600
C	2.25284100	0.71284200	4.86092400
C	2.72204900	-1.72620900	5.21557200
C	4.30546100	-0.00227400	6.06872700
H	2.68422900	1.70327000	4.67793300
H	1.52352800	0.51055300	4.06880000
H	1.71479400	0.75018100	5.81498100
H	3.49311400	-2.50065000	5.28672000
H	2.17818500	-1.69668600	6.16673200
H	2.01462200	-2.02462900	4.43577900
H	3.74279100	0.04309000	7.00685800
H	5.09141300	-0.75459400	6.19008400
H	4.78161900	0.97242300	5.91777500

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C	-4.11980400	-2.72489300	-0.19269000
C	-4.83670700	-3.51981000	0.70462400
C	-4.18839800	-4.48359500	1.46663100
C	-2.81063400	-4.63195100	1.33204800
C	-2.06158600	-3.81706300	0.47217000
C	-2.74070800	-2.85392800	-0.28781600
C	-6.24458000	-1.72802300	0.04670700
C	-6.29252300	-3.11689600	0.70810700
H	-4.74063400	-5.10473500	2.16586800
H	-2.28841500	-5.38359600	1.91757200
H	-6.00885900	-0.97288900	0.80493000
H	-6.89198400	-3.81907400	0.11544000
C	-5.05487400	-1.80954100	-0.95590800
C	-4.63923600	-0.42439800	-1.41749500
C	-5.53691900	-2.42479700	-2.29846400
C	-5.37505700	-0.06251800	-2.55189700
C	-3.75274500	0.48644900	-0.85593200
C	-6.17517500	-1.24367500	-3.05348400
H	-6.21962300	-3.26583200	-2.14615200
C	-5.29931700	1.22489500	-3.06607000
C	-3.71336900	1.81266600	-1.31197000
H	-6.11824600	-1.35409700	-4.14001700
C	-4.49553500	2.16205500	-2.41763000
H	-5.86740100	1.50548800	-3.94829700
H	-4.45982300	3.18836200	-2.77149000
H	-6.71885800	-3.09421600	1.71473500
H	-7.17995100	-1.44143800	-0.44264800
H	-4.66290200	-2.78646300	-2.85092900
H	-7.23513200	-1.13172300	-2.79448400
O	-2.89003800	0.08734200	0.14850200
O	-2.05205600	-1.97940900	-1.10465500
P	-1.48566200	-0.61444800	-0.36407800
O	-0.76356000	-1.00406700	0.89538400
O	-0.81917000	0.17977500	-1.43583600
C	-2.90928100	2.85697200	-0.61689100
C	-1.90625200	3.49759500	-1.27207400
C	-3.26569200	3.26862400	0.73207200
C	-1.18194700	4.58613300	-0.68003700
H	-1.63055400	3.18054400	-2.27506000
C	-2.57412800	4.34405900	1.34946200
C	-4.29826900	2.62160700	1.44803200
C	-0.16201800	5.24028000	-1.40567700
C	-1.50312300	5.01995000	0.62841200

C	-2.94033000	4.71833900	2.66165600
H	-4.84004800	1.80879400	0.97730900
C	-4.63326800	3.00590900	2.72769700
C	0.53743100	6.28990000	-0.85210900
H	0.05869800	4.89714800	-2.41297300
C	-0.76774200	6.09606200	1.17304800
C	-3.94616800	4.06492400	3.34173800
H	-2.42555000	5.53420900	3.15649700
H	-5.42814400	2.49054300	3.25751700
C	0.23146600	6.71657400	0.45186900
H	1.31806500	6.79004900	-1.41734500
H	-0.98506000	6.45393900	2.17289300
H	-4.20616700	4.37182300	4.35012900
H	0.77987900	7.54176400	0.89542000
C	-0.59470400	-4.04161100	0.34304900
C	-0.08273000	-4.39978200	-0.86586600
C	0.26956200	-4.02501900	1.51175400
C	1.28906600	-4.79200300	-1.02956300
H	-0.73343800	-4.43719100	-1.73648400
C	1.61322500	-4.46990700	1.40218400
C	-0.19859500	-3.56208400	2.76172500
C	1.77841700	-5.17543800	-2.30014900
C	2.15178900	-4.82330000	0.09415500
C	2.39498000	-4.54967900	2.57585600
H	-1.19635100	-3.14278500	2.82231100
C	0.59792700	-3.61905800	3.88505700
C	3.09377400	-5.54951300	-2.46740500
H	1.09300300	-5.17088500	-3.14416300
C	3.50150400	-5.18622200	-0.11191200
C	1.89526000	-4.14755000	3.79623100
H	3.40685900	-4.93676300	2.52704200
H	0.21998300	-3.25705000	4.83606500
C	3.96350900	-5.54014000	-1.36235900
H	3.45886200	-5.84464400	-3.44612100
H	4.20004800	-5.17186100	0.71635800
H	2.51670200	-4.21778500	4.68409100
H	5.00633100	-5.81123800	-1.49255900
H	0.82347800	-1.20357600	0.65605100
C	2.51589100	3.92117000	-4.54337100
C	2.16551600	2.62279800	-4.88330100
C	2.02704000	1.64773700	-3.88560900
C	2.22293800	1.98807200	-2.54109200
C	2.57211500	3.29160600	-2.20463900
C	2.72515800	4.25069000	-3.20342400

H	1.55384900	0.05988900	-5.28666500
H	2.63351000	4.67416200	-5.31540700
H	2.00675600	2.34446100	-5.92126500
C	1.73364300	0.27437600	-4.23481000
C	2.04385900	0.95090900	-1.44728500
H	2.73014300	3.55776200	-1.16319100
H	3.00935900	5.26250500	-2.93146900
C	1.88332600	-0.47057700	-1.95510900
C	1.68416300	-0.75685300	-3.35613100
H	1.05532000	1.14344000	-0.99706700
N	1.84838400	-1.47010400	-1.11199100
N	1.79136600	-1.31649700	0.24994400
C	2.93138900	-1.56579500	0.96770200
O	4.00811400	-1.84865800	0.48662200
O	2.67204300	-1.40848300	2.26735900
C	3.81446700	-1.49301900	3.11789700
H	4.55490400	-0.74248000	2.83015100
H	4.26323500	-2.48754500	3.06482100
C	1.37550700	-2.16154600	-3.78131700
H	2.20873800	-2.83941900	-3.56811800
H	0.48679600	-2.53254500	-3.25500400
H	1.17580000	-2.19458300	-4.85318200
C	2.82351500	2.20680400	3.53731200
C	1.58901500	1.92979400	2.90298100
C	1.58541500	1.56089400	1.56159100
C	2.80839700	1.47463600	0.89348500
C	4.04000300	1.73075900	1.52449400
C	4.03431700	2.10909200	2.87207800
H	2.82566400	2.49892100	4.58353900
H	0.66076200	1.29648700	1.05830500
H	4.96605300	2.31626700	3.39128000
C	4.41993600	1.10940800	-0.65204300
C	5.11962500	0.80478100	-1.81905900
C	6.50568500	0.89093300	-1.77484000
C	7.17755800	1.26941700	-0.60252500
C	6.47187100	1.57304500	0.55519800
C	5.07726000	1.49760500	0.53661100
H	4.60274100	0.50622900	-2.72685500
H	7.07886100	0.65728500	-2.66662600
H	8.26136500	1.32367100	-0.60274900
H	6.99559300	1.86438700	1.46114500
N	3.04980400	1.09474400	-0.42464300
C	0.29207100	2.02756700	3.71224200
C	-0.93400200	1.64923800	2.87635600

C	0.37191500	1.06881500	4.91177500
C	0.12075700	3.47069500	4.21300900
H	-1.02138400	2.28450100	1.98960700
H	-0.89556300	0.60799400	2.54407600
H	-1.84375000	1.79070200	3.47064400
H	1.19717800	1.32162300	5.58486500
H	-0.55799600	1.11224400	5.48952800
H	0.51310400	0.03880900	4.56686100
H	0.06541000	4.16601700	3.36719900
H	-0.80584100	3.56031400	4.79154100
H	0.95203900	3.78158400	4.85422900
H	3.44649600	-1.29474400	4.12433200
H	1.76237400	-2.42690600	-1.46141800

TSII-2Value of imaginary frequency = -1249.2 cm⁻¹

C	-1.51216900	4.46605400	0.11004100
C	-1.66215100	5.55713800	-0.74927400
C	-0.63032300	5.93482200	-1.59881800
C	0.55526600	5.20676700	-1.57737000
C	0.72199400	4.09041200	-0.74670000
C	-0.34082200	3.71924400	0.08821100
C	-3.80895500	5.01382200	0.09917500
C	-3.04554400	6.14682800	-0.60774000
H	-0.74369200	6.77747400	-2.27448200
H	1.37932500	5.49205300	-2.22536000
H	-4.16913500	4.29706400	-0.64714300
H	-3.01794800	7.05378300	0.00875000
C	-2.73826500	4.30918400	0.98405800
C	-3.23464100	2.95292000	1.44407600
C	-2.60497000	5.04476800	2.34540200
C	-3.92760900	3.08670200	2.65262600
C	-3.17379800	1.71433500	0.82139100
C	-3.76300600	4.48883100	3.19563300
H	-2.63060700	6.13218200	2.22924400
C	-4.62687300	2.01447800	3.18821900
C	-3.93512500	0.63801500	1.29746800
H	-3.54507700	4.49734400	4.26711600
C	-4.65435300	0.81065100	2.48459100
H	-5.15965500	2.11128300	4.12980700
H	-5.23935000	-0.02524500	2.85703200
H	-3.48525000	6.42072700	-1.57048200
H	-4.66622100	5.35796100	0.68477600
H	-1.64728400	4.77003500	2.80072500
H	-4.68100400	5.07027200	3.04629500
O	-2.32918300	1.53046400	-0.26969300
O	-0.27621200	2.56992600	0.86955000
P	-0.76953300	1.20395400	0.10294900
O	0.00001600	1.01851100	-1.15819300
O	-0.75227500	0.12381100	1.17524900
C	-4.05950000	-0.64478600	0.54840500
C	-3.59239600	-1.80261100	1.08387500
C	-4.78587300	-0.67341200	-0.71112000
C	-3.81409300	-3.07501300	0.45547400
H	-3.03599500	-1.77850100	2.01802200
C	-5.02616400	-1.91406300	-1.35955500
C	-5.25566400	0.51464500	-1.31383200
C	-3.32410200	-4.25696100	1.05261900

C	-4.54019800	-3.14836800	-0.75680100
C	-5.70995500	-1.90790700	-2.59485600
H	-5.09085800	1.46317200	-0.81424800
C	-5.91895700	0.49137300	-2.52139800
C	-3.53819200	-5.48580500	0.46987800
H	-2.77887900	-4.17193400	1.98780400
C	-4.75244800	-4.42271700	-1.32999000
C	-6.14573700	-0.73273900	-3.16979300
H	-5.89549000	-2.84086800	-3.11500600
H	-6.26568900	1.41804900	-2.96777100
C	-4.25989000	-5.56530100	-0.73405200
H	-3.15460400	-6.38862400	0.93492800
H	-5.30592700	-4.51842700	-2.25723500
H	-6.66539800	-0.75711500	-4.12254700
H	-4.43279500	-6.53096800	-1.19881600
C	2.05216100	3.41822400	-0.72339200
C	2.81409300	3.52622300	0.39762400
C	2.61168900	2.81316600	-1.91899000
C	4.17207900	3.06059100	0.44672600
H	2.40870800	4.01773500	1.27969100
C	3.96341800	2.37784500	-1.92190400
C	1.82838900	2.63736200	-3.08058000
C	4.93251800	3.19858600	1.63087900
C	4.75490900	2.46914400	-0.70079200
C	4.49891200	1.85417400	-3.11874100
H	0.78004700	2.91219300	-3.04881200
C	2.37166300	2.10010400	-4.22781400
C	6.22898000	2.73757200	1.69406100
H	4.47139900	3.67757000	2.49116300
C	6.07892400	1.98719800	-0.60005900
C	3.72406300	1.72370600	-4.25178100
H	5.53939800	1.55149600	-3.15915900
H	1.75341900	1.96737500	-5.11021200
C	6.79936200	2.11689700	0.56875300
H	6.80524100	2.84665500	2.60747800
H	6.54249300	1.49083600	-1.44459000
H	4.15922300	1.31624300	-5.15941700
H	7.81305000	1.73263200	0.61996300
H	1.62196900	0.31926800	-0.74607800
C	-0.77243800	-3.46686900	5.06373500
C	-0.14955700	-2.24602200	5.23226500
C	0.51166200	-1.63428900	4.15041800
C	0.52423700	-2.25353800	2.88816600
C	-0.10718300	-3.49409200	2.72995200

C	-0.73933200	-4.09257500	3.80902800
H	1.22780900	0.04804300	5.31126300
H	-1.27600000	-3.94547000	5.89686600
H	-0.15023600	-1.74827800	6.19812400
C	1.24791300	-0.41273100	4.32543300
C	1.16623500	-1.57488000	1.73610900
H	-0.09453500	-3.98295400	1.75994400
H	-1.21400600	-5.06087500	3.67872700
C	1.97943100	-0.40029200	2.03157600
C	1.97610400	0.19157000	3.34889200
H	0.18297800	-0.81809700	1.30522600
N	2.60683100	0.26796100	1.06673500
N	2.47422200	-0.01201100	-0.26706400
C	3.48503600	-0.65758500	-0.92738600
O	4.54044100	-0.99436600	-0.43690300
O	3.11123500	-0.85476200	-2.19605000
C	4.05953100	-1.55868300	-2.99424700
H	4.26574400	-2.53984700	-2.55914300
H	4.99140500	-0.99283700	-3.07521600
C	2.74465300	1.45694600	3.59539000
H	3.81171000	1.32451300	3.38459100
H	2.37290400	2.26993800	2.95955900
H	2.64076200	1.76429400	4.63707500
C	0.84549800	-3.70772700	-3.07012900
C	-0.02274200	-2.73549400	-2.52039200
C	0.19444400	-2.28556100	-1.22024700
C	1.27267600	-2.81000300	-0.50530100
C	2.13116200	-3.78655900	-1.04963400
C	1.90487100	-4.23629400	-2.35374100
H	0.67324800	-4.05480900	-4.08476100
H	-0.44315400	-1.53524300	-0.76853200
H	2.55574900	-4.98440600	-2.79844200
C	2.83203100	-3.26603400	1.06554800
C	3.59577400	-3.29501200	2.23236600
C	4.68047800	-4.16282500	2.26464300
C	4.99842500	-4.97884400	1.16762300
C	4.22822300	-4.94662700	0.01177600
C	3.13063000	-4.08448200	-0.04424300
H	3.35401100	-2.66483700	3.08404500
H	5.29493500	-4.20722800	3.15850700
H	5.85458800	-5.64300700	1.22660500
H	4.47388400	-5.58028500	-0.83578400
N	1.71553300	-2.48891700	0.77445000
C	-1.16815900	-2.19829800	-3.38405300

C	-2.00093100	-1.15370900	-2.63951300
C	-0.57714900	-1.54134600	-4.64199300
C	-2.09017900	-3.36078700	-3.78561900
H	-2.39103900	-1.55970300	-1.70117000
H	-1.41280200	-0.26185200	-2.41061100
H	-2.85995800	-0.85628100	-3.25185600
H	-0.02734700	-2.25974500	-5.25857900
H	-1.37816200	-1.11464900	-5.25628000
H	0.10935200	-0.73498400	-4.36193600
H	-2.51309100	-3.83961400	-2.89579000
H	-2.91909500	-2.98782700	-4.39848500
H	-1.56087000	-4.12473300	-4.36427100
H	3.59744700	-1.66981000	-3.97475600
H	3.13712200	1.10491200	1.29738800

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C	-4.73452500	1.80622700	-0.55724000
C	-5.40403100	2.31063200	-1.67608200
C	-4.86493600	3.36029500	-2.40925000
C	-3.64542600	3.90352800	-2.01454300
C	-2.93374100	3.39452400	-0.92071700
C	-3.49337000	2.32196600	-0.21734500
C	-6.45303800	0.27147100	-1.06402600
C	-6.67866300	1.53503400	-1.91190500
H	-5.38201300	3.75302200	-3.27978000
H	-3.21528000	4.73511100	-2.56551300
H	-5.88124800	-0.46138900	-1.64417400
H	-7.54697000	2.10366800	-1.55729900
C	-5.57657500	0.75221700	0.13005400
C	-4.97195800	-0.42891000	0.86303300
C	-6.48195200	1.34529200	1.24547100
C	-5.85411700	-0.86974500	1.85717000
C	-3.80020400	-1.13522800	0.64122800
C	-6.99169800	0.11348300	2.01687100
H	-7.28332000	1.96778500	0.83765100
C	-5.61404100	-2.05067400	2.54566600
C	-3.56105200	-2.36019400	1.27358100
H	-7.20603000	0.32999800	3.06684300
C	-4.48894500	-2.80687100	2.21808000
H	-6.29612000	-2.39124900	3.31911100
H	-4.30757500	-3.75805100	2.70965500
H	-6.84389700	1.31395000	-2.96957500
H	-7.37871500	-0.20373200	-0.72795000
H	-5.86575600	1.96609100	1.90467600
H	-7.91214000	-0.28396600	1.57276700
O	-2.81222200	-0.60796600	-0.20189500
O	-2.78908400	1.72572500	0.83548300
P	-1.82795700	0.49337600	0.44026800
O	-0.70243900	0.81468100	-0.45381300
O	-1.46870800	-0.03102700	1.89047800
C	-2.41096500	-3.23307900	0.89632600
C	-1.27351000	-3.26776600	1.63662000
C	-2.56521300	-4.12280800	-0.24214300
C	-0.21029700	-4.19201300	1.35071000
H	-1.16128700	-2.60062900	2.48783900
C	-1.54226300	-5.05755800	-0.54675900
C	-3.71481000	-4.06714900	-1.06299700
C	0.95371200	-4.20973400	2.14922000
C	-0.34343200	-5.10893000	0.27994400

C	-1.71315100	-5.89847300	-1.66759900
H	-4.49966100	-3.35510800	-0.82792500
C	-3.85050700	-4.89596200	-2.15593300
C	1.95681500	-5.12276100	1.90889000
H	1.04654200	-3.49303100	2.96259400
C	0.70119100	-6.03281000	0.05709600
C	-2.83893400	-5.82035400	-2.46014100
H	-0.94321400	-6.61540300	-1.92949100
H	-4.73759600	-4.83468500	-2.77841600
C	1.82550700	-6.04286300	0.85573900
H	2.84624000	-5.12930600	2.52951500
H	0.62897600	-6.75555800	-0.74756700
H	-2.93943900	-6.47545500	-3.31989900
H	2.61347200	-6.76501600	0.66667100
C	-1.66133800	4.03879300	-0.48918600
C	-1.63566100	4.70380200	0.69685500
C	-0.48961200	4.03608900	-1.34452400
C	-0.46015200	5.37689100	1.16707600
H	-2.52335200	4.72203000	1.32492800
C	0.68029600	4.72709600	-0.93253000
C	-0.49005800	3.36296100	-2.58807600
C	-0.45270300	5.99876500	2.43470100
C	0.71530000	5.36838300	0.37720500
C	1.78517000	4.76609000	-1.81328100
H	-1.36632600	2.79394800	-2.87931100
C	0.60119300	3.41970000	-3.42661300
C	0.69641400	6.57510300	2.92919900
H	-1.36824100	5.99805800	3.02038200
C	1.88415900	5.95146200	0.91535700
C	1.74111100	4.14523200	-3.04252900
H	2.68586700	5.29847400	-1.53097200
H	0.58406300	2.89643300	-4.37756800
C	1.87647000	6.53847100	2.16410800
H	0.69760700	7.04393500	3.90819000
H	2.81245100	5.92590000	0.35634400
H	2.60061300	4.20092100	-3.70365000
H	2.79025800	6.97144100	2.55863500
H	1.15798600	1.13351600	-1.20160500
C	2.93036500	-2.60672000	4.88389100
C	2.07791400	-1.53108500	4.84203400
C	2.04504300	-0.68190400	3.70670100
C	2.87159700	-0.96966100	2.58850400
C	3.72993700	-2.10005700	2.64948200
C	3.76901300	-2.88262800	3.77817700

H	0.59613100	0.70415900	4.52072800
H	2.96617100	-3.24358700	5.76193400
H	1.43188700	-1.29847100	5.68444600
C	1.23092200	0.48001700	3.66598800
C	2.85731100	-0.08614700	1.46463500
H	4.36105800	-2.33589100	1.79858600
H	4.44664100	-3.73021200	3.81934800
C	2.06794500	1.05472500	1.45681600
C	1.23673800	1.34186100	2.59730700
H	-0.50763300	-0.05974900	2.05971300
N	2.09170100	1.99487300	0.42064300
N	2.02658700	1.55194600	-0.88082000
C	3.08641000	1.71770600	-1.71672900
O	4.13792000	2.25900000	-1.45148200
O	2.78839400	1.17137500	-2.91364600
C	3.82703100	1.26039700	-3.88241300
H	4.76543100	0.87130000	-3.48111600
H	3.97611700	2.29766100	-4.19796100
C	0.38974400	2.58404500	2.60839700
H	1.01322400	3.48663500	2.62513700
H	-0.24884000	2.64845100	1.71896200
H	-0.25514700	2.60292200	3.48943700
C	3.32584900	-2.32543900	-3.20153500
C	2.13632200	-2.12857500	-2.45863500
C	2.21270400	-1.52149800	-1.21071000
C	3.46036100	-1.08913100	-0.75570300
C	4.64334000	-1.27164200	-1.49532500
C	4.56338600	-1.91517100	-2.73599900
H	3.26590900	-2.80643500	-4.17377500
H	1.32786000	-1.32769300	-0.61288000
H	5.45687100	-2.07377800	-3.33424100
C	5.11669200	-0.11298500	0.42595400
C	5.86214600	0.54986000	1.40038800
C	7.22821800	0.67562200	1.18238300
C	7.83863500	0.15469500	0.02997400
C	7.08876800	-0.51121700	-0.93096900
C	5.71314900	-0.65675900	-0.73434400
H	5.38663500	0.95757600	2.28687300
H	7.83614200	1.19050700	1.92013300
H	8.90837200	0.27498800	-0.10860500
H	7.56254600	-0.91642800	-1.82078700
N	3.75124700	-0.36719900	0.39616000
C	0.79719900	-2.54233000	-3.07584700
C	-0.38316600	-2.22289600	-2.15387100

C	0.59861900	-1.77055600	-4.39159100
C	0.80636400	-4.05184000	-3.36151600
H	-0.27818600	-2.71747400	-1.18268100
H	-0.48232100	-1.14626400	-1.98035900
H	-1.31432200	-2.58114600	-2.60761200
H	1.38053200	-2.00196700	-5.12189300
H	-0.36763100	-2.03023100	-4.83875900
H	0.61322100	-0.69073000	-4.20739900
H	0.93386400	-4.61575200	-2.43070200
H	-0.14172700	-4.35577400	-3.81951100
H	1.61683800	-4.33018400	-4.04246500
H	3.49884000	0.65465400	-4.72727300
H	1.47725700	2.78705000	0.56733900

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C	2.85817800	-0.09537700	5.34225800
C	3.76513000	-0.91928300	4.72010700
C	3.54599500	-1.34956600	3.38683600
C	2.37359700	-0.90591300	2.71165100
C	1.44568700	-0.06230700	3.38029000
C	1.68660300	0.33517900	4.67061600
H	5.32546500	-2.57111200	3.24589100
H	3.03534400	0.22757000	6.36393000
H	4.65850300	-1.25329300	5.24102900
C	4.44973800	-2.21359200	2.70891900
C	2.17060900	-1.29994100	1.37331900
H	0.55544600	0.25112100	2.84046000
H	0.98225500	0.98185700	5.18425100
C	3.08164600	-2.11502300	0.73511700
C	4.23524800	-2.62353300	1.41609300
H	1.26544500	-0.98307900	0.86938200
N	2.93592800	-2.53050600	-0.60439800
N	2.09873800	-1.91726100	-1.29525000
C	2.04391200	-2.46495000	-2.63917400
O	2.55740200	-3.47658700	-3.03168700
O	1.29131800	-1.64001200	-3.35665400
C	1.12484700	-2.01384600	-4.72803300
H	0.58286700	-2.95962700	-4.79505200
H	0.55048800	-1.21105900	-5.18667700
H	2.09936900	-2.11863300	-5.21087300
C	5.16202500	-3.59022900	0.73285000
H	4.63395200	-4.51440500	0.47864800
H	5.54832000	-3.18252600	-0.20434700
H	6.00132500	-3.83817700	1.38601600
C	-3.24802400	2.69812000	0.44982600
C	-4.03651800	3.11687800	1.52650600
C	-4.85096400	2.21447800	2.19874500
C	-4.85974700	0.88031500	1.79878800
C	-4.03263300	0.41744300	0.76766000
C	-3.22223800	1.35266400	0.11224800
C	-2.50644200	4.86460900	1.02154500
C	-3.80264800	4.58379600	1.80467200
H	-5.46666800	2.53739700	3.03311400
H	-5.49702700	0.16480600	2.31054900
H	-1.63968800	4.59869800	1.63650600
H	-4.63575600	5.18968500	1.42838700
C	-2.57041700	3.89496900	-0.19179400
C	-1.23992200	3.79357200	-0.91511400

C	-3.45404300	4.51386400	-1.31370300
C	-1.17735600	4.74535900	-1.93983000
C	-0.15107600	2.96193900	-0.69845300
C	-2.50463500	5.45303300	-2.07674800
H	-4.33818100	5.01582000	-0.91097000
C	-0.01998500	4.90848900	-2.68824000
C	1.03229200	3.10176900	-1.43575900
H	-2.79467000	5.59686700	-3.12094600
C	1.07891600	4.09576100	-2.41990800
H	0.02833500	5.64826900	-3.48200300
H	1.99429800	4.20888200	-2.99299200
H	-3.70609900	4.79271600	2.87345300
H	-2.40023700	5.90754000	0.71006300
H	-3.78832200	3.71016000	-1.97862300
H	-2.46418900	6.44440800	-1.60923200
O	-0.24366500	1.94374800	0.24858600
O	-2.29911200	0.91413500	-0.84418500
P	-0.87284000	0.52250900	-0.20045900
O	-0.89684000	-0.38342800	0.95945900
O	-0.13579700	0.05775300	-1.51009300
C	2.19069300	2.18077900	-1.26717900
C	2.59757700	1.46206700	-2.34821000
C	2.91274600	2.06608600	-0.01214800
C	3.70571700	0.55718000	-2.29055900
H	2.04659600	1.53754600	-3.28266400
C	4.03741700	1.20168700	0.07310900
C	2.54146600	2.82224100	1.12270500
C	4.04664900	-0.21893500	-3.42114100
C	4.43132800	0.41134500	-1.08551700
C	4.74440500	1.13373400	1.29392600
H	1.69149700	3.49331500	1.05618200
C	3.24424200	2.72717000	2.30366200
C	5.06932300	-1.13911500	-3.36169300
H	3.47373300	-0.08250100	-4.33524600
C	5.48580700	-0.52660500	-1.05657400
C	4.35775400	1.87598100	2.38876400
H	5.60958300	0.48621400	1.38203500
H	2.93903800	3.31067200	3.16666300
C	5.79328200	-1.28974800	-2.16571800
H	5.31604600	-1.74540000	-4.22744600
H	6.05831200	-0.67700400	-0.14763400
H	4.91444900	1.80083900	3.31767300
H	6.60295200	-2.01133600	-2.11307900
C	-4.05683000	-1.01555700	0.36097700

C	-4.40487300	-1.33570600	-0.91352400
C	-3.77757700	-2.07157500	1.31772000
C	-4.56185000	-2.69435200	-1.34379000
H	-4.60308700	-0.54547100	-1.63351200
C	-3.95271900	-3.42824400	0.93803900
C	-3.30214400	-1.77675200	2.61553200
C	-4.94347700	-2.98082400	-2.67311100
C	-4.36610000	-3.75064300	-0.42215000
C	-3.69538800	-4.43296800	1.89776800
H	-3.10935600	-0.74341400	2.88090200
C	-3.04808900	-2.77797700	3.52614200
C	-5.13148500	-4.28005500	-3.08815900
H	-5.08760600	-2.15346100	-3.36283300
C	-4.56931900	-5.07334900	-0.87400400
C	-3.26029500	-4.11883500	3.16693300
H	-3.83006600	-5.47669400	1.63809800
H	-2.67459700	-2.53076700	4.51486500
C	-4.94382400	-5.33346500	-2.17575300
H	-5.42361700	-4.49229700	-4.11182600
H	-4.43144400	-5.90754300	-0.19596800
H	-3.06732500	-4.91134900	3.88322300
H	-5.09317800	-6.35965800	-2.49688500
H	0.66771900	-0.49715400	-1.36551100

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C	-4.51956400	5.58252500	-0.94134900
C	-4.80877100	4.21276800	-1.06012300
C	-3.81091800	3.24913900	-1.00571200
C	-2.49777300	3.68769000	-0.82672700
C	-2.18952900	5.06422700	-0.70424700
C	-3.21291300	6.01431500	-0.76329300
H	-5.32698100	6.30617800	-0.99073200
H	-4.03632100	2.19289800	-1.10139100
H	-2.98609000	7.07283300	-0.67078800
C	-0.27005800	3.81732200	-0.55958200
C	1.08570800	3.53045200	-0.41531300
C	1.98279600	4.58381000	-0.22750700
C	1.49809900	5.90697800	-0.20141600
C	0.14763000	6.19390200	-0.35243000
C	-0.75525900	5.14654500	-0.53041000
H	1.42815300	2.50003900	-0.45464800
H	2.19008800	6.72859600	-0.05896400
H	-0.19937800	7.22326000	-0.32816000
N	-1.33095500	2.95425300	-0.74059100
H	-1.25536500	1.94177600	-0.77123000
C	-1.21853500	-4.02527500	-0.79204900
C	-1.86241600	-4.66570500	-1.85510100
C	-3.13337500	-4.26897900	-2.24448900
C	-3.74566500	-3.21789800	-1.57099500
C	-3.09103600	-2.49033100	-0.56365500
C	-1.80006800	-2.91051400	-0.20707700
C	0.36830700	-5.48171800	-1.75836400
C	-0.99506000	-5.76952600	-2.41193500
H	-3.65421100	-4.77889200	-3.04944200
H	-4.76086700	-2.93948200	-1.83290000
H	0.92446900	-4.75720100	-2.36348900
H	-1.38087200	-6.75270900	-2.11731500
C	0.00796500	-4.82112600	-0.39747600
C	1.22694200	-4.21819400	0.27033700
C	-0.36832200	-5.92220200	0.63659400
C	1.83991400	-5.18162000	1.08117900
C	1.81014500	-2.96598700	0.14045600
C	0.98335400	-6.42092300	1.17138600
H	-0.98366000	-6.70990700	0.19367900
C	3.06069100	-4.92635700	1.68568100
C	3.06939900	-2.69356200	0.69445300
H	0.92201300	-6.80975400	2.19121300
C	3.67581600	-3.69926800	1.45997100

H	3.53711500	-5.67217000	2.31502700
H	4.65357200	-3.49770600	1.88609200
H	-0.95441200	-5.75126700	-3.50438500
H	0.98978000	-6.37252800	-1.63255400
H	-0.93816200	-5.45758000	1.44861900
H	1.39265200	-7.21975900	0.54127700
O	1.12068600	-1.95728600	-0.54362700
O	-1.06972800	-2.21506800	0.76662100
P	-0.01018600	-1.12320400	0.25087400
O	-0.51929700	-0.02126600	-0.58278900
O	0.61073100	-0.75207300	1.66201500
C	3.83346300	-1.42632500	0.51007300
C	4.29548200	-0.78440800	1.61893100
C	4.26443700	-0.98191100	-0.80640100
C	5.26028000	0.27434000	1.54928700
H	3.97386200	-1.11792300	2.60294000
C	5.20326000	0.08006600	-0.91416500
C	3.80398600	-1.60745800	-1.98730800
C	5.76475300	0.85822700	2.73265000
C	5.74871700	0.69403100	0.28996000
C	5.59902700	0.50196400	-2.20322300
H	3.11940500	-2.44452400	-1.91564000
C	4.21109900	-1.17679700	-3.23061900
C	6.74979600	1.81930800	2.67953200
H	5.37078200	0.52173700	3.68797200
C	6.76421000	1.67646000	0.26448100
C	5.10971700	-0.10407800	-3.33982200
H	6.29889800	1.32280600	-2.31062300
H	3.83652200	-1.66728000	-4.12334800
C	7.25635900	2.22514000	1.43159900
H	7.13896200	2.25669500	3.59339900
H	7.18264700	2.00393200	-0.68076800
H	5.42659500	0.24470600	-4.31749300
H	8.04170900	2.97317700	1.38317300
C	-3.82442900	-1.41600700	0.16037100
C	-3.82050100	-1.40494400	1.52204900
C	-4.67880300	-0.47934400	-0.55656600
C	-4.65636700	-0.52569200	2.28575400
H	-3.20070800	-2.11120600	2.06761500
C	-5.59825400	0.32655500	0.16693800
C	-4.61876500	-0.34338200	-1.96401100
C	-4.60018000	-0.53884000	3.69697200
C	-5.57376600	0.32329800	1.62402400
C	-6.50544900	1.13046300	-0.55935000

H	-3.85726600	-0.88398200	-2.51442900
C	-5.49721200	0.47143500	-2.64489700
C	-5.42495700	0.27401700	4.44179500
H	-3.89033900	-1.20338100	4.18222800
C	-6.40660300	1.14827000	2.41171700
C	-6.47397900	1.18909400	-1.93640000
H	-7.24386600	1.72177700	-0.03010500
H	-5.42903600	0.56017200	-3.72439400
C	-6.33395700	1.12494300	3.78899900
H	-5.37355100	0.26159900	5.52585300
H	-7.10897700	1.82636500	1.94089900
H	-7.18565100	1.81277800	-2.46857900
H	-6.98123600	1.77230700	4.37230400
H	1.04252900	0.11813200	1.66799300
H	-5.83759900	3.89526400	-1.19973600
C	3.46630400	4.25874000	-0.03578400
C	3.62378100	3.37564500	1.21209300
C	3.98846700	3.50575900	-1.26908100
C	4.32487000	5.51199100	0.15815900
H	3.21041500	3.87604600	2.09457200
H	3.10845500	2.41692200	1.09184100
H	4.68132900	3.16585100	1.39838700
H	3.87129200	4.11276200	-2.17328600
H	5.05207100	3.27508600	-1.14354200
H	3.45803300	2.56125700	-1.42375000
H	5.37000400	5.21351300	0.29316500
H	4.27612700	6.17764500	-0.70992300
H	4.02366600	6.07868700	1.04524500

COMIII

C	4.70270300	-3.59713000	1.30344000
C	3.61912300	-4.43107900	1.40314500
C	2.32164900	-3.90055700	1.62305900
C	2.16387900	-2.48772600	1.71720200
C	3.30184400	-1.64424500	1.58100300
C	4.54308100	-2.19058300	1.39205300
H	1.33060100	-5.81580900	1.72323100
H	5.69260400	-4.01188900	1.13995500
H	3.73692300	-5.50810300	1.31953500
C	1.19143800	-4.74011300	1.80008400
C	0.88176100	-1.96826500	1.98024100
H	3.16561200	-0.56580900	1.62552500
H	5.40980500	-1.54631600	1.28838200
C	-0.19414000	-2.81766700	2.17891800
C	-0.05096700	-4.24211600	2.09946800
H	0.76625400	-0.89599000	2.10663900
N	-1.44638400	-2.35990400	2.61341000
N	-1.71112100	-1.14945300	2.46888600
C	-2.96145000	-0.81779600	3.12287200
O	-3.88331100	-1.56296700	3.31101200
O	-2.88248300	0.45515000	3.48774400
C	-3.94784300	0.92815500	4.32307600
H	-3.93589100	0.38949800	5.27317200
H	-3.75008000	1.98674000	4.47994500
H	-4.91844300	0.78597800	3.84310700
C	-1.21861800	-5.16091600	2.32285200
H	-1.82551600	-4.84303700	3.17379600
H	-1.86920400	-5.17745400	1.44293300
H	-0.86526000	-6.17994100	2.49534600
C	5.01458800	-4.30529200	-2.22689600
C	5.16073700	-2.91133700	-2.10925700
C	4.07681600	-2.08676800	-1.84578900
C	2.82571000	-2.68971900	-1.69558700
C	2.65986800	-4.09296900	-1.80953100
C	3.76968600	-4.90068000	-2.07965400
H	5.88534500	-4.91772900	-2.43965200
H	4.19219700	-1.01295900	-1.73956900
H	3.65632300	-5.97754500	-2.17221200
C	0.64120600	-3.09380700	-1.38215500
C	-0.73387900	-2.96522600	-1.18483500
C	-1.52731800	-4.11332500	-1.19564700
C	-0.91004500	-5.37251200	-1.36423200
C	0.45762200	-5.49925300	-1.56822800

C	1.25204500	-4.35187400	-1.59994100
H	-1.16831000	-1.97665600	-1.06099300
H	-1.51593600	-6.27129000	-1.35390200
H	0.89980200	-6.48177700	-1.71128100
N	1.60296300	-2.10891000	-1.44138900
H	1.42863200	-1.12520400	-1.25560500
C	0.62542000	4.72972500	-0.67119200
C	1.09034500	5.57771800	-1.67941200
C	2.35546100	5.39607500	-2.21994200
C	3.14906000	4.36238600	-1.73713700
C	2.69273700	3.45837100	-0.76328700
C	1.39548500	3.65067700	-0.26369600
C	-1.20636600	6.06379700	-1.33573600
C	0.05688700	6.62843900	-2.00558700
H	2.73262200	6.06075300	-2.99140800
H	4.15973900	4.24730400	-2.11499300
H	-1.70613100	5.36941600	-2.02018400
H	0.34143400	7.59561400	-1.57349300
C	-0.67593500	5.25926500	-0.11089700
C	-1.77871600	4.38065500	0.44308500
C	-0.44465100	6.22116600	1.08715200
C	-2.53925200	5.11979900	1.35525600
C	-2.18464700	3.10149200	0.08766400
C	-1.84895700	6.42268300	1.68591900
H	0.03628300	7.15381900	0.77957300
C	-3.75774100	4.63656400	1.80924900
C	-3.46413100	2.63590400	0.43031500
H	-1.82821900	6.61810600	2.76154900
C	-4.22884400	3.43031900	1.29926600
H	-4.35683600	5.20669800	2.51316600
H	-5.22310400	3.08526500	1.56637200
H	-0.06271700	6.77696800	-3.08215100
H	-1.92857500	6.82991200	-1.04115900
H	0.20456300	5.72387900	1.81581900
H	-2.36840800	7.26470300	1.21329500
O	-1.30496500	2.27130100	-0.61313800
O	0.85508000	2.79016800	0.69164900
P	-0.09019500	1.57466300	0.20700900
O	0.55734300	0.55126000	-0.63387400
O	-0.64270200	1.16891800	1.61259400
C	-4.10357200	1.40746600	-0.12201900
C	-4.76604800	0.58127100	0.73446400
C	-4.21914400	1.17760000	-1.55635600
C	-5.61838700	-0.48057800	0.29386100

