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Supporting information

Chiral Phosphoric Acid Catalyzed Asymmetric Arylation of Indole via Nucleophilic Aromatic Substitution: Mechanisms and Origin of Enantioselectivity

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1. QTAIM Analyses

QTAIM analyses were carried out on some optimized complexes, transition states and intermediates to figure out the intermolecular interactions.

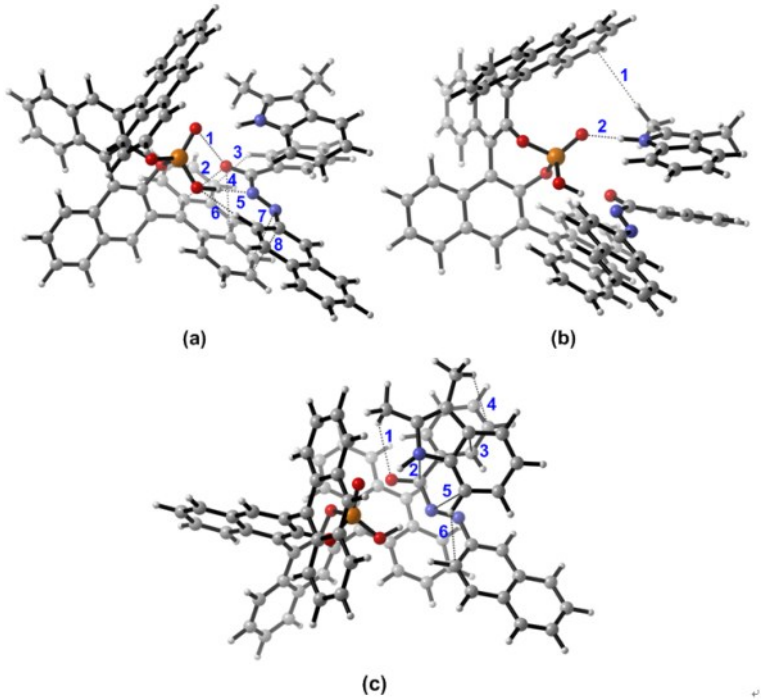

Figure S1 Intermolecular interactions in **COMI** and numbers of bond critical points (BCPs No.).

Table S1 Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.), the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **COMI**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
COMI(a)	1	lp…π	2.97	0.0113	0.0412	0.0094	-0.0085	0.0009
	2	π…π	3.05	0.0086	0.0300	0.0066	-0.0056	0.0010
	3	C-H…π	2.71	0.0074	0.0239	0.0048	-0.0037	0.0011
	4	π…π	3.38	0.0069	0.0232	0.0047	-0.0035	0.0012
	5	O-H…N	1.68	0.0546	0.1049	0.0338	-0.0413	-0.0075
	6	C-H…O	2.40	0.0099	0.0396	0.0086	-0.0073	0.0013
	7	π…π	3.19	0.0081	0.0234	0.0051	-0.0043	0.0008
	8	π…π	3.25	0.0075	0.0232	0.0048	-0.0038	0.0010
COMI(b)	1	C-H…π	3.14	0.0031	0.0091	0.0018	-0.0012	0.0006
	2	N-H…O	1.88	0.0283	0.0929	0.0230	-0.0229	0.0001
COMI(c)	1	C-H…O	2.72	0.0057	0.0211	0.0044	-0.0036	0.0008
	2	lp…π	2.99	0.0101	0.0326	0.0071	-0.0061	0.0010
	3	π…π	3.10	0.0095	0.0318	0.0065	-0.0051	0.0014
	4	C-H…π	2.97	0.0054	0.0158	0.0032	-0.0024	0.0008
	5	π…π	3.20	0.0076	0.0238	0.0052	-0.0044	0.0008
	6	C-H…π	2.83	0.0060	0.0199	0.0039	-0.0029	0.0010

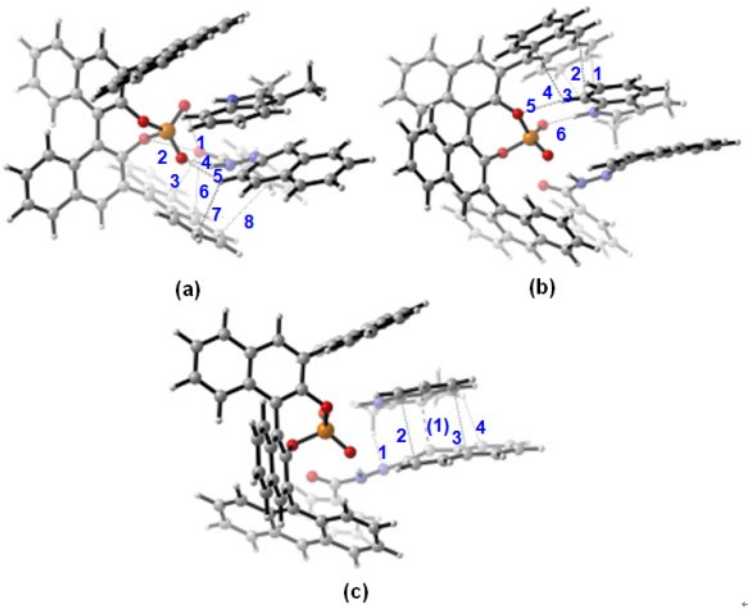

Figure S2 Intermolecular interactions in**TSI-1** and numbers of bond critical points (BCPs No.).