H	-4.70009800	0.76575200	1.80080300
C	-5.01952400	0.10100300	-2.03005900
C	-3.59752800	2.02430800	-2.50255500
C	-6.32547400	-1.26219700	1.23415900
C	-5.76435800	-0.72667300	-1.08964800
C	-5.09272100	-0.12601600	-3.42259800
H	-3.03047900	2.88256100	-2.16384900
C	-3.70069400	1.78805100	-3.85555500
C	-7.17020400	-2.26645000	0.81697400
H	-6.17629200	-1.06551400	2.29193700
C	-6.64468100	-1.75671600	-1.49002800
C	-4.44130000	0.69074900	-4.32048800
H	-5.67041700	-0.96152800	-3.80111600
H	-3.20729600	2.45097200	-4.55917000
C	-7.32965300	-2.51145800	-0.55906800
H	-7.70997200	-2.86611000	1.54289900
H	-6.80215200	-1.96462300	-2.54239100
H	-4.51079800	0.48974100	-5.38480200
H	-8.00023200	-3.29657700	-0.89443700
C	3.65387000	2.47254100	-0.19669900
C	3.81224300	2.40231600	1.15388700
C	4.55924600	1.72796600	-1.05971500
C	4.90465100	1.69848700	1.76136400
H	3.14230700	2.95574300	1.80658000
C	5.69018100	1.07762000	-0.49746900
C	4.33809000	1.63013800	-2.45373800
C	5.03970500	1.67121700	3.16745200
C	5.88823400	1.08949800	0.94652500
C	6.58941400	0.41933600	-1.36650500
H	3.44001000	2.06582600	-2.87751200
C	5.22989000	0.97694900	-3.27672500
C	6.12869700	1.07132500	3.75905400
H	4.26826300	2.14038300	3.77229200
C	7.00759700	0.50332400	1.57869000
C	6.37831400	0.38378600	-2.72877200
H	7.46369700	-0.07832000	-0.96207800
H	5.03586500	0.90975200	-4.34228400
C	7.12478900	0.49169900	2.95339400
H	6.22435900	1.05250200	4.83992300
H	7.79137600	0.04482800	0.98619600
H	7.08737200	-0.12690400	-3.37305700
H	7.99227000	0.03029000	3.41465500
H	-1.00220400	0.24091600	1.76375400
H	6.14433000	-2.46520900	-2.22493100

C	-3.05105500	-3.96544600	-1.12336600
C	-3.46795200	-3.08131300	0.06133500
C	-3.51840100	-3.30712900	-2.43386500
C	-3.76947400	-5.31221200	-0.98646700
H	-3.14551000	-3.50682100	1.01718500
H	-3.05435500	-2.06952800	-0.01211100
H	-4.55810700	-2.99410400	0.08605400
H	-3.21825900	-3.91004200	-3.29784200
H	-4.60995400	-3.21145000	-2.44122100
H	-3.08771400	-2.30788000	-2.55185800
H	-4.84827100	-5.13845200	-0.91389800
H	-3.59529600	-5.95724400	-1.85352600
H	-3.45793700	-5.85500700	-0.08715400

TSIII-1Value of imaginary frequency = -237.8 cm⁻¹

C	5.04958400	-3.15590400	2.27070000
C	4.10030000	-4.13946300	2.02142700
C	2.77171700	-3.78822200	1.75764800
C	2.43231500	-2.41396700	1.70479500
C	3.40576100	-1.42863400	1.94033800
C	4.70527300	-1.79903400	2.24548400
H	2.03835700	-5.82986100	1.51297800
H	6.07392300	-3.44232900	2.49040600
H	4.37654700	-5.18959100	2.04839200
C	1.73377600	-4.78800900	1.57173100
C	1.08379900	-2.05641400	1.36376600
H	3.12416300	-0.37877200	1.88051800
H	5.45367600	-1.04223900	2.45070400
C	0.05539800	-3.04491000	1.64731900
C	0.42236400	-4.46478600	1.55458400
H	0.82372400	-1.00053900	1.41671600
N	-1.15393500	-2.78250700	2.06418700
N	-1.56309800	-1.54597100	2.27567500
C	-2.67650500	-1.39610700	3.10469500
O	-3.44605800	-2.26677500	3.42340700
O	-2.70741300	-0.12881200	3.52810900
C	-3.67669700	0.15563500	4.54034200
H	-3.44040500	-0.40023800	5.45072200
H	-3.60366000	1.22751300	4.71932500
H	-4.68408000	-0.10680200	4.21063500
C	-0.67549000	-5.47951500	1.46811600
H	-1.30333500	-5.44887400	2.36382800
H	-1.32510400	-5.26085800	0.61376200
H	-0.26238700	-6.48402400	1.35699100
C	4.43438400	-4.24891000	-1.96061100
C	4.65760500	-2.96959200	-1.44544500
C	3.59834500	-2.14133500	-1.07211200
C	2.31701200	-2.65513500	-1.19923300
C	2.07471300	-3.92688100	-1.74917200
C	3.13866900	-4.73351600	-2.13546100
H	5.28145900	-4.86713200	-2.24033200
H	3.76983100	-1.14123400	-0.69040300
H	2.96504900	-5.71671200	-2.56197700
C	0.06597400	-2.93270100	-1.23431300
C	-1.29696500	-2.74323200	-1.12924600
C	-2.15098900	-3.76058400	-1.59787800
C	-1.59012300	-4.91920900	-2.14890300

C	-0.20878800	-5.09954500	-2.24921900
C	0.62749000	-4.09604300	-1.78900800
H	-1.69209600	-1.82343100	-0.70500700
H	-2.23844100	-5.70994500	-2.50768600
H	0.19669900	-6.00694400	-2.68664400
N	1.09966400	-2.07771000	-0.75359600
H	0.96116400	-1.04057100	-0.85329400
C	0.84286600	4.60383100	-0.59570400
C	1.23312100	5.43750100	-1.64553800
C	2.40078500	5.17998900	-2.35160100
C	3.18294300	4.09563800	-1.97133300
C	2.80103500	3.22672100	-0.93689100
C	1.58476700	3.47177700	-0.28299600
C	-0.97353000	6.05106300	-1.02363200
C	0.23507300	6.55554300	-1.82931300
H	2.71212500	5.82085600	-3.17122500
H	4.12564400	3.91044400	-2.47781300
H	-1.59113500	5.40563300	-1.65801900
H	0.62811300	7.49261100	-1.41580700
C	-0.35819600	5.18273100	0.11555300
C	-1.43752400	4.33536700	0.75630800
C	0.04739700	6.08807100	1.31009600
C	-2.05628200	5.06701600	1.77441300
C	-1.93849200	3.09419600	0.37903100
C	-1.26898400	6.32290500	2.07468300
H	0.53229700	7.01179700	0.98090100
C	-3.24394500	4.61931800	2.33557600
C	-3.20958900	2.69118900	0.82472900
H	-1.11514000	6.46922200	3.14760100
C	-3.83069400	3.47034100	1.81390600
H	-3.73559600	5.17548600	3.12843000
H	-4.81047800	3.16036600	2.16442800
H	-0.00059400	6.73945300	-2.88118700
H	-1.60829900	6.85261300	-0.63524500
H	0.75133900	5.53652200	1.94273400
H	-1.79686400	7.20831500	1.70030600
O	-1.18759200	2.28291500	-0.45688300
O	1.10108200	2.61774300	0.69084100
P	0.05381400	1.43405500	0.22662100
O	0.64872200	0.61589300	-0.87871700
O	-0.38549000	0.79759800	1.50962500
C	-4.01270000	1.57052000	0.25171300
C	-4.62822200	0.70342600	1.10192800
C	-4.35879600	1.53407000	-1.16421200

C	-5.64802700	-0.21139300	0.68151300
H	-4.38528800	0.74012200	2.15761100
C	-5.36231600	0.63386200	-1.61927400
C	-3.75558900	2.40288300	-2.10253600
C	-6.27920100	-1.05672900	1.62088300
C	-6.04793500	-0.23707500	-0.67324100
C	-5.67652500	0.61081400	-2.99663800
H	-3.01423000	3.11686800	-1.76680800
C	-4.08672100	2.36164500	-3.43875300
C	-7.30329200	-1.89426600	1.23966500
H	-5.93035700	-1.04614400	2.64958900
C	-7.10245800	-1.10481100	-1.03827700
C	-5.05051200	1.44844800	-3.89315300
H	-6.42059100	-0.08444700	-3.36815000
H	-3.60076200	3.03558800	-4.13713700
C	-7.71970200	-1.91188300	-0.10400400
H	-7.78281400	-2.54064100	1.96785900
H	-7.45182100	-1.14020600	-2.06420900
H	-5.30789100	1.40463500	-4.94678000
H	-8.53206600	-2.56360500	-0.41042500
C	3.79453300	2.21366200	-0.48630400
C	4.24383200	2.24866300	0.79788700
C	4.45167700	1.34621700	-1.44842400
C	5.41329900	1.52787800	1.21524200
H	3.76249700	2.90236000	1.52119700
C	5.64928600	0.67198000	-1.09286400
C	3.90263900	1.14523500	-2.73529600
C	5.87675200	1.63536400	2.54612600
C	6.15260000	0.77216100	0.27205000
C	6.30288500	-0.09613100	-2.08199500
H	2.95335900	1.61172000	-2.97684700
C	4.54234500	0.35656300	-3.66659000
C	7.04506700	1.01960400	2.93966500
H	5.29696500	2.22457400	3.25161200
C	7.34128300	0.14375800	0.70438600
C	5.76823000	-0.24654200	-3.34442200
H	7.23762000	-0.59496600	-1.85077700
H	4.09929700	0.20436700	-4.64551000
C	7.78141000	0.26666600	2.00706600
H	7.39650300	1.11315800	3.96230500
H	7.93138300	-0.44377300	0.01014500
H	6.28635400	-0.85260800	-4.08113900
H	8.70179600	-0.22163200	2.31197700
H	-1.03124100	-0.68245500	2.02986400

H	5.67272200	-2.60519900	-1.32925800
C	-3.65978400	-3.55130700	-1.50414000
C	-4.03251800	-3.12770300	-0.07464200
C	-4.05049700	-2.44787100	-2.50010600
C	-4.45007900	-4.81798800	-1.84657700
H	-3.71980400	-3.88416800	0.65425400
H	-3.57105100	-2.17644200	0.20852400
H	-5.11671100	-3.00237300	0.00228100
H	-3.77046400	-2.73093600	-3.52065300
H	-5.13245700	-2.28180300	-2.47127000
H	-3.55740400	-1.49982600	-2.26311700
H	-5.51850400	-4.61862200	-1.71476400
H	-4.29690000	-5.12926300	-2.88496500
H	-4.18008700	-5.65245100	-1.19022200

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C	5.23762400	-2.57078000	2.73465700
C	4.62433000	-3.65707000	2.11224900
C	3.36817900	-3.51623400	1.52066800
C	2.75251500	-2.25071100	1.53754900
C	3.34987500	-1.17624100	2.18214700
C	4.59745100	-1.33502800	2.78742900
H	3.23853500	-5.54609600	0.66951600
H	6.21635900	-2.69246900	3.18903600
H	5.11887100	-4.62436800	2.08761300
C	2.66802300	-4.64818000	0.89458100
C	1.46171600	-2.09446100	0.76676500
H	2.85512600	-0.20697500	2.18412400
H	5.06874800	-0.49247100	3.28268500
C	0.65782400	-3.34654200	1.07567300
C	1.33962000	-4.60897400	0.68647900
H	0.95014400	-1.19039100	1.09739600
N	-0.42725600	-3.44491500	1.74532600
N	-1.03162900	-2.32201800	2.21983300
C	-1.87262100	-2.46868000	3.29361900
O	-2.26896100	-3.50743500	3.76935400
O	-2.19927000	-1.24422100	3.75320300
C	-3.01565700	-1.23097900	4.92615600
H	-2.51202400	-1.74704400	5.74623300
H	-3.15667000	-0.17870600	5.16973700
H	-3.98250600	-1.70483500	4.74046500
C	0.51100400	-5.73226100	0.14918300
H	-0.28381900	-5.98596000	0.85787100
H	0.02361500	-5.42741700	-0.78511400
H	1.12041800	-6.61867300	-0.03933100
C	5.06073700	-3.07929200	-2.98143500
C	5.29178500	-2.40559500	-1.77692000
C	4.25093600	-1.96572300	-0.96570100
C	2.94231300	-2.27133500	-1.35040000
C	2.70637500	-2.92834800	-2.57522600
C	3.76093200	-3.32535600	-3.39795900
H	5.89971700	-3.39459700	-3.59370100
H	4.47493500	-1.41046500	-0.06406200
H	3.55979200	-3.82758400	-4.33979500
C	0.69339700	-2.48777400	-1.57791200
C	-0.68392300	-2.45096000	-1.39800300
C	-1.50549900	-3.04406400	-2.36514700
C	-0.91783100	-3.63329600	-3.49793400
C	0.45842600	-3.64104500	-3.68826600

C	1.27310000	-3.06790100	-2.71723900
H	-1.11577200	-1.96361200	-0.52594900
H	-1.54718600	-4.08923800	-4.25303900
H	0.88979600	-4.09313700	-4.57669100
N	1.69876000	-1.97583100	-0.71693500
H	0.89355900	-0.05053800	-0.99627200
C	0.15747400	4.43599100	-0.78773100
C	0.49105000	5.23371000	-1.88547700
C	1.72160500	5.08289200	-2.50971300
C	2.62331400	4.15108900	-2.00410200
C	2.29782900	3.30050200	-0.93566700
C	1.01728600	3.42969100	-0.37984400
C	-1.79659800	5.62833600	-1.36030000
C	-0.63312400	6.19436700	-2.19541700
H	1.99548200	5.70010600	-3.36012400
H	3.61540800	4.07864100	-2.43794000
H	-2.32132400	4.85697500	-1.93487800
H	-0.36920500	7.21018600	-1.87739800
C	-1.10662500	4.95380600	-0.14050200
C	-2.07113400	4.07179200	0.62233800
C	-0.77416600	6.01963900	0.94269900
C	-2.71158200	4.81847300	1.61763900
C	-2.45268000	2.75689800	0.39658600
C	-2.08216300	6.18700300	1.73410500
H	-0.40431100	6.94992300	0.50288400
C	-3.77195900	4.27885000	2.33060700
C	-3.58154300	2.22056600	1.02688700
H	-1.91480400	6.48167100	2.77358100
C	-4.21961900	3.00357700	1.99758800
H	-4.26686900	4.84729900	3.11240700
H	-5.09470300	2.58846200	2.48860800
H	-0.86054300	6.23751400	-3.26393700
H	-2.52477600	6.38456900	-1.05385400
H	0.00479900	5.61708800	1.59943700
H	-2.73046300	6.94626700	1.28030400
O	-1.68884800	1.97405900	-0.48479700
O	0.58345200	2.53692100	0.60744100
P	-0.36911700	1.31208400	0.15993300
O	0.26002600	0.68633800	-1.14473200
O	-0.58835500	0.42162000	1.31681100
C	-4.28438200	0.96800700	0.61348900
C	-4.22995800	-0.16646800	1.35710700
C	-5.22190200	1.06826400	-0.49524300
C	-5.12459900	-1.26889100	1.11885800

H	-3.52713200	-0.23938100	2.18322600
C	-6.12756700	0.00687200	-0.74917600
C	-5.25912200	2.21433400	-1.32177600
C	-5.07581400	-2.41921900	1.93652600
C	-6.09113100	-1.18514600	0.08823600
C	-7.02806700	0.13394200	-1.82955600
H	-4.57679300	3.03399700	-1.12251700
C	-6.14281400	2.30766800	-2.37481400
C	-5.95681800	-3.46158900	1.74973000
H	-4.32259600	-2.48284700	2.71505400
C	-6.97752800	-2.27072500	-0.08858100
C	-7.03633300	1.25610900	-2.63045800
H	-7.72605500	-0.66544800	-2.04993900
H	-6.14760100	3.19300600	-3.00261500
C	-6.91628600	-3.38303200	0.72588500
H	-5.90492600	-4.34029000	2.38455800
H	-7.73085000	-2.23873400	-0.86749400
H	-7.73548500	1.32399900	-3.45798900
H	-7.61349400	-4.20072500	0.57187500
C	3.37010500	2.47325400	-0.31385800
C	3.59400700	2.60171400	1.02394000
C	4.32326500	1.73806000	-1.12891300
C	4.78237400	2.10187900	1.65233900
H	2.90069600	3.17308100	1.63618200
C	5.55370000	1.31335100	-0.56057400
C	4.06155900	1.45433700	-2.48902400
C	4.99045400	2.29933000	3.03610200
C	5.78791800	1.48735700	0.86793000
C	6.52201200	0.73870800	-1.41273800
H	3.09180300	1.71282900	-2.90229700
C	5.01293600	0.85961200	-3.28889100
C	6.16686300	1.90530400	3.63548000
H	4.20803100	2.78252900	3.61532300
C	6.97469400	1.07326200	1.51198500
C	6.26799100	0.53367100	-2.75210600
H	7.48673700	0.44517600	-1.01381300
H	4.79158900	0.64536800	-4.32954300
C	7.16365700	1.28180500	2.86318600
H	6.32338500	2.06949300	4.69694500
H	7.75887300	0.58256100	0.94685800
H	7.02926700	0.08656000	-3.38417400
H	8.08843200	0.96010100	3.33209800
H	-0.72693100	-1.37439400	1.98767100
H	6.31074000	-2.19527100	-1.46856700

C	-3.01939400	-3.00146800	-2.16877800
C	-3.37825600	-3.61629700	-0.80789900
C	-3.47657000	-1.53536700	-2.21831300
C	-3.77373500	-3.77523200	-3.25496100
H	-3.06604400	-4.66581300	-0.76129600
H	-2.89997400	-3.08714200	0.02297100
H	-4.46135700	-3.57206800	-0.65084300
H	-3.13966400	-1.05369800	-3.14253600
H	-4.56826500	-1.48458400	-2.18652100
H	-3.08466800	-0.95796500	-1.37276500
H	-4.84620900	-3.74261300	-3.03669200
H	-3.62351900	-3.33753900	-4.24732800
H	-3.47055800	-4.82702700	-3.28949300

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C	-1.40268000	3.79747300	3.04102700
C	-1.93859200	4.27655700	1.84682900
C	-2.17058500	3.41199900	0.77373900
C	-1.87550900	2.04572600	0.93202000
C	-1.33996700	1.56740400	2.12353800
C	-1.09393700	2.44572800	3.18158900
H	-3.18355900	4.87900500	-0.51297200
H	-1.22100800	4.48366200	3.86253200
H	-2.17642400	5.33208300	1.73798800
C	-2.74101100	3.88558600	-0.49417700
C	-2.18529500	1.10660800	-0.21022400
H	-1.13448900	0.50343100	2.22327900
H	-0.67855800	2.07165600	4.11207500
C	-1.94709400	1.86043100	-1.51239700
C	-2.65925400	3.15590000	-1.62164800
H	-1.53165100	0.23957400	-0.12205900
N	-1.14366100	1.56672700	-2.46822900
N	-0.31971600	0.49746200	-2.34793700
C	0.41495100	0.11452200	-3.44121500
O	0.39987200	0.62932900	-4.53628700
O	1.13723500	-0.97110100	-3.10974400
C	1.79749100	-1.60565500	-4.20400800
H	2.61579300	-0.98496700	-4.57837200
H	2.17838700	-2.54676800	-3.80788200
H	1.09208600	-1.79489900	-5.01708700
C	-3.14296000	3.60607600	-2.96379500
H	-2.33764300	3.52877500	-3.69979600
H	-3.95753000	2.95992100	-3.31021900
H	-3.50210200	4.63734800	-2.92844200
C	-7.07611000	0.86249800	2.05390400
C	-6.06554000	1.79313000	2.32885300
C	-4.85380400	1.79426500	1.64913600
C	-4.64740200	0.82657800	0.65453200
C	-5.66948200	-0.11860900	0.37569500
C	-6.87876000	-0.09808200	1.07359700
H	-8.00843700	0.89552500	2.60798600
H	-4.10567700	2.52802400	1.90831000
H	-7.64884500	-0.83059400	0.84710000
C	-3.87487600	-0.53388200	-0.97516900
C	-3.09035400	-1.18046100	-1.92797400
C	-3.59685800	-2.30263700	-2.58806400
C	-4.88800500	-2.76256100	-2.26429700
C	-5.67164100	-2.11727900	-1.31240800

C	-5.17056000	-0.99007300	-0.66288800
H	-2.09755700	-0.82552100	-2.17034700
H	-5.29360700	-3.63443600	-2.76447100
H	-6.66445800	-2.49205900	-1.07789600
N	-3.56165100	0.57055900	-0.18961100
H	1.29393400	1.41540000	1.86897100
C	4.84106500	-0.26786000	-0.37867200
C	6.12128600	0.13233000	0.01539900
C	6.37393700	1.45493900	0.36002100
C	5.33257200	2.38000500	0.32454200
C	4.02849600	1.99963500	-0.01620600
C	3.81242700	0.65956800	-0.35616600
C	6.07677000	-2.24486000	-0.00854000
C	7.05512500	-1.05555500	0.02639800
H	7.36870100	1.76678800	0.66410700
H	5.51934300	3.41733400	0.58723700
H	5.75060100	-2.48164900	1.01009600
H	7.70302900	-1.04658900	-0.85844400
C	4.85339400	-1.72128200	-0.81419900
C	3.64118100	-2.62362100	-0.66526500
C	5.11867100	-1.86154400	-2.34040100
C	3.62762400	-3.58666000	-1.68164400
C	2.62512100	-2.63324700	0.27605200
C	4.74148700	-3.31690700	-2.66658000
H	6.14801400	-1.60448200	-2.60501600
C	2.64632600	-4.56843000	-1.71495800
C	1.62886600	-3.61855600	0.28525800
H	4.42350100	-3.45105200	-3.70477800
C	1.66749200	-4.58863100	-0.72148600
H	2.63058000	-5.30870500	-2.51010500
H	0.89826100	-5.35537400	-0.72844400
H	7.70483800	-1.06664700	0.90536200
H	6.50450100	-3.14932400	-0.44997800
H	4.44422800	-1.18023300	-2.87158400
H	5.58546600	-3.99586300	-2.49505300
O	2.54150800	-1.57453400	1.19552800
O	2.50674000	0.23018200	-0.60804900
P	1.68360700	-0.33394900	0.65062500
O	1.89728000	0.64926600	1.87011400
O	0.29744000	-0.61399000	0.23052200
C	0.52280600	-3.59154000	1.28302300
C	-0.75192600	-3.42242800	0.84476900
C	0.78537600	-3.71727700	2.70488400
C	-1.86284100	-3.32726400	1.74522200

H	-0.94550200	-3.29191100	-0.21683600
C	-0.28888300	-3.62311900	3.62943400
C	2.09289900	-3.94508600	3.19060600
C	-3.16642800	-3.12333300	1.24075700
C	-1.64703100	-3.41065500	3.14165800
C	-0.00070200	-3.75008700	5.00668200
H	2.91078400	-4.03461900	2.48265200
C	2.34286200	-4.06735100	4.53938800
C	-4.23791500	-2.99499900	2.09626300
H	-3.30798600	-3.06578900	0.16349300
C	-2.76499400	-3.27928000	3.99485900
C	1.28442000	-3.96482600	5.45638900
H	-0.80115900	-3.68321100	5.73456800
H	3.35434700	-4.24460900	4.89117500
C	-4.03057800	-3.07368600	3.48471700
H	-5.23425300	-2.82653400	1.69872200
H	-2.64129400	-3.33200500	5.07052000
H	1.47563300	-4.05966000	6.52072400
H	-4.87135200	-2.96892300	4.16331900
C	2.91290100	2.98691600	-0.05362300
C	2.21223700	3.15744800	-1.20860900
C	2.58581300	3.79822600	1.10731800
C	1.22930700	4.19027400	-1.36248500
H	2.43414500	2.53459800	-2.07250600
C	1.62873200	4.84198000	0.98751000
C	3.17090500	3.54304100	2.37034900
C	0.57590000	4.36894700	-2.60260300
C	0.96520700	5.07413000	-0.28883700
C	1.33125300	5.61319300	2.13297500
H	3.87134000	2.72054400	2.46956400
C	2.84778100	4.30420700	3.47311000
C	-0.29472300	5.41895400	-2.79050700
H	0.77522300	3.66237800	-3.40411100
C	0.06210700	6.13827900	-0.50791800
C	1.92891600	5.35808700	3.34885400
H	0.60248400	6.41343500	2.06934900
H	3.30241400	4.08682300	4.43445600
C	-0.54903900	6.31081300	-1.73279200
H	-0.78285900	5.55923700	-3.74969900
H	-0.14929500	6.84775900	0.28441000
H	1.67366200	5.96268100	4.21367800
H	-1.23282600	7.14144100	-1.88008300
H	-0.13436900	0.03053700	-1.45508300
H	-6.22402800	2.54104300	3.09988400

C	-2.72114400	-2.96576300	-3.65993600
C	-2.42791100	-1.94184500	-4.77019100
C	-1.39103500	-3.42569800	-3.03753900
C	-3.40200400	-4.18350900	-4.29109700
H	-3.35581400	-1.59803100	-5.23920300
H	-1.90589400	-1.05937600	-4.38532800
H	-1.80105400	-2.39435200	-5.54707400
H	-1.56756000	-4.17196600	-2.25490400
H	-0.75614100	-3.88650900	-3.80419400
H	-0.82953500	-2.59240100	-2.60002800
H	-2.73930400	-4.62220400	-5.04383600
H	-3.61836200	-4.95659900	-3.54635300
H	-4.33834200	-3.91225800	-4.78925400

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C	6.38708500	-1.58670400	-0.60118500
C	5.47383900	-1.54828800	-1.64531800
C	4.24827300	-0.88664800	-1.48296100
C	3.92590400	-0.29786700	-0.25321100
C	4.84206600	-0.34626400	0.79206800
C	6.07155500	-0.97528600	0.61227200
H	3.63844400	-1.19743700	-3.53995200
H	7.34500600	-2.07957300	-0.73221800
H	5.70417900	-2.00349300	-2.60459500
C	3.36084500	-0.70335100	-2.61046600
C	2.57203300	0.36302800	-0.06517600
H	4.60266000	0.11568200	1.74513900
H	6.78571400	-0.99137500	1.42974900
C	1.85884600	0.70238800	-1.36531000
C	2.25809300	0.08820600	-2.61269600
H	1.89554100	-0.41235300	0.34615600
N	0.78732900	1.45363300	-1.38860400
N	0.11362400	1.93904100	-0.29331400
C	0.40881500	3.22376600	0.12486700
O	1.12288700	3.98999700	-0.47840900
O	-0.22184600	3.47173400	1.27165100
C	0.05833300	4.75534400	1.83705300
H	1.12870700	4.85999100	2.02560000
H	-0.27197800	5.54847100	1.16461400
H	-0.50111200	4.79206500	2.77089900
C	1.46120400	0.34498100	-3.86046100
H	0.42144900	0.02505500	-3.72667900
H	1.47366000	1.41058500	-4.11922200
H	1.89501100	-0.20918700	-4.69410700
C	5.14361100	4.73691900	1.11374100
C	5.19201700	3.98027300	-0.06747300
C	4.39859300	2.85351400	-0.23884000
C	3.54854200	2.50167300	0.80868400
C	3.48605700	3.24798200	2.00505300
C	4.29293800	4.37955300	2.15183900
H	5.77699100	5.61259900	1.21176400
H	4.43311300	2.27594300	-1.15812100
H	4.25475500	4.96848300	3.06386300
C	1.99156700	1.50398400	2.11828900
C	0.93756400	0.71490100	2.58150700
C	0.30831000	1.07995300	3.77184700
C	0.81055700	2.17712000	4.50530300
C	1.88574500	2.93159700	4.05911600

C	2.47848000	2.61428900	2.83514300
H	0.56784700	-0.11420000	1.98622100
H	0.33319000	2.45970000	5.43680800
H	2.23641700	3.78162400	4.63831200
N	2.64670200	1.44382600	0.88686200
H	-0.23783000	1.22024300	0.34275100
H	5.86104300	4.28203100	-0.86719900
C	-1.00377100	0.40368300	4.18908000
C	-2.15242000	1.18790300	3.52538400
C	-1.08449100	-1.05488300	3.71847100
C	-1.19616600	0.42450600	5.71224400
H	-2.11967200	2.24657500	3.80493000
H	-2.09205100	1.12014100	2.43336600
H	-3.12003100	0.77977600	3.84138900
H	-0.27058500	-1.65302400	4.14530300
H	-2.03085500	-1.49003000	4.05726400
H	-1.06134400	-1.14705600	2.62582600
H	-2.09379400	-0.14436600	5.97501700
H	-0.34355500	-0.03017000	6.22802600
H	-1.33224800	1.43743900	6.10169800
C	-3.23402600	-3.06365500	0.97555000
C	-3.35384900	-3.57522800	2.27068900
C	-2.29947600	-4.26371300	2.85840800
C	-1.10849400	-4.40816600	2.15021500
C	-0.93484000	-3.84271800	0.87938800
C	-2.02223700	-3.16541500	0.30597200
C	-5.18178500	-2.10593100	1.89261900
C	-4.70218400	-3.21324200	2.85040500
H	-2.39182800	-4.67159900	3.86108200
H	-0.27828300	-4.94663400	2.59848900
H	-4.76220900	-1.14331800	2.20676500
H	-5.38027000	-4.07541800	2.83547400
C	-4.56141700	-2.48845700	0.51862400
C	-4.66355600	-1.36086500	-0.49360100
C	-5.44514800	-3.56670300	-0.17219600
C	-5.85297400	-1.47735200	-1.22270200
C	-3.80797600	-0.29464500	-0.74606000
C	-6.55950500	-2.76466100	-0.86606700
H	-5.81801200	-4.31105500	0.53725300
C	-6.22099700	-0.50788000	-2.14593900
C	-4.16675600	0.70446800	-1.66247700
H	-6.96929700	-3.27334000	-1.74302100
C	-5.38086100	0.58697800	-2.34461200
H	-7.14285900	-0.60190900	-2.71279800

H	-5.65293300	1.36222400	-3.05530800
H	-4.63139000	-2.87560800	3.88863600
H	-6.27034500	-2.00821000	1.84431100
H	-4.84095000	-4.08318200	-0.92594900
H	-7.39466500	-2.57233400	-0.18093500
O	-2.58531900	-0.22943600	-0.11181600
O	-1.87759300	-2.53994300	-0.91345000
P	-1.31502600	-0.99367000	-0.85690500
O	-0.20891200	-0.85913800	0.14913300
O	-1.15642100	-0.55982500	-2.27158900
C	-3.27070200	1.86821600	-1.91947700
C	-2.57089900	1.93380200	-3.08092600
C	-3.18734400	2.95549900	-0.96369200
C	-1.69141300	3.02815300	-3.37882800
H	-2.62949700	1.11183600	-3.78780700
C	-2.38945700	4.09252500	-1.25944800
C	-3.91145100	2.92013300	0.24839500
C	-0.91666800	3.02137300	-4.56180800
C	-1.57947000	4.10858600	-2.47045400
C	-2.41083800	5.17997200	-0.36083100
H	-4.50550500	2.04192500	0.48176000
C	-3.88091800	3.98152100	1.12802500
C	-0.04314400	4.05114600	-4.83801600
H	-1.02268000	2.18487700	-5.24816900
C	-0.66677800	5.14290300	-2.77268400
C	-3.13997900	5.13044300	0.80944000
H	-1.85392100	6.08134100	-0.59271200
H	-4.44345100	3.93471400	2.05540200
C	0.08399300	5.11673200	-3.92911400
H	0.54964400	4.03788700	-5.74745000
H	-0.52134100	5.96059400	-2.07635900
H	-3.13666300	5.98161100	1.48384100
H	0.78523000	5.91994500	-4.13212300
C	0.35345200	-3.98076900	0.14472800
C	0.36278500	-4.48118900	-1.12023800
C	1.61541700	-3.65500300	0.78664700
C	1.57989400	-4.71565000	-1.84220600
H	-0.57543400	-4.72270200	-1.61215500
C	2.84177400	-3.97924600	0.14939500
C	1.65033100	-2.99820600	2.03708000
C	1.53915600	-5.18990900	-3.17201800
C	2.82839900	-4.49212800	-1.21348000
C	4.04349500	-3.77252900	0.86204500
H	0.71653100	-2.66754900	2.47475100

C	2.84073200	-2.76399700	2.69112500
C	2.70050800	-5.42792500	-3.87318400
H	0.56956900	-5.35655800	-3.63355700
C	4.00437600	-4.74351600	-1.95471700
C	4.04570900	-3.19697200	2.11447400
H	4.99052500	-4.06170300	0.42068100
H	2.84213600	-2.25139400	3.64874700
C	3.94362800	-5.19925100	-3.25614400
H	2.65864100	-5.78767700	-4.89645600
H	4.97730700	-4.56786500	-1.50871800
H	4.98573900	-3.04611800	2.63657300
H	4.86211100	-5.38395600	-3.80505600
H	0.25966400	1.52666900	-2.26000800

TSIII-2Value of imaginary frequency = -1140.8 cm⁻¹

C	-4.81605100	-3.50781100	-0.70358200
C	-4.09303200	-3.10676900	-1.80749100
C	-2.75276900	-2.69783200	-1.66312600
C	-2.15624600	-2.66502500	-0.39046100
C	-2.90766000	-3.05814800	0.72508600
C	-4.21392800	-3.48741800	0.56357300
H	-2.43761200	-2.40439300	-3.78249100
H	-5.84480800	-3.83710600	-0.81175300
H	-4.53798900	-3.10982300	-2.79890500
C	-1.94885300	-2.38964200	-2.81013900
C	-0.75347600	-2.20258400	-0.24333200
H	-2.45603800	-3.03768500	1.71229700
H	-4.78215700	-3.80000700	1.43367900
C	0.01730800	-2.03983400	-1.47312000
C	-0.62026100	-2.09598700	-2.76308600
H	-0.86458400	-0.92019800	-0.09995800
N	1.29185500	-1.65287400	-1.44528400
N	1.92850100	-1.25164000	-0.30256400
C	2.77797300	-2.11792600	0.34715000
O	2.95931900	-3.27147300	0.03366600
O	3.32714300	-1.48922100	1.38824400
C	4.12005300	-2.32190200	2.23516900
H	3.52980000	-3.17020000	2.58899500
H	5.00151900	-2.68373300	1.70049700
H	4.41865200	-1.69150800	3.07208400
C	0.17059700	-1.78148000	-3.99900200
H	0.54540200	-0.75264500	-3.94140200
H	1.01916500	-2.46404900	-4.12082000
H	-0.46361100	-1.86747600	-4.88292500
C	0.59715800	-6.83116400	1.60170400
C	0.08988500	-6.48440400	0.33996200
C	-0.17262000	-5.16252200	0.00198700
C	0.09051500	-4.18840500	0.96479600
C	0.59369200	-4.51863700	2.24075900
C	0.85199600	-5.85456800	2.55614200
H	0.79229800	-7.87383900	1.83078000
H	-0.56322200	-4.89874100	-0.97688300
H	1.24380400	-6.12387700	3.53301800
C	0.31069500	-2.24031700	2.08816500
C	0.38446700	-0.89699800	2.44932900
C	0.90253600	-0.56003300	3.69907000
C	1.30534600	-1.58516900	4.57936600

C	1.22456900	-2.92487600	4.22108800
C	0.73839700	-3.26735200	2.95817500
H	0.09209000	-0.12653200	1.74665300
H	1.69800500	-1.33431200	5.55824900
H	1.55561200	-3.69694100	4.91056800
N	-0.07824300	-2.80945300	0.87559200
H	1.93905700	-0.25516500	-0.09478100
H	-0.10069900	-7.26464000	-0.39043000
C	1.11341900	0.92351000	4.02326100
C	2.30268500	1.42374700	3.18268500
C	-0.13038800	1.75043100	3.65820200
C	1.42720000	1.15389600	5.50544900
H	3.19955300	0.82634800	3.37996200
H	2.07937300	1.35735500	2.11202300
H	2.52674200	2.47045100	3.42432100
H	-1.00854100	1.41496800	4.22149700
H	0.04628100	2.80412500	3.90377600
H	-0.36625400	1.70163900	2.58846100
H	1.51170600	2.22822800	5.69866300
H	0.63754200	0.75569500	6.15162900
H	2.37600100	0.69348100	5.79854400
C	-0.93746800	4.16162800	0.80296600
C	-1.31490200	4.61456000	2.07020300
C	-2.49603700	4.17169900	2.64827000
C	-3.27515400	3.24622900	1.95990100
C	-2.88467500	2.71238400	0.72202100
C	-1.69686100	3.20095700	0.15250400
C	0.93598000	5.26884600	1.70331100
C	-0.26282100	5.54403400	2.62862400
H	-2.80929200	4.52930000	3.62494400
H	-4.20915300	2.90772600	2.39695300
H	1.48476400	4.39121000	2.06559000
H	-0.58738100	6.58978000	2.56305300
C	0.29200500	4.90969100	0.33378200
C	1.31268300	4.32073700	-0.62402100
C	-0.09362100	6.21124000	-0.42391400
C	1.91293700	5.35362900	-1.35596600
C	1.74139000	3.01018400	-0.81220700
C	1.21393100	6.66648900	-1.09072100
H	-0.53301400	6.95994700	0.24112300
C	2.98274800	5.10321200	-2.20255100
C	2.84462800	2.74009400	-1.63389000
H	1.04805400	7.23951900	-2.00715100
C	3.45744100	3.79925700	-2.31131300

H	3.44311300	5.90636700	-2.77052800
H	4.30960600	3.57809800	-2.94721500
H	-0.04407900	5.33895400	3.68085300
H	1.63516800	6.10639700	1.62694000
H	-0.83166600	5.95992800	-1.19339400
H	1.80994000	7.29427200	-0.41703000
O	1.05594700	1.96171900	-0.20822100
O	-1.23899800	2.71828100	-1.06451900
P	-0.27691900	1.40205500	-1.02202000
O	-0.88323400	0.42436800	-0.02690800
O	0.05637500	1.00624000	-2.40959400
C	3.42440500	1.37553900	-1.79805000
C	3.19957200	0.67842600	-2.94256000
C	4.35882900	0.86571400	-0.80917700
C	3.83301800	-0.58578100	-3.19895100
H	2.51106300	1.07607300	-3.68341200
C	5.03183100	-0.36263300	-1.04592200
C	4.63249900	1.58212400	0.37661700
C	3.56166400	-1.29342800	-4.39261100
C	4.72229100	-1.13447400	-2.24271200
C	5.99812500	-0.79177200	-0.11235400
H	4.10861200	2.51500300	0.56327300
C	5.56222600	1.12310700	1.28644700
C	4.12705200	-2.52853400	-4.62447200
H	2.89405700	-0.84383600	-5.12329600
C	5.26860800	-2.41184800	-2.49578200
C	6.26329200	-0.06510200	1.02986300
H	6.55633700	-1.70360200	-0.29350400
H	5.76260900	1.69049600	2.19015700
C	4.97699600	-3.09488400	-3.65822800
H	3.91133700	-3.06568900	-5.54268500
H	5.91636900	-2.88142700	-1.76448300
H	7.01342600	-0.41765600	1.73129100
H	5.40631900	-4.07772000	-3.82458700
C	-3.76579200	1.73278800	0.02885400
C	-4.08100000	1.91522100	-1.28271200
C	-4.41680500	0.66248500	0.77237900
C	-5.06088800	1.11246300	-1.95403300
H	-3.60710000	2.71369500	-1.84622000
C	-5.49980000	-0.04246300	0.18460000
C	-4.00236300	0.30280800	2.07613200
C	-5.31849400	1.30360800	-3.32954100
C	-5.80883000	0.15783800	-1.22479400
C	-6.23583800	-0.93881800	0.99106200

H	-3.10551700	0.75537600	2.48606700
C	-4.71278500	-0.60960700	2.82662500
C	-6.28329300	0.56421100	-3.97668000
H	-4.73612800	2.04625600	-3.86822600
C	-6.79309200	-0.58622100	-1.91189700
C	-5.87095900	-1.19826400	2.29467300
H	-7.10710500	-1.43872700	0.58219900
H	-4.37919500	-0.86562500	3.82746900
C	-7.02577000	-0.38981000	-3.25796300
H	-6.47157300	0.71562400	-5.03495200
H	-7.37206000	-1.33792600	-1.38656800
H	-6.45918200	-1.88553900	2.89539800
H	-7.78629400	-0.97655800	-3.76397000
H	1.76677800	-1.44558500	-2.32023600

IMIII-4

C	-5.45382700	3.63249500	-0.13539500
C	-4.61541000	3.41330300	-1.20061100
C	-3.75292400	2.28841300	-1.22210600
C	-3.73787100	1.38974900	-0.12498900
C	-4.58687000	1.66202800	0.98155800
C	-5.42988800	2.74759100	0.96640800
H	-2.98128900	2.66180100	-3.20504700
H	-6.12931200	4.48241200	-0.13304200
H	-4.61436300	4.08229700	-2.05775700
C	-2.95689900	1.98194000	-2.35638300
C	-2.94133400	0.19911300	-0.19885200
H	-4.57646300	0.99598800	1.83809400
H	-6.08325700	2.92974100	1.81447900
C	-2.17434200	-0.07592900	-1.32675400
C	-2.20084100	0.84464100	-2.44068000
H	-0.19751800	1.57362100	-0.48562400
N	-1.42444600	-1.23172200	-1.52028100
N	-0.89598300	-1.95482500	-0.48179800
C	-1.53343400	-3.08741200	-0.04485900
O	-2.50092600	-3.60030600	-0.56015900
O	-0.90856500	-3.55370600	1.05022200
C	-1.55366300	-4.66878600	1.66146100
H	-2.56367700	-4.39749600	1.97750400
H	-1.60766600	-5.51222400	0.97088000
H	-0.94355400	-4.92856700	2.52650400
C	-1.48072200	0.50496800	-3.71912200
H	-0.40248200	0.38888400	-3.56853100
H	-1.86721400	-0.42857500	-4.14461100
H	-1.63479100	1.29851300	-4.45296300
C	-6.59673500	-3.02152100	1.46020700
C	-6.51196700	-2.30933100	0.25206800
C	-5.40672400	-1.52677300	-0.05443900
C	-4.37629000	-1.47500700	0.88466700
C	-4.44644100	-2.17645000	2.10574800
C	-5.56781400	-2.96185000	2.39015300
H	-7.47590400	-3.62370900	1.66518200
H	-5.33728300	-0.98108000	-0.98989000
H	-5.63209300	-3.51137200	3.32509000
C	-2.46390900	-1.01380800	1.99470500
C	-1.17665400	-0.60305200	2.34646600
C	-0.59058500	-1.14054900	3.49445900
C	-1.34965400	-2.00157800	4.31601200
C	-2.64742100	-2.36693100	3.99218400

C	-3.21152100	-1.89418700	2.80710100
H	-0.62749000	0.07033000	1.69591000
H	-0.90999200	-2.40792300	5.21934800
H	-3.20394100	-3.04335400	4.63542800
N	-3.17369000	-0.77417000	0.81930600
H	-0.19624000	-1.52549600	0.11619500
H	-7.32823100	-2.37227400	-0.46089300
C	0.90637900	-0.93814900	3.75789900
C	1.65828700	-1.94859900	2.87010700
C	1.37081400	0.47825600	3.39740300
C	1.28154000	-1.19846700	5.22331400
H	1.34984700	-2.97408700	3.09888800
H	1.45615600	-1.76630900	1.80964500
H	2.74079800	-1.87015800	3.03168000
H	0.82386100	1.23207900	3.97528600
H	2.43499300	0.58146400	3.63333200
H	1.25539600	0.69940200	2.33065900
H	2.34052400	-0.96475400	5.37488500
H	0.69633700	-0.57424700	5.90684500
H	1.14018900	-2.24526800	5.50651700
C	4.07658600	1.82180500	1.16922500
C	4.30468500	2.21708200	2.49119300
C	3.56357800	3.24400500	3.06184200
C	2.55700600	3.84888300	2.31456700
C	2.26049800	3.43345100	1.00941700
C	3.05002600	2.41824500	0.45536000
C	5.40539000	0.14347200	2.15310900
C	5.35372400	1.33502600	3.12592000
H	3.74421900	3.55477700	4.08655400
H	1.96070100	4.64390200	2.75234300
H	4.61474000	-0.57157900	2.40698600
H	6.32024400	1.85006900	3.18119900
C	5.08169500	0.76278100	0.76210300
C	4.78329400	-0.31259100	-0.27029000
C	6.37116500	1.38491500	0.15643000
C	5.97835700	-0.71486700	-0.88131700
C	3.60136900	-0.94545400	-0.63480700
C	7.11450100	0.18831800	-0.46168500
H	6.95671200	1.92559000	0.90482600
C	6.00475700	-1.78499300	-1.76445300
C	3.59627300	-2.03123900	-1.51754300
H	7.74866900	0.47180500	-1.30570700
C	4.81696000	-2.45255100	-2.05364100
H	6.93436500	-2.09219600	-2.23422200

H	4.81546500	-3.29757700	-2.73554300
H	5.08379800	1.04034400	4.14419800
H	6.36192400	-0.38570100	2.15729500
H	6.08433800	2.08934300	-0.63144800
H	7.75583700	-0.30854400	0.27586700
O	2.37444300	-0.45689800	-0.15829800
O	2.77378500	1.96647200	-0.83567500
P	1.74689800	0.74630700	-1.02506100
O	0.48911400	1.00605300	-0.08859700
O	1.49965800	0.52020000	-2.45550400
C	2.34301900	-2.74662300	-1.90072400
C	1.69852800	-2.41378600	-3.04827900
C	1.88779500	-3.87415400	-1.11124600
C	0.52691700	-3.11656800	-3.49013100
H	2.05422100	-1.57817800	-3.64260900
C	0.77483500	-4.63631500	-1.55486300
C	2.55441000	-4.24979300	0.07526100
C	-0.15189700	-2.70313900	-4.65868900
C	0.04226100	-4.21643700	-2.74258600
C	0.41876300	-5.78883000	-0.82342100
H	3.39201800	-3.65103900	0.42046700
C	2.16636900	-5.36644200	0.78545100
C	-1.29831500	-3.34742500	-5.07032500
H	0.24554300	-1.86228500	-5.22169400
C	-1.14365600	-4.84640100	-3.17816800
C	1.10257700	-6.15363700	0.31850600
H	-0.40230700	-6.41106300	-1.16226000
H	2.69365600	-5.64263800	1.69326600
C	-1.79969200	-4.42189300	-4.31464300
H	-1.81871800	-3.02208700	-5.96562200
H	-1.57090700	-5.65867700	-2.60231700
H	0.80923500	-7.04715800	0.86113600
H	-2.71526500	-4.91707600	-4.62147000
C	1.14529800	4.05981400	0.24751900
C	1.37691400	4.61670100	-0.97215200
C	-0.18612300	4.12908900	0.82714800
C	0.35334000	5.31021500	-1.69982900
H	2.36898500	4.56295500	-1.41275200
C	-1.19735900	4.88488800	0.17831700
C	-0.50723200	3.43262900	2.01581800
C	0.62891000	5.85062500	-2.97561900
C	-0.93066700	5.47495200	-1.12649100
C	-2.44935800	5.01708300	0.81930100
H	0.24047500	2.79202300	2.46735400

C	-1.75099400	3.54495000	2.59593000
C	-0.34062900	6.53215500	-3.67649000
H	1.62222200	5.71385000	-3.39422700
C	-1.90719300	6.17746500	-1.86757500
C	-2.71870100	4.37642300	2.00942900
H	-3.22531000	5.62484900	0.36986200
H	-1.97909600	2.99055500	3.50114900
C	-1.61983900	6.69385100	-3.11428800
H	-0.12194400	6.94157700	-4.65744000
H	-2.90432400	6.31242300	-1.46401500
H	-3.69086600	4.49301000	2.47634800
H	-2.38819700	7.22777500	-3.66453800
H	-0.82904500	-1.24159900	-2.33949400

DIV

C	4.32652400	4.05462600	2.30119700
C	4.72266000	4.03762900	0.98569200
C	4.11661200	3.14399300	0.06629100
C	3.09676900	2.27125700	0.54108500
C	2.71306300	2.29733300	1.90872200
C	3.31477600	3.17891900	2.76914400
H	5.29814800	3.73503100	-1.64723600
H	4.79412500	4.74580700	2.99606700
H	5.50101200	4.70814100	0.63212600
C	4.50673600	3.07491300	-1.30039500
C	2.49254000	1.37745800	-0.36480000
H	1.94074800	1.60652900	2.24234300
H	3.02556400	3.20295900	3.81507600
C	2.87788300	1.35786000	-1.69004400
C	3.92456100	2.19921700	-2.18228800
H	1.77933800	0.65538000	0.02286600
N	2.34144400	0.41346400	-2.58959000
N	1.18504800	0.03592600	-2.32111400
C	0.72210800	-1.04994500	-3.15197800
O	1.40945600	-1.91863400	-3.61988300
O	-0.59263500	-0.94467200	-3.23484900
C	-1.25796200	-2.02921300	-3.89407600
H	-1.03989600	-2.96494800	-3.37428600
H	-2.32008300	-1.79577200	-3.84096900
H	-0.92744800	-2.09957800	-4.93262800
C	4.34041400	2.11812400	-3.62382900
H	4.58657100	1.08746100	-3.89606500
H	3.53339100	2.44394000	-4.28786200
H	5.21180700	2.75015200	-3.80643700
C	-1.30278900	-3.53525400	0.79725500
C	-1.24669600	-4.51096200	1.79636800
C	-0.06040000	-4.75381900	2.47781100
C	1.06946400	-4.00271800	2.16104000
C	1.02667700	-2.97612700	1.20890600
C	-0.18577000	-2.75175500	0.54680500
C	-3.53459900	-4.14503900	1.25891300
C	-2.60898100	-5.13809400	1.98739600
H	-0.01041000	-5.51205300	3.25389600
H	2.00612600	-4.18755000	2.67928000
H	-3.80525700	-3.32787200	1.93672800
H	-2.64885200	-6.13216200	1.52582100
C	-2.65560100	-3.56841300	0.11313300
C	-3.28095500	-2.34183300	-0.52725000

C	-2.64988400	-4.55236900	-1.09225800
C	-4.07157500	-2.71900200	-1.61935400
C	-3.21957200	-1.00202700	-0.17123600
C	-3.90927200	-4.19429200	-1.90062100
H	-2.62243300	-5.59621700	-0.76794500
C	-4.83971700	-1.78169500	-2.29830300
C	-3.99876200	-0.03504900	-0.82050500
H	-3.80101600	-4.40387400	-2.96903500
C	-4.81089400	-0.45197700	-1.88111800
H	-5.45347700	-2.07597100	-3.14487500
H	-5.41776900	0.29256100	-2.38769600
H	-2.86461200	-5.25999100	3.04335500
H	-4.45554600	-4.59915100	0.88178500
H	-1.75454800	-4.36292000	-1.69395400
H	-4.78361300	-4.75418700	-1.54733900
O	-2.34977200	-0.60075800	0.84137700
O	-0.31928500	-1.65757100	-0.31243900
P	-0.81269100	-0.30629700	0.45484400
O	-0.02574000	0.03376400	1.65208600
O	-0.87158200	0.71335200	-0.73265100
C	-3.94817100	1.40314700	-0.43823100
C	-3.57001700	2.31593600	-1.37129200
C	-4.32615900	1.84698500	0.89199600
C	-3.49849900	3.71868400	-1.08386800
H	-3.27423500	1.97964700	-2.36205900
C	-4.26274000	3.22806200	1.21625600
C	-4.78435400	0.93390600	1.86855900
C	-3.08419000	4.62949400	-2.08043000
C	-3.83121800	4.18921700	0.20857600
C	-4.63913800	3.63121800	2.51695700
H	-4.85635000	-0.11896200	1.61637300
C	-5.14836900	1.35657000	3.12744700
C	-2.99869500	5.97720300	-1.81254200
H	-2.82986900	4.24328900	-3.06397500
C	-3.73198900	5.57614500	0.45679700
C	-5.06858000	2.71924400	3.45626600
H	-4.59639700	4.67890900	2.79123000
H	-5.49824200	0.63792000	3.86177600
C	-3.32642700	6.45065700	-0.52989000
H	-2.67714500	6.67061800	-2.58323400
H	-3.97276300	5.97475000	1.43563500
H	-5.35164400	3.05732500	4.44813500
H	-3.25795800	7.51185200	-0.31168900
C	2.25173500	-2.19154000	0.88671900

C	2.75477900	-2.23764300	-0.37721600
C	2.96077300	-1.45411300	1.91788900
C	3.99782600	-1.61272200	-0.72488200
H	2.22710100	-2.78814600	-1.15355400
C	4.21011900	-0.84915100	1.61878600
C	2.41894900	-1.30856700	3.21589100
C	4.47499000	-1.67845500	-2.05203200
C	4.73602000	-0.91412900	0.26074400
C	4.89987800	-0.18320300	2.65671600
H	1.43354300	-1.71172600	3.42033200
C	3.10995700	-0.64313500	4.20484900
C	5.65457800	-1.05926800	-2.40517400
H	3.87851500	-2.20405400	-2.79260300
C	5.93016300	-0.27227900	-0.13417100
C	4.37180900	-0.09297300	3.92651500
H	5.86073900	0.27857500	2.45997100
H	2.67589100	-0.53979600	5.19440700
C	6.38034100	-0.34326300	-1.43738500
H	6.01704700	-1.11398500	-3.42720900
H	6.50911700	0.29684600	0.58434500
H	4.92239500	0.42698700	4.70451500
H	7.29912600	0.16410400	-1.71566900
H	-0.08373900	0.59835900	-1.34990100

DIV_{R2}

C	-2.26420700	-0.10430500	4.50228900
C	-1.10975100	-0.44337900	3.75340500
C	-0.88631200	0.18029000	2.53054200
C	-1.82288800	1.11651000	2.07784700
C	-2.96195200	1.47020900	2.83123100
C	-3.17588300	0.84063500	4.06230300
H	-2.44231500	-0.59835500	5.45296400
H	-0.02916100	-0.05082400	1.90744500
H	-4.05150000	1.07922500	4.66040000
C	-2.98634100	2.56247400	0.81527100
C	-3.46544900	3.35941600	-0.22771600
C	-4.68786200	3.99385600	-0.04522200
C	-5.42494600	3.84265000	1.14189400
C	-4.94524100	3.04956700	2.17684300
C	-3.71579700	2.40298800	2.02154500
H	-2.90843200	3.46543000	-1.15355900
H	-5.08510900	4.61430900	-0.84347200
H	-6.37824100	4.35065700	1.24784600
H	-5.51850800	2.92779600	3.09204700
N	-1.84838400	1.79143700	0.87793400
H	-1.10617700	1.72611900	0.18890700
C	-0.16314700	-1.51691500	4.29808800
C	-0.89356300	-2.86991800	4.30510800
C	1.09926500	-1.65648400	3.44418100
C	0.26841800	-1.16184100	5.73042300
H	-1.80395000	-2.83508300	4.91192400
H	-1.17579800	-3.15962600	3.28688900
H	-0.24443300	-3.65261700	4.71486300
H	1.68144900	-0.72838900	3.43133800
H	1.73860100	-2.44196900	3.86182600
H	0.87030100	-1.92664100	2.40723900
H	0.97668400	-1.90840900	6.10656300
H	0.75931500	-0.18327500	5.75755500
H	-0.57971600	-1.13382400	6.42038800
C	2.88754300	-2.46283400	0.18110500
C	3.50476600	-2.79573000	1.39146600
C	4.23185100	-1.84998000	2.10377500
C	4.31594200	-0.55002100	1.61370100
C	3.67635700	-0.17224700	0.42637100
C	2.96865100	-1.15402600	-0.27555100
C	1.97054500	-4.52653300	0.87188800
C	3.18392800	-4.22251600	1.76635900
H	4.70690800	-2.11056300	3.04524000

H	4.86540300	0.20612700	2.16703000
H	1.05704900	-4.16274700	1.35664500
H	4.02614300	-4.88534100	1.53323300
C	2.22179100	-3.69033500	-0.41760000
C	0.97113400	-3.60925500	-1.27509900
C	3.16406600	-4.47739100	-1.37178800
C	0.93349700	-4.69053000	-2.16500300
C	-0.07567300	-2.70314000	-1.28228600
C	2.23097200	-5.46239900	-2.09987800
H	3.98067400	-4.96604100	-0.83332600
C	-0.16999900	-4.90140200	-2.98002300
C	-1.20611400	-2.88625000	-2.09017500
H	2.59661800	-5.74019800	-3.09194600
C	-1.24008800	-4.00876500	-2.92334000
H	-0.19644200	-5.74126200	-3.66807100
H	-2.11171300	-4.16063100	-3.55308800
H	2.96636200	-4.33401800	2.83232500
H	1.84071000	-5.58995700	0.65320400
H	3.59846000	-3.77832100	-2.09436700
H	2.10418800	-6.38953300	-1.52806300
O	0.01862900	-1.52748100	-0.53202700
O	2.27914400	-0.80013000	-1.44191600
P	0.77939400	-0.28146700	-1.21570400
O	0.58821900	0.92806200	-0.39725800
O	0.35584900	-0.21932600	-2.74017500
C	-2.28435700	-1.85845700	-2.14111300
C	-2.54478500	-1.24846400	-3.33174100
C	-3.05099400	-1.49509900	-0.96211600
C	-3.52946200	-0.21248800	-3.46327500
H	-1.97094900	-1.52664000	-4.21365400
C	-4.04198300	-0.48140900	-1.05752300
C	-2.84854400	-2.14803900	0.27541800
C	-3.73587000	0.42178500	-4.70869500
C	-4.27701300	0.18968600	-2.33026400
C	-4.78350800	-0.15714600	0.10004300
H	-2.09665900	-2.92810600	0.34492800
C	-3.59480800	-1.81814500	1.38509300
C	-4.65870100	1.43537100	-4.83717000
H	-3.14860400	0.09608800	-5.56328800
C	-5.21876700	1.23108700	-2.49177300
C	-4.57082300	-0.81291700	1.29295100
H	-5.53246200	0.62654100	0.06408300
H	-3.42147100	-2.32142200	2.33174000
C	-5.40467800	1.84035000	-3.71552100

H	-4.81043800	1.92019700	-5.79628600
H	-5.80524900	1.57263900	-1.64675700
H	-5.15297100	-0.54063200	2.16762700
H	-6.13319600	2.63937600	-3.81130100
C	3.77855700	1.23261100	-0.06242100
C	4.43394500	1.49763100	-1.22258000
C	3.23445300	2.32227600	0.72619300
C	4.66473400	2.84036100	-1.67367300
H	4.83162200	0.68041800	-1.81980400
C	3.46465800	3.66349800	0.32721600
C	2.43833000	2.06811700	1.86556100
C	5.37105400	3.07615500	-2.87337600
C	4.21666700	3.93307100	-0.89204600
C	2.92824200	4.70015700	1.12354400
H	2.21652100	1.03963200	2.12970100
C	1.91357100	3.09740000	2.61388000
C	5.63517300	4.35970500	-3.29615700
H	5.70284200	2.22145800	-3.45686900
C	4.50705400	5.23855600	-1.34578800
C	2.17454300	4.42786200	2.24508700
H	3.09387700	5.73516700	0.84750300
H	1.28946600	2.87749200	3.47472900
C	5.20093600	5.44851200	-2.51943500
H	6.17748200	4.53263000	-4.22037100
H	4.18748100	6.09973800	-0.77001700
H	1.76713700	5.24467900	2.83267600
H	5.41190800	6.46270000	-2.84418100
H	-0.53748700	0.14243600	-2.87306000

COMIV

C	-5.42671900	-0.34789500	-0.64300100
C	-5.16207300	-1.25384900	-1.64511500
C	-3.82767600	-1.51458100	-2.03888600
C	-2.77621400	-0.81026900	-1.38371400
C	-3.07446000	0.11834500	-0.35351600
C	-4.37790100	0.34307800	0.00876900
H	-4.31501300	-2.98670100	-3.54703400
H	-6.45401900	-0.16152000	-0.34123200
H	-5.97051000	-1.78446200	-2.14065900
C	-3.50344000	-2.45462100	-3.05645900
C	-1.44568100	-1.06816800	-1.76138500
H	-2.24962600	0.64098700	0.12778900
H	-4.60393500	1.05754700	0.79342600
C	-1.16083900	-1.99217600	-2.75230900
C	-2.20787600	-2.71365200	-3.41925500
H	-0.65706100	-0.54434500	-1.23149900
N	0.13209400	-2.32928400	-3.15835500
N	1.09282800	-1.68497900	-2.68434200
C	2.35660100	-2.20121800	-3.16340000
O	2.55870500	-3.30991400	-3.58105100
O	3.25636400	-1.23703200	-3.02834800
C	4.57991800	-1.56670000	-3.46487300
H	4.59075100	-1.71442200	-4.54713700
H	5.20064700	-0.71654800	-3.18693100
H	4.92899700	-2.47688100	-2.97203500
C	-1.87122900	-3.72993500	-4.47473500
H	-1.32360300	-3.27559300	-5.30569000
H	-1.23184500	-4.51770600	-4.06513000
H	-2.78325100	-4.18542800	-4.86597700
C	-5.09088700	-2.01684200	2.64345400
C	-4.47540400	-0.88771900	3.23649300
C	-3.12294600	-0.65654700	3.00466600
C	-2.42162300	-1.54295900	2.18225300
C	-3.03465500	-2.66913000	1.59094300
C	-4.39246200	-2.89745300	1.83330200
H	-6.14488800	-2.20296500	2.82846400
H	-2.60842400	0.20038000	3.42549100
H	-4.89730100	-3.74881300	1.38482800
C	-0.83805700	-2.54955200	0.94725100
C	0.34937900	-2.88147300	0.29167200
C	0.34253400	-4.01156300	-0.51558600
C	-0.81745200	-4.78580000	-0.68382300
C	-1.99970100	-4.44509500	-0.03691600

C	-2.01592600	-3.32327000	0.79611900
H	1.24098800	-2.27034300	0.40493600
H	1.25046000	-4.28845500	-1.04542600
H	-0.78694000	-5.65881500	-1.32840600
H	-2.89873700	-5.03931000	-0.17652100
N	-1.09831300	-1.49344700	1.79514300
H	-0.51037400	-0.66836200	1.86078800
C	-5.31712300	0.03519700	4.12559200
C	-5.78916200	-0.75314500	5.35876200
C	-4.52651000	1.25670100	4.60374400
C	-6.54494500	0.53927600	3.34907900
H	-6.39466800	-1.61896100	5.07398200
H	-4.93287200	-1.11534500	5.93704800
H	-6.39708200	-0.11390900	6.00886600
H	-4.16973700	1.85882700	3.76079100
H	-5.17133500	1.89080000	5.22066900
H	-3.66258700	0.97008500	5.21164100
H	-7.15829300	1.17908600	3.99345000
H	-6.24274000	1.12934800	2.47696200
H	-7.17551700	-0.28371000	3.00078000
C	2.34758500	4.24387400	0.29786200
C	2.08797500	5.47567200	0.90674500
C	0.85635600	6.09313600	0.73987500
C	-0.13415500	5.44188700	0.01126200
C	0.04651200	4.15070800	-0.50988600
C	1.32372000	3.57987300	-0.36303200
C	4.15465100	4.66758400	1.75528000
C	3.28969100	5.93986000	1.69497300
H	0.66080300	7.06921300	1.17425000
H	-1.08989500	5.93225800	-0.13970200
H	3.83916700	4.04352900	2.59852900
H	3.80925700	6.75373900	1.17547700
C	3.82629000	3.91960000	0.43211900
C	4.39958900	2.51135900	0.41754300
C	4.63379200	4.56031900	-0.73470500
C	5.69795500	2.54045700	-0.10755700
C	3.87001400	1.29975300	0.84037300
C	6.02543200	3.91698800	-0.63285600
H	4.64831100	5.65173700	-0.67402200
C	6.48123000	1.39579400	-0.13145600
C	4.63140900	0.11944900	0.82188200
H	6.55213300	3.88147200	-1.59019200
C	5.94801300	0.20362300	0.34996200
H	7.49146200	1.42329200	-0.52934600

H	6.54958500	-0.70010800	0.34446000
H	3.01301400	6.31227300	2.68509100
H	5.22394100	4.87075000	1.86001600
H	4.16367000	4.27466700	-1.68193100
H	6.66536800	4.46118400	0.07242700
O	2.53699400	1.25095100	1.24946900
O	1.59869800	2.31125100	-0.87434000
P	1.39930500	1.05938400	0.12572200
O	0.06697800	0.97118400	0.75772200
O	1.93314300	-0.12842200	-0.72575100
C	4.08745200	-1.22391100	1.17150900
C	4.22896300	-2.21799900	0.25155300
C	3.46584900	-1.52139400	2.44932500
C	3.79265500	-3.56109400	0.48868400
H	4.67869800	-1.99138400	-0.71187400
C	2.98604100	-2.83487800	2.70821100
C	3.34917000	-0.53811600	3.45847100
C	3.97479000	-4.55529300	-0.49937600
C	3.16562500	-3.88648400	1.71448400
C	2.35130300	-3.08607500	3.94512300
H	3.75413900	0.45211700	3.28058100
C	2.73899100	-0.81751600	4.66076300
C	3.55147200	-5.84763300	-0.28258300
H	4.45021400	-4.28024100	-1.43773000
C	2.73558300	-5.21772600	1.90709800
C	2.22190200	-2.10116700	4.89983800
H	1.95423900	-4.07188700	4.15670700
H	2.65578200	-0.04636800	5.42005000
C	2.92484100	-6.17627600	0.93271800
H	3.69227500	-6.60620200	-1.04589700
H	2.24104200	-5.50468400	2.82777300
H	1.72633400	-2.32197800	5.83992900
H	2.58148900	-7.19140300	1.10577200
C	-1.06498900	3.46034600	-1.22332100
C	-0.81760600	2.77611700	-2.37533400
C	-2.44329200	3.56896100	-0.75209500
C	-1.85720300	2.15109100	-3.13836500
H	0.19783700	2.69259300	-2.74963300
C	-3.50612600	3.13265900	-1.58743500
C	-2.76432700	4.06597000	0.53362900
C	-1.53270500	1.31681500	-4.23038100
C	-3.21012200	2.35820600	-2.78531700
C	-4.83545800	3.37235600	-1.17601000
H	-1.96318700	4.29972600	1.22498200

C	-4.07253900	4.24075600	0.93311600
C	-2.52214000	0.68533200	-4.95149400
H	-0.48418500	1.16248700	-4.47399000
C	-4.20606000	1.71589600	-3.55257800
C	-5.12008300	3.93162500	0.05059800
H	-5.65728400	3.09060900	-1.82441500
H	-4.28798800	4.62181200	1.92663000
C	-3.86960400	0.89291900	-4.60850800
H	-2.26512400	0.02650800	-5.77540400
H	-5.25307700	1.83097100	-3.29628400
H	-6.15139900	4.10114000	0.34454200
H	-4.65303600	0.38867000	-5.16608600
H	1.42654700	-0.55632400	-1.49051600

TSIV-1Value of imaginary frequency = -242.9 cm⁻¹

C	-4.63855100	-2.84687200	-2.16652500
C	-3.71353500	-3.88075600	-2.09692900
C	-2.35331200	-3.59998800	-1.92233600
C	-1.95586600	-2.25020700	-1.76767500
C	-2.90524300	-1.21616300	-1.80527400
C	-4.23922400	-1.51111600	-2.03090800
H	-1.68286500	-5.67692000	-1.95954400
H	-5.68744100	-3.07640700	-2.33120500
H	-4.03427000	-4.91284100	-2.20616500
C	-1.34370200	-4.64438500	-1.94642600
C	-0.56297300	-1.96392000	-1.55627600
H	-2.57948100	-0.18738900	-1.66318000
H	-4.97246800	-0.71383400	-2.08879900
C	0.39183800	-2.95623700	-2.02487200
C	-0.02547200	-4.36334200	-2.04020200
H	-0.26760200	-0.91702100	-1.56377700
N	1.59735600	-2.70622800	-2.46527600
N	2.07020400	-1.48063200	-2.53924000
C	3.29291400	-1.31291700	-3.18572000
O	4.02299700	-2.19590800	-3.56248100
O	3.50827600	-0.00288400	-3.33894800
C	4.70386100	0.33441200	-4.04767000
H	4.69656200	-0.12203500	-5.03975900
H	4.69998800	1.41999900	-4.12684800
H	5.58965200	-0.00387800	-3.50247900
C	1.03053600	-5.41719700	-2.17725700
H	1.53796400	-5.33613400	-3.14343200
H	1.79619900	-5.29279300	-1.40463600
H	0.59124800	-6.41301800	-2.09052000
C	-3.34116900	-4.48481900	2.15621600
C	-3.72831200	-3.18994600	1.76552600
C	-2.76706000	-2.32657700	1.22259400
C	-1.46144000	-2.79048200	1.10369500
C	-1.07582900	-4.06694200	1.53586800
C	-2.03012300	-4.93168400	2.05730600
H	-4.08734600	-5.15364700	2.57483800
H	-3.01382500	-1.31417600	0.92257300
H	-1.75493400	-5.92605600	2.39556800
C	0.78870500	-2.94298300	0.80435900
C	2.11770400	-2.69293700	0.50782100
C	3.03011100	-3.72039000	0.76862100
C	2.62374300	-4.93990300	1.31127700

C	1.28236500	-5.17654700	1.60967700
C	0.36394700	-4.16833600	1.34741900
H	2.44159700	-1.74328200	0.08819200
H	4.07434800	-3.57178000	0.52926600
H	3.36505300	-5.71102300	1.49605400
H	0.96055900	-6.12202300	2.03578200
N	-0.34280800	-2.11820200	0.53172800
H	-0.26701700	-1.08747200	0.70982300
C	-5.18435400	-2.77090100	1.98132200
C	-5.50166400	-2.81634800	3.48561300
C	-5.45567500	-1.35409000	1.47754000
C	-6.11580800	-3.74079300	1.23640400
H	-5.36938300	-3.82142300	3.89750500
H	-4.85137200	-2.13344000	4.04174500
H	-6.54102300	-2.51595500	3.65905800
H	-5.26321400	-1.25843000	0.40352600
H	-6.50596000	-1.10330000	1.65464200
H	-4.84787000	-0.60977000	2.00290300
H	-7.15813900	-3.42630800	1.35812600
H	-5.88279800	-3.75479000	0.16700800
H	-6.03105000	-4.76371700	1.61558100
C	0.17665700	4.72317500	0.41131500
C	-0.20553100	5.74503900	1.28463500
C	-1.49831400	5.79599200	1.78528600
C	-2.40296300	4.81825800	1.39254000
C	-2.03913500	3.74747400	0.55819400
C	-0.71108300	3.69883900	0.09719000
C	2.14063600	5.90462800	0.99007400
C	0.93860200	6.70014000	1.52098600
H	-1.81024100	6.59656800	2.44957900
H	-3.43264400	4.88497200	1.72757800
H	2.52366500	5.24877100	1.77980900
H	0.78816300	7.62664300	0.95275700
C	1.55341100	5.01882200	-0.14852600
C	2.55334600	3.95145000	-0.53677200
C	1.48614000	5.83921600	-1.46643200
C	3.42890300	4.46109300	-1.50041600
C	2.75624700	2.68319300	-0.00911600
C	2.92329500	5.78833200	-2.01947700
H	1.11761800	6.85589200	-1.30220100
C	4.57627800	3.76012100	-1.84476200
C	3.95651600	1.99849800	-0.26228100
H	2.95906200	5.84514600	-3.11106300
C	4.84873700	2.56411900	-1.18608200

H	5.26802800	4.14799900	-2.58724500
H	5.78024100	2.04187500	-1.38447200
H	1.04194500	6.97885700	2.57335100
H	2.96487300	6.53306200	0.64150900
H	0.80373900	5.33292400	-2.15783900
H	3.53140500	6.61507900	-1.63286100
O	1.75472300	2.09861200	0.75025800
O	-0.27115000	2.67960700	-0.72591900
P	0.53659400	1.38848600	-0.10330600
O	-0.30931100	0.64309300	0.88163500
O	1.09925200	0.69274900	-1.30458700
C	4.36573200	0.73569700	0.41324600
C	4.87606200	-0.26983100	-0.35037100
C	4.40408300	0.60949300	1.86380800
C	5.47870100	-1.44235300	0.20685900
H	4.86704700	-0.17137000	-1.43034900
C	4.95378400	-0.56208000	2.45399400
C	3.95441200	1.64699900	2.71180200
C	6.03130600	-2.42735000	-0.64277500
C	5.52576000	-1.60483600	1.61087700
C	4.96640100	-0.66732500	3.86255200
H	3.57813800	2.56402500	2.27591100
C	3.99199000	1.52212800	4.08266800
C	6.62979400	-3.55116500	-0.11657800
H	5.95720400	-2.28780400	-1.71851900
C	6.13896600	-2.77038400	2.12236900
C	4.48999100	0.34612000	4.66442300
H	5.36223700	-1.55976300	4.33250000
H	3.63712300	2.33358600	4.70998700
C	6.68082100	-3.72007000	1.27935400
H	7.05096200	-4.30554100	-0.77336600
H	6.19491800	-2.93663200	3.19183600
H	4.51102300	0.23730100	5.74418000
H	7.14724700	-4.60553500	1.69992900
C	-3.12409200	2.85536900	0.05838600
C	-3.24916200	2.64063000	-1.28065000
C	-4.18960900	2.41245200	0.94846400
C	-4.43015100	2.06203000	-1.85631700
H	-2.46921100	2.97971000	-1.95695900
C	-5.42037500	1.95894200	0.40546900
C	-4.03854900	2.44438900	2.35425900
C	-4.51382500	1.85418100	-3.25141200
C	-5.54371000	1.76364000	-1.03339600
C	-6.49295600	1.70379300	1.28851000

H	-3.07364200	2.71184300	2.77131300
C	-5.08953800	2.14533900	3.19483700
C	-5.66859900	1.36959300	-3.82595500
H	-3.64743200	2.09005800	-3.86365900
C	-6.71531100	1.26777300	-1.64757700
C	-6.34105300	1.81062500	2.65410000
H	-7.45677800	1.40292500	0.89344600
H	-4.94890600	2.17714700	4.27054800
C	-6.77887400	1.07669200	-3.01370500
H	-5.72229800	1.21257300	-4.89851400
H	-7.58338900	1.02082400	-1.04667800
H	-7.18143200	1.60410800	3.30966800
H	-7.69056600	0.69252700	-3.46045900
H	1.61540100	-0.63195900	-2.13283500

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C	4.63505500	-2.73508700	2.37445600
C	3.85128400	-3.81502900	1.97239000
C	2.53061000	-3.61653300	1.56573200
C	2.02248700	-2.30594300	1.52327400
C	2.80384600	-1.23156600	1.93013300
C	4.11217700	-1.44376500	2.36516800
H	2.08357700	-5.71251100	1.05507100
H	5.65727400	-2.90255200	2.70063000
H	4.25392200	-4.82412400	1.99840000
C	1.63818100	-4.74031500	1.25207900
C	0.60866600	-2.11146300	1.02614600
H	2.39231200	-0.22454200	1.89535400
H	4.71834800	-0.60476000	2.68937700
C	-0.21113500	-3.23946400	1.62708700
C	0.30235700	-4.59939100	1.32754000
H	0.25261600	-1.13664700	1.35580500
N	-1.23753900	-3.14499800	2.38708400
N	-1.73638400	-1.92704700	2.70335900
C	-2.77271100	-1.86829500	3.59900200
O	-3.32203200	-2.80486700	4.13296400
O	-3.09777700	-0.57642300	3.79307100
C	-4.21944800	-0.35933800	4.65033300
H	-4.01358600	-0.73297300	5.65572200
H	-4.36744100	0.71970300	4.66848200
H	-5.11127700	-0.85393500	4.25595500
C	-0.68829700	-5.70867500	1.15641500
H	-1.31152900	-5.80108500	2.05112600
H	-1.36212300	-5.48974100	0.31926900
H	-0.18560300	-6.66046700	0.97217200
C	3.24419800	-3.67722700	-3.25546500
C	3.77559200	-2.83550000	-2.25872700
C	2.92097100	-2.27514200	-1.30688900
C	1.56358200	-2.60262400	-1.33634500
C	1.04631700	-3.42036000	-2.35052500
C	1.89117400	-3.95959500	-3.32039400
H	3.90878400	-4.10330300	-4.00148200
H	3.30582700	-1.59690000	-0.55813100
H	1.49082700	-4.58914300	-4.10964000
C	-0.69194400	-2.71764400	-1.03600400
C	-2.00230700	-2.58307900	-0.58603200
C	-2.98565900	-3.31433200	-1.24835200
C	-2.68822600	-4.11190700	-2.35926500
C	-1.38633100	-4.20244300	-2.83292100

C	-0.38529900	-3.50923800	-2.15364800
H	-2.26271200	-1.94328900	0.25238200
H	-4.00569700	-3.26925500	-0.88968900
H	-3.48744400	-4.65560000	-2.85302000
H	-1.14402500	-4.80747000	-3.70150500
N	0.49828000	-2.13477000	-0.49357000
H	0.29191300	-0.39562400	-0.84947500
C	5.28095000	-2.55550900	-2.25635800
C	5.67362000	-1.88055700	-3.58012400
C	5.68504500	-1.63829900	-1.10245400
C	6.04482200	-3.88172800	-2.11139300
H	5.45397300	-2.51931400	-4.44127000
H	5.13041800	-0.93864400	-3.70704900
H	6.74751300	-1.66129000	-3.58874400
H	5.46141900	-2.09311000	-0.13242000
H	6.76164600	-1.44410700	-1.14629700
H	5.17108400	-0.67399100	-1.15831900
H	7.12407700	-3.69333200	-2.09584900
H	5.77174500	-4.38671800	-1.17865400
H	5.83699100	-4.56520100	-2.94003700
C	-0.11707100	4.52206600	-0.73728200
C	0.33059000	5.41558000	-1.71493000
C	1.64677100	5.37463700	-2.14870300
C	2.51048300	4.44650000	-1.58004200
C	2.08101200	3.48614500	-0.64773700
C	0.72368800	3.51603000	-0.27992900
C	-2.01793900	5.70446200	-1.49945200
C	-0.77365600	6.36203200	-2.11947900
H	2.01388800	6.07888200	-2.88927500
H	3.56010700	4.47353100	-1.84974700
H	-2.42780000	4.96203200	-2.19289600
H	-0.59650900	7.35987400	-1.70047100
C	-1.47869300	4.96434200	-0.24234100
C	-2.51643400	4.01672800	0.31142800
C	-1.34388800	5.96358400	0.94306500
C	-3.32574800	4.68358900	1.23769300
C	-2.80018300	2.70478600	-0.02795800
C	-2.76370300	6.05455700	1.53101200
H	-0.93879200	6.92781300	0.62397700
C	-4.45396300	4.06766400	1.75808300
C	-3.97484700	2.08594300	0.41404000
H	-2.76691300	6.28542800	2.59960700
C	-4.78672800	2.79065900	1.31126300
H	-5.08079900	4.57465800	2.48574000

H	-5.69653900	2.31145300	1.66028300
H	-0.84810700	6.47440600	-3.20453000
H	-2.81112600	6.41416400	-1.24873900
H	-0.66244600	5.53370600	1.68508600
H	-3.35393500	6.83036300	1.02862800
O	-1.86805100	1.98409400	-0.79074400
O	0.20500700	2.57059500	0.61068600
P	-0.68524300	1.32768500	0.09363400
O	0.17616700	0.59195300	-0.98989900
O	-1.15266800	0.53913700	1.25238800
C	-4.46165300	0.76752500	-0.08005900
C	-4.61504300	-0.26470100	0.78943300
C	-4.95604100	0.64939100	-1.44225000
C	-5.30478700	-1.46950200	0.42413100
H	-4.22599300	-0.17411800	1.80098000
C	-5.66942900	-0.51575700	-1.82934300
C	-4.77027800	1.68379500	-2.38687200
C	-5.42520500	-2.53072900	1.34776500
C	-5.87643100	-1.58926900	-0.86602800
C	-6.15701500	-0.59820400	-3.15212700
H	-4.24101700	2.58341500	-2.09198200
C	-5.25251500	1.57331700	-3.67259600
C	-6.10683900	-3.68124400	1.01570300
H	-4.96424000	-2.43544200	2.32734500
C	-6.58729300	-2.77066700	-1.17271400
C	-5.95372000	0.42009100	-4.05819900
H	-6.70120700	-1.47859500	-3.47364400
H	-5.09298600	2.37728700	-4.38394300
C	-6.70025500	-3.79461400	-0.25396600
H	-6.18588100	-4.49367400	1.73072500
H	-7.04836600	-2.89389700	-2.14576700
H	-6.33698900	0.32791800	-5.06948700
H	-7.24766600	-4.69428300	-0.51698000
C	3.11252500	2.66717700	0.05243600
C	3.07124600	2.57262500	1.41109500
C	4.29878300	2.19356600	-0.65196800
C	4.18374200	2.09560100	2.18157300
H	2.20415200	2.93684800	1.95502700
C	5.46629300	1.85666500	0.08408600
C	4.33137700	2.08391200	-2.06151700
C	4.08353600	1.99613300	3.58726900
C	5.40796500	1.79382300	1.53911100
C	6.65443700	1.57613100	-0.62685400
H	3.41921500	2.25545000	-2.62305300

C	5.49798700	1.77590000	-2.72915100
C	5.16894900	1.61705100	4.34651700
H	3.13243700	2.22832300	4.05910200
C	6.50721600	1.41594600	2.34103400
C	6.68035300	1.55723500	-2.00456100
H	7.56805000	1.35774200	-0.08568300
H	5.50032300	1.70724000	-3.81251500
C	6.39189800	1.33040900	3.71409800
H	5.08284300	1.54020300	5.42569000
H	7.45941400	1.17481900	1.88281300
H	7.60713100	1.33961600	-2.52655400
H	7.25121700	1.03480800	4.30770500
H	-1.40574100	-1.04866900	2.29622700

IMIV-2

C	1.88272200	1.87039700	-2.88517000
C	2.35661500	2.59193800	-1.79059100
C	2.40482400	2.01066000	-0.52067500
C	1.97115400	0.67951100	-0.37032600
C	1.51373600	-0.04702200	-1.46415100
C	1.46582500	0.54817500	-2.72787900
H	3.50867100	3.63578000	0.47472800
H	1.83890800	2.34109000	-3.86277100
H	2.68518900	3.62094100	-1.91522000
C	2.91309800	2.74275600	0.64904000
C	2.03556100	0.05589200	1.00667900
H	1.19453300	-1.07716700	-1.32031900
H	1.10335400	-0.02009100	-3.57923900
C	1.71249900	1.16794300	1.99804800
C	2.61095800	2.34754800	1.89731400
H	1.31424000	-0.76491000	1.04941800
N	0.72149700	1.27071500	2.80015000
N	-0.21596500	0.28790900	2.83264000
C	-1.38617200	0.56190300	3.50480800
O	-1.63359700	1.54694300	4.16322200
O	-2.22102100	-0.47380900	3.32652600
C	-3.51369600	-0.30060500	3.90123900
H	-3.98052900	0.61245000	3.52353200
H	-4.08709000	-1.17914200	3.60552400
H	-3.44580800	-0.24358200	4.99059900
C	3.07114500	3.01132200	3.15557200
H	2.22699200	3.16575600	3.83266200
H	3.78845100	2.36364500	3.67434700
H	3.55007800	3.97145700	2.94892000
C	7.14083700	-0.97775000	-0.31353400
C	6.19088200	-0.32399800	-1.12835000
C	4.89847300	-0.11680400	-0.65363200
C	4.55520300	-0.56117900	0.63512600
C	5.51656900	-1.22587600	1.43337500
C	6.81210300	-1.42892500	0.95092000
H	8.14782600	-1.13671600	-0.68750800
H	4.17364900	0.36791900	-1.28713700
H	7.54819000	-1.94006100	1.56535300
C	3.53180900	-1.16179900	2.55934100
C	2.60116300	-1.41271200	3.57479900
C	3.03887800	-2.12004500	4.68799300
C	4.36417800	-2.56710000	4.80488600
C	5.28173700	-2.31897200	3.79374800

C	4.86536700	-1.61198100	2.66223400
H	1.56857000	-1.08717400	3.50856600
H	2.33351800	-2.32804300	5.48668300
H	4.66780300	-3.11605100	5.69031900
H	6.30628000	-2.67108400	3.87439900
N	3.35205300	-0.51041800	1.34565700
H	-0.82516900	0.94883300	-1.69328000
C	6.61308800	0.13644800	-2.52902500
C	7.06774600	-1.08146100	-3.35064400
C	5.47325900	0.82751100	-3.28329400
C	7.78246800	1.12785700	-2.40595800
H	7.91034100	-1.59578900	-2.87914600
H	6.25108300	-1.80226900	-3.46312000
H	7.38454200	-0.76588900	-4.35098500
H	5.12192600	1.72013500	-2.75500200
H	5.82577200	1.14040000	-4.27149100
H	4.61841600	0.15826800	-3.42835100
H	8.09522500	1.46945700	-3.39891300
H	7.49041800	2.00453900	-1.81886800
H	8.65047100	0.67141600	-1.92108300
C	-5.21119700	0.59732800	-0.22538700
C	-6.21424800	1.23791500	-0.96165700
C	-6.03329900	2.53216200	-1.43225900
C	-4.81760600	3.17317600	-1.20805800
C	-3.76168400	2.53097000	-0.54834400
C	-3.99375000	1.24206800	-0.05221100
C	-6.76082000	-1.06841200	-0.85589200
C	-7.38058100	0.30266100	-1.18071600
H	-6.81836100	3.03217500	-1.99177300
H	-4.65652600	4.17846200	-1.58642600
H	-6.24099600	-1.45598300	-1.73898000
H	-8.20697100	0.53944700	-0.49995300
C	-5.71029800	-0.75988500	0.24847800
C	-4.77494700	-1.93008300	0.48809300
C	-6.42573700	-0.67641500	1.62852600
C	-5.27492500	-2.75810500	1.50041600
C	-3.58962000	-2.28052100	-0.13564900
C	-6.50604500	-2.13484100	2.11753000
H	-7.40271100	-0.19134700	1.55331200
C	-4.62359500	-3.93882900	1.83628200
C	-2.90791700	-3.46550000	0.17500500
H	-6.51346200	-2.21696400	3.20822700
C	-3.45398700	-4.29051100	1.16192900
H	-5.00924200	-4.57814700	2.62514300

H	-2.93047400	-5.20718900	1.41611100
H	-7.77161100	0.36195100	-2.19971900
H	-7.48986900	-1.81519200	-0.52892700
H	-5.80847200	-0.08825800	2.31339800
H	-7.41466000	-2.62714900	1.75039200
O	-3.01388700	-1.39541000	-1.05569200
O	-2.93613100	0.55930100	0.55679000
P	-2.00359800	-0.32724900	-0.40972800
O	-1.69568200	0.50910500	-1.71427900
O	-0.85065500	-0.84980500	0.34380100
C	-1.58619600	-3.74603600	-0.44972800
C	-0.48533800	-3.76720000	0.34487200
C	-1.44242500	-3.88315100	-1.88632800
C	0.84137800	-3.80750100	-0.19659600
H	-0.59577600	-3.63689600	1.41888200
C	-0.14598900	-3.96239900	-2.45878300
C	-2.57319800	-3.95348700	-2.73067500
C	1.96003100	-3.69303800	0.65819000
C	1.02803900	-3.87235700	-1.59891200
C	-0.03833100	-4.12244800	-3.85822000
H	-3.56382500	-3.89773900	-2.28952800
C	-2.43817400	-4.10421300	-4.09283100
C	3.23616600	-3.63114900	0.14305900
H	1.79683200	-3.63558300	1.73195200
C	2.34721100	-3.80145900	-2.10014300
C	-1.15653600	-4.19151000	-4.66138400
H	0.94027000	-4.20897300	-4.31680700
H	-3.31961200	-4.16015300	-4.72368700
C	3.42713600	-3.67941900	-1.24914400
H	4.08877200	-3.52960600	0.80765100
H	2.52596500	-3.82007700	-3.16938700
H	-1.04441300	-4.31941300	-5.73351600
H	4.43141900	-3.61018900	-1.65565600
C	-2.44092400	3.20654300	-0.39895700
C	-1.89306700	3.38315100	0.83471700
C	-1.75080300	3.73022400	-1.56949200
C	-0.72011400	4.18530600	1.04015400
H	-2.37828900	2.96480300	1.71411200
C	-0.59660500	4.54060700	-1.40242600
C	-2.17740700	3.41155000	-2.88078200
C	-0.24427100	4.41848200	2.34980800
C	-0.09245700	4.81187900	-0.06301300
C	0.04144200	5.05047400	-2.55543600
H	-3.02290900	2.74530900	-3.01187100

C	-1.52350200	3.90854400	-3.98709100
C	0.80152300	5.28788600	2.56839300
H	-0.72227500	3.89786300	3.17597600
C	0.99523000	5.67662800	0.18926200
C	-0.41232200	4.75104900	-3.82189400
H	0.91616200	5.68293500	-2.45293800
H	-1.86473500	3.64367400	-4.98281600
C	1.42381000	5.92074600	1.47782600
H	1.14975200	5.48023100	3.57839800
H	1.49537600	6.17986200	-0.63066700
H	0.09942400	5.15523200	-4.68991700
H	2.24948000	6.60502200	1.64940800
H	-0.32190500	-0.35861600	2.04628800

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C	5.10060500	0.62525500	0.92922600
C	5.68031200	1.02512200	2.13628300
C	5.32655300	2.23443900	2.72109300
C	4.37812600	3.03494500	2.08882400
C	3.73882100	2.63042500	0.90876100
C	4.10475400	1.39706200	0.34637000
C	6.25586700	-1.25116300	1.77004400
C	6.64595700	-0.03060800	2.62453300
H	5.77849500	2.55663300	3.65490600
H	4.11076800	3.99535600	2.52035500
H	5.41996400	-1.77752700	2.24420400
H	7.68296500	0.27255200	2.43332900
C	5.75873300	-0.64268200	0.42698800
C	5.02017600	-1.66479100	-0.41471900
C	6.97338200	-0.33839700	-0.49555000
C	5.91837100	-2.32869800	-1.25757100
C	3.68014500	-2.03232800	-0.41156600
C	7.28275700	-1.68224300	-1.17997300
H	7.82015100	0.07670100	0.05909000
C	5.50337800	-3.40264400	-2.03284700
C	3.25139500	-3.15098500	-1.13893300
H	7.74369500	-1.56236200	-2.16427800
C	4.17756600	-3.82447500	-1.94109900
H	6.19729900	-3.91309000	-2.69462700
H	3.84059900	-4.68745100	-2.50818200
H	6.55548500	-0.21661900	3.69826400
H	7.07256700	-1.96455000	1.62570500
H	6.66435700	0.39535700	-1.24796400
H	7.96541600	-2.28943400	-0.57266300
O	2.75919600	-1.28261400	0.29260600
O	3.46781100	0.92073100	-0.78027200
P	2.11577400	0.00761300	-0.52647100
O	1.19685600	0.67420900	0.44652000
O	1.66703900	-0.40366400	-1.89504600
C	1.86388600	-3.68512500	-1.02513200
C	1.00046800	-3.59927500	-2.06986900
C	1.48183900	-4.42137600	0.16853600
C	-0.26860000	-4.27114700	-2.06353300
H	1.27751800	-3.01882800	-2.94548400
C	0.23376000	-5.09712400	0.21239600
C	2.34343100	-4.49731200	1.28669400
C	-1.12076500	-4.19111500	-3.18770300
C	-0.64874700	-5.05234900	-0.94668900

C	-0.09889100	-5.81963600	1.37987600
H	3.30086200	-3.98809600	1.25018700
C	1.99408300	-5.21354300	2.41112800
C	-2.29957000	-4.90142500	-3.23107200
H	-0.81684800	-3.57065400	-4.02689100
C	-1.86234700	-5.77175200	-1.01786300
C	0.76036700	-5.88238000	2.45652900
H	-1.05045300	-6.33496500	1.44395400
H	2.67265800	-5.26120700	3.25714200
C	-2.66335100	-5.70985900	-2.13834800
H	-2.94134100	-4.84712200	-4.10523000
H	-2.17454000	-6.39658000	-0.18864100
H	0.47973700	-6.44863600	3.33948600
H	-3.58614600	-6.28144100	-2.17201700
C	2.77631600	3.53437400	0.22320400
C	2.98293300	3.84053400	-1.08652600
C	1.68574700	4.17228900	0.94096100
C	2.18351900	4.80125600	-1.78610300
H	3.79299100	3.36064800	-1.62879300
C	0.93420000	5.19854200	0.30821200
C	1.33833000	3.78268200	2.25454100
C	2.40772500	5.05306400	-3.15828400
C	1.17339900	5.51115800	-1.09521300
C	-0.05801800	5.86595800	1.05891500
H	1.86232800	2.95016000	2.71059300
C	0.33988500	4.43013600	2.95166900
C	1.64528000	5.97481800	-3.84084400
H	3.19138900	4.49803600	-3.66686500
C	0.41052700	6.45651100	-1.81740500
C	-0.34366800	5.50216400	2.35760400
H	-0.61722800	6.67988600	0.61000900
H	0.08378300	4.11136600	3.95717000
C	0.63606300	6.68082400	-3.16063500
H	1.82055100	6.15799300	-4.89619300
H	-0.37539600	7.01582900	-1.32112900
H	-1.11843800	6.02716400	2.90787900
H	0.03299200	7.40935800	-3.69360400
C	-3.88101100	4.64995800	1.76220500
C	-3.11728400	4.62782400	0.60607400
C	-2.44396800	3.45746700	0.22659700
C	-2.57040500	2.29786500	0.99997000
C	-3.30248200	2.33727700	2.18508200
C	-3.95403000	3.50683000	2.56177600
H	-1.45266400	4.38274000	-1.46854400

H	-4.40741400	5.55332600	2.05219800
H	-3.02140800	5.51563500	-0.01341200
C	-1.60092800	3.43703800	-0.94955400
C	-1.86651300	1.02844600	0.56615500
H	-3.38032000	1.44953900	2.80487500
H	-4.53244900	3.52265800	3.47975200
C	-1.31533300	1.05795100	-0.84869400
C	-1.00140700	2.33187200	-1.45908300
H	-0.88074700	1.03591000	1.07797600
N	-0.94563800	-0.01368900	-1.49916500
N	-1.30635400	-1.30622800	-1.19857500
C	-2.61344900	-1.64224800	-1.50297200
O	-3.31590600	-1.00645200	-2.25637700
O	-2.96043600	-2.74817600	-0.85505200
C	-4.31528300	-3.15560900	-1.07637400
H	-4.45809100	-3.44129200	-2.12070400
H	-4.47226400	-4.01411700	-0.42488700
H	-4.99865500	-2.34390500	-0.81682800
C	-0.17188400	2.38156700	-2.71089700
H	0.82783200	1.96404600	-2.54465500
H	-0.64432100	1.81080400	-3.51933000
H	-0.06399200	3.41648200	-3.04189600
C	-6.59156900	-1.09556000	1.07600500
C	-6.22371900	-0.02552900	0.23634000
C	-4.87900700	0.34482000	0.16151700
C	-3.94569600	-0.35293600	0.91850400
C	-4.30709100	-1.44014000	1.74074500
C	-5.65108400	-1.80374800	1.81749500
H	-7.63205800	-1.39061800	1.14531000
H	-4.55920600	1.15732500	-0.48430600
H	-5.96174100	-2.63590100	2.44275400
C	-2.03170400	-1.13512700	1.84149100
C	-0.69410000	-1.37990000	2.15941800
C	-0.43048600	-2.46189600	2.99447000
C	-1.45882800	-3.27192200	3.49675400
C	-2.78469800	-3.02712600	3.16110600
C	-3.07899600	-1.95222300	2.32027300
H	0.11266600	-0.76949100	1.75712600
H	0.60099500	-2.68787600	3.24633500
H	-1.20988500	-4.11183300	4.13729100
H	-3.57982300	-3.66490800	3.53646900
N	-2.56682900	-0.15671300	0.99951400
C	-7.23844600	0.75168800	-0.60846100
C	-7.23211600	2.22702800	-0.17358400

C	-6.83959600	0.65593000	-2.09076000
C	-8.66126200	0.20729600	-0.45403000
H	-7.50913600	2.32385400	0.88148300
H	-6.24596400	2.68438200	-0.30444500
H	-7.95067900	2.80015500	-0.77001600
H	-6.81630500	-0.38703500	-2.42362300
H	-7.56154100	1.19824400	-2.71132000
H	-5.85042700	1.08581200	-2.27334800
H	-9.34321800	0.78849500	-1.08258700
H	-8.72932800	-0.83987300	-0.76658200
H	-9.01605500	0.28286400	0.57900700
H	-0.81782700	-1.76611900	-0.43352500
H	-0.18745800	0.04605800	-2.18953900

TSIV-2Value of imaginary frequency = -1154.0 cm⁻¹

C	-4.82488300	-0.99169600	-0.89088900
C	-5.60453600	-0.74600100	-2.02471500
C	-5.79989600	0.55333400	-2.47125300
C	-5.18918300	1.59871000	-1.78444800
C	-4.31915200	1.37543100	-0.70623900
C	-4.13315200	0.04758100	-0.28387500
C	-5.30817900	-3.09968200	-1.83349600
C	-6.14005500	-2.04356300	-2.58605300
H	-6.42748800	0.76059400	-3.33318600
H	-5.38028100	2.62099900	-2.09418500
H	-4.36311700	-3.27224100	-2.36020500
H	-7.21027300	-2.14982000	-2.37154900
C	-4.99611000	-2.43507900	-0.46411200
C	-3.95060800	-3.19732500	0.32458600
C	-6.22501000	-2.57785800	0.48160100
C	-4.57168400	-4.13768900	1.15428400
C	-2.56330900	-3.11210900	0.29369800
C	-6.07220900	-3.97464600	1.10460600
H	-7.17183600	-2.43206700	-0.04597800
C	-3.82016300	-5.03341200	1.90068700
C	-1.78322100	-4.02638600	1.01450000
H	-6.53404800	-4.05521000	2.09250800
C	-2.43241600	-4.98283900	1.80366100
H	-4.30000700	-5.75960300	2.55042200
H	-1.82175100	-5.68807500	2.35990700
H	-6.02042200	-2.10438500	-3.67134600
H	-5.81955100	-4.06014400	-1.72108300
H	-6.14874600	-1.81565200	1.26482300
H	-6.52483400	-4.74626800	0.46979500
O	-1.96412100	-2.09722200	-0.43928400
O	-3.26095800	-0.24751100	0.75142200
P	-1.72958300	-0.68100800	0.36685800
O	-1.20669200	0.26916700	-0.70240800
O	-0.97939200	-0.87927100	1.63222500
C	-0.29364400	-4.08811000	0.95057500
C	0.45391100	-3.64042500	1.99256700
C	0.34171100	-4.80289500	-0.13994900
C	1.86461800	-3.89148800	2.07784200
H	-0.02687500	-3.09738100	2.80120000
C	1.74080500	-5.04482000	-0.10636400
C	-0.41824200	-5.29196600	-1.22662700
C	2.58927000	-3.47513700	3.21721400

C	2.51958700	-4.60017600	1.04283800
C	2.32350800	-5.74948500	-1.18276900
H	-1.48903000	-5.11418300	-1.24196900
C	0.17611400	-5.99070500	-2.25518300
C	3.92736800	-3.77043000	3.34826400
H	2.06270800	-2.92544000	3.99320900
C	3.89539100	-4.88115500	1.19858400
C	1.56219100	-6.21595100	-2.23406700
H	3.39216800	-5.93118000	-1.19496700
H	-0.42496800	-6.36041700	-3.08026000
C	4.58101000	-4.48569800	2.32778900
H	4.47626000	-3.45872800	4.23176800
H	4.42972000	-5.43173300	0.43256600
H	2.03858100	-6.75696900	-3.04601000
H	5.63593800	-4.72455900	2.42621900
C	-3.72886100	2.52726600	0.03035800
C	-3.79916100	2.55032900	1.39068200
C	-3.22208000	3.69833300	-0.67203500
C	-3.40505000	3.69087400	2.16243300
H	-4.19236500	1.69088300	1.92556900
C	-2.94764600	4.88999500	0.05185700
C	-3.00236800	3.69086300	-2.06964800
C	-3.45255600	3.64533800	3.57381000
C	-2.99356200	4.87600300	1.50866300
C	-2.62322700	6.06042100	-0.67161800
H	-3.10394200	2.75779300	-2.61210500
C	-2.65906200	4.84003500	-2.74720000
C	-3.07744600	4.73487400	4.32805600
H	-3.78359300	2.72716300	4.05190900
C	-2.60599600	5.97691400	2.30563100
C	-2.50953000	6.04670400	-2.04539400
H	-2.46815000	6.99538500	-0.14436400
H	-2.49873100	4.80883500	-3.82026000
C	-2.64327400	5.90790000	3.68408300
H	-3.11104800	4.68988000	5.41200700
H	-2.26120300	6.89367000	1.83993000
H	-2.26919900	6.96179400	-2.57845600
H	-2.33819800	6.76698600	4.27344200
C	0.93622700	4.77447600	-2.95800900
C	0.52970700	4.82644900	-1.63836900
C	0.60730700	3.68135500	-0.82776600
C	1.12799800	2.48415100	-1.34582700
C	1.52388800	2.43886300	-2.68771700
C	1.42564700	3.57139600	-3.48179400

H	-0.25045700	4.63833200	0.91812700
H	0.87513200	5.65833200	-3.58488400
H	0.13784300	5.74390000	-1.21109800
C	0.20218000	3.71892900	0.55106000
C	1.24606700	1.28157900	-0.47093800
H	1.92448300	1.51969300	-3.10358600
H	1.74401400	3.52339200	-4.51846400
C	1.05648600	1.50140300	0.96450300
C	0.36911300	2.69197800	1.42459600
H	0.08300700	0.72457300	-0.60568900
N	1.34019700	0.60319400	1.89627600
N	1.95048200	-0.60789200	1.68212200
C	3.33618000	-0.58209600	1.71491100
O	3.97411100	0.24132500	2.33125400
O	3.84065700	-1.58311800	1.00082100
C	5.27131400	-1.62160400	0.98341600
H	5.65377300	-1.89668300	1.96908800
H	5.53567700	-2.38233300	0.24975300
H	5.66746400	-0.64688300	0.69049400
C	-0.06307400	2.80401200	2.86014200
H	-0.78036700	2.01537600	3.11764300
H	0.78710100	2.73490500	3.54905400
H	-0.55111400	3.76709300	3.02363300
C	6.31676000	1.40827400	-1.27412600
C	5.53559000	2.27309900	-0.48086400
C	4.17679800	1.99690800	-0.31567000
C	3.63972300	0.87303800	-0.93179800
C	4.41762200	0.00751600	-1.72463500
C	5.77352300	0.28726500	-1.89275200
H	7.37133400	1.61530300	-1.41407500
H	3.54589900	2.64115600	0.29192400
H	6.40057200	-0.36023000	-2.49943800
C	2.23806300	-0.72803500	-1.68894200
C	1.13037400	-1.51586600	-2.00690700
C	1.33880400	-2.61218300	-2.83599900
C	2.60904900	-2.93046600	-3.33667300
C	3.70688100	-2.14092000	-3.02220000
C	3.52277500	-1.02650300	-2.20217600
H	0.13699400	-1.27766100	-1.64760200
H	0.48994700	-3.23721900	-3.09408100
H	2.73007600	-3.80077000	-3.97395400
H	4.69277900	-2.37534900	-3.41383600
N	2.32192000	0.41510200	-0.89007200
C	6.11912000	3.50999800	0.21020500

C	5.40279200	4.76727800	-0.30988000
C	5.90076800	3.39138300	1.72768900
C	7.61998200	3.66722700	-0.05032300
H	5.54860900	4.88095500	-1.38909300
H	4.32563100	4.72778700	-0.11913700
H	5.79980200	5.66050700	0.18536800
H	6.37714200	2.48794700	2.12181300
H	6.33053700	4.26016300	2.23884800
H	4.83745600	3.34442300	1.98086700
H	7.98703700	4.56023500	0.46534500
H	8.18668100	2.80872300	0.32465300
H	7.83651100	3.78618300	-1.11698500
H	1.45402400	-1.25028200	1.06758700
H	0.93733800	0.71533900	2.81841600

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C	5.01248900	-1.39052300	0.63058300
C	5.89272200	-1.28672400	1.71174700
C	6.23132900	-0.04117000	2.22008500
C	5.66535400	1.09575100	1.65280000
C	4.70861200	1.02466500	0.62724600
C	4.39020700	-0.25331600	0.13908000
C	5.36589000	-3.58595400	1.42259700
C	6.35381700	-2.65670900	2.14993900
H	6.93760900	0.05341900	3.03953500
H	5.96568100	2.07312000	2.01488800
H	4.45748700	-3.70312400	2.02398100
H	7.38628500	-2.83983800	1.82912400
C	5.00274300	-2.81732600	0.12034800
C	3.81712700	-3.44406200	-0.58461900
C	6.11443400	-3.03253200	-0.94739600
C	4.26297100	-4.41419900	-1.49042400
C	2.45467000	-3.24644800	-0.41689400
C	5.76916900	-4.38394500	-1.59396800
H	7.11616400	-2.99597700	-0.51053600
C	3.35883600	-5.21982500	-2.16592300
C	1.51719400	-4.07049100	-1.05005400
H	6.11613000	-4.46230200	-2.62771100
C	1.99814100	-5.05924600	-1.91714000
H	3.70277700	-5.96754500	-2.87443600
H	1.27503900	-5.70250800	-2.40916700
H	6.32614400	-2.77457800	3.23651100
H	5.77133000	-4.57995800	1.21495200
H	6.03698100	-2.23603100	-1.69542200
H	6.21221200	-5.21842600	-1.03713000
O	2.01654500	-2.16200900	0.36144900
O	3.43477700	-0.40327100	-0.87050600
P	1.92046900	-0.78402100	-0.46675300
O	1.51515100	0.17326300	0.72899400
O	1.07383300	-0.80706600	-1.67062400
C	0.04441200	-4.01062300	-0.81759600
C	-0.78483700	-3.67818000	-1.84186500
C	-0.51007200	-4.52135400	0.42417500
C	-2.20667800	-3.85944600	-1.76152200
H	-0.36625700	-3.30283800	-2.77241400
C	-1.91318500	-4.71060600	0.54135200
C	0.32593900	-4.88389300	1.50474100
C	-3.02235600	-3.56914100	-2.87803600
C	-2.78421400	-4.38080000	-0.58064500

C	-2.41659000	-5.25953200	1.74115700
H	1.39893600	-4.75054500	1.41183000
C	-0.19485200	-5.42053800	2.66259100
C	-4.37605300	-3.81307000	-2.84315100
H	-2.55568800	-3.15716600	-3.76892400
C	-4.18061600	-4.59726300	-0.56330100
C	-1.58082200	-5.61183600	2.77962400
H	-3.48389000	-5.40803300	1.85979000
H	0.46515000	-5.69779100	3.47862000
C	-4.95647400	-4.33427700	-1.67212100
H	-4.99390600	-3.59915600	-3.71008400
H	-4.65901300	-4.99117200	0.32615400
H	-1.99738100	-6.03487500	3.68867300
H	-6.02527200	-4.52378300	-1.63715500
C	4.18888100	2.28217400	0.01723200
C	4.16491700	2.40697600	-1.34022300
C	3.88870400	3.44868100	0.84032300
C	3.91695400	3.65894000	-1.99330500
H	4.40407400	1.55246000	-1.96678000
C	3.75721000	4.72571800	0.22952100
C	3.72903900	3.35018100	2.24240700
C	3.88966000	3.72960200	-3.40429400
C	3.74950000	4.83496600	-1.22435400
C	3.61768700	5.86052800	1.06053700
H	3.73193900	2.36970200	2.70589500
C	3.56367000	4.47139500	3.02689800
C	3.68710200	4.93150700	-4.04509400
H	4.02563400	2.81280700	-3.97212400
C	3.54308600	6.05409400	-1.90681000
C	3.54568100	5.74310900	2.43268900
H	3.56111000	6.84860100	0.61851300
H	3.44328900	4.36720400	4.10058100
C	3.51111800	6.10168800	-3.28521000
H	3.66121000	4.97770400	-5.12905600
H	3.39403900	6.97344700	-1.35245300
H	3.44547800	6.63239200	3.04719500
H	3.34557300	7.05074600	-3.78519400
C	-0.17826300	4.45112500	2.98830200
C	0.39013800	4.29576000	1.74882300
C	-0.11170000	3.33227900	0.84175600
C	-1.21384100	2.52258200	1.21119900
C	-1.78630500	2.70395200	2.49850700
C	-1.27700700	3.64461400	3.36150300
H	1.26890200	3.81536800	-0.75571700

H	0.21395900	5.18950600	3.68098200
H	1.23199000	4.90742300	1.43944200
C	0.44900500	3.16599400	-0.45520600
C	-1.71170900	1.54764900	0.28433600
H	-2.63158400	2.09531100	2.80185700
H	-1.72612300	3.76927100	4.34204400
C	-1.12408600	1.38134200	-0.96244400
C	-0.03311700	2.24822100	-1.34999400
H	1.27678000	1.07265200	0.43047000
N	-1.51100300	0.47035400	-1.94710400
N	-2.32599400	-0.59977200	-1.62537300
C	-3.68094800	-0.41530400	-1.79381600
O	-4.19450700	0.37617600	-2.55278200
O	-4.34752400	-1.26730300	-1.00442400
C	-5.76654200	-1.19285300	-1.11684600
H	-6.09151200	-1.54186400	-2.10131700
H	-6.16023800	-1.84710900	-0.33918500
H	-6.10791200	-0.16587000	-0.96057800
C	0.53115200	2.17662700	-2.74450800
H	1.07626300	1.24206600	-2.91814500
H	-0.27136900	2.23705300	-3.48737300
H	1.21814400	3.00928500	-2.90951700
C	-6.82578300	1.77589700	1.07564500
C	-6.06324000	2.57283500	0.19703800
C	-4.70141000	2.29994500	0.04248700
C	-4.14450300	1.24408000	0.75494600
C	-4.90698000	0.44064800	1.63053700
C	-6.26415900	0.72042500	1.78578100
H	-7.88229400	1.97968700	1.20545900
H	-4.08197700	2.87968200	-0.63564700
H	-6.87970900	0.11983400	2.44986300
C	-2.73519100	-0.29487700	1.60898500
C	-1.60927000	-1.05436900	1.93095400
C	-1.78100700	-2.09018200	2.84105100
C	-3.03314600	-2.36326700	3.41411200
C	-4.14813000	-1.60241200	3.08616700
C	-4.00271900	-0.55219700	2.17688700
H	-0.63708600	-0.83356200	1.49857700
H	-0.92718300	-2.70680800	3.10633900
H	-3.12721800	-3.18348300	4.11883500
H	-5.11558800	-1.81285700	3.53350200
N	-2.83009800	0.78000900	0.73076000
C	-6.68100400	3.71376600	-0.61921200
C	-5.95410400	5.02983100	-0.29810000

C	-6.52166900	3.39794300	-2.11579900
C	-8.17106600	3.90265200	-0.32049300
H	-6.04274200	5.27520500	0.76533600
H	-4.88994700	4.97402500	-0.54491200
H	-6.39006900	5.85184200	-0.87672200
H	-7.01673000	2.45464100	-2.36956500
H	-6.97010000	4.19497000	-2.71984000
H	-5.46911000	3.30974000	-2.39966000
H	-8.55902700	4.73293600	-0.91916000
H	-8.75205800	3.00995900	-0.57379300
H	-8.34583000	4.14071900	0.73394000
H	-2.04939600	-1.17460800	-0.83182500
H	-0.71915300	0.14895400	-2.49283600

P

H	-0.47596500	2.42790200	1.34939200
C	-2.37263500	-3.86354700	-2.27519500
C	-3.01453800	-3.61073000	-1.08860300
C	-2.75664900	-2.41846900	-0.36566800
C	-1.81881700	-1.48370100	-0.87718800
C	-1.17714800	-1.76112600	-2.11307600
C	-1.44900800	-2.92426100	-2.79148800
H	-4.13757600	-2.84462800	1.24041600
H	-2.57439000	-4.77876800	-2.82258200
H	-3.73160600	-4.31940700	-0.68286500
C	-3.42024200	-2.12451200	0.85378000
C	-1.56772600	-0.28939200	-0.13663700
H	-0.47361400	-1.04184900	-2.51933200
H	-0.95182900	-3.12403900	-3.73572300
C	-2.21268000	-0.04195000	1.06317600
C	-3.17476000	-0.98021200	1.56486100
N	-2.01776000	1.14669600	1.79190600
N	-0.73705000	1.65052200	1.94424200
C	0.24560100	0.86075000	2.47895300
O	0.05867800	-0.21061400	3.01626600
O	1.43363600	1.46818100	2.35195400
C	2.53344600	0.74805500	2.90803400
H	2.55773900	-0.26969100	2.51363600
H	3.42673900	1.29552900	2.60936100
H	2.45670200	0.71455800	3.99810700
C	-3.86618400	-0.71940900	2.87634000
H	-3.13782400	-0.63102500	3.69111700
H	-4.45891200	0.20230000	2.85361000
H	-4.54057100	-1.54247200	3.11899100
C	3.46629100	0.71920900	-0.85586300
C	2.88680700	-0.48984900	-0.40287900
C	1.49990500	-0.57626400	-0.29803300
C	0.73345400	0.53122000	-0.66985000
C	1.30826500	1.73807800	-1.11256700
C	2.70124000	1.82229200	-1.20029800
H	4.54586100	0.78645200	-0.94943500
H	1.00552500	-1.47514600	0.05379200
H	3.17900500	2.73740900	-1.53870000
C	-0.97647400	1.94730200	-1.07002000
C	-2.23600900	2.54027700	-1.17314100
C	-2.28647700	3.86047200	-1.60070900
C	-1.11810000	4.57556200	-1.91307300
C	0.13153200	3.98197300	-1.79816100

C	0.21280900	2.65428800	-1.36532100
H	-3.13550700	1.98483600	-0.92840100
H	-3.25101400	4.35000400	-1.69360900
H	-1.19619900	5.60590400	-2.24457200
H	1.03288700	4.53900700	-2.03669100
N	-0.65216100	0.65868000	-0.66660600
C	3.79184700	-1.69303600	-0.11073400
C	3.02106700	-2.84461100	0.54303600
C	4.37290300	-2.18927300	-1.44670500
C	4.95136700	-1.30081000	0.81872900
H	2.54773600	-2.53350800	1.48120300
H	2.24258400	-3.23925300	-0.11736800
H	3.70992200	-3.66496300	0.76801100
H	4.97188100	-1.41226100	-1.93201600
H	5.01568000	-3.06111300	-1.28098400
H	3.57197600	-2.47865800	-2.13488100
H	5.59496100	-2.16979100	0.99278300
H	5.57491800	-0.51096400	0.39103700
H	4.58508400	-0.95579400	1.79045100
H	-2.49841900	1.14763300	2.68249300

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H	0.47598800	2.42758700	1.34902600
C	2.37236600	-3.86369100	-2.27512000
C	3.01424900	-3.61089800	-1.08852300
C	2.75639900	-2.41861700	-0.36560400
C	1.81864300	-1.48380100	-0.87714700
C	1.17699400	-1.76119400	-2.11307000
C	1.44881400	-2.92434800	-2.79145600
H	4.13726300	-2.84488600	1.24051400
H	2.57407800	-4.77893200	-2.82249200
H	3.73130200	-4.31957600	-0.68276300
C	3.41999400	-2.12471400	0.85386000
C	1.56761800	-0.28947800	-0.13657400
H	0.47354200	-1.04185800	-2.51936300
H	0.95168500	-3.12411300	-3.73572000
C	2.21265300	-0.04201800	1.06318200
C	3.17463300	-0.98037400	1.56491000
N	2.01803500	1.14678900	1.79176200
N	0.73728400	1.65065300	1.94434600
C	-0.24529400	0.86070400	2.47905800
O	-0.05818700	-0.21061600	3.01639600
O	-1.43336900	1.46795700	2.35210300
C	-2.53316900	0.74729100	2.90754400
H	-2.55724200	-0.27019100	2.51243300
H	-3.42648300	1.29483000	2.60904200
H	-2.45664400	0.71321000	3.99760900
C	3.86613200	-0.71966800	2.87636800
H	3.13782000	-0.63108300	3.69117000
H	4.45907100	0.20190200	2.85362200
H	4.54027600	-1.54291200	3.11907200
C	-3.46633700	0.71961900	-0.85565400
C	-2.88696900	-0.48947000	-0.40262300
C	-1.50007000	-0.57598300	-0.29774400
C	-0.73352000	0.53138700	-0.66970400
C	-1.30821100	1.73827500	-1.11250900
C	-2.70118500	1.82260700	-1.20017800
H	-4.54589600	0.78695300	-0.94929000
H	-1.00571800	-1.47485700	0.05413900
H	-3.17889000	2.73774000	-1.53862700
C	0.97655500	1.94723600	-1.07006400
C	2.23618000	2.54001600	-1.17327000
C	2.28683400	3.86013400	-1.60103600
C	1.11853800	4.57532300	-1.91350200
C	-0.13117200	3.98192900	-1.79848000

C	-0.21264900	2.65431500	-1.36544500
H	3.13556400	1.98443800	-0.92843200
H	3.25142800	4.34952900	-1.69405500
H	1.19676700	5.60560500	-2.24515800
H	-1.03244500	4.53907800	-2.03705500
N	0.65211900	0.65871100	-0.66646700
C	-3.79209300	-1.69262100	-0.11061500
C	-3.02148500	-2.84434900	0.54311400
C	-4.37302700	-2.18865800	-1.44672600
C	-4.95174100	-1.30046200	0.81871900
H	-2.54798300	-2.53332900	1.48121700
H	-2.24316500	-3.23918300	-0.11736800
H	-3.71049500	-3.66454200	0.76818000
H	-4.97199400	-1.41156400	-1.93192200
H	-5.01578500	-3.06054900	-1.28122700
H	-3.57201300	-2.47785100	-2.13487700
H	-5.59561200	-2.16935200	0.99221000
H	-5.57496600	-0.51026500	0.39120300
H	-4.58565300	-0.95599400	1.79070800
H	2.49850800	1.14739500	2.68244700

TCE

C	-0.00003500	0.67806200	-0.00001300
C	0.00003500	-0.67806200	-0.00000100
C	1.22701300	1.42237800	0.00001200
N	2.21284400	2.02513700	0.00002300
C	-1.22693400	1.42239200	-0.00003200
N	-2.21256500	2.02542000	-0.00004800
C	-1.22701300	-1.42237800	-0.00001300
N	-2.21284400	-2.02513700	-0.00002600
C	1.22693400	-1.42239200	0.00003400
N	2.21256500	-2.02542000	0.00006200

Table 4 系列 CPA 催化的过渡态结构

(S) -C1

TSI

Value of imaginary frequency = -269.2 cm⁻¹

C	-4.53375600	-0.16466700	-0.65818900
C	-5.69930700	-0.65542700	-0.06410500
C	-5.79610300	-1.97766100	0.37073600
C	-4.67189300	-2.79320200	0.21497300
C	-3.46973500	-2.31748900	-0.32180900
C	-3.41586900	-0.98309500	-0.74671100
C	-5.88673700	1.71201400	-0.18513100
C	-6.72882800	0.44447700	0.05439800
H	-4.71668700	-3.82952800	0.54160100
H	-5.43155600	2.03298000	0.75838400
H	-7.51329500	0.33330500	-0.70526600
C	-4.75876500	1.25431400	-1.15211600
C	-3.63779700	2.27507700	-1.25422000
C	-5.28889600	1.27213000	-2.61436500
C	-3.89205100	3.16679000	-2.29969000
C	-2.49133100	2.42952200	-0.48550000
C	-5.11396500	2.73112400	-3.07392200
H	-6.31902200	0.91094300	-2.68226900
C	-3.05617300	4.25595300	-2.54929000
C	-1.62134200	3.50734500	-0.70519700
H	-4.97681200	2.82056100	-4.15584800
C	-1.93597300	4.41000000	-1.72918800
H	-1.26329200	5.24705000	-1.90110400
H	-7.22551900	0.44477400	1.02958100
H	-6.46072200	2.54968300	-0.59200500
H	-4.65583700	0.61867900	-3.22492500
H	-5.98532500	3.34355800	-2.80841700
O	-2.18297800	1.47181700	0.46590600
O	-2.21909500	-0.45480400	-1.19957300
P	-1.26340200	0.21746000	-0.04785100
O	-1.12378700	-0.68118200	1.14253100
O	-0.04632000	0.68875900	-0.78980500
H	-0.10825900	-1.82355400	2.03268300
C	-0.34485600	3.65531000	0.05035800
C	0.83750700	3.69540700	-0.65834300
C	-0.30731300	3.75474900	1.47980800
C	2.08851400	3.80143500	-0.00940400
H	0.80482300	3.60307200	-1.74014400
C	0.95747700	3.86404800	2.13020500
C	-1.48158800	3.76839500	2.28341800

C	2.14911200	3.87340100	1.35861500
C	1.00663700	3.96348000	3.54727100
H	-2.45156100	3.70100400	1.80138900
C	-1.40194200	3.86990800	3.64921400
C	-0.14364200	3.96439200	4.29249600
H	1.98040300	4.03276600	4.02615000
H	-2.31025000	3.87957900	4.24383000
H	-0.09559500	4.03869200	5.37472300
C	3.53177700	-2.37784400	-3.51996000
C	4.24224200	-2.68625000	-2.36768400
C	3.66978700	-2.48048200	-1.10526800
C	2.35821000	-1.94828100	-1.03228200
C	1.64882800	-1.63698900	-2.20809800
C	2.23289200	-1.85467500	-3.44426800
H	5.39936000	-3.18418600	0.02964100
H	3.98961800	-2.54187100	-4.49125900
H	5.24540400	-3.09760800	-2.43429200
C	4.37308600	-2.84003500	0.11496400
C	1.76467100	-1.71926200	0.25743900
H	0.64889700	-1.21852500	-2.12272200
H	1.68577200	-1.62236800	-4.35190000
C	2.36338800	-2.37859400	1.40579300
C	3.74882300	-2.81262300	1.30865300
H	0.69789000	-1.51896400	0.27494600
N	1.74799600	-2.64503300	2.53133600
N	0.47929300	-2.35883600	2.70138400
C	-0.07667000	-2.65733900	3.94653500
O	0.48892600	-3.21901800	4.84960100
O	-1.33413600	-2.21669200	3.95683400
C	-2.04419200	-2.45439200	5.17859200
H	-1.54637200	-1.94977600	6.00888400
H	-3.03853900	-2.04017400	5.02403100
H	-2.10341600	-3.52555900	5.38153200
C	6.05477500	1.27066000	-0.47305500
C	5.12715100	1.13455000	-1.52293700
C	3.80279500	0.79864200	-1.21337500
C	3.45472300	0.64728200	0.12382700
C	4.36776100	0.84487400	1.17008800
C	5.69198300	1.14080100	0.86430300
H	7.08690400	1.51424500	-0.70757200
H	3.04670300	0.68968500	-1.98269900
H	6.42556100	1.29255000	1.65028100
C	2.27034300	0.52642100	2.05518700
C	1.24765200	0.50946900	2.99347200

C	1.60337300	0.68940200	4.32970200
C	2.93511100	0.89132900	4.70788800
C	3.94918100	0.94286800	3.75339200
C	3.60950700	0.76162000	2.41502900
H	0.21275200	0.36338400	2.69596600
H	0.82493600	0.68288500	5.08696600
H	3.17814500	1.02613300	5.75713700
H	4.97882500	1.12912800	4.04330800
N	2.18219000	0.31069100	0.65135700
H	1.32350800	0.62592500	0.12842000
C	5.58967700	1.37138200	-2.96444700
C	4.42377400	1.32331800	-3.95503300
C	6.25222700	2.75519600	-3.07185400
C	6.60813600	0.28760900	-3.35169600
H	3.93570900	0.34362800	-3.95740500
H	3.66839000	2.08289600	-3.72522900
H	4.79703000	1.51451700	-4.96602400
H	7.14229700	2.83311400	-2.44125500
H	6.55988600	2.94177600	-4.10649200
H	5.55441700	3.54594100	-2.77627100
H	6.95677200	0.44571700	-4.37821100
H	7.48144300	0.30157700	-2.69214400
H	6.15343000	-0.70685600	-3.29248000
H	4.23072100	-3.14518400	2.22228400
C	-3.34575600	5.20920700	-3.67780500
H	-3.32613300	4.69161700	-4.64324300
H	-4.33878300	5.65920900	-3.57411400
H	-2.60930500	6.01534100	-3.71162000
C	-7.06280100	-2.49304000	0.99938900
H	-7.28015000	-1.96837100	1.93642600
H	-7.92386600	-2.34073600	0.34009300
H	-6.98722700	-3.56042000	1.21966600
C	-2.26678300	-3.19628900	-0.37289300
C	-1.60169500	-3.49701400	-1.60775100
C	-1.78884100	-3.74127200	0.79907300
C	-2.05297400	-3.00585000	-2.86425100
C	-0.45361000	-4.34359100	-1.58673300
C	-0.64152100	-4.57020700	0.81663300
H	-2.27942500	-3.48883500	1.73526800
C	-1.40306500	-3.33611500	-4.02729900
H	-2.93032800	-2.36801300	-2.89707900
C	0.19973100	-4.66402000	-2.80711600
C	0.01996800	-4.85702700	-0.34966200
H	-0.28248200	-4.96411000	1.76332300

C	-0.26386500	-4.17690000	-4.00168500
H	-1.76746100	-2.95447700	-4.97615300
H	1.07951000	-5.30184500	-2.77144800
H	0.90779600	-5.48427700	-0.34909400
H	0.24384900	-4.42567000	-4.92873400
H	2.99909500	3.81223000	-0.60155300
H	3.10404100	3.94647300	1.87303500

(S)-C1

TSII, TSII-1' Ar=naphthyl

Value of imaginary frequency = -282.7 cm⁻¹

C	-4.02515800	-1.17393400	0.74628500
C	-4.81635800	-1.40765100	1.87423900
C	-4.37412500	-2.21552300	2.92151800
C	-3.10079300	-2.77870700	2.80411600
C	-2.26446000	-2.52255700	1.71136900
C	-2.73503100	-1.68572400	0.69206100
C	-5.83172300	0.34316100	0.62718900
C	-6.12091000	-0.65347000	1.76477700
H	-2.73153400	-3.42936700	3.59338600
H	-5.34921200	1.23717900	1.03779200
H	-6.94424900	-1.33192300	1.50569300
C	-4.81569100	-0.39556300	-0.28860700
C	-4.16014800	0.54597600	-1.28088300
C	-5.58015400	-1.34199600	-1.25808800
C	-4.90665500	0.59292200	-2.46094200
C	-3.02789400	1.33975000	-1.15327100
C	-6.01257500	-0.43469000	-2.42461900
H	-6.41353200	-1.85039100	-0.76489300
C	-4.58860400	1.47659900	-3.49196700
C	-2.68610600	2.25599800	-2.15514600
H	-6.10792000	-0.97800100	-3.36981700
C	-3.48500200	2.31157400	-3.30442200
H	-3.21836900	3.02306400	-4.08243100
H	-6.39587200	-0.15807400	2.70104200
H	-6.72565200	0.65555700	0.07971800
H	-4.88276100	-2.10261300	-1.62690400
H	-6.98220900	0.04094900	-2.22831900
O	-2.21125400	1.18855000	-0.04413100
O	-1.90017700	-1.33414800	-0.35564100
P	-1.03377200	0.05556500	-0.16562200
O	-0.33401000	0.06782600	1.16074800
O	-0.25841100	0.18852400	-1.44188200
H	1.19131600	-0.31111500	1.93970900
C	-1.49453000	3.14503400	-2.05038400
C	-0.49581300	3.03115300	-2.99219600
C	-1.40303800	4.16602000	-1.04843900
C	0.62391400	3.89425000	-2.99261100
H	-0.56950100	2.24790900	-3.74056400
C	-0.29320200	5.06124900	-1.07983300
C	-2.39149800	4.35135300	-0.04161500
C	0.72005500	4.89501400	-2.06121300

C	-0.22805900	6.12005100	-0.13364300
H	-3.24396900	3.68042100	-0.00711400
C	-2.28653100	5.36894500	0.87385600
C	-1.19580000	6.27047600	0.82604900
H	0.60944200	6.81061300	-0.18877200
H	-3.05054200	5.49127300	1.63538400
H	-1.13052300	7.07936600	1.54740900
C	-0.90773200	-3.13878700	1.66869200
C	0.02040600	-2.79098600	2.62428000
C	-0.58359900	-4.15398100	0.70859700
C	1.29647500	-3.40249600	2.67202100
H	-0.23179000	-2.01440500	3.34183400
C	0.69689400	-4.77947100	0.77289400
C	-1.50021800	-4.59295100	-0.28667300
C	1.63078700	-4.37103900	1.76257300
C	1.01527400	-5.81382100	-0.14708200
H	-2.48009100	-4.12864800	-0.34478300
C	-1.16634200	-5.60157500	-1.15657300
C	0.10395300	-6.22286600	-1.08635100
H	1.99705900	-6.27671400	-0.08494300
H	-1.88229100	-5.92965400	-1.90419800
H	0.35408600	-7.01760500	-1.78281500
C	2.43431800	-4.30660100	-3.24531500
C	3.56268000	-4.02708000	-2.48906100
C	3.50244100	-3.09484800	-1.44309800
C	2.26560700	-2.45969600	-1.17236800
C	1.12421200	-2.75680900	-1.94365000
C	1.21091900	-3.67347400	-2.97533400
H	5.61436800	-3.23999800	-0.90174700
H	2.49828700	-5.02688300	-4.05554400
H	4.50609700	-4.52059600	-2.70435900
C	4.66847300	-2.77883600	-0.63412200
C	2.19984600	-1.46489400	-0.13951600
H	0.19112400	-2.24376500	-1.72324600
H	0.33420300	-3.90932400	-3.56921000
C	3.29384000	-1.38585600	0.81145700
C	4.57312300	-1.97182500	0.44104200
H	1.21073900	-1.16660400	0.19234200
N	3.20767600	-0.88405100	2.01839500
N	2.07263900	-0.41705600	2.48379000
C	2.03559900	-0.06452800	3.83265700
O	2.95766300	-0.13892900	4.60548100
O	0.80243100	0.35494300	4.11765300
C	0.59798900	0.77777400	5.47114500

H	1.24188700	1.62833500	5.70585100
H	-0.44935600	1.06819300	5.52882400
H	0.80613000	-0.04362200	6.15965800
C	5.75292200	-0.10534400	-3.70975300
C	4.58340900	-0.76848900	-4.08684000
C	3.41284900	-0.66254200	-3.33160600
C	3.46226300	0.12261400	-2.18879500
C	4.62374900	0.82738400	-1.81697500
C	5.78112800	0.70857700	-2.57573100
H	6.64676300	-0.20917900	-4.31657900
H	2.50326700	-1.17253800	-3.63086900
H	6.68245900	1.24724600	-2.29983500
C	2.92927100	1.35757400	-0.35914700
C	2.22615000	2.02784300	0.63355200
C	2.90259300	2.98967800	1.38891700
C	4.26772700	3.22610700	1.12935100
C	4.95868500	2.56283800	0.12316700
C	4.27462600	1.62194300	-0.64360700
H	1.18090700	1.79415800	0.80779500
H	4.79917200	3.96214300	1.72552800
H	6.00348300	2.78555400	-0.07081700
N	2.44857800	0.32992200	-1.21716400
H	1.43724800	0.35517400	-1.48391000
H	4.57793400	-1.37982400	-4.98363600
C	2.19840000	3.78872100	2.48862100
C	0.70251100	3.46301400	2.55336600
C	2.84541300	3.46265300	3.84441200
C	2.36501600	5.29123800	2.21001700
H	0.19778200	3.69229000	1.60702700
H	0.52590600	2.40732700	2.78667900
H	0.23174900	4.06563500	3.33752300
H	3.89823200	3.76226700	3.86489900
H	2.32703400	3.99868700	4.64745600
H	2.80434300	2.39078100	4.06127800
H	1.80196800	5.87503000	2.94704800
H	3.41319400	5.60031200	2.26740900
H	1.98809800	5.54103700	1.21479500
H	5.41975200	-1.76791600	1.08847000
C	-5.40543600	1.51629700	-4.75564600
H	-5.35491400	0.55919200	-5.28646600
H	-6.46152500	1.70872000	-4.53873700
H	-5.04843400	2.29708600	-5.43126400
C	-5.24025700	-2.46191100	4.12735700
H	-5.43347100	-1.52974600	4.66966700

H	-6.21334700	-2.87321000	3.83810700
H	-4.76531700	-3.16306500	4.81740300
H	2.00977700	-3.09047900	3.43042800
H	2.60868600	-4.84569800	1.78686800
H	1.56806500	5.57492300	-2.05632300
H	1.39976000	3.76167800	-3.74029500

(S)-C2**TSI**Value of imaginary frequency = -336.2 cm⁻¹

C	5.05461100	-0.82861000	-0.84132700
C	6.28233000	-0.28522100	-0.45766500
C	6.48744100	1.09501700	-0.41518100
C	5.40711600	1.91938200	-0.74120500
C	4.14568700	1.40761600	-1.07005600
C	3.98704700	0.01538500	-1.11570300
C	6.30537500	-2.59448000	0.10131700
C	7.24455900	-1.38738600	-0.08036000
H	5.53867200	2.99894400	-0.71893400
H	5.89586500	-2.58760700	1.11743900
H	7.97520300	-1.56216500	-0.88084700
C	5.14508900	-2.34344500	-0.90433400
C	3.94753400	-3.23834800	-0.63307600
C	5.55972100	-2.84894200	-2.31570500
C	4.05672800	-4.42503000	-1.36225600
C	2.85726600	-3.05056700	0.20697500
C	5.24228900	-4.35605100	-2.29697500
H	6.60614400	-2.62487300	-2.54225200
C	3.13320800	-5.46204300	-1.21653600
C	1.91112500	-4.06940300	0.38442700
H	5.01454200	-4.75175700	-3.29150800
C	2.07763500	-5.26573300	-0.32204800
H	1.34472500	-6.05701700	-0.18016000
H	7.81136000	-1.15376200	0.82606300
H	6.79344800	-3.55909600	-0.06534000
H	4.93253400	-2.35347100	-3.06494500
H	6.08511000	-4.93955100	-1.90363300
O	2.66739100	-1.82299300	0.81881900
O	2.74319800	-0.53354000	-1.37134400
P	1.78315500	-0.74343800	-0.05160500
O	1.72749400	0.50021800	0.78063300
O	0.53005700	-1.36804300	-0.58124700
H	0.51743800	1.73166300	1.36127500
C	-2.02208100	1.13129300	-4.78419900
C	-2.76486700	1.95619900	-3.95122400
C	-2.48395200	2.02477200	-2.57825800
C	-1.40796100	1.25899900	-2.06858500
C	-0.67389900	0.41308200	-2.91940100
C	-0.98237500	0.34510000	-4.26795500
H	-4.11378000	3.40318800	-2.10312100
H	-2.25418600	1.09047400	-5.84433300

H	-3.57103900	2.56180100	-4.35617500
C	-3.24661300	2.89247500	-1.69492900
C	-1.06561700	1.35281300	-0.66294100
H	0.13129500	-0.18138700	-2.49479300
H	-0.41179700	-0.30327000	-4.92460500
C	-1.66046400	2.44654300	0.09774400
C	-2.85331100	3.09654600	-0.42378400
H	-0.06413700	1.03224500	-0.39094000
N	-1.21213300	2.90249700	1.24110100
N	-0.10463800	2.45223500	1.77618500
C	0.18572900	2.88025300	3.07456300
O	-0.44140300	3.69679300	3.69994700
O	1.25584500	2.21437700	3.50559100
C	1.66232400	2.54147400	4.83640600
H	0.86787800	2.29970300	5.54656600
H	2.54547500	1.93595900	5.03278800
H	1.90397700	3.60431100	4.91233700
C	-5.96273600	0.11783100	-0.58643800
C	-5.19198200	-0.36117400	-1.66185000
C	-3.81499200	-0.54285900	-1.47877600
C	-3.27923300	-0.26770500	-0.22829400
C	-4.05862000	0.15005500	0.85922500
C	-5.42029200	0.36153700	0.67105800
H	-7.02681100	0.28054900	-0.73107100
H	-3.17612700	-0.90957500	-2.27492400
H	-6.05048800	0.69315300	1.49067000
C	-1.90317400	-0.17353500	1.58781100
C	-0.84687200	-0.36987700	2.46652300
C	-1.08399200	-0.10245900	3.81275000
C	-2.33382800	0.34871100	4.25679400
C	-3.39751500	0.49561700	3.37171600
C	-3.17932500	0.21385500	2.02371400
H	0.12673900	-0.70314800	2.12628600
H	-0.28040700	-0.25024100	4.52801900
H	-2.48131100	0.56006200	5.31133800
H	-4.37670300	0.80745400	3.72118600
N	-1.90663400	-0.29569100	0.16336900
H	-1.23155100	-0.96933700	-0.24407500
C	-5.88196300	-0.65697900	-2.99760700
C	-4.92590100	-1.29156000	-4.01116000
C	-7.05509200	-1.62664900	-2.77723500
C	-6.41728300	0.66068000	-3.58156800
H	-4.09377500	-0.62445400	-4.25732900
H	-4.51242400	-2.23481700	-3.63663400

H	-5.46833800	-1.50735400	-4.93692600
H	-7.80575300	-1.21648600	-2.09616100
H	-7.54917700	-1.83341300	-3.73272000
H	-6.70369400	-2.57812000	-2.36423700
H	-6.91044600	0.47541900	-4.54218000
H	-7.14485300	1.12870300	-2.91126600
H	-5.59922000	1.37000000	-3.74608600
H	-3.36627100	3.78630200	0.23921600
C	3.27082900	-6.73502600	-2.00818700
H	3.16151700	-6.54480000	-3.08179700
H	4.25630000	-7.18929800	-1.86082600
H	2.51192700	-7.46437800	-1.71561700
C	7.82097000	1.66564700	-0.01246000
H	8.06963500	1.39391900	1.01949900
H	8.62544600	1.28197400	-0.64889900
H	7.82025200	2.75573500	-0.08413100
C	3.00088600	2.30271100	-1.39606300
C	2.51684000	3.27121000	-0.48958100
C	2.39121900	2.17263300	-2.64855100
C	1.42933900	4.10616000	-0.88017300
C	3.05371000	3.43347400	0.83983100
C	1.33446200	2.98553400	-3.03254400
H	2.76374000	1.41658900	-3.33382500
C	0.91888600	5.09472200	0.01921700
C	0.83326900	3.95793200	-2.16255900
C	2.58278400	4.38534000	1.68249300
H	3.83768900	2.76007800	1.16702400
H	0.87544900	2.86067600	-4.00996400
C	1.49893000	5.25423200	1.30581400
C	-0.18270100	5.91007100	-0.36292000
C	-0.27796300	4.79891800	-2.52622900
H	3.00224600	4.49002800	2.68028500
C	0.97610800	6.21378700	2.18077300
C	-0.67543900	6.85947200	0.54077300
C	-0.76395300	5.72880000	-1.66894500
H	-0.72454600	4.65830000	-3.50743600
C	-0.09999700	7.00844400	1.79906700
H	1.41494600	6.32164700	3.16907400
H	-1.51942600	7.47795900	0.24772900
H	-1.60995600	6.35210300	-1.94611100
H	-0.49808600	7.74475500	2.49025600
C	0.78244000	-3.88252500	1.34026900
C	-0.56287200	-3.83392900	0.92065900
C	1.08254700	-3.75012300	2.69970100

C	-1.58679300	-3.64715800	1.89200900
C	-0.94563700	-3.91684700	-0.46867100
C	0.08516900	-3.59039600	3.65223600
H	2.12353500	-3.77806400	3.00886700
C	-2.95366600	-3.53614100	1.48413000
C	-1.25812700	-3.53294500	3.26965600
C	-2.24420800	-3.83902200	-0.84990400
H	-0.16256800	-4.01626000	-1.21162300
H	0.34306700	-3.49341800	4.70360500
C	-3.29888400	-3.64861000	0.11208600
C	-3.97130600	-3.29527100	2.44873000
C	-2.30940600	-3.30182700	4.22658200
H	-2.51355000	-3.90316400	-1.90140000
C	-4.64119600	-3.53523000	-0.26953700
C	-5.29901000	-3.16922100	2.02502500
C	-3.60073800	-3.17970500	3.83643500
H	-2.03468300	-3.20738100	5.27405400
C	-5.62973500	-3.29126600	0.67735500
H	-4.89690400	-3.62376000	-1.32268300
H	-6.07216700	-2.97646300	2.76402300
H	-4.38542400	-2.98928600	4.56387000
H	-6.66445500	-3.18891100	0.36290100

(S)-C2**TSII**Value of imaginary frequency = -275.6 cm⁻¹

C	-4.45708200	2.28031600	-0.14348100
C	-5.64597100	2.21283800	0.58589900
C	-6.33995100	1.01153600	0.74192300
C	-5.80006800	-0.13004200	0.14063000
C	-4.57924000	-0.10507600	-0.54204300
C	-3.89486600	1.11420200	-0.64408500
C	-4.68083900	4.36132800	0.94607900
C	-5.99233300	3.57489800	1.14312500
H	-6.33316300	-1.07526300	0.21657300
H	-4.01854900	4.19058100	1.80186200
H	-6.82133600	4.02788900	0.58413100
C	-4.03564000	3.72773400	-0.31760500
C	-2.58585100	4.13219900	-0.51442800
C	-4.67480600	4.34301500	-1.59776900
C	-2.50077000	5.25741900	-1.33717900
C	-1.42427200	3.56847200	-0.00217900
C	-3.86774800	5.62579900	-1.86276500
H	-5.74826700	4.51631700	-1.47851600
C	-1.27755600	5.86940400	-1.61568100
C	-0.17742700	4.15401800	-0.25297600
H	-3.85018800	5.90259600	-2.92127600
C	-0.13218400	5.30610700	-1.04897200
H	0.83558300	5.76668200	-1.23537600
H	-6.30168500	3.52887600	2.19188400
H	-4.83059300	5.43944900	0.83600700
H	-4.53057200	3.64449800	-2.42941400
H	-4.27963400	6.48175000	-1.31225200
O	-1.50438700	2.38358800	0.70912000
O	-2.63478600	1.15198700	-1.21807800
P	-1.36041200	1.01763700	-0.18828100
O	-1.54447100	-0.11168300	0.77864000
O	-0.15430700	1.08042000	-1.08151100
H	-0.77188000	-1.52344300	1.50434900
C	0.97991700	-2.95378600	-4.75069300
C	1.69667300	-3.67893400	-3.80926500
C	1.55566500	-3.40101100	-2.44256500
C	0.67784000	-2.36171200	-2.04791400
C	-0.04382700	-1.63559800	-3.01152900
C	0.10076000	-1.93565800	-4.35581600
H	2.96027500	-4.93128100	-1.76276300
H	1.09951100	-3.18044100	-5.80604600

H	2.37072800	-4.47124200	-4.12198300
C	2.25899200	-4.17195200	-1.43012600
C	0.57504700	-2.01548900	-0.65356100
H	-0.69640100	-0.83090000	-2.67977700
H	-0.45900800	-1.38056100	-5.10169200
C	1.03116500	-3.00068200	0.31547200
C	1.99586700	-3.99973200	-0.11947500
H	-0.25068700	-1.36666200	-0.37648000
N	0.59784600	-3.10990000	1.54617500
N	-0.32873500	-2.30865500	2.02145300
C	-0.82774800	-2.60456200	3.28677600
O	-0.50696100	-3.54891300	3.96701800
O	-1.71700000	-1.66930500	3.62109000
C	-2.27569600	-1.80890300	4.93112600
H	-1.48909000	-1.74626800	5.68733800
H	-2.97504200	-0.98204000	5.04025300
H	-2.79619500	-2.76491300	5.02496200
C	5.36755600	-1.35798900	-2.64599100
C	4.23266300	-0.97639700	-3.36549500
C	3.04846000	-0.62363900	-2.71576500
C	3.04066100	-0.68029600	-1.32944500
C	4.18858000	-1.01906600	-0.59113100
C	5.36186700	-1.36580000	-1.25046300
H	6.27434500	-1.62483700	-3.17980700
H	2.17394700	-0.30969700	-3.27403200
H	6.25599200	-1.62554600	-0.69187000
C	2.49979700	-0.45594100	0.86705900
C	1.86155400	-0.13388100	2.05750700
C	2.57816700	-0.27025200	3.25507300
C	3.90509000	-0.73686200	3.20231100
C	4.54700600	-1.02709600	2.00402700
C	3.83730100	-0.87383700	0.81793200
H	0.83157300	0.21220100	2.04105500
H	4.45633500	-0.86556700	4.12900200
H	5.58263000	-1.35369500	1.99501200
N	1.94750200	-0.46074000	-0.44810500
H	1.22447500	0.26541500	-0.69565400
H	4.26729100	-0.95005300	-4.45030100
C	1.95062900	0.02495000	4.62247500
C	0.57285600	0.67908300	4.48824200
C	1.80767200	-1.29925800	5.39152100
C	2.85347300	0.96599200	5.43664600
H	0.63213200	1.62494000	3.93846500
H	-0.14045100	0.03234000	3.96933000

H	0.16927800	0.88914200	5.48438000
H	2.78466400	-1.76134900	5.56697900
H	1.34051900	-1.12024000	6.36679300
H	1.19411700	-2.01809400	4.84022400
H	2.39101900	1.17008400	6.40849600
H	3.83891900	0.53085100	5.62524400
H	2.99645500	1.91959500	4.92101200
H	2.44792500	-4.62011000	0.64767300
C	-1.20552200	7.08310200	-2.50317700
H	-1.54409400	6.84824300	-3.51844700
H	-1.84784800	7.88689800	-2.12807600
H	-0.18389300	7.46449600	-2.56724800
C	-7.62357900	0.95945100	1.52662600
H	-7.44903400	1.20127200	2.58093300
H	-8.35052300	1.68461900	1.14589300
H	-8.07534000	-0.03409800	1.47783700
C	-4.00548100	-1.30456900	-1.21607400
C	-3.50392100	-2.41142300	-0.50578000
C	-3.91806900	-1.28787800	-2.61344100
C	-2.83386800	-3.44586900	-1.22262100
C	-3.61331700	-2.53283600	0.92810700
C	-3.32858100	-2.32577000	-3.31867900
H	-4.31546700	-0.42998600	-3.14863700
C	-2.19085900	-4.50842600	-0.51215900
C	-2.74863400	-3.40277300	-2.63920300
C	-3.08720600	-3.59403300	1.58540200
H	-4.12694300	-1.75058600	1.47624100
H	-3.26985300	-2.28762100	-4.40326900
C	-2.30634000	-4.59231600	0.90090400
C	-1.40621700	-5.46426800	-1.21423600
C	-2.00570300	-4.42452900	-3.33139000
H	-3.20085300	-3.68524500	2.66340500
C	-1.61533900	-5.59651400	1.58835200
C	-0.72130600	-6.44843800	-0.48950400
C	-1.34371200	-5.39236000	-2.65170500
H	-1.95807100	-4.37540500	-4.41605800
C	-0.82011000	-6.50684500	0.89682300
H	-1.68481200	-5.63777400	2.67166600
H	-0.10739700	-7.16623000	-1.02717900
H	-0.75422400	-6.13816500	-3.17874600
H	-0.27664900	-7.27091200	1.44390800
C	1.06839000	3.63253800	0.37698500
C	2.17802600	3.20729900	-0.38149400
C	1.16950800	3.67649800	1.77175200

C	3.39688100	2.88800400	0.28453400
C	2.12936400	3.07437200	-1.81855500
C	2.35176700	3.35799500	2.42375000
H	0.30778700	4.00152900	2.34816500
C	4.55530500	2.52166700	-0.47142800
C	3.48497500	2.97023000	1.70024800
C	3.22522800	2.71663500	-2.53123300
H	1.18223600	3.24996400	-2.31644500
H	2.41104600	3.44075000	3.50521800
C	4.48696000	2.44943900	-1.88851500
C	5.78307600	2.24606700	0.19138900
C	4.73451600	2.66525600	2.34755200
H	3.17077700	2.61605800	-3.61232800
C	5.63777100	2.11847400	-2.61288000
C	6.91313200	1.92051200	-0.57057900
C	5.83101700	2.32245000	1.62874900
H	4.77537700	2.72066900	3.43247200
C	6.84029400	1.86526600	-1.95839200
H	5.58084800	2.06126100	-3.69677900
H	7.85147000	1.71717900	-0.06139200
H	6.77209000	2.09850500	2.12430600
H	7.72461100	1.61174900	-2.53519600

(S)-C3**TS1**Value of imaginary frequency = -324.2 cm⁻¹

C	4.64957700	0.65545600	-1.15472000
C	5.78519300	1.28768900	-0.64606600
C	5.73168500	2.58986500	-0.14602300
C	4.48724800	3.22214300	-0.13104500
C	3.31395500	2.59042600	-0.56598100
C	3.41768600	1.29471100	-1.09171500
C	6.30375300	-1.01331900	-0.92263400
C	6.97286300	0.35567800	-0.69968400
H	4.41371600	4.23418300	0.26064800
H	6.00381400	-1.43518600	0.04312900
H	7.64031400	0.61804700	-1.53074300
C	5.02231600	-0.69249200	-1.74475300
C	4.06279700	-1.87112200	-1.77331900
C	5.38825400	-0.59009600	-3.25229500
C	4.35685600	-2.69521700	-2.86425100
C	3.03488700	-2.22623000	-0.90914700
C	5.39935700	-2.04828300	-3.74588700
H	6.33519500	-0.06604500	-3.41090800
C	3.70204000	-3.91052500	-3.06335700
C	2.35668200	-3.44264600	-1.07196600
H	5.15609100	-2.13576200	-4.80936500
C	2.71607100	-4.27062300	-2.14039200
H	2.18772600	-5.21287500	-2.26489900
H	7.57137400	0.38926400	0.21575900
H	6.94668600	-1.73851400	-1.42967700
H	4.59693600	-0.03539200	-3.76822800
H	6.38190300	-2.51611000	-3.60211700
O	2.63890400	-1.34939100	0.08789900
O	2.28931800	0.60938600	-1.50690200
P	1.50686600	-0.23793000	-0.33767500
O	1.30115400	0.60922900	0.88057400
O	0.34129900	-0.87115300	-1.03653900
H	0.06454700	1.42377100	1.90169400
C	1.22578000	-3.80548300	-0.17132500
C	-0.03185900	-3.85068800	-0.68227700
C	1.43760200	-4.07551600	1.23888100
C	-1.18233700	-4.09585500	0.13813400
H	-0.19254100	-3.62005000	-1.73181000
C	0.32723300	-4.36127400	2.07728300
C	2.73635300	-4.06871000	1.79646600
C	-2.47881300	-4.03235500	-0.41931800

C	-1.02066100	-4.34599700	1.52215400
C	0.56762400	-4.63156000	3.44307600
H	3.58319900	-3.85399600	1.15205000
C	2.94062400	-4.33315600	3.13316400
C	-3.59534400	-4.20176800	0.36979300
H	-2.58000600	-3.82789900	-1.48273200
C	-2.18125600	-4.52533700	2.30707300
C	1.84428800	-4.61833700	3.96421300
H	-0.26283900	-4.85809200	4.10262400
H	3.94626400	-4.32336300	3.54175800
C	-3.44017200	-4.45136700	1.74492600
H	-4.58937700	-4.12503200	-0.06167500
H	-2.09753300	-4.70128300	3.37374500
H	2.00094100	-4.83095600	5.01720300
H	-4.31697400	-4.57363400	2.37421700
C	2.00145000	3.29451900	-0.48725600
C	1.29041700	3.51329800	-1.62687000
C	1.49412600	3.80147600	0.77873600
C	0.04896100	4.23181100	-1.63163400
H	1.67150900	3.14771100	-2.57758900
C	0.27017600	4.52310000	0.81182900
C	2.18917600	3.58863600	1.99145300
C	-0.64058300	4.45664000	-2.84402800
C	-0.49015500	4.71470000	-0.41644100
C	-0.17204500	5.05277900	2.04535300
H	3.08701300	2.98177600	1.98365300
C	1.74222500	4.12996700	3.17775900
C	-1.84926700	5.11606700	-2.85611800
H	-0.20274400	4.08585600	-3.76708200
C	-1.74000900	5.37408100	-0.45411900
C	0.55443900	4.87904400	3.20375900
H	-1.09432200	5.62058300	2.09006900
H	2.30055300	3.95994700	4.09392900
C	-2.40726200	5.56724000	-1.64552600
H	-2.37579300	5.27727100	-3.79188700
H	-2.19744700	5.72985000	0.46216400
H	0.19574100	5.30195300	4.13687100
H	-3.36960100	6.07040200	-1.64738600
C	-3.24589500	2.02162700	-3.92610300
C	-3.97899700	2.41531200	-2.81684200
C	-3.46663800	2.23644900	-1.52256600
C	-2.18082100	1.66435200	-1.37278800
C	-1.44405100	1.27563600	-2.50697500
C	-1.97551300	1.44736500	-3.77424400

H	-5.22222900	3.04119100	-0.50016900
H	-3.66020800	2.16041600	-4.92054200
H	-4.95854300	2.86968800	-2.93800100
C	-4.22011900	2.65061100	-0.35092900
C	-1.65172100	1.43522600	-0.04297300
H	-0.46530900	0.82452700	-2.36652700
H	-1.40705600	1.14572000	-4.64794300
C	-2.32658200	2.08507300	1.07540500
C	-3.67738600	2.58704100	0.87999800
H	-0.57703000	1.29143200	0.03091000
N	-1.82543200	2.23363300	2.27653100
N	-0.60599100	1.85238900	2.56713500
C	-0.24294000	1.87808800	3.91489700
O	-0.90501500	2.33985900	4.80956500
O	0.94304500	1.28586400	4.04085200
C	1.45412900	1.25185500	5.37563700
H	0.79390700	0.66778100	6.02089400
H	2.43168200	0.77829100	5.30328300
H	1.54829100	2.26453200	5.77446200
C	-6.07948700	-1.20295400	-0.33918800
C	-5.28873000	-1.11755500	-1.49946300
C	-3.91591100	-0.86887900	-1.36341600
C	-3.39024600	-0.76431300	-0.08335300
C	-4.16823200	-0.92212000	1.07062400
C	-5.53767000	-1.12141100	0.94054500
H	-7.14745200	-1.37263400	-0.43990300
H	-3.26225700	-0.79716200	-2.22596600
H	-6.16858800	-1.24347100	1.81592200
C	-1.95271200	-0.87054500	1.67716300
C	-0.82022400	-1.09370200	2.44925300
C	-1.01588300	-1.38460800	3.79796800
C	-2.30125500	-1.44352900	4.35120500
C	-3.42964100	-1.25582000	3.55870200
C	-3.24825700	-0.98743500	2.20317400
H	0.17965400	-1.01705700	2.03626100
H	-0.14954000	-1.57202200	4.42494200
H	-2.41868600	-1.66103800	5.40825700
H	-4.42722600	-1.34399500	3.97774000
N	-2.03024300	-0.53465900	0.28647100
H	-1.24752000	-0.87208500	-0.31701400
C	-5.94687800	-1.31678900	-2.86890100
C	-4.91774800	-1.33305100	-4.00233800
C	-6.69827700	-2.65848500	-2.89105100
C	-6.93990400	-0.17123200	-3.12089800

H	-4.37670100	-0.38454400	-4.07044100
H	-4.18614300	-2.13788100	-3.87038900
H	-5.42920700	-1.49696400	-4.95596100
H	-7.49500900	-2.69806700	-2.14273500
H	-7.15679000	-2.80952800	-3.87419300
H	-6.01186900	-3.49142900	-2.70395200
H	-7.42285300	-0.29875500	-4.09584200
H	-7.72226100	-0.14214800	-2.35596100
H	-6.42220800	0.79387800	-3.11695600
H	-4.20632400	2.93053800	1.76338700
C	4.03881700	-4.78486700	-4.24148700
H	3.82189600	-4.27312800	-5.18572500
H	5.10323400	-5.04240600	-4.25279400
H	3.46361000	-5.71337200	-4.22040100
C	6.97019000	3.26858100	0.37463800
H	7.39607400	2.71571700	1.21926700
H	7.74586100	3.32403800	-0.39672900
H	6.75137400	4.28483300	0.71039300

(S)-C3**TSII**Value of imaginary frequency = -296.6 cm⁻¹

C	0.96619500	4.39349200	-0.13163400
C	0.95247200	5.37055100	0.86560700
C	-0.21676100	5.68646900	1.55901500
C	-1.37253700	4.97056300	1.23434400
C	-1.37375400	3.93568300	0.29128700
C	-0.17845000	3.65317700	-0.38391000
C	3.22136200	4.91118100	0.31980700
C	2.34000500	5.93724000	1.05870000
H	-2.30045400	5.20023500	1.75336200
H	3.46440200	4.08185100	0.99336600
H	2.42364500	6.93606400	0.61110600
C	2.31426400	4.37286300	-0.82380300
C	2.89766100	3.13006900	-1.48057000
C	2.34441700	5.36635000	-2.01988200
C	3.72873600	3.50873900	-2.53821900
C	2.77725100	1.78022100	-1.15042300
C	3.61217400	4.99039000	-2.80445500
H	2.32705300	6.40885100	-1.68988200
C	4.52429000	2.58573400	-3.21763300
C	3.57334800	0.82833200	-1.79930300
H	3.53010000	5.21499200	-3.87249200
C	4.44587400	1.25516300	-2.80883900
H	5.06395500	0.50821200	-3.30211500
H	2.60389000	6.03693600	2.11615900
H	4.15734600	5.33130800	-0.05944600
H	1.46080500	5.18881900	-2.64269400
H	4.49429600	5.52644300	-2.43105100
O	1.88795300	1.39144600	-0.16432300
O	-0.10255800	2.57785200	-1.25417700
P	0.30502500	1.15492300	-0.54663700
O	-0.37526800	1.01195400	0.78217600
O	0.12708500	0.10741500	-1.60436600
H	-1.14784500	-0.04904600	1.94155400
C	3.55627000	-0.62828100	-1.46142700
C	2.65225200	-1.45521800	-2.04582700
C	4.60688300	-1.18744500	-0.62740500
C	2.67875100	-2.87602800	-1.84432400
H	1.87743300	-1.04024100	-2.68209000
C	4.69822500	-2.59453500	-0.44987900
C	5.56586800	-0.35310000	-0.00820900
C	1.70424600	-3.69278400	-2.45528400

C	3.68708600	-3.46141100	-1.04177100
C	5.78502000	-3.10907200	0.29139100
H	5.47827700	0.72243000	-0.12718800
C	6.60465100	-0.88297200	0.72779900
C	1.69914400	-5.05642700	-2.25700200
H	0.94805800	-3.22195200	-3.07909300
C	3.66046900	-4.86058900	-0.85336500
C	6.72413800	-2.27596700	0.86354400
H	5.89262400	-4.18031900	0.41931400
H	7.33221700	-0.22485000	1.19246200
C	2.68426700	-5.64053400	-1.44147600
H	0.93052200	-5.67281500	-2.71514900
H	4.40465900	-5.34097300	-0.22788500
H	7.54993600	-2.69985100	1.42654100
H	2.67926000	-6.71283500	-1.27144600
C	-2.61352000	3.17004000	-0.02411400
C	-3.10115100	3.20757500	-1.29346900
C	-3.31873700	2.40305000	0.98988700
C	-4.30018800	2.52159400	-1.67888800
H	-2.57818900	3.78267100	-2.05383100
C	-4.48972500	1.67743300	0.63675500
C	-2.85869700	2.35172000	2.32579800
C	-4.78631500	2.62541600	-3.00087900
C	-4.99655800	1.73624700	-0.72946000
C	-5.14139900	0.91963100	1.63618800
H	-1.94101900	2.86611000	2.58738300
C	-3.54446700	1.64281100	3.28819800
C	-5.92910500	1.95952500	-3.38565800
H	-4.23757700	3.23996500	-3.70982100
C	-6.15680500	1.05102500	-1.15427800
C	-4.68840700	0.90715700	2.93854100
H	-6.01919600	0.33574600	1.38455600
H	-3.18644000	1.63086200	4.31423100
C	-6.61257500	1.15972100	-2.45253900
H	-6.29756200	2.04388700	-4.40337400
H	-6.71218800	0.42928200	-0.46098600
H	-5.21236500	0.32465900	3.68997300
H	-7.50596800	0.62062500	-2.75283800
C	-4.79854100	-1.65227000	-3.38847500
C	-5.04152400	-2.46421500	-2.29102400
C	-4.25137600	-2.35376700	-1.13738100
C	-3.21638100	-1.38739300	-1.11417000
C	-2.98771500	-0.56044500	-2.23105600
C	-3.76825200	-0.69962800	-3.36433500

H	-5.24077600	-3.96853400	-0.04744700
H	-5.41417100	-1.75234700	-4.27769900
H	-5.83929200	-3.20114900	-2.31775300
C	-4.47200100	-3.20481000	0.02006500
C	-2.35096700	-1.29729800	0.03417000
H	-2.17294800	0.15920300	-2.19074000
H	-3.59279500	-0.06627900	-4.22743700
C	-2.76776500	-1.97606900	1.25111100
C	-3.76809600	-3.02834400	1.15522800
H	-1.75450800	-0.39307000	0.12152900
N	-2.36527200	-1.66928000	2.45964000
N	-1.54526200	-0.67051800	2.67513600
C	-1.30425300	-0.32192100	4.00327400
O	-1.74162200	-0.88871600	4.97267200
O	-0.51591800	0.75322100	4.01154400
C	-0.20280700	1.27540800	5.30596100
H	0.25490200	0.50852900	5.93372000
H	0.49689200	2.09073900	5.13015800
H	-1.10766000	1.65023300	5.79119500
C	-2.05322200	-6.18731100	-1.58193000
C	-2.29748000	-5.15684600	-2.49338200
C	-1.86072400	-3.85246500	-2.24697700
C	-1.18194600	-3.62588100	-1.05940200
C	-0.88998300	-4.66025800	-0.15272900
C	-1.33517500	-5.95139500	-0.40856600
H	-2.40857900	-7.18927500	-1.80052800
H	-2.03982300	-3.05545500	-2.96167200
H	-1.11522600	-6.76044800	0.28113400
C	0.12108700	-2.72998100	0.57956900
C	0.95315900	-1.89092300	1.31187400
C	1.62810800	-2.42024100	2.41319800
C	1.45471400	-3.78381800	2.72844300
C	0.63506300	-4.61988600	1.98275200
C	-0.04324100	-4.08475400	0.88796100
H	1.05382600	-0.84533600	1.05215100
H	1.98238800	-4.20073400	3.58169000
H	0.53287100	-5.66968300	2.24022200
N	-0.69288600	-2.39193700	-0.54361100
H	-0.32944100	-1.65202500	-1.17215400
H	-2.83715600	-5.36779400	-3.41117600
C	2.53008200	-1.55064300	3.29450100
C	2.53946800	-0.08998700	2.83289800
C	2.02649600	-1.61808700	4.74597500
C	3.96977400	-2.07858100	3.23050900

H	2.94994100	0.00570100	1.82161300
H	1.53674600	0.34968500	2.83322200
H	3.17089400	0.49854500	3.50732100
H	2.13368000	-2.62311600	5.16574700
H	2.60357200	-0.93145500	5.37551600
H	0.96886900	-1.34360400	4.81296600
H	4.61661900	-1.49374900	3.89471200
H	4.03394400	-3.12912300	3.53240800
H	4.35655700	-1.98909100	2.21224500
H	-3.95469400	-3.61745200	2.04731600
C	5.41629600	3.01754400	-4.35014600
H	4.82632800	3.37675800	-5.20088700
H	6.07512400	3.83824100	-4.04713800
H	6.03933700	2.19014600	-4.69755100
C	-0.21829500	6.74997000	2.62399200
H	0.45262500	6.48111100	3.44752800
H	0.12887200	7.71023500	2.22816500
H	-1.21942100	6.89342900	3.03711300

(S)-C6-40°C, TSI_{Ar}-1

TSI

Value of imaginary frequency = -332.6 cm⁻¹

C	4.77975500	0.84695600	-1.27799600
C	5.92882700	1.41482500	-0.71936400
C	5.86256700	2.63060100	-0.05015900
C	4.62640100	3.25842700	0.09001400
C	3.44753600	2.68144800	-0.40068800
C	3.54951800	1.46604800	-1.09702100
C	6.44099100	-0.82976800	-1.29452000
C	7.11621500	0.50519800	-0.93136100
H	6.75526900	3.07986400	0.37528900
H	4.56004300	4.20732600	0.61502300
H	6.16530100	-1.36263900	-0.37771400
H	7.74330500	0.86892200	-1.75464500
C	5.13915200	-0.41657100	-2.04061000
C	4.18126100	-1.58713900	-2.18834400
C	5.46213900	-0.12854900	-3.53441100
C	4.44256300	-2.26956500	-3.38331800
C	3.17624800	-2.04829000	-1.34833600
C	5.46843000	-1.51708700	-4.19947400
H	6.40166900	0.41847500	-3.65522300
C	3.76411600	-3.43973300	-3.69747400
C	2.48780100	-3.23794900	-1.63364500
H	5.21101400	-1.48251000	-5.26159300
C	2.80462800	-3.92564300	-2.80868400
H	3.96559400	-3.96537500	-4.62657000
H	2.26710900	-4.84216300	-3.03425900
H	7.75176300	0.43493100	-0.04453900
H	7.07101700	-1.48861100	-1.89874700
H	4.65357400	0.47789500	-3.95706000
H	6.45415500	-1.99122400	-4.11755800
O	2.80736200	-1.30226700	-0.24248300
O	2.41480100	0.83339700	-1.57244200
P	1.65741200	-0.15640500	-0.50236700
O	1.47738800	0.53229800	0.81519100
O	0.48004200	-0.71126200	-1.24461000
H	0.27228900	1.17520100	1.95808400
C	1.39483200	-3.71740800	-0.74161900
C	0.11964700	-3.72577700	-1.20862800
C	1.66597000	-4.15789300	0.61408900
C	-0.99301700	-4.10239600	-0.38596100
H	-0.08447900	-3.37210100	-2.21556300
C	0.59519700	-4.57682700	1.44819900

C	2.98506500	-4.18660900	1.12083700
C	-2.31076600	-3.99672900	-0.88351600
C	-0.77314200	-4.52592900	0.94732400
C	0.89495400	-5.01153800	2.75862000
H	3.80222200	-3.87180100	0.47938100
C	3.24728700	-4.61219900	2.40443400
C	-3.39279100	-4.29521000	-0.08477800
H	-2.45657100	-3.65555000	-1.90589300
C	-1.89907400	-4.83620200	1.74130800
C	2.19058400	-5.02947400	3.23104800
H	0.09675300	-5.34037300	3.41471400
H	4.26754100	-4.62741800	2.77456900
C	-3.18004000	-4.72032900	1.23853300
H	-4.40358000	-4.18538800	-0.46714900
H	-1.77205300	-5.14991000	2.77134100
H	2.39235900	-5.36843000	4.24247700
H	-4.02967500	-4.94798100	1.87553200
C	2.12995600	3.35336900	-0.21027300
C	1.38726800	3.68214700	-1.30165700
C	1.64333600	3.70477300	1.11538000
C	0.13404600	4.37176900	-1.19990800
H	1.74905500	3.42956100	-2.29556900
C	0.40898100	4.39602700	1.25431900
C	2.36685500	3.36725300	2.28248300
C	-0.58868500	4.70851300	-2.36625800
C	-0.38144500	4.71382500	0.07208300
C	-0.01783500	4.76766900	2.54942300
H	3.27401800	2.78170800	2.18939400
C	1.93576400	3.75987800	3.53149800
C	-1.80539500	5.34667500	-2.28174000
H	-0.16830400	4.44030000	-3.33209900
C	-1.63970300	5.35656700	0.13208700
C	0.73520400	4.47554700	3.66633900
H	-0.95329600	5.29992000	2.67741600
H	2.51682100	3.49857000	4.41111800
C	-2.33694500	5.66322600	-1.01769000
H	-2.35878400	5.59463200	-3.18215700
H	-2.07898500	5.61196200	1.08994300
H	0.38811300	4.77925400	4.64884900
H	-3.30453700	6.15082400	-0.94446800
C	-3.29659800	2.41715500	-3.59589900
C	-3.98387900	2.66314500	-2.41657100
C	-3.41627400	2.33159900	-1.17691100
C	-2.12163000	1.76117100	-1.15264100

C	-1.43248900	1.52217700	-2.35575700
C	-2.01938300	1.84020500	-3.56926500
H	-5.13536300	2.97555100	0.00802700
H	-3.75404900	2.67322000	-4.54730300
H	-4.97006600	3.11876900	-2.44009100
C	-4.12328600	2.58648100	0.06695600
C	-1.53306300	1.37772600	0.11620800
H	-0.44591700	1.06835900	-2.31065500
H	-1.48800800	1.65140400	-4.49637200
C	-2.16378300	1.88035700	1.33223300
C	-3.52669400	2.38135000	1.25659300
H	-0.45532900	1.24132300	0.12620000
N	-1.60922300	1.89524300	2.51894700
N	-0.37260300	1.50348800	2.70235400
C	0.05911600	1.36563700	4.02286100
O	-0.55876700	1.69933800	5.00233100
O	1.25393500	0.77727000	4.00982600
C	1.82946000	0.56325400	5.30065600
H	1.18967600	-0.08740300	5.90134600
H	2.79202600	0.08799100	5.11989200
H	1.96603200	1.51490800	5.81977000
C	-5.94211200	-1.28049000	-0.24613900
C	-5.22594400	-1.02683800	-1.43006700
C	-3.85006900	-0.77133900	-1.34538100
C	-3.24729600	-0.82598800	-0.09626000
C	-3.95182000	-1.14318600	1.07180300
C	-5.32410000	-1.35105500	0.99882200
H	-7.01174000	-1.45980600	-0.30358100
H	-3.25427800	-0.56737000	-2.22870100
H	-5.89771700	-1.59802200	1.88700100
C	-1.70419800	-1.12370500	1.55354900
C	-0.52668400	-1.41751600	2.22856400
C	-0.64222500	-1.88103600	3.53768600
C	-1.89273300	-2.03841100	4.14866400
C	-3.06693500	-1.77615300	3.44923100
C	-2.96561800	-1.33309400	2.13158700
H	0.44851800	-1.27048600	1.77806800
H	0.26158800	-2.12681700	4.08678400
H	-1.94596000	-2.39048100	5.17412700
H	-4.03842500	-1.93489000	3.90701300
N	-1.86899000	-0.61954000	0.22057600
H	-1.12512100	-0.87003000	-0.46367300
C	-5.97055400	-1.04568500	-2.76879200
C	-5.01859600	-0.89270200	-3.95740700

C	-6.71794400	-2.38034300	-2.92648100
C	-6.98210700	0.11144700	-2.79271100
H	-4.48750500	0.06339600	-3.92929400
H	-4.27635400	-1.69815000	-3.98347800
H	-5.59041400	-0.93194000	-4.88975500
H	-7.45910600	-2.53311600	-2.13707800
H	-7.24535900	-2.39984200	-3.88629400
H	-6.01859700	-3.22303100	-2.90578900
H	-7.52128800	0.12291800	-3.74625900
H	-7.71880300	0.01792800	-1.98861300
H	-6.47133600	1.07299100	-2.67505200
H	-4.02028000	2.60575500	2.19699400

(S)-C6-40°C, TSII_{Ar}-1

TSII

Value of imaginary frequency = -286.3 cm⁻¹

C	-0.07756900	4.60366700	-0.03717800
C	-0.25403600	5.51375300	1.00946100
C	-1.40768900	5.48293800	1.78336300
C	-2.38475300	4.52655900	1.50623700
C	-2.20601300	3.56700600	0.50229600
C	-1.02231100	3.61269200	-0.25021900
C	2.00596800	5.66013800	0.28201000
C	0.95743500	6.41040200	1.12622800
H	-1.55100300	6.19127800	2.59416700
H	-3.29967100	4.50380500	2.09178200
H	2.49957600	4.90004500	0.89764200
H	0.74791700	7.40310300	0.70931500
C	1.17426200	4.94409800	-0.82118600
C	1.99617500	3.91217700	-1.57847100
C	0.85902000	5.94854200	-1.96752500
C	2.62170300	4.52375100	-2.67037700
C	2.24414000	2.56634400	-1.31169100
C	2.12217500	5.93854100	-2.84389300
H	0.59867600	6.94006900	-1.58681800
C	3.55651900	3.83784100	-3.43547100
C	3.20065100	1.86023100	-2.05584100
H	1.91755000	6.18160500	-3.89013000
C	3.85668100	2.52042800	-3.10265100
H	4.04322500	4.31732100	-4.27980200
H	4.59791300	1.96992400	-3.67550000
H	1.27146800	6.55429000	2.16369100
H	2.77535700	6.31366900	-0.13916800
H	0.00787800	5.56718400	-2.54247400
H	2.86481100	6.65913700	-2.48057700
O	1.56398200	1.93967100	-0.28494100
O	-0.74296900	2.61588500	-1.16987000
P	0.05816100	1.32944300	-0.53955400
O	-0.44841200	1.02535800	0.83911000
O	0.04019000	0.27633300	-1.60624800
H	-0.88333800	-0.16284600	2.05229900
C	3.55749500	0.43491800	-1.78047600
C	2.82166200	-0.56675300	-2.32559300
C	4.77052000	0.11896200	-1.04578000
C	3.17778100	-1.94744500	-2.16369400
H	1.92602900	-0.32773700	-2.88866600
C	5.18629600	-1.23380600	-0.91438400

C	5.56764100	1.14035100	-0.47999600
C	2.36683600	-2.95540200	-2.72585200
C	4.34433100	-2.29928700	-1.44339600
C	6.41949800	-1.50013900	-0.27891600
H	5.23456000	2.17044000	-0.56052900
C	6.75580200	0.84826600	0.15625000
C	2.67691300	-4.28732000	-2.55744000
H	1.48420900	-2.65964400	-3.28797000
C	4.63382300	-3.67096200	-1.27367400
C	7.19428000	-0.48363600	0.24033400
H	6.77320200	-2.52166400	-0.19538200
H	7.35466700	1.64721400	0.58223700
C	3.81518700	-4.64391500	-1.81272000
H	2.03393900	-5.05538100	-2.97813100
H	5.50223700	-3.97696300	-0.70086900
H	8.13841900	-0.71556100	0.72335400
H	4.05387600	-5.69198100	-1.65901300
C	-3.26449400	2.56567200	0.18497500
C	-3.81501000	2.57981300	-1.05933800
C	-3.75134600	1.61418300	1.16983700
C	-4.88950800	1.70868200	-1.43716300
H	-3.45158100	3.28902900	-1.79912700
C	-4.80545700	0.72290700	0.82745600
C	-3.18511200	1.54160000	2.46288600
C	-5.44888700	1.78762300	-2.73141600
C	-5.39967300	0.77576600	-0.50277400
C	-5.24676800	-0.20423100	1.79766400
H	-2.34818000	2.18634900	2.70799400
C	-3.65892700	0.64577200	3.39804800
C	-6.48838500	0.96226700	-3.10139100
H	-5.04262400	2.51467000	-3.42965300
C	-6.46134600	-0.06246400	-0.90914100
C	-4.69396700	-0.24049300	3.06052000
H	-6.03772600	-0.90465000	1.55534700
H	-3.22165500	0.61228400	4.39242000
C	-6.99527100	0.02886100	-2.17894000
H	-6.91562700	1.03135400	-4.09698300
H	-6.87310800	-0.79431200	-0.22340000
H	-5.05635800	-0.95865300	3.78941500
H	-7.81291000	-0.62511400	-2.46622100
C	-4.54704400	-2.54429400	-2.95502700
C	-4.47574500	-3.40505400	-1.86997300
C	-3.61986300	-3.12298000	-0.79491100
C	-2.84988300	-1.93463700	-0.83556700

C	-2.93701400	-1.06490500	-1.94069300
C	-3.77466700	-1.37294400	-2.99721500
H	-4.06991200	-4.94353400	0.32671900
H	-5.20890900	-2.77923100	-3.78334000
H	-5.07350600	-4.31152600	-1.84752000
C	-3.50889100	-4.01421400	0.34758000
C	-1.92740200	-1.64976400	0.23009300
H	-2.31720400	-0.17108600	-1.95505100
H	-3.84153600	-0.70764500	-3.85110700
C	-2.04410700	-2.41728300	1.45767100
C	-2.76095100	-3.68244800	1.41832800
H	-1.54106900	-0.63546800	0.28352800
N	-1.60050000	-2.03714800	2.63173800
N	-1.03668300	-0.86726500	2.80091300
C	-0.74008200	-0.48288300	4.10862300
O	-0.82145500	-1.18321700	5.08615100
O	-0.36349900	0.79570100	4.08660600
C	0.03814100	1.33994800	5.34899000
H	0.90837100	0.80421200	5.73462800
H	0.29142400	2.37928400	5.14832300
H	-0.78077400	1.27779100	6.06881200
C	-0.62292000	-6.29590000	-1.73165000
C	-1.20180100	-5.31348300	-2.53860300
C	-1.06824200	-3.95576500	-2.23639000
C	-0.34565700	-3.62726800	-1.09898000
C	0.28331600	-4.60219400	-0.30323400
C	0.13733700	-5.94887200	-0.61317700
H	-0.74853400	-7.34240200	-1.99056300
H	-1.50560300	-3.19270800	-2.87252400
H	0.61926600	-6.71212900	-0.00979200
C	0.86253400	-2.51956400	0.47824600
C	1.52091100	-1.53659400	1.20817700
C	2.42295500	-1.93251600	2.19671300
C	2.63875300	-3.31008700	2.40920300
C	1.97949800	-4.28661600	1.67485700
C	1.07240200	-3.88609300	0.69421500
H	1.31195200	-0.48881300	1.03279500
H	3.34668700	-3.62346600	3.17114200
H	2.17373300	-5.33959300	1.85457600
N	-0.11009600	-2.33776000	-0.54793600
H	0.01168500	-1.50920900	-1.16056700
H	-1.76864300	-5.60397800	-3.41739000
C	3.16820400	-0.90791000	3.05722900
C	2.75462600	0.52753400	2.71864300

C	2.86832500	-1.18057800	4.54038200
C	4.67818000	-1.03612100	2.80986900
H	3.00386300	0.78234400	1.68250900
H	1.68075800	0.69171900	2.85419800
H	3.28990100	1.22312800	3.37399400
H	3.24642800	-2.15737400	4.85794200
H	3.34926500	-0.41944800	5.16485800
H	1.79139100	-1.16327300	4.73940600
H	5.22731300	-0.34071400	3.45529500
H	5.04192100	-2.04809000	3.01631500
H	4.91071400	-0.79291100	1.76981800
H	-2.70797100	-4.31087800	2.30132900

(S)-C7**TSI**Value of imaginary frequency = -327.8 cm⁻¹

C	4.26921700	-0.29253900	-0.85272100
C	5.41623200	-0.99028800	-0.46275600
C	5.35978800	-2.36855400	-0.33909100
C	4.17089200	-3.05616300	-0.55407400
C	2.99918300	-2.36389900	-0.87793600
C	3.07010100	-0.96947700	-1.03321400
C	5.82557000	1.30897000	-0.07720600
C	6.55475900	-0.04221500	-0.19076400
H	4.14068600	-4.13577700	-0.44771200
H	5.45749400	1.44031600	0.94601000
H	7.27315500	-0.05004500	-1.01962800
C	4.60559300	1.17800000	-1.03372700
C	3.58913500	2.28226000	-0.79516600
C	5.04728600	1.50653000	-2.48770200
C	3.90370000	3.38398200	-1.59970600
C	2.50568000	2.34580200	0.06939000
C	5.01001300	3.04442400	-2.56532400
H	6.02695500	1.08249800	-2.72403300
C	3.18381500	4.55738900	-1.45615800
C	1.76740800	3.53207300	0.21278000
H	4.80028700	3.41481800	-3.57254800
C	2.12971600	4.64365400	-0.55062900
H	1.57061400	5.56752700	-0.44735000
H	7.10336700	-0.31036900	0.71599900
H	6.45375400	2.16693600	-0.33078100
H	4.31242400	1.08741400	-3.18288000
H	5.95790000	3.49324600	-2.24420900
O	2.11609000	1.21586500	0.76039900
O	1.93363000	-0.24018500	-1.31642600
P	1.04664500	0.23421700	-0.01321800
O	0.81074200	-0.91617500	0.91393800
O	-0.09508800	1.01090700	-0.59342500
H	-0.49137900	-2.03601000	1.54834100
C	0.57673800	3.58364000	1.10646600
C	-0.65084100	3.76147500	0.55366200
C	0.70538800	3.41846100	2.54192600
C	-1.85115300	3.73453500	1.33807000
H	-0.74562500	3.85876700	-0.52455000
C	-0.45757200	3.42065700	3.35638800
C	1.97178500	3.26247800	3.15000300
C	-3.11284600	3.82835000	0.70973900

C	-1.77120200	3.55951500	2.74107900
C	-0.30112700	3.26345700	4.75186600
H	2.86096600	3.27032100	2.52740500
C	2.09395700	3.10775300	4.51319400
C	-4.27437600	3.75006200	1.44645600
H	-3.14989500	3.94842600	-0.37049300
C	-2.97681100	3.48867100	3.47354900
C	0.94464600	3.10750800	5.32186700
H	-1.17375400	3.26653700	5.39530400
H	3.07536500	2.98899500	4.96138800
C	-4.20047800	3.57873000	2.84056900
H	-5.24102400	3.80543400	0.95402900
H	-2.95540500	3.33568300	4.54684700
H	1.03629500	2.98882100	6.39706400
H	-5.11344800	3.50550600	3.42426000
C	1.72163300	-3.10480600	-1.08491800
C	1.10596100	-3.03416500	-2.29580800
C	1.15924000	-3.94742700	-0.04124000
C	-0.09663800	-3.75958200	-2.58699700
H	1.53393600	-2.41854200	-3.08369400
C	-0.02609700	-4.68854500	-0.29835500
C	1.76200500	-4.04868600	1.23362600
C	-0.69322600	-3.66515600	-3.86382700
C	-0.69355700	-4.56302800	-1.58780900
C	-0.52020600	-5.54680800	0.70981900
H	2.62578000	-3.43445900	1.46131500
C	1.26669600	-4.90665600	2.19239400
C	-1.87102200	-4.32223600	-4.14134900
H	-0.20988600	-3.04994500	-4.61823400
C	-1.91209100	-5.21209600	-1.89241300
C	0.12070000	-5.67275200	1.92365300
H	-1.41375000	-6.13334700	0.52939800
H	1.75741900	-4.97866100	3.15880200
C	-2.48961100	-5.09233800	-3.13913600
H	-2.32872900	-4.23623900	-5.12205900
H	-2.41777300	-5.80600500	-1.13966300
H	-0.27405900	-6.34741500	2.67663500
H	-3.42964500	-5.59522900	-3.34550500
C	-3.28098100	-1.05975500	-4.47880500
C	-4.09500700	-1.74148300	-3.58654100
C	-3.70110800	-1.91446100	-2.25114600
C	-2.45118800	-1.39508300	-1.83801000
C	-1.63290400	-0.70905500	-2.75423700
C	-2.04720300	-0.53791700	-4.06410000

H	-5.50953100	-2.98097800	-1.64444400
H	-3.60276500	-0.93018000	-5.50815500
H	-5.04517900	-2.15427200	-3.91406000
C	-4.53483900	-2.64126300	-1.30747200
C	-2.04373500	-1.53586200	-0.45593600
H	-0.68395000	-0.30762200	-2.40945100
H	-1.41569500	-0.00789400	-4.76963300
C	-2.77843800	-2.48445900	0.37378600
C	-4.09277100	-2.92367600	-0.06714900
H	-0.98603900	-1.39781900	-0.24954200
N	-2.36538700	-2.95688100	1.52282900
N	-1.18632400	-2.65119900	2.00760100
C	-0.93113800	-3.03209600	3.32652400
O	-1.63528900	-3.74387600	3.99693800
O	0.20259800	-2.45374100	3.71801700
C	0.60184300	-2.76762800	5.05467200
H	-0.14025600	-2.40407200	5.76914900
H	1.55353100	-2.26068200	5.20420400
H	0.72156900	-3.84678000	5.17411900
C	-6.51684700	1.06375700	-0.46583600
C	-5.60956300	1.30316400	-1.51366900
C	-4.25001900	1.03150200	-1.30487800
C	-3.85463800	0.58063300	-0.05311700
C	-4.75152700	0.40982000	1.00900800
C	-6.10655000	0.63186100	0.79236300
H	-7.57383700	1.25198900	-0.62958300
H	-3.51056200	1.20041100	-2.08004300
H	-6.82813300	0.50479200	1.59362600
C	-2.60957500	0.18038600	1.80975400
C	-1.56920700	0.16181200	2.72994100
C	-1.91214800	0.05689300	4.07676500
C	-3.24969300	-0.02751800	4.48357000
C	-4.28464700	0.02958000	3.55482400
C	-3.95572200	0.15252100	2.20613300
H	-0.52940500	0.19309700	2.41989700
H	-1.12042700	0.04187200	4.81975400
H	-3.48143600	-0.11776100	5.54027100
H	-5.32234100	0.00440400	3.87261500
N	-2.53334700	0.25809600	0.38096100
H	-1.70981100	0.76221200	-0.01762400
C	-6.13230900	1.86867500	-2.83878800
C	-4.99621600	2.20814100	-3.80638800
C	-6.92909000	3.15646100	-2.56893300
C	-7.05174200	0.83122400	-3.50201300

H	-4.41790400	1.32044000	-4.07934100
H	-4.31015700	2.94811800	-3.37982600
H	-5.41509600	2.62933000	-4.72551000
H	-7.80609700	2.97281700	-1.94206800
H	-7.28081600	3.58132300	-3.51523900
H	-6.30331600	3.90522000	-2.07140500
H	-7.45029200	1.22693800	-4.44264700
H	-7.89844500	0.57468700	-2.85745200
H	-6.50038200	-0.08835500	-3.72482800
H	-4.67847400	-3.50619400	0.63681100
Br	3.63364600	6.06313000	-2.51752300
Br	6.92096400	-3.32692400	0.15212900

(S)-C7**TSII**Value of imaginary frequency = -291.5 cm⁻¹

C	2.95368400	-2.71024200	-0.11005600
C	3.40860700	-3.61476400	0.85259200
C	2.56160300	-4.62151200	1.28481800
C	1.26236200	-4.72331700	0.79597900
C	0.77537400	-3.77909100	-0.11306600
C	1.64147800	-2.76389500	-0.54913600
C	4.98560400	-1.84646800	0.72600300
C	4.81010200	-3.27217200	1.28613100
H	0.61224100	-5.52275700	1.13695000
H	4.59558500	-1.11921100	1.44597800
H	5.53310900	-3.97403700	0.85288800
C	4.09433400	-1.81621100	-0.54954900
C	3.88429700	-0.40163300	-1.06853200
C	4.87098800	-2.44787900	-1.74007100
C	4.90601700	-0.09301700	-1.97211400
C	2.93775800	0.56399200	-0.73186300
C	5.74364400	-1.30500600	-2.28283700
H	5.44456300	-3.32699500	-1.43474400
C	5.02554000	1.20027500	-2.45282600
C	3.07007700	1.87946400	-1.20118300
H	5.95112100	-1.39534000	-3.35253400
C	4.13314200	2.18734800	-2.05714000
H	4.24617600	3.20491500	-2.41691800
H	4.92371600	-3.32091400	2.37257400
H	6.02613600	-1.59271000	0.50624700
H	4.15073000	-2.75477800	-2.50594800
H	6.71070700	-1.24647500	-1.76821500
O	1.88876500	0.22587700	0.09648000
O	1.17033300	-1.74904000	-1.36040900
P	0.53849400	-0.47503200	-0.53723100
O	-0.21497800	-0.95812000	0.66441100
O	-0.12212900	0.39580000	-1.56110900
H	-1.53388500	-0.70751900	1.78348500
C	2.16837000	2.99562200	-0.78086700
C	0.98985200	3.21929900	-1.41663700
C	2.63318000	3.92823800	0.23218900
C	0.16861800	4.35664600	-1.10872200
H	0.64702300	2.52427400	-2.17656700
C	1.87341100	5.09238200	0.52372100
C	3.84490200	3.70689700	0.92710800
C	-1.05613200	4.54557500	-1.78351900

C	0.59150500	5.29696900	-0.13885600
C	2.39574600	6.02183200	1.45108300
H	4.41110500	2.80330500	0.72421600
C	4.31582000	4.61808800	1.84832600
C	-1.86674400	5.62099300	-1.49071200
H	-1.35294700	3.81920500	-2.53633800
C	-0.25849300	6.38768000	0.14657100
C	3.59298700	5.79592800	2.09808800
H	1.84945700	6.93252800	1.66914800
H	5.24813700	4.42890500	2.37101600
C	-1.46329700	6.54388200	-0.51003900
H	-2.81619000	5.74559800	-2.00375900
H	0.02247900	7.11510700	0.89985900
H	3.97052200	6.52585300	2.80727900
H	-2.10129400	7.38756800	-0.26541600
C	-0.61266300	-3.86390300	-0.64899400
C	-0.78061400	-4.00726600	-1.99099300
C	-1.77491400	-3.81796700	0.22102200
C	-2.07513600	-4.14882100	-2.59140600
H	0.08954100	-4.03549900	-2.64216400
C	-3.07592800	-3.93367500	-0.34044400
C	-1.64387900	-3.63898400	1.61688900
C	-2.19737300	-4.32858300	-3.98693300
C	-3.23291800	-4.11769100	-1.77798600
C	-4.19203600	-3.85912800	0.52290100
H	-0.65579600	-3.49561600	2.04011500
C	-2.75097700	-3.60898400	2.43764300
C	-3.43621700	-4.47544100	-4.57170800
H	-1.29324800	-4.35058200	-4.58959700
C	-4.49028800	-4.26500100	-2.40364200
C	-4.03809100	-3.71071700	1.88512500
H	-5.19476000	-3.92156600	0.11570300
H	-2.63090200	-3.48757000	3.51119400
C	-4.59066600	-4.44115100	-3.76863200
H	-3.52335900	-4.61674200	-5.64456000
H	-5.39957000	-4.24337100	-1.81383500
H	-4.91199800	-3.66454800	2.52729500
H	-5.56961100	-4.55382600	-4.22454200
C	-5.04294500	-0.85037500	-3.87493100
C	-5.79205700	-0.47859600	-2.76881100
C	-5.17013500	-0.25734100	-1.53138500
C	-3.76923600	-0.44013100	-1.43381700
C	-3.02070700	-0.82475200	-2.56301100
C	-3.65366300	-1.02098500	-3.77792500

H	-6.99300500	0.33740400	-0.48306700
H	-5.53714900	-1.01184000	-4.82840700
H	-6.86658300	-0.34308900	-2.85212000
C	-5.93009500	0.15209700	-0.36190700
C	-3.09984200	-0.16222600	-0.18693000
H	-1.94241500	-0.93128500	-2.46598300
H	-3.07933200	-1.31261700	-4.65066900
C	-3.92373100	-0.02346600	1.00570000
C	-5.34087000	0.26316000	0.84405500
H	-2.09588900	-0.56305900	-0.07614100
N	-3.50854600	-0.19916300	2.23572200
N	-2.27269600	-0.54894100	2.49626400
C	-1.96610200	-0.88506000	3.81348300
O	-2.71275600	-0.80410500	4.75613100
O	-0.70659500	-1.32209900	3.84355900
C	-0.22783600	-1.73528500	5.12813700
H	-0.33075100	-0.92898600	5.85689700
H	0.82182500	-1.98341400	4.98000600
H	-0.78145700	-2.61242400	5.47132100
C	-5.61982400	4.13238000	-1.50205300
C	-5.11002400	3.28922100	-2.49213100
C	-4.00806300	2.46630600	-2.24539900
C	-3.44797900	2.52251400	-0.97893300
C	-3.91941600	3.39838000	0.01483500
C	-5.02202500	4.20438100	-0.24234900
H	-6.48103500	4.75457000	-1.72359700
H	-3.60771900	1.81492300	-3.01594600
H	-5.39977500	4.88676200	0.51278500
C	-2.02692900	2.34777800	0.79241100
C	-0.92617200	2.06999300	1.59437700
C	-0.80676000	2.73950200	2.81359900
C	-1.79593700	3.67653900	3.17517300
C	-2.88211700	3.96380100	2.35983500
C	-2.99915900	3.29048800	1.14389900
H	-0.19296000	1.33353900	1.29180700
H	-1.70477400	4.19883800	4.12312000
H	-3.61752700	4.70458500	2.65846300
N	-2.37152400	1.74754700	-0.45770000
H	-1.58420900	1.45750700	-1.06610500
H	-5.57615400	3.26632400	-3.47206000
C	0.35343400	2.46047700	3.77361000
C	1.29267600	1.37984300	3.22990000
C	-0.21601100	2.00378000	5.12727000
C	1.17265500	3.74241400	3.97799200

H	1.75902900	1.69802600	2.29082900
H	0.77273600	0.43383700	3.04550100
H	2.09035500	1.19578500	3.95746300
H	-0.78095800	2.80308200	5.61686600
H	0.60001000	1.71261400	5.79807000
H	-0.88939700	1.14901200	5.00979300
H	1.97657500	3.56359500	4.70139600
H	0.55684300	4.56668800	4.35277100
H	1.62577200	4.05445800	3.03356000
H	-5.89994500	0.51707400	1.73873200
Br	3.19249200	-5.87206300	2.56401900
Br	6.43771800	1.62244000	-3.64638000

(S)-C8**TSI**Value of imaginary frequency = -315.3 cm⁻¹

H	-0.29327900	1.69608200	1.84644700
C	-3.25257300	2.09090100	-4.12080400
C	-4.07896500	2.46139100	-3.06909200
C	-3.67353500	2.26410400	-1.74134800
C	-2.39946700	1.69424400	-1.49766000
C	-1.57471700	1.31587400	-2.57362900
C	-2.00027600	1.50998500	-3.87668100
H	-5.51157000	3.03534100	-0.84249400
H	-3.58160200	2.25099600	-5.14342500
H	-5.04550600	2.91769200	-3.26362200
C	-4.51080400	2.67396900	-0.62583900
C	-1.94893800	1.50783400	-0.13722400
H	-0.61111300	0.86118900	-2.35918400
H	-1.36333500	1.22261500	-4.70658500
C	-2.68233400	2.20187700	0.91092700
C	-4.03725000	2.65448900	0.63453600
H	-0.88264200	1.35709800	-0.00108100
N	-2.21799300	2.47077300	2.10631300
N	-0.99165300	2.16908900	2.45268000
C	-0.63171100	2.40601100	3.78265300
O	-1.28664600	3.02022100	4.58586000
O	0.54150900	1.82093000	4.00419900
C	1.06873400	2.01281100	5.31897500
H	1.18641800	3.07806900	5.53105600
H	2.03618600	1.51361000	5.32451100
H	0.40445300	1.56427600	6.06129100
C	-6.40459600	-0.98140000	-0.35491800
C	-5.60875100	-0.95982200	-1.51573600
C	-4.22453800	-0.79195000	-1.38226800
C	-3.69723200	-0.68878400	-0.10209800
C	-4.48365800	-0.77470700	1.05484400
C	-5.86243400	-0.90367900	0.92401600
H	-7.48027800	-1.09211100	-0.45553300
H	-3.56480800	-0.77014100	-2.24285400
H	-6.50174700	-0.96191500	1.79963400
C	-2.27063800	-0.70765200	1.67202300
C	-1.14231100	-0.84945400	2.47093300
C	-1.34634900	-1.01476200	3.83829900
C	-2.63665400	-1.04569100	4.38304800
C	-3.76010400	-0.94555700	3.56813300
C	-3.57102800	-0.78821600	2.19561400

H	-0.13815500	-0.80962900	2.06467500
H	-0.48536300	-1.13142200	4.48894400
H	-2.76051900	-1.17518900	5.45371500
H	-4.76019200	-1.00524800	3.98587700
N	-2.33986100	-0.46919100	0.26589900
H	-1.55284800	-0.82864200	-0.30952900
C	-6.27867700	-1.13001800	-2.88317900
C	-5.25448300	-1.18823900	-4.01962200
C	-7.22180100	0.05757500	-3.13281900
C	-7.08957200	-2.43659600	-2.90051800
H	-4.55480300	-2.02164400	-3.89098400
H	-4.67576600	-0.26178000	-4.08895000
H	-5.77410100	-1.33106900	-4.97217100
H	-8.00108000	0.12203600	-2.36714300
H	-7.71268900	-0.04922300	-4.10632500
H	-6.66357200	0.99991900	-3.13180200
H	-7.56066600	-2.56868100	-3.88039600
H	-7.88184700	-2.43697100	-2.14645300
H	-6.44274300	-3.30042100	-2.71381100
H	-4.62055000	3.01000900	1.47789200
C	6.22117100	-3.07773400	-3.69178600
C	5.67989200	-2.17730100	-2.80867400
C	4.61798600	-2.55369700	-1.94040400
C	4.10114300	-3.87827400	-2.04139000
C	4.69145600	-4.79043500	-2.95725000
C	5.73192100	-4.40420600	-3.76189600
H	7.02870200	-2.76822600	-4.34789600
H	6.05577700	-1.16018700	-2.77476400
C	4.02278400	-1.64240000	-1.00778200
C	2.98071600	-4.26294300	-1.25869800
H	4.29028200	-5.79881700	-3.01297100
H	6.17260000	-5.10640700	-4.46235400
C	2.36711700	-3.37732300	-0.40842500
C	2.91299500	-2.06806200	-0.30016300
H	2.58982200	-5.27208900	-1.36368500
C	4.48968300	-0.23705200	-0.81490500
C	5.82155800	0.10563900	-0.41014200
C	3.56333900	0.78081500	-0.93734500
C	6.15170700	1.47925100	-0.21822200
C	6.82541300	-0.86912400	-0.15470500
C	3.85578800	2.14996200	-0.67802200
C	7.47385700	1.83332900	0.16417500
C	5.14959900	2.47591900	-0.35435800
C	8.09104200	-0.49577100	0.22324100

H	6.58035800	-1.92127000	-0.25131500
C	8.42718000	0.87083500	0.37325800
H	7.70755600	2.88636500	0.29673100
H	5.41353500	3.51213100	-0.15674100
H	8.84134900	-1.25693900	0.41328000
H	9.43388300	1.15064100	0.66683000
O	2.28054300	0.45833900	-1.31935100
O	2.28625900	-1.19006400	0.55649000
P	1.28161900	-0.09471200	-0.14335700
O	1.02238500	0.94208500	0.90337900
O	0.14784800	-0.75686100	-0.86048400
C	2.73449000	3.13421100	-0.70455600
C	2.07115300	3.36657800	-1.86682000
C	2.26582800	3.74690000	0.52771000
C	0.90490100	4.19891200	-1.92959400
H	2.40448300	2.88651600	-2.78381900
C	1.09784000	4.55582500	0.50943200
C	2.91918400	3.51717600	1.75970400
C	0.23632000	4.39442000	-3.15869000
C	0.39684500	4.78943300	-0.74747700
C	0.63052800	5.09380600	1.73064100
H	3.79251400	2.87547400	1.78204300
C	2.45393500	4.07271600	2.93068300
C	-0.90995900	5.15501000	-3.22576600
H	0.64101800	3.92297300	-4.05068100
C	-0.77786500	5.56945400	-0.84547400
C	1.29469800	4.86677800	2.91746700
H	-0.27073100	5.69572100	1.74705500
H	2.97219800	3.88015400	3.86552400
C	-1.41789600	5.74722800	-2.05515200
H	-1.42211200	5.29312500	-4.17292900
H	-1.19908500	6.03756000	0.03685300
H	0.91137000	5.29168800	3.84070000
H	-2.32201700	6.34642100	-2.09995800
C	1.15230200	-3.72104400	0.39079400
C	1.26170000	-3.89277400	1.73404200
C	-0.15068500	-3.80241900	-0.24472300
C	0.12132300	-4.15611200	2.56500800
H	2.23477800	-3.81171700	2.21261100
C	-1.30599900	-4.03012800	0.54885900
C	-0.29937500	-3.61735000	-1.63777100
C	0.27804300	-4.32817200	3.95826000
C	-1.17018500	-4.21351600	1.98798400
C	-2.56713000	-4.05824000	-0.08916100

H	0.58076300	-3.41181700	-2.23676500
C	-1.53964500	-3.66121200	-2.23544900
C	-0.81414200	-4.55003700	4.76835800
H	1.27908500	-4.27721400	4.37847800
C	-2.27329500	-4.43551600	2.84193600
C	-2.68462600	-3.88401600	-1.45179400
H	-3.46702700	-4.22055000	0.49367300
H	-1.63290600	-3.51297800	-3.30709200
C	-2.10012100	-4.60280900	4.20058000
H	-0.68553700	-4.68108100	5.83831500
H	-3.27800600	-4.47584000	2.43655200
H	-3.66610300	-3.91454800	-1.91578600
H	-2.96486200	-4.77158700	4.83515400

(S)-C8**TSII**Value of imaginary frequency = -238.4 cm⁻¹

H	1.29508600	-0.36695100	2.03434900
C	5.37989200	-1.16397600	-3.11989500
C	5.90810400	-0.32647700	-2.14926200
C	5.12068000	0.08328600	-1.06282800
C	3.78022100	-0.37198000	-0.98988600
C	3.25230900	-1.21589800	-1.98830900
C	4.05107100	-1.61414400	-3.04368100
H	6.65532800	1.31786700	-0.11705000
H	6.00228700	-1.47596700	-3.95320400
H	6.93590700	0.01755700	-2.21871400
C	5.64834600	0.92769200	-0.00533100
C	2.95527500	0.06419700	0.09346000
H	2.21250500	-1.52599700	-1.91694700
H	3.65547300	-2.27227300	-3.80956800
C	3.60198800	0.60406300	1.26753000
C	4.93688100	1.16150000	1.11726300
H	1.98753500	-0.41543300	0.20161300
N	3.11522000	0.55928800	2.48570800
N	1.96139100	-0.00542000	2.74556800
C	1.62701100	-0.16768800	4.09365600
O	2.31531700	0.15922900	5.02698800
O	0.42952500	-0.74484400	4.16400900
C	-0.06648300	-0.94299400	5.49199000
H	0.60333900	-1.59485700	6.05812100
H	-1.04217700	-1.41034200	5.37228700
H	-0.16204300	0.01556300	6.00712500
C	4.71559300	4.15611400	-2.88961800
C	4.36180900	2.91994500	-3.43658300
C	3.45427700	2.07636600	-2.79368500
C	2.92620400	2.50959800	-1.58391300
C	3.24670500	3.76812100	-1.03826400
C	4.15311300	4.59647400	-1.69048800
H	5.42400100	4.78957300	-3.41386800
H	3.16593400	1.12560500	-3.22986200
H	4.40677700	5.57075000	-1.28355000
C	1.64824300	2.75664100	0.27092600
C	0.68287000	2.59743900	1.25250700
C	0.46164500	3.65050600	2.15586000
C	1.24236600	4.81194400	2.04309300
C	2.21442500	4.96351700	1.05474300
C	2.41782600	3.92757900	0.15226000

H	0.10808200	1.67569800	1.30612400
H	1.09041600	5.62816900	2.73941000
H	2.78909800	5.88249600	0.98794400
N	2.02426600	1.82973400	-0.73435800
H	1.27138900	1.22820700	-1.15399800
H	5.34520800	1.71889300	1.95398000
C	-6.31602900	-3.44077400	-2.91995600
C	-5.24605800	-3.21253900	-2.09039900
C	-4.77013600	-1.89264900	-1.85795600
C	-5.41625500	-0.81817900	-2.53106400
C	-6.52944900	-1.08352000	-3.37194900
C	-6.97524100	-2.36610300	-3.56218100
H	-6.65651600	-4.45755700	-3.08975000
H	-4.74476600	-4.04933200	-1.61637500
C	-3.65269400	-1.61397000	-0.99869400
C	-4.93570600	0.50527400	-2.35585900
H	-7.01287500	-0.24648300	-3.86837500
H	-7.82297000	-2.56293900	-4.21073600
C	-3.81398500	0.76859100	-1.61142100
C	-3.15098100	-0.32351600	-0.97277900
H	-5.46380300	1.32456200	-2.83668100
C	-3.02853000	-2.68606800	-0.16716500
C	-3.76152000	-3.46766600	0.78845800
C	-1.67601700	-2.91251200	-0.28091500
C	-3.07642900	-4.48760600	1.51203200
C	-5.13458500	-3.24216800	1.07792400
C	-0.96789000	-3.91610800	0.43628800
C	-3.79228400	-5.27435800	2.45367900
C	-1.68575200	-4.69691500	1.30713100
C	-5.79531600	-4.01089100	2.00382400
H	-5.65921000	-2.44228300	0.56715200
C	-5.12326700	-5.04800800	2.69285900
H	-3.25697500	-6.05566000	2.98648500
H	-1.18683200	-5.48403500	1.86739500
H	-6.84257000	-3.81736500	2.21407800
H	-5.66082300	-5.65151800	3.41729000
O	-0.95382700	-2.09754600	-1.12399900
O	-2.05063500	-0.01101900	-0.21042000
P	-0.55866400	-0.65487300	-0.46831200
O	0.03425000	-0.80262200	0.90007300
O	0.20851600	0.04601300	-1.54597700
C	0.49187700	-4.09401700	0.17862300
C	0.88999500	-4.46436600	-1.06792300
C	1.48727100	-3.85495900	1.20911900

C	2.27069800	-4.63721200	-1.41434500
H	0.14641200	-4.63273200	-1.84316900
C	2.86753300	-4.00525500	0.89983700
C	1.11760900	-3.45502500	2.51343100
C	2.63421700	-5.03197100	-2.72142200
C	3.27288300	-4.40268700	-0.44274900
C	3.81826500	-3.75446900	1.91461900
H	0.06939100	-3.29375500	2.73989300
C	2.06844400	-3.24770500	3.48986600
C	3.95825500	-5.19216200	-3.06611900
H	1.84672900	-5.20713800	-3.44953800
C	4.62321500	-4.56324600	-0.82634400
C	3.43147300	-3.39148100	3.18689200
H	4.87614800	-3.85319200	1.70072900
H	1.76366200	-2.95985500	4.49159000
C	4.95924600	-4.95053200	-2.10712900
H	4.23027200	-5.49742900	-4.07177100
H	5.41859200	-4.38513800	-0.11194200
H	4.18129400	-3.21334000	3.95130800
H	6.00470900	-5.06785800	-2.37533900
C	-3.38246300	2.17609800	-1.35536800
C	-4.16789700	2.95430400	-0.56443200
C	-2.16681500	2.72680000	-1.92518300
C	-3.80097300	4.29735500	-0.21027900
H	-5.08579500	2.54829500	-0.14634900
C	-1.75051500	4.03762200	-1.56876200
C	-1.40456000	1.99172800	-2.85473800
C	-4.62461700	5.05718100	0.64892300
C	-2.57659300	4.83620000	-0.67223000
C	-0.54993000	4.53474000	-2.12046500
H	-1.72893000	0.99384300	-3.13032000
C	-0.25020600	2.51225900	-3.40036600
C	-4.24515500	6.31773800	1.05700300
H	-5.55906800	4.62232000	0.99402500
C	-2.20861800	6.12767900	-0.23508800
C	0.18702600	3.78994500	-3.01945700
H	-0.19572800	5.52267900	-1.84883000
H	0.32831700	1.92483700	-4.10681300
C	-3.02218500	6.85185100	0.61336000
H	-4.88099000	6.89414000	1.72163700
H	-1.26968000	6.56508300	-0.55525000
H	1.10599500	4.19677400	-3.43222700
H	-2.71402400	7.84058500	0.93899100
C	-0.64190100	3.51554600	3.21141700

C	-2.00488300	3.51693400	2.50322800
C	-0.47778800	2.19426000	3.97253400
C	-0.62269000	4.66584700	4.22250700
H	-2.17306600	4.47356000	2.00079200
H	-2.07022100	2.71963400	1.75447500
H	-2.80910300	3.36624100	3.23304100
H	0.49359200	2.15074700	4.47951900
H	-1.26281300	2.10372800	4.73177200
H	-0.56564200	1.33268500	3.30527000
H	-1.40184600	4.49954100	4.97303600
H	0.33849400	4.73182900	4.74347700
H	-0.82594800	5.62971500	3.74443100
H	4.79630700	2.60560600	-4.38039100

(R)-C10**TSI**Value of imaginary frequency = -307.5 cm⁻¹

H	-0.55592300	1.46338500	1.90445300
C	-3.76393400	1.86967700	-3.96153400
C	-4.56663500	2.15328900	-2.86588900
C	-4.07869300	1.98178400	-1.56183400
C	-2.74798400	1.53037700	-1.38876000
C	-1.94359300	1.24925100	-2.50889400
C	-2.45043300	1.41040300	-3.78733900
H	-5.92711100	2.59021400	-0.56844700
H	-4.15945900	2.00311500	-4.96427300
H	-5.58059800	2.51713000	-3.00660000
C	-4.89494900	2.29713600	-0.40193600
C	-2.22870000	1.33402700	-0.05438700
H	-0.93045900	0.88861000	-2.34910900
H	-1.83152600	1.19045300	-4.65095100
C	-2.98401900	1.89823200	1.05545800
C	-4.37323600	2.26852800	0.83981600
H	-1.14810500	1.28678300	0.04076300
N	-2.51369600	2.09914100	2.26242300
N	-1.26699400	1.83624200	2.56353200
C	-0.90488800	1.93959300	3.90863800
O	-1.58813400	2.40857400	4.78312700
O	0.30719200	1.40955100	4.05400800
C	0.83227200	1.47234000	5.38266200
H	0.85019900	2.50532100	5.73752400
H	1.84275500	1.07247100	5.31859200
H	0.22394500	0.86659600	6.05832900
C	-6.32622400	-1.81542500	-0.53801300
C	-5.51592200	-1.59101200	-1.66611600
C	-4.18689500	-1.18886900	-1.47469500
C	-3.71563500	-1.06969100	-0.17363600
C	-4.50644200	-1.36220100	0.94607300
C	-5.83763300	-1.71844400	0.76149800
H	-7.36298400	-2.10625200	-0.68097800
H	-3.52180200	-1.00700500	-2.31189700
H	-6.47545400	-1.94852500	1.60960100
C	-2.33796400	-1.04392400	1.63584800
C	-1.21404300	-1.14164400	2.44752500
C	-1.41556900	-1.50274400	3.77801500
C	-2.69922400	-1.75908400	4.27667900
C	-3.81367900	-1.69365300	3.44582300
C	-3.62376600	-1.34950100	2.10853500

H	-0.21884500	-0.91832700	2.07941400
H	-0.55462000	-1.58910900	4.43398400
H	-2.82311700	-2.03141700	5.32014100
H	-4.80480100	-1.92911500	3.82130900
N	-2.40830600	-0.69267000	0.25034800
H	-1.57121300	-0.93116200	-0.33045400
C	-6.10573600	-1.80652400	-3.06395300
C	-5.05043800	-1.65258800	-4.16226700
C	-7.22082700	-0.77542200	-3.30143700
C	-6.69211300	-3.22484700	-3.16382200
H	-4.23417700	-2.37248900	-4.03781200
H	-4.62318400	-0.64546500	-4.17382700
H	-5.51218500	-1.83274900	-5.13808300
H	-8.02312600	-0.87702500	-2.56407900
H	-7.65598600	-0.91253000	-4.29731800
H	-6.82400400	0.24326000	-3.23593200
H	-7.10695200	-3.38522800	-4.16475900
H	-7.49526500	-3.38890700	-2.44023100
H	-5.91747700	-3.97948400	-2.99059100
H	-4.95023900	2.54685700	1.71577800
C	7.00875100	-1.66142300	-3.57709000
C	5.68199700	-0.90002900	-3.36485500
C	4.75718800	-1.57662900	-2.38226700
C	4.54216700	-2.94929100	-2.60051600
C	5.36661100	-3.60857200	-3.67658800
C	6.83660900	-3.19460500	-3.52278700
H	7.41776100	-1.35919200	-4.54582900
H	5.86599000	0.14224300	-3.09704600
C	4.04070200	-0.90446900	-1.37795800
C	3.60597500	-3.65124800	-1.84384300
H	5.25899400	-4.69584000	-3.62351100
H	7.44504100	-3.67433100	-4.29498000
C	2.83807000	-2.99836100	-0.88123100
C	3.07390600	-1.63908300	-0.67225600
H	3.44782200	-4.71164400	-2.02551600
C	4.19742200	0.54744100	-1.04024600
C	5.40799400	1.11222300	-0.58474900
C	3.04554000	1.34335200	-1.05142800
C	5.43359200	2.46840500	-0.21580400
C	6.64934100	0.25549900	-0.42898700
C	3.03498800	2.67484700	-0.62602900
C	6.69140000	3.14233600	0.30292900
C	4.25714200	3.22149000	-0.24360700
C	7.66614000	0.86046900	0.53635600

H	6.35712400	-0.75113100	-0.11162000
C	7.95336800	2.30235200	0.13015600
H	6.80311200	4.11606200	-0.18654800
H	4.29043200	4.25965700	0.08171900
H	7.27019500	0.84069100	1.55989100
H	8.27549900	2.32000600	-0.91901000
O	1.85771300	0.75855900	-1.45053600
O	2.29877800	-0.99650900	0.27479900
P	1.06872400	-0.06905400	-0.27936500
O	0.70032500	0.81420300	0.87214600
O	0.00551700	-0.84722700	-0.99620200
C	1.74480500	3.42027400	-0.54011700
C	1.01200000	3.63399700	-1.66516600
C	1.23007400	3.86881800	0.74519800
C	-0.28118200	4.25557100	-1.63340300
H	1.39149400	3.29842900	-2.62733600
C	-0.04268100	4.49832300	0.81419100
C	1.95443100	3.67251700	1.94276000
C	-1.01771100	4.43376900	-2.82568600
C	-0.84061800	4.65244200	-0.39589400
C	-0.50474400	4.96027000	2.06749100
H	2.89927700	3.14229600	1.90785600
C	1.47788700	4.13025100	3.15217300
C	-2.29015900	4.96033600	-2.79750100
H	-0.56628900	4.12668000	-3.76579200
C	-2.15768800	5.16570900	-0.39093900
C	0.24234900	4.79577600	3.21444800
H	-1.46368900	5.46093500	2.13838000
H	2.05770300	3.97009100	4.05651400
C	-2.86816100	5.31377500	-1.56449400
H	-2.85265400	5.08288400	-3.71800600
H	-2.63354100	5.43979700	0.54416700
H	-0.13483800	5.16256900	4.16412300
H	-3.88245900	5.70025900	-1.53294800
C	1.72115700	-3.62807800	-0.11609100
C	0.50297400	-3.73927900	-0.70303300
C	1.87820900	-3.95984800	1.28654400
C	-0.67000600	-4.10186000	0.04147000
H	0.37594100	-3.44965200	-1.74186200
C	0.74829100	-4.35192800	2.05098800
C	3.14280200	-3.88672800	1.91149800
C	-1.93866300	-4.08295400	-0.57992000
C	-0.56586300	-4.39770400	1.42144200
C	0.93522100	-4.65867000	3.41681600

H	4.00279600	-3.58607200	1.32066100
C	3.29666200	-4.19445200	3.24624900
C	-3.08204100	-4.35205600	0.14099000
H	-1.99688400	-3.83272300	-1.63679000
C	-1.75160500	-4.68064000	2.13510900
C	2.18065100	-4.58405200	4.00546200
H	0.08804500	-4.96115500	4.02238600
H	4.27672700	-4.13404900	3.70914900
C	-2.98230400	-4.65604900	1.51098100
H	-4.05625900	-4.30964500	-0.33907600
H	-1.70976600	-4.90019700	3.19620100
H	2.29667700	-4.82668500	5.05721800
H	-3.88119100	-4.85974100	2.08549300
H	7.73743000	-1.35296300	-2.82153100
H	7.19134700	-3.57285700	-2.55825300
H	5.00495100	-3.29653200	-4.66660400
H	5.14956600	-0.87695900	-4.32559000
H	7.13728900	0.13982000	-1.40418800
H	8.57962300	0.25815000	0.52846100
H	8.76609200	2.73008900	0.72501900
H	6.54682000	3.35311700	1.37093900

(R)-C10**TSII**Value of imaginary frequency = -270.5 cm⁻¹

H	1.41017600	-1.15751600	1.63493600
C	2.46345700	-2.71592200	-4.78232600
C	3.61659700	-2.75598500	-4.01401300
C	3.59764800	-2.32016400	-2.67995200
C	2.37742600	-1.84473100	-2.14033400
C	1.21173100	-1.80962300	-2.93137800
C	1.25503100	-2.24520700	-4.24312300
H	5.71861300	-2.68181100	-2.30303100
H	2.49493700	-3.05320800	-5.81400300
H	4.54783700	-3.12190600	-4.43707800
C	4.78682400	-2.36075200	-1.84717500
C	2.35965100	-1.33253100	-0.79937300
H	0.29346300	-1.42113800	-2.49691200
H	0.35947400	-2.22331200	-4.85529500
C	3.46693900	-1.66407600	0.07444200
C	4.72635500	-2.06224800	-0.53360200
H	1.38852000	-1.16175300	-0.34771800
N	3.41435800	-1.70669800	1.38429300
N	2.31289400	-1.46310700	2.04944400
C	2.36733500	-1.63835000	3.43920800
O	3.35148800	-1.94421600	4.06362000
O	1.16125700	-1.39543400	3.93871900
C	1.07205400	-1.46710100	5.36386600
H	1.33624000	-2.46719300	5.71308500
H	0.03503400	-1.23892300	5.60454500
H	1.73999700	-0.73420100	5.82215800
C	5.77668400	1.35845800	-3.79151300
C	4.59003200	0.84765000	-4.32101500
C	3.47182400	0.62706900	-3.51365700
C	3.58994400	0.92535800	-2.16329300
C	4.76452200	1.48678000	-1.62587300
C	5.87056500	1.69624400	-2.44047400
H	6.62948900	1.51575400	-4.44418000
H	2.54679200	0.24457900	-3.93110700
H	6.78204700	2.12692200	-2.03750000
C	3.15268500	1.40158200	0.01265800
C	2.49331600	1.68152000	1.19707400
C	3.17549900	2.41185200	2.18345200
C	4.51159900	2.77695900	1.95634700
C	5.16993900	2.48233100	0.76316100
C	4.47521300	1.80664000	-0.23138700

H	1.46651500	1.35364800	1.34015600
H	5.05378700	3.32578800	2.71747400
H	6.19417100	2.80677500	0.60588900
N	2.63331800	0.73458000	-1.13216900
H	1.61137900	0.85732500	-1.32027100
H	5.58814600	-2.15047000	0.11987400
C	-6.59960700	-0.04556700	-3.57756000
C	-5.96880300	-0.36747800	-2.22480500
C	-4.99674800	0.70029100	-1.75762600
C	-5.00602200	1.97621400	-2.34206900
C	-6.00780600	2.36681500	-3.41325800
C	-7.15651000	1.37385300	-3.55836300
H	-5.84680500	-0.12992900	-4.37194000
H	-6.77409200	-0.47943800	-1.48961700
C	-4.03255200	0.40027400	-0.76948500
C	-4.03735300	2.91510700	-1.97394100
H	-6.38629200	3.37193800	-3.19693000
H	-7.72207400	1.59235700	-4.46923800
C	-3.03245300	2.61747200	-1.06104600
C	-3.05210700	1.35105500	-0.47279700
H	-4.04895000	3.89802100	-2.44058000
C	-3.96549600	-0.92964900	-0.08811800
C	-5.01972900	-1.46796000	0.66572400
C	-2.76562400	-1.65715100	-0.16852900
C	-4.88753100	-2.75024500	1.22845000
C	-6.26966300	-0.70951500	1.04666300
C	-2.60060800	-2.91384700	0.41914500
C	-6.07678700	-3.30621900	1.96929500
C	-3.70257500	-3.46163400	1.08340600
C	-7.57112100	-1.53739300	0.92918100
H	-6.14117800	-0.43743000	2.10305800
C	-7.34660300	-3.04463700	1.14992600
H	-5.93904500	-4.37540000	2.15486400
H	-3.61525000	-4.45259300	1.52327700
H	-8.27954100	-1.15216000	1.66884100
H	-7.23090800	-3.54719700	0.18325300
O	-1.71543900	-1.09833200	-0.87054700
O	-2.05502600	1.02701000	0.43165200
P	-0.84340600	0.08102400	-0.13119100
O	-0.12512000	-0.44103900	1.07653000
O	-0.07349800	0.72829900	-1.24362400
C	-1.28630100	-3.61449400	0.34769700
C	-0.77314700	-3.97514500	-0.85957900
C	-0.53743500	-3.91019400	1.55959300

C	0.51992700	-4.58292200	-0.99415000
H	-1.34183900	-3.78209200	-1.76643500
C	0.76609300	-4.46741500	1.45966500
C	-1.07879200	-3.67335400	2.84519300
C	1.00001900	-4.97940500	-2.26264500
C	1.33487700	-4.75210600	0.14877900
C	1.46345700	-4.78035700	2.64865600
H	-2.05628100	-3.21382800	2.93245200
C	-0.39282400	-4.02599100	3.98586000
C	2.27700600	-5.47266400	-2.41018900
H	0.34487000	-4.87127400	-3.12274800
C	2.65745900	-5.21785900	-0.03497300
C	0.89264700	-4.58374700	3.88772100
H	2.45580500	-5.21356100	2.59220700
H	-0.83968900	-3.85565600	4.96087400
C	3.12049300	-5.56495500	-1.28690400
H	2.63984900	-5.77018700	-3.38914900
H	3.32911500	-5.29808800	0.81285400
H	1.44147400	-4.85722400	4.78406300
H	4.14134900	-5.91581100	-1.40397000
C	-1.92803500	3.57160000	-0.74946900
C	-0.85163000	3.62809600	-1.57435500
C	-1.97369400	4.40052200	0.43776300
C	0.27873400	4.46589000	-1.29209100
H	-0.80470700	2.97952800	-2.44363600
C	-0.89278800	5.27353600	0.73017100
C	-3.07869200	4.34990800	1.31705000
C	1.41025300	4.44087200	-2.13730500
C	0.27075700	5.29822000	-0.14725200
C	-0.97279800	6.07393900	1.89154700
H	-3.89945500	3.67637700	1.08993300
C	-3.12615000	5.13774900	2.44673900
C	2.51531400	5.21524200	-1.85993000
H	1.39630700	3.78657300	-3.00540100
C	1.41079800	6.09422300	0.10497400
C	-2.06313200	6.01026100	2.73400900
H	-0.16314600	6.75190100	2.13805600
H	-3.98228400	5.08502600	3.11194400
C	2.50876600	6.05298000	-0.72988300
H	3.38677100	5.17972700	-2.50635600
H	1.43961500	6.74597300	0.97133800
H	-2.09613400	6.63475300	3.62132100
H	3.37612100	6.66627900	-0.50622000
H	-7.38470900	-0.77613700	-3.79509100

H	-7.84983100	1.47588000	-2.71326400
H	-5.47629300	2.44063000	-4.37152700
H	-5.45220500	-1.33252000	-2.25746300
H	-6.35295400	0.23279100	0.50219200
H	-8.03105200	-1.38036300	-0.05098600
H	-8.21723900	-3.49035800	1.63976100
H	-6.17181800	-2.81726400	2.94940200
H	4.52924800	0.61594600	-5.37969500
C	2.42397700	2.81389300	3.45574800
C	1.24193900	3.71943200	3.07097900
C	1.88751200	1.55214000	4.14270200
C	3.31514500	3.56820700	4.44617000
H	1.59670300	4.63113500	2.57764500
H	0.55097200	3.21379400	2.38819700
H	0.68100200	4.00774800	3.96721500
H	2.71253400	0.87733500	4.40195400
H	1.36017500	1.81878300	5.06581800
H	1.18582800	1.01224400	3.50091800
H	2.73151300	3.82050900	5.33705200
H	4.16913300	2.96173300	4.76607000
H	3.69501500	4.50321000	4.02153600

(S)-C6-50°C

TSI

Value of imaginary frequency = -325.8 cm⁻¹

C	4.76696100	0.81221700	-1.30553000
C	5.92095400	1.38840300	-0.76666100
C	5.86235300	2.61510300	-0.11739600
C	4.62853500	3.24653800	0.02354300
C	3.44497200	2.66160300	-0.44495000
C	3.53901100	1.43518700	-1.12235200
C	6.42641400	-0.86562400	-1.30914100
C	7.10588000	0.47379600	-0.97189300
H	6.75950900	3.07045800	0.29187800
H	4.56693000	4.20434600	0.53268500
H	6.15527600	-1.38287600	-0.38218800
H	7.72955700	0.82325300	-1.80406700
C	5.11955400	-0.46306200	-2.05190800
C	4.16238400	-1.63713300	-2.17562400
C	5.43162100	-0.19800200	-3.55216100
C	4.41830300	-2.33838700	-3.36016200
C	3.16394100	-2.08642700	-1.32216200
C	5.43694000	-1.59671900	-4.19513800
H	6.36855800	0.34978300	-3.68852900
C	3.74185700	-3.51574400	-3.64941000
C	2.47534100	-3.28178900	-1.58295300
H	5.17260100	-1.57941800	-5.25600200
C	2.78873200	-3.98884700	-2.74723300
H	3.93994400	-4.05684300	-4.57022400
H	2.25299200	-4.91082400	-2.95412900
H	7.74630800	0.41662100	-0.08752000
H	7.05097800	-1.53598000	-1.90664300
H	4.61837900	0.39945200	-3.97831300
H	6.42475100	-2.06674100	-4.11294600
O	2.80406500	-1.32225800	-0.22604900
O	2.39927200	0.79794700	-1.57827500
P	1.65118700	-0.18284500	-0.49322900
O	1.47113400	0.51974800	0.81663300
O	0.47328500	-0.74762000	-1.22821000
H	0.26932300	1.20244700	1.96113500
C	1.38437200	-3.74155800	-0.67807700
C	0.10923400	-3.76615800	-1.14454900
C	1.65508400	-4.13927200	0.69112700
C	-1.00405000	-4.11014600	-0.30866900
H	-0.09419100	-3.44516500	-2.16261100
C	0.58367300	-4.52690000	1.53876100

C	2.97427000	-4.15958700	1.19729800
C	-2.32187900	-4.01841600	-0.80832800
C	-0.78513600	-4.48337900	1.03934500
C	0.88299300	-4.92313800	2.86113400
H	3.79188700	-3.86817600	0.54562700
C	3.23600900	-4.54727300	2.49258300
C	-3.40436800	-4.27615400	0.00337400
H	-2.46796700	-3.71883900	-1.84365300
C	-1.91164600	-4.74956300	1.84783300
C	2.17872900	-4.93412800	3.33251300
H	0.08348400	-5.23109800	3.52564000
H	4.25679000	-4.55631100	2.86152000
C	-3.19233600	-4.64318700	1.34361200
H	-4.41499300	-4.17512600	-0.38165100
H	-1.78452600	-5.01369300	2.89162900
H	2.38027100	-5.24490300	4.35306600
H	-4.04220300	-4.83272100	1.99281400
C	2.13017500	3.33813200	-0.25172800
C	1.37961800	3.65824600	-1.34017300
C	1.65691900	3.70686600	1.07379300
C	0.12910600	4.35227000	-1.23537900
H	1.73365900	3.39351400	-2.33369900
C	0.42599700	4.40337000	1.21584900
C	2.39063800	3.38041600	2.23750800
C	-0.60304600	4.67998200	-2.39817900
C	-0.37659600	4.70480900	0.03760700
C	0.01386400	4.79338200	2.51003900
H	3.29225900	2.78623100	2.14289400
C	1.97401700	3.79259700	3.48511100
C	-1.82098900	5.31468000	-2.30891600
H	-0.19020500	4.40626500	-3.36564600
C	-1.63689900	5.34228200	0.10236100
C	0.77829100	4.51552300	3.62269600
H	-0.91929400	5.32873800	2.64114600
H	2.56319200	3.53992100	4.36183900
C	-2.34491000	5.63676800	-1.04353700
H	-2.38084200	5.55620300	-3.20711900
H	-2.07003000	5.60073400	1.06207500
H	0.44110200	4.83261900	4.60439300
H	-3.31474700	6.11915000	-0.96572500
C	-3.26318100	2.36799100	-3.64401200
C	-3.95866600	2.62708200	-2.47283700
C	-3.39759800	2.31546600	-1.22507600
C	-2.10204500	1.74827200	-1.18486700

C	-1.40457100	1.49464900	-2.38013100
C	-1.98427400	1.79588300	-3.60121900
H	-5.12651800	2.96886900	-0.06008700
H	-3.71513900	2.60930600	-4.60195400
H	-4.94619400	3.07913000	-2.50890100
C	-4.11271600	2.58631200	0.01022000
C	-1.51969900	1.38695500	0.09366900
H	-0.41726500	1.04389200	-2.32332400
H	-1.44631300	1.59552000	-4.52207700
C	-2.15729200	1.90995600	1.29683700
C	-3.52146100	2.40439100	1.20584200
H	-0.44184500	1.25157700	0.11227100
N	-1.61119900	1.94718700	2.48674300
N	-0.37825300	1.55594500	2.69084000
C	0.03460500	1.44773200	4.02025400
O	-0.59392900	1.81032100	4.98212700
O	1.22643800	0.85235900	4.04066100
C	1.76977100	0.65486300	5.34692200
H	1.11255600	0.01458700	5.94009700
H	2.73485600	0.17467500	5.19472200
H	1.89557100	1.61260300	5.85752600
C	-5.91927000	-1.27432300	-0.29293100
C	-5.18079600	-1.05306500	-1.46929900
C	-3.80667400	-0.79722300	-1.36510600
C	-3.22730200	-0.82120200	-0.10428100
C	-3.95396600	-1.10503200	1.05857000
C	-5.32473700	-1.31285100	0.96472800
H	-6.98782000	-1.45503200	-0.36586500
H	-3.19373800	-0.61619000	-2.24171200
H	-5.91581800	-1.53650600	1.84769900
C	-1.71559000	-1.08262100	1.57845900
C	-0.55093500	-1.36930400	2.27838100
C	-0.69045100	-1.79714500	3.59720900
C	-1.95138200	-1.92673100	4.19260800
C	-3.11221400	-1.67582600	3.46768000
C	-2.98764200	-1.26917300	2.14077500
H	0.43194200	-1.24431700	1.83714300
H	0.20327400	-2.03933100	4.16420700
H	-2.02349700	-2.25031900	5.22633400
H	-4.09138100	-1.81642300	3.91486900
N	-1.85532800	-0.61102500	0.23178100
H	-1.09722900	-0.87423900	-0.43510000
C	-5.89774300	-1.11376100	-2.82200900
C	-4.92383600	-0.97662500	-3.99478900

C	-6.62254900	-2.46311500	-2.96005900
C	-6.92447000	0.02741200	-2.89733900
H	-4.40502300	-0.01351100	-3.97800600
H	-4.17167400	-1.77317400	-3.98733500
H	-5.47564600	-1.04491900	-4.93749900
H	-7.38097200	-2.60422300	-2.18489300
H	-7.12543200	-2.51854900	-3.93158900
H	-5.91193300	-3.29427000	-2.89740900
H	-7.44969100	0.00205200	-3.85843900
H	-7.67173100	-0.05196300	-2.10179600
H	-6.42777000	0.99857600	-2.80141700
H	-4.01997100	2.64184500	2.14019100

(S)-C6-50°C

TSH

Value of imaginary frequency = -279.8 cm⁻¹

C	-0.03554300	4.60433200	-0.04284400
C	-0.20483100	5.51785700	1.00157000
C	-1.35922800	5.49891100	1.77441100
C	-2.34404000	4.55044300	1.49900400
C	-2.17258000	3.58710300	0.49778800
C	-0.98829600	3.62094300	-0.25405600
C	2.05644200	5.64381100	0.27357500
C	1.01459200	6.40398100	1.11733900
H	-1.49712700	6.21059800	2.58323800
H	-3.25985600	4.53661500	2.08338300
H	2.54385000	4.88045500	0.88986800
H	0.81427000	7.39883000	0.70075000
C	1.21871200	4.93260400	-0.82798000
C	2.03200400	3.89305200	-1.58413000
C	0.91036200	5.93660100	-1.97645000
C	2.66185900	4.49755600	-2.67713600
C	2.26803200	2.54542700	-1.31657800
C	2.17292100	5.91576600	-2.85341300
H	0.65583500	6.93086900	-1.59867500
C	3.58989600	3.80282800	-3.44208400
C	3.21731200	1.83007600	-2.06082700
H	1.96895000	6.15805000	-3.90003400
C	3.87837400	2.48323400	-3.10851600
H	4.07956700	4.27708100	-4.28767500
H	4.61333800	1.92476800	-3.68165400
H	1.33058300	6.54559600	2.15460200
H	2.83165200	6.29005200	-0.14848200
H	0.05659300	5.55883700	-2.54970200
H	2.92091000	6.63251100	-2.49310700
O	1.58311200	1.92579400	-0.28883500
O	-0.71788700	2.62061300	-1.17253200
P	0.07250900	1.32818400	-0.54119200
O	-0.43517000	1.03055000	0.83847500
O	0.04123000	0.27274000	-1.60549400
H	-0.88198900	-0.14611200	2.04548600
C	3.55954800	0.40164500	-1.78408900
C	2.81451200	-0.59219400	-2.33033400
C	4.76659400	0.07382800	-1.04546800
C	3.15445300	-1.97626800	-2.16471400
H	1.92396500	-0.34272100	-2.89696600
C	5.16603200	-1.28317700	-0.90927200

C	5.57386400	1.08751700	-0.48090400
C	2.33439500	-2.97621600	-2.72733400
C	4.31345100	-2.33982900	-1.43838300
C	6.39403200	-1.56132200	-0.26937700
H	5.25240600	2.12090200	-0.56588700
C	6.75673300	0.78380100	0.15917700
C	2.62659400	-4.31113700	-2.55297600
H	1.45815900	-2.67201600	-3.29489200
C	4.58481500	-3.71415900	-1.26321400
C	7.17918900	-0.55259000	0.24881700
H	6.73556600	-2.58657700	-0.18148100
H	7.36384900	1.57704300	0.58409700
C	3.75683200	-4.67883200	-1.80210400
H	1.97423500	-5.07216800	-2.97196800
H	5.44639600	-4.02867200	-0.68478600
H	8.11898700	-0.79422300	0.73553100
H	3.98154100	-5.72919700	-1.64291600
C	-3.23772000	2.59253300	0.18252600
C	-3.78557800	2.60513100	-1.06275200
C	-3.73102400	1.64715900	1.16976900
C	-4.86147200	1.73608000	-1.44057600
H	-3.41570400	3.30964500	-1.80376900
C	-4.78734900	0.75864900	0.82792200
C	-3.16720700	1.57699600	2.46384000
C	-5.41514300	1.80956700	-2.73726900
C	-5.37638700	0.80766000	-0.50449800
C	-5.23331200	-0.16347600	1.80040800
H	-2.32628300	2.21762000	2.70625400
C	-3.64663400	0.68668500	3.40127300
C	-6.45192200	0.98202200	-3.10910400
H	-5.00605900	2.53396000	-3.43664000
C	-6.43535600	-0.03225200	-0.91274900
C	-4.68371800	-0.19706200	3.06448500
H	-6.02497600	-0.86322200	1.55854700
H	-3.21027300	0.65282500	4.39612600
C	-6.96197800	0.05193300	-2.18565600
H	-6.87444400	1.04704500	-4.10703700
H	-6.84987600	-0.76149300	-0.22596700
H	-5.04867400	-0.91253500	3.79467200
H	-7.77712500	-0.60462300	-2.47430400
C	-4.58193200	-2.50560600	-2.93872900
C	-4.50956600	-3.36834300	-1.85568700
C	-3.64735700	-3.09263100	-0.78402400
C	-2.86964000	-1.90966500	-0.82857700

C	-2.95608800	-1.03878000	-1.93267700
C	-3.80334200	-1.33881300	-2.98359200
H	-4.10456500	-4.90876000	0.34198200
H	-5.25130100	-2.73438900	-3.76282200
H	-5.11290900	-4.27115900	-1.83144800
C	-3.53889700	-3.98221900	0.35961000
C	-1.94224400	-1.62970100	0.23414200
H	-2.33044300	-0.14900400	-1.94984200
H	-3.87427200	-0.66920300	-3.83361200
C	-2.06250500	-2.39227400	1.46357800
C	-2.78812800	-3.65194500	1.42886200
H	-1.54774400	-0.61839100	0.28347300
N	-1.61584900	-2.01071800	2.63644000
N	-1.04372700	-0.84477200	2.79865300
C	-0.74679400	-0.45319100	4.10378500
O	-0.83442800	-1.14409700	5.08719100
O	-0.36205400	0.82362800	4.07225200
C	0.05069100	1.37043200	5.32863700
H	0.92171800	0.83243700	5.70993300
H	0.30664400	2.40805800	5.12214500
H	-0.76228800	1.31329200	6.05576900
C	-0.67685900	-6.28243800	-1.73922800
C	-1.24768600	-5.29356500	-2.54348200
C	-1.10342200	-3.93806800	-2.23728000
C	-0.37806700	-3.61804200	-1.09928100
C	0.24234900	-4.60000600	-0.30536200
C	0.08511400	-5.94421500	-0.61946700
H	-0.81057700	-7.32726600	-2.00093400
H	-1.53570300	-3.16994900	-2.87082800
H	0.56041800	-6.71328800	-0.01820300
C	0.83772000	-2.52444500	0.48159500
C	1.50223000	-1.54837200	1.21463700
C	2.39821800	-1.95352300	2.20456300
C	2.60142800	-3.33300400	2.41514800
C	1.93684600	-4.30244800	1.67691100
C	1.03585200	-3.89292400	0.69475500
H	1.30473700	-0.49859000	1.03863500
H	3.30459300	-3.65375800	3.17836600
H	2.12242800	-5.35717900	1.85553300
N	-0.13125500	-2.33221200	-0.54607500
H	-0.00192500	-1.50173000	-1.15536700
H	-1.81682900	-5.57706800	-3.42305400
C	3.15259900	-0.93673600	3.06641100
C	2.75443700	0.50327400	2.72831100

C	2.84986800	-1.20722600	4.54944000
C	4.66110400	-1.08003200	2.81812400
H	3.00743800	0.75641600	1.69283300
H	1.68277600	0.68128200	2.86339800
H	3.29765100	1.19293700	3.38349300
H	3.21889300	-2.18724400	4.86787200
H	3.33850500	-0.45130700	5.17447300
H	1.77333900	-1.18162300	4.74974600
H	5.21853400	-0.39104200	3.46337600
H	5.01512200	-2.09577600	3.02321100
H	4.89554000	-0.83871000	1.77830100
H	-2.73725200	-4.27765500	2.31380700

TSI_H-1Value of imaginary frequency = -303.1 cm⁻¹

C	-4.98926700	-0.65514400	0.98905200
C	-6.13355400	0.03674300	1.40723900
C	-6.14255100	0.76614900	2.58990900
C	-4.97613900	0.82823900	3.35489500
C	-3.81448400	0.19469400	2.92257200
C	-3.82477100	-0.53830500	1.73722500
C	-6.46086500	-0.60551300	-0.85575900
C	-7.23366000	-0.11363400	0.38093400
H	-7.03583800	1.29935900	2.90259800
H	-4.96056700	1.40195600	4.27629000
H	-6.04043800	0.25299800	-1.39095100
H	-7.97264000	-0.85508700	0.70851100
C	-5.29113000	-1.44784800	-0.27033700
C	-4.22575800	-1.74900500	-1.30764300
C	-5.79138800	-2.88746700	0.04001400
C	-4.52044800	-2.94840000	-1.96861800
C	-3.08875700	-1.04070200	-1.67368700
C	-5.70557200	-3.62101200	-1.31163400
H	-6.79416400	-2.89087000	0.47688300
C	-3.74359600	-3.39148200	-3.03245200
C	-2.29655900	-1.47333800	-2.73545000
H	-5.56307300	-4.69954800	-1.20211800
C	-2.63735600	-2.63386500	-3.42424700
H	-3.97946900	-4.32313400	-3.53877400
H	-2.01482600	-2.96741800	-4.24867400
H	-7.76816400	0.82363500	0.20406800
H	-7.07414100	-1.18082600	-1.55520200
H	-5.10278200	-3.35158300	0.75449400
H	-6.61707100	-3.46976400	-1.90275200
O	-2.69932300	0.07623600	-0.95076100
O	-2.64868100	-1.12305400	1.29278800
P	-1.69996900	-0.20792400	0.32158300
O	-1.43267900	1.14050900	0.92095600
O	-0.56074800	-1.09847500	-0.07861100
H	-0.18094600	2.45298100	0.83599500
C	3.55553400	-2.33029000	3.50105700
C	4.27997900	-1.19649800	3.16266800
C	3.68424300	-0.16773300	2.41905300
C	2.32613700	-0.30594100	2.03920500
C	1.60858500	-1.47206500	2.37035200
C	2.21963100	-2.47754100	3.09736500
H	5.47448400	1.08021300	2.30564600

H	4.03171900	-3.11691600	4.07875700
H	5.31371800	-1.09085400	3.47910600
C	4.41535700	1.03885300	2.07018500
C	1.68342100	0.75255600	1.30740000
H	0.57947400	-1.56639300	2.03274500
H	1.66811100	-3.37400100	3.35937400
C	2.35740000	2.03781600	1.24208000
C	3.78561200	2.09133300	1.51306200
H	0.59813100	0.72512100	1.27192300
N	1.77627400	3.17551500	0.95030800
N	0.47812300	3.25306100	0.78247800
C	-0.03206400	4.47039000	0.32098100
O	0.60360300	5.48022400	0.16271100
O	-1.33041900	4.30670300	0.08026100
C	-2.00078000	5.47209000	-0.41461300
H	-1.55117900	5.79710100	-1.35518900
H	-3.03505300	5.17106700	-0.56988300
H	-1.94350100	6.28058400	0.31697700
C	5.77950000	-0.57702000	-1.47927900
C	5.11063900	-1.58869400	-0.76558400
C	3.75363600	-1.41781800	-0.46163000
C	3.12031600	-0.26716000	-0.91364100
C	3.77351600	0.70871600	-1.68116100
C	5.12981800	0.55980000	-1.94970900
H	6.83634700	-0.69797600	-1.69790400
H	3.19474000	-2.16580600	0.09010300
H	5.66793700	1.30259100	-2.53063800
C	1.54266900	1.24400400	-1.54531100
C	0.33595800	1.86747600	-1.84448800
C	0.38124700	2.97457200	-2.68769800
C	1.59468300	3.44405700	-3.20844800
C	2.79274700	2.79758600	-2.92357800
C	2.76136300	1.67766600	-2.09289200
H	-0.60784900	1.53578800	-1.42498200
H	-0.54432400	3.48248600	-2.94035600
H	1.59593300	4.31640500	-3.85387900
H	3.72913900	3.14697000	-3.34701600
N	1.77830300	0.13623500	-0.68395300
H	0.99951500	-0.54660300	-0.56559300
C	5.88519500	-2.84619800	-0.35754600
C	4.98763300	-3.87705000	0.33170000
C	6.49254600	-3.50150500	-1.60972100
C	7.01292900	-2.45146000	0.60866900
H	4.55521100	-3.48215300	1.25639600

H	4.16971800	-4.20054500	-0.32085800
H	5.58036200	-4.76022800	0.58956300
H	7.19525900	-2.83633700	-2.11957800
H	7.03621500	-4.40936700	-1.32724400
H	5.70883800	-3.78036900	-2.32173400
H	7.58295400	-3.33891400	0.90453100
H	7.70726600	-1.74158100	0.14874900
H	6.60207800	-1.99002000	1.51294700
H	-2.88435300	0.27702000	3.47500400
H	-1.40718300	-0.90495600	-2.98788700
H	4.29744600	3.02270700	1.29328100

TSII_H-1Value of imaginary frequency = -250.7 cm⁻¹

C	4.50974600	-0.71051200	-1.05162600
C	5.54938200	0.10421100	-1.51899800
C	5.52963000	0.63050300	-2.80486600
C	4.43642400	0.35884000	-3.63005400
C	3.36899900	-0.40074200	-3.15958900
C	3.40771700	-0.92590100	-1.86925300
C	5.79166500	-0.10411400	0.83394800
C	6.57006800	0.31889400	-0.42454600
H	6.34156800	1.26139500	-3.15519700
H	4.39800000	0.76768000	-4.63496800
H	5.18746800	0.73710700	1.19153900
H	7.44894300	-0.31869600	-0.58048700
C	4.83578100	-1.22711200	0.33748400
C	3.75580700	-1.54346900	1.35468400
C	5.59605700	-2.58395500	0.30782100
C	4.19757300	-2.54278200	2.23051500
C	2.49154500	-0.99938400	1.53849200
C	5.52572500	-3.09214800	1.76007200
H	6.61706900	-2.47811900	-0.06978900
C	3.43071400	-2.93040200	3.32292000
C	1.70885000	-1.37599700	2.62870300
H	5.57297600	-4.18217700	1.83213500
C	2.18926500	-2.32429200	3.52809900
H	3.78277100	-3.70574200	3.99733800
H	1.57537800	-2.61659600	4.37429500
H	6.92159800	1.35325600	-0.38065500
H	6.43358100	-0.43910000	1.65366300
H	5.05588000	-3.27428800	-0.34941400
H	6.34943500	-2.68959500	2.36219500
O	1.97735400	-0.10768200	0.60949400
O	2.31613300	-1.63855400	-1.39465900
P	1.14802300	-0.77145000	-0.64568100
O	0.71334500	0.39607300	-1.48087400
O	0.14149400	-1.77156400	-0.15866700
H	-0.60199100	1.51396800	-1.68990100
C	-4.44553400	-3.80498800	-2.72814400
C	-5.17416800	-2.66864100	-2.41351400
C	-4.52064700	-1.50046700	-1.99305100
C	-3.10594900	-1.51339300	-1.90039000
C	-2.37808900	-2.68089600	-2.20819100
C	-3.04411800	-3.81668100	-2.62727800
H	-6.33622700	-0.32611300	-1.68284900

H	-4.96598900	-4.70076800	-3.05327000
H	-6.25760600	-2.67157600	-2.48866100
C	-5.25133400	-0.28826000	-1.66905300
C	-2.42492900	-0.34083300	-1.44067700
H	-1.29759300	-2.66838900	-2.08871900
H	-2.49013800	-4.71640100	-2.87248900
C	-3.14784900	0.91227600	-1.44258800
C	-4.60156900	0.86580300	-1.41442500
H	-1.34232100	-0.32886000	-1.53234700
N	-2.60771700	2.10371800	-1.54797500
N	-1.31978800	2.26909200	-1.71715900
C	-0.88392000	3.57103100	-1.99413400
O	-1.57625100	4.55653400	-1.97737700
O	0.41214900	3.52145500	-2.28611400
C	1.02199400	4.79150600	-2.54591400
H	0.91825600	5.44729900	-1.67854700
H	2.07156100	4.57674100	-2.73758500
H	0.56174500	5.26018300	-3.41821200
C	-5.91909700	-2.02010700	2.14865400
C	-5.20225000	-2.91996800	1.35678400
C	-3.95177800	-2.58747100	0.83199300
C	-3.45581800	-1.32402600	1.12240100
C	-4.14816900	-0.42132400	1.95361700
C	-5.39346900	-0.76641000	2.46497100
H	-6.89006800	-2.30832800	2.53851600
H	-3.39105800	-3.29264900	0.22739300
H	-5.94021500	-0.08074500	3.10504000
C	-2.12048700	0.49419800	1.37020700
C	-1.03826700	1.35825300	1.36783800
C	-1.09236400	2.50629500	2.17321900
C	-2.26334100	2.76675900	2.90182200
C	-3.35795500	1.90268500	2.88171100
C	-3.28136200	0.74154600	2.12264000
H	-0.16000800	1.14905100	0.76451300
H	-2.32525700	3.65809200	3.51511700
H	-4.24237100	2.12586500	3.47063500
N	-2.26133100	-0.72353700	0.65562300
H	-1.40132200	-1.28759000	0.49099200
H	2.48784900	-0.57768100	-3.76720900
H	0.72259600	-0.93531600	2.74030800
H	-5.62112700	-3.89818700	1.14265300
C	0.14899500	3.39919700	2.25973700
C	1.29906900	2.57904700	2.87019400
C	0.55733300	3.85568400	0.85115700

C	-0.08702000	4.63803600	3.12715800
H	1.02850900	2.20410700	3.86320600
H	1.55635000	1.72427500	2.23607500
H	2.19227100	3.20564300	2.97179000
H	-0.24736100	4.43649200	0.38545100
H	1.44885900	4.49031700	0.90788700
H	0.79846700	3.00498600	0.20555900
H	0.82231000	5.24678000	3.14300500
H	-0.89931700	5.25853600	2.73409000
H	-0.32606400	4.36976200	4.16133900
H	-5.12682500	1.79918300	-1.24035200

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H	-1.35131500	-2.42282900	0.90342200
C	1.29646900	5.39481200	-2.14936800
C	0.54088200	4.04546500	-2.13200400
C	1.32048600	2.92230500	-1.49170600
C	2.65171900	2.78040900	-1.91799800
C	3.20147000	3.85207900	-2.82316200
C	2.82456300	5.22800300	-2.25797900
H	0.92047200	5.97569100	-2.99686400
H	-0.44957900	4.15771100	-1.68737600
C	0.76726400	1.97258700	-0.61760200
C	3.41893800	1.70382500	-1.48622600
H	4.28585700	3.74734400	-2.91849000
H	3.25079500	6.02212300	-2.87761200
C	2.87904200	0.71080500	-0.66474100
C	1.55336000	0.86760700	-0.26621800
H	4.45395500	1.61520700	-1.80683000
C	-0.62652900	2.05199600	-0.08680800
C	-1.07446300	3.12317800	0.71337200
C	-1.48913300	0.98102000	-0.32532800
C	-2.40135700	3.12249400	1.17395600
C	-0.11815900	4.22853500	1.11719000
C	-2.80485100	0.94927900	0.13407800
C	-2.95071800	4.23316900	2.04973100
C	-3.24182100	2.05004900	0.86706900
C	-0.60169300	5.01469100	2.33391100
H	0.87234300	3.79860900	1.29992900
C	-2.04428800	5.45906200	2.11582300
H	-3.94994900	4.50582100	1.69341300
H	-4.26532700	2.05835000	1.23657400
H	-0.54556700	4.38777800	3.23317900
H	-2.10791400	6.02358100	1.17661100
O	-1.00083700	-0.11678300	-1.03543600
O	0.97806600	-0.13403900	0.52127300
P	-0.03883300	-1.12916800	-0.23007600
O	-0.83809900	-1.61098800	1.05495100
O	0.50692300	-2.16005300	-1.12074900
C	-3.69075100	-0.21679700	-0.14374200
C	-4.07345900	-0.48277100	-1.42010700
C	-4.14481900	-1.07094900	0.93956500
C	-4.93959600	-1.57987900	-1.74366900
H	-3.72548200	0.15060100	-2.23258600
C	-5.00585800	-2.16594000	0.65872600
C	-3.71979800	-0.85411500	2.27116400

C	-5.31873600	-1.81436700	-3.08406300
C	-5.41903000	-2.42594800	-0.71501000
C	-5.42644200	-2.98276300	1.73261400
H	-3.03880100	-0.03638600	2.48028900
C	-4.14249100	-1.67131900	3.29665700
C	-6.15096800	-2.86268300	-3.40739700
H	-4.93717500	-1.15034600	-3.85492300
C	-6.27064900	-3.49447500	-1.07500000
C	-5.00961000	-2.74236600	3.02435800
H	-6.08778000	-3.82117000	1.54632200
H	-3.80200700	-1.48962000	4.31112100
C	-6.62869300	-3.70829400	-2.38999100
H	-6.43617700	-3.03869000	-4.43976800
H	-6.65557000	-4.16647800	-0.31664700
H	-5.34700700	-3.38744600	3.82954300
H	-7.28234900	-4.53805400	-2.64002600
C	3.67184200	-0.49228600	-0.28888200
C	4.12924500	-1.30723700	-1.27611100
C	3.97751900	-0.79649600	1.09797900
C	4.88739400	-2.49286900	-0.99711100
H	3.89705500	-1.08109900	-2.31392700
C	4.72510100	-1.96193500	1.41305600
C	3.56434700	0.05875900	2.14441100
C	5.32381600	-3.32267700	-2.05330500
C	5.18267600	-2.83995800	0.34269600
C	5.01245100	-2.22970400	2.77026100
H	3.00882200	0.95931800	1.90300600
C	3.86079400	-0.22666700	3.45901000
C	6.03719200	-4.47249200	-1.79670900
H	5.08048300	-3.03716300	-3.07319300
C	5.91297900	-4.02593500	0.57793400
C	4.58918200	-1.38562100	3.77432200
H	5.58249700	-3.11186800	3.03753700
H	3.53383800	0.44345300	4.24778000
C	6.33129500	-4.82418500	-0.46704000
H	6.36785000	-5.10643600	-2.61335300
H	6.15340600	-4.32819500	1.59082800
H	4.82483100	-1.61582200	4.80861300
H	6.88974100	-5.73144300	-0.25859100
H	1.05714900	5.96884400	-1.24945000
H	3.27940700	5.31840500	-1.26564600
H	2.77443500	3.74440900	-3.83003500
H	0.37413400	3.74106100	-3.17412500
H	0.00265400	4.93007200	0.28316200

H	0.05632900	5.87377100	2.49550600
H	-2.38049200	6.12428100	2.91674100
H	-3.08617300	3.83264200	3.06307000

TSI'_(R)-C10-1Value of imaginary frequency = -333.7 cm⁻¹

C	7.41575800	-2.27542800	-0.94656200
C	6.28820900	-1.24607300	-1.17264900
C	4.91345900	-1.84769000	-1.01602400
C	4.69376600	-3.04432200	-1.71963100
C	5.86689300	-3.62743900	-2.46368300
C	7.09613300	-3.66553500	-1.54357300
H	8.33402100	-1.87294400	-1.38474600
H	6.42596300	-0.37665400	-0.52683200
C	3.86557700	-1.25956800	-0.28856700
C	3.44427000	-3.65591500	-1.69156800
H	5.62499300	-4.62893400	-2.83085100
H	7.95893100	-4.05489900	-2.09150800
C	2.37350900	-3.07001900	-1.01493200
C	2.60183200	-1.87042600	-0.34098800
H	3.28966500	-4.59619800	-2.21553600
C	4.00712800	0.00015900	0.50435700
C	4.92549100	0.15670900	1.55465300
C	3.13302000	1.06386300	0.22055200
C	4.98310400	1.37242000	2.25769700
C	5.84487000	-0.92648400	2.06169000
C	3.19690900	2.28796200	0.88899800
C	6.00036800	1.47672900	3.36395300
C	4.14269200	2.42347200	1.90869300
C	7.29248000	-0.42522300	2.24411400
H	5.46526100	-1.24283000	3.04275100
C	7.36882800	0.99117100	2.86181400
H	6.06372300	2.50617600	3.72791200
H	4.21142600	3.36899400	2.44205600
H	7.82575200	-1.14632200	2.87092800
H	7.72123300	1.70281600	2.10845600
O	2.19021700	0.88354000	-0.77384100
O	1.55218400	-1.28208800	0.33372000
P	0.84983400	0.04418200	-0.35341800
O	0.12136300	0.68488300	0.79669100
O	0.12754900	-0.30920000	-1.61522600
H	-0.88814800	1.80482100	0.34808900
C	-2.74161700	-1.51556500	0.00195700
C	-4.12637200	-1.56936100	0.25497200
C	-4.59375700	-2.28371200	1.35870100
C	-3.65953400	-2.90188900	2.18786900
C	-2.28325800	-2.80826600	1.93344000
C	-1.79751800	-2.11559100	0.82762400

C	-3.72950500	-0.36506000	-1.65666100
C	-4.75412400	-0.71931300	-0.74014400
H	-5.65732700	-2.34658400	1.57172500
H	-4.00263400	-3.46366400	3.05148400
H	-1.58002400	-3.30273700	2.59674200
H	-0.73497800	-2.07012500	0.61044000
H	-1.60224000	-0.56160400	-1.52419200
N	-2.55339100	-0.77103100	-1.16138700
C	-3.84773600	0.32146800	-2.99747400
C	-2.46871900	0.72906100	-3.52402000
C	-4.75593600	1.55559100	-2.90790200
C	-4.47778100	-0.69160100	-3.97261900
H	-1.82562900	-0.14088400	-3.69353600
H	-1.94971800	1.39317500	-2.82697700
H	-2.58522600	1.25246600	-4.47742500
H	-4.89707000	1.96509400	-3.91313200
H	-4.30759200	2.32853700	-2.27827300
H	-5.74406100	1.29616800	-2.51235100
H	-4.59040100	-0.22515900	-4.95681900
H	-5.46491500	-1.01421200	-3.62759200
H	-3.84152800	-1.57450800	-4.07911700
C	-7.17192500	-0.21112600	3.75584800
C	-5.80098900	-0.08720900	3.90465400
C	-5.00440500	0.36574300	2.83966700
C	-5.62971200	0.70305400	1.61484200
C	-7.02408600	0.57117800	1.47973400
C	-7.78961600	0.11900100	2.53843900
H	-3.11672400	0.18278900	3.91788700
H	-7.77468500	-0.56682700	4.58556900
H	-5.32391500	-0.34508900	4.84590700
C	-3.56502700	0.50149900	2.98119800
C	-4.81387600	1.15493200	0.51432600
H	-7.48801400	0.82897500	0.53106900
H	-8.86467200	0.02008500	2.43136200
C	-3.42946000	1.47305500	0.76875900
C	-2.79855900	1.01377600	1.99616600
H	-5.29554100	1.68646600	-0.29877500
H	-1.72461400	1.11230600	2.11553900
N	-2.87017500	2.17468300	-0.19479800
N	-1.58433400	2.42104700	-0.17650100
C	-1.03267400	3.07930100	-1.28276100
O	0.10396400	2.87756900	-1.63231400
O	-1.88685400	3.92185400	-1.85840700
C	-1.38465900	4.53836600	-3.05200600

H	-0.39214300	4.95810900	-2.87773100
H	-2.09720600	5.32315400	-3.30102300
H	-1.33495600	3.80110500	-3.85779900
H	-5.80940800	-0.69513400	-0.98036000
H	6.09243500	-3.00749800	-3.34237100
H	6.88738400	-4.37439700	-0.73578500
H	7.60286200	-2.37667700	0.12703100
H	6.36288100	-0.87804900	-2.20486800
H	7.79728300	-0.42453100	1.27302300
H	8.09246700	1.01395600	3.68160400
H	5.68604000	0.85361600	4.21250900
H	5.82169700	-1.81181300	1.42333700
C	1.02674100	-3.71154000	-0.97166500
C	0.09971400	-3.43391500	-1.92375300
C	0.70385100	-4.62597400	0.10774300
C	-1.21771600	-4.00486600	-1.88794300
H	0.33218700	-2.72539600	-2.71330400
C	-0.58096700	-5.22818400	0.16428800
C	1.64864800	-4.91913000	1.11809200
C	-2.17331500	-3.64831500	-2.86544800
C	-1.57555700	-4.89420400	-0.84635100
C	-0.85947500	-6.11757700	1.22639200
H	2.62656000	-4.45037700	1.07434400
C	1.34550600	-5.78372000	2.14740000
C	-3.45836200	-4.14275500	-2.81010200
H	-1.87395800	-2.96726600	-3.65900200
C	-2.90113300	-5.38089800	-0.80858400
C	0.07998000	-6.39210200	2.19812400
H	-1.82897000	-6.59881900	1.28863200
H	2.08285500	-5.99521000	2.91527000
C	-3.82284200	-5.01325500	-1.76717500
H	-4.18864200	-3.86143800	-3.56259200
H	-3.21611300	-6.04377500	-0.01082500
H	-0.16108800	-7.07871200	3.00354100
H	-4.83704400	-5.39635300	-1.71258200
C	2.33250700	3.44138600	0.49454000
C	2.66708400	4.16992100	-0.60093100
C	1.16586800	3.80995300	1.27300400
C	1.90043100	5.30539000	-1.02724300
H	3.53816800	3.89305400	-1.18982600
C	0.37158000	4.91960500	0.87590200
C	0.78855100	3.06776800	2.41518400
C	2.28256300	6.03304200	-2.17586300
C	0.75159900	5.69590000	-0.29770400

C	-0.78618300	5.22263200	1.62844500
H	1.38820300	2.21105900	2.70132600
C	-0.33869800	3.39466300	3.13743900
C	1.55425700	7.12532500	-2.59628300
H	3.16519700	5.71322900	-2.72330800
C	0.02354300	6.82039900	-0.74866900
C	-1.13826600	4.47801700	2.73400500
H	-1.42070200	6.05151400	1.33652600
H	-0.61600900	2.80786600	4.00800600
C	0.41598400	7.52163900	-1.87122100
H	1.85645000	7.67846900	-3.48002100
H	-0.85876000	7.15165500	-0.21283900
H	-2.03494300	4.72953800	3.29205600
H	-0.15969200	8.38295500	-2.19559300

TSII_(R)-C10-1Value of imaginary frequency = -317.2 cm⁻¹

C	-7.78228300	-0.22957000	-0.27404700
C	-6.39847900	-0.77865100	-0.68095400
C	-5.31126000	0.26444100	-0.59570100
C	-5.60710000	1.48887800	-1.21828700
C	-6.98484100	1.65076300	-1.80553500
C	-8.03851600	1.20817100	-0.78086100
H	-8.54378800	-0.91347900	-0.66120200
H	-6.15362700	-1.67104200	-0.10264800
C	-4.04915100	0.05958300	-0.01522400
C	-4.64814900	2.49089900	-1.26853100
H	-7.14919100	2.68845300	-2.11024800
H	-9.03874300	1.28938900	-1.21608800
C	-3.36349100	2.29469000	-0.75346600
C	-3.08028400	1.07457200	-0.13606200
H	-4.88296900	3.43987500	-1.74599400
C	-3.66998300	-1.21651100	0.66406400
C	-4.36975400	-1.75479900	1.75682300
C	-2.53619100	-1.90110400	0.19438700
C	-3.95478600	-2.97309300	2.31981300
C	-5.53040900	-1.08526800	2.45036200
C	-2.14232300	-3.13699200	0.71062300
C	-4.74021800	-3.49205900	3.49584600
C	-2.87565500	-3.66056600	1.77793600
C	-6.70226500	-2.05701500	2.70095900
H	-5.16724500	-0.72654600	3.42305400
C	-6.24317000	-3.45368000	3.18243600
H	-4.42274300	-4.50791100	3.74828700
H	-2.58062400	-4.61963900	2.19864400
H	-7.37318000	-1.59951100	3.43446000
H	-6.44218200	-4.19551800	2.40247300
O	-1.78560200	-1.31279200	-0.80969000
O	-1.83790500	0.87765600	0.43059700
P	-0.75778500	-0.14709000	-0.28344700
O	0.09773400	-0.65674800	0.84273200
O	-0.11810900	0.49927700	-1.47325800
H	1.46630400	-1.45172800	0.26344400
C	3.25667700	0.94247200	-1.79799700
C	4.56890800	1.30498200	-1.45163600
C	5.62363300	0.88979400	-2.27270200
C	5.32344700	0.16533600	-3.41975100
C	3.99807700	-0.17265400	-3.74661300
C	2.93568000	0.20149300	-2.93227200

C	3.09079000	2.15862100	0.08433400
C	4.48580600	1.96771500	-0.16505400
H	6.65211800	1.13892200	-2.02678500
H	6.12673300	-0.14544100	-4.08020600
H	3.80281900	-0.73603700	-4.65379200
H	1.90389800	-0.06486700	-3.14526600
H	1.37720800	1.33446900	-0.90209300
N	2.40063400	1.46936900	-0.83195500
C	2.40499000	3.14521600	0.99635500
C	0.94250400	2.75024700	1.22933900
C	2.45801100	4.48202700	0.22319000
C	3.12675700	3.32707900	2.33325500
H	0.86417200	1.74505800	1.65756400
H	0.36060600	2.77402500	0.30056100
H	0.48108700	3.46244100	1.92069000
H	1.87974900	5.23417000	0.77090400
H	2.02821500	4.37183200	-0.77538800
H	3.48831500	4.83961800	0.12506300
H	2.77961800	4.25640200	2.79560100
H	4.21346800	3.39573400	2.21166600
H	2.90290500	2.50901500	3.01801100
C	6.39567100	1.68531600	4.72627900
C	5.12867200	1.13049600	4.65803700
C	4.64109900	0.61821100	3.44500400
C	5.46198300	0.67797500	2.29622600
C	6.74963600	1.23724000	2.38298700
C	7.21298600	1.73743600	3.58594900
H	2.67688900	0.08245900	4.22374900
H	6.76109100	2.08215000	5.66818000
H	4.49599500	1.09265900	5.54032800
C	3.30872700	0.05676600	3.33970800
C	4.96025000	0.15632800	1.04483900
H	7.37037600	1.27145800	1.49110300
H	8.20626200	2.16911100	3.65134400
C	3.73287500	-0.59362600	1.04356000
C	2.84841400	-0.49003600	2.19250600
H	5.68349200	-0.09534500	0.27641400
H	1.84834800	-0.90402200	2.14494400
N	3.50765300	-1.28580600	-0.05766800
N	2.31665300	-1.81223300	-0.23554500
C	2.01970200	-2.42738000	-1.45585800
O	0.89530400	-2.42111500	-1.89574800
O	3.07367500	-3.01178700	-2.01499600
C	2.81299200	-3.54526200	-3.31848200

H	1.95606000	-4.22137800	-3.29213800
H	3.71706900	-4.08055800	-3.60544100
H	2.61364900	-2.73136100	-4.02055100
H	5.25488900	2.58850200	0.27603400
H	-7.07578800	1.03118700	-2.70853300
H	-8.00145700	1.90757200	0.06076700
H	-7.87304300	-0.24971000	0.81642700
H	-6.45342900	-1.09872200	-1.73045800
H	-7.28010200	-2.16637000	1.77806900
H	-6.81182700	-3.76158700	4.06459700
H	-4.53891100	-2.86395600	4.37469500
H	-5.87366900	-0.20307600	1.90608500
C	-2.33731400	3.36431900	-0.91893600
C	-1.36653900	3.21732300	-1.85728500
C	-2.40518300	4.58268300	-0.13489500
C	-0.40441700	4.24835600	-2.12217600
H	-1.29855600	2.29445500	-2.42330700
C	-1.47932800	5.63253600	-0.37964600
C	-3.37182000	4.74099300	0.88467100
C	0.59766900	4.04769200	-3.09923000
C	-0.46898600	5.47469900	-1.41843700
C	-1.56385000	6.80069800	0.41041100
H	-4.07140900	3.93325900	1.07420900
C	-3.43109800	5.89333800	1.63827500
C	1.50056600	5.04527300	-3.39681000
H	0.63831700	3.08957900	-3.61152900
C	0.46095200	6.48495900	-1.75217100
C	-2.51737600	6.93283300	1.39783500
H	-0.86482900	7.61346500	0.24964200
H	-4.17863900	5.99542500	2.41866900
C	1.42151300	6.27741400	-2.72132500
H	2.26638000	4.88572800	-4.14933400
H	0.43256300	7.44335900	-1.24565500
H	-2.55677000	7.84059100	1.99174600
H	2.12430400	7.07010500	-2.95867600
C	-1.01567200	-3.91945000	0.12459200
C	-1.17707100	-4.50804600	-1.08849900
C	0.22462800	-4.10338100	0.85204400
C	-0.16567800	-5.34016200	-1.67415200
H	-2.10243400	-4.36246800	-1.64066700
C	1.25778800	-4.90544800	0.29802700
C	0.43724300	-3.47261500	2.09973000
C	-0.37989100	-5.94801500	-2.93127500
C	1.04979400	-5.56518200	-0.98444000

C	2.47584400	-5.01820300	1.00530300
H	-0.34796700	-2.84535200	2.50744100
C	1.62829400	-3.61951000	2.77749900
C	0.57379700	-6.77098600	-3.49090800
H	-1.31659500	-5.75615400	-3.44792000
C	2.00692600	-6.42116400	-1.57507000
C	2.66131300	-4.39167000	2.21925400
H	3.29134400	-5.59882800	0.58936100
H	1.77480900	-3.12502100	3.73315200
C	1.77446500	-7.01378700	-2.79968100
H	0.39877300	-7.23519900	-4.45651300
H	2.94160200	-6.62958700	-1.06679600
H	3.60833300	-4.49258500	2.74047100
H	2.52406700	-7.67021800	-3.23078600