Table S2 Numbers of bond critical point (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **TSI-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSI-1(a)	1	lp…π	3.08	0.0093	0.0352	0.0078	-0.0068	0.0010
	2	lp…lp	2.96	0.0093	0.0342	0.0080	-0.0074	0.0006
	3	π…π	3.10	0.0082	0.0291	0.0064	-0.0055	0.0009
	4	N-H…O	1.63	0.0542	0.1515	0.0418	-0.0458	-0.0040
	5	C-H…O	2.29	0.0137	0.0481	0.0113	-0.0107	0.0006
	6	π…π	3.20	0.0083	0.0292	0.0060	-0.0048	0.0012
	7	C-H…π	2.96	0.0047	0.0144	0.0028	-0.0020	0.0008
	8	π…π	3.59	0.0041	0.0127	0.0025	-0.0019	0.0006
TSI-1(b)	1	π…π	3.47	0.0055	0.0161	0.0036	-0.0031	0.0005
	2	π…π	3.34	0.0070	0.0205	0.0043	-0.0034	0.0009
	3	C-H…π	3.14	0.0034	0.0109	0.0021	-0.0015	0.0006
	4	C-H…π	2.93	0.0060	0.0196	0.0039	-0.0029	0.0010
	5	C-H…O	2.35	0.0122	0.0377	0.0093	-0.0092	0.0001
	6	N-H…O	1.65	0.0506	0.1484	0.0395	-0.0420	-0.0025
TSI-1(c)	(1)	C…C	2.32	0.0476	0.0433	0.0185	-0.0262	-0.0077
	1	C-H…N	2.56	0.0103	0.0317	0.0070	-0.0060	0.0010
	2	π…π	3.15	0.0092	0.0282	0.0059	-0.0048	0.0011
	3	π…π	3.08	0.0100	0.0303	0.0063	-0.0051	0.0012
	4	C-H…π	2.53	0.0109	0.0368	0.0076	-0.0059	0.0017

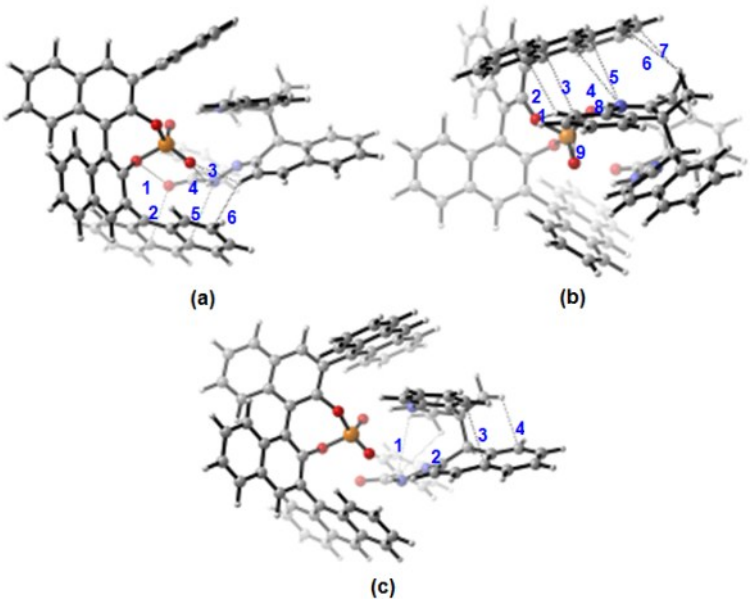

Figure S3 Intermolecular interactions in **IMI-1** and numbers of bond critical points (BCPs No.).

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 **IMI-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMI-1(a)	1	lp…lp	2.97	0.0088	0.0318	0.0075	-0.0071	0.0004
	2	lp…π	2.98	0.0099	0.0364	0.0079	-0.0067	0.0012
	3	C-H…O	2.47	0.0097	0.0357	0.0079	-0.0069	0.0010
	4	N-H…O	1.98	0.0255	0.0769	0.0202	-0.0212	-0.0010
	5	lp…π	3.53	0.0044	0.0145	0.0029	-0.0022	0.0007
	6	C-H…π	2.90	0.0054	0.0166	0.0033	-0.0025	0.0008
IMI-1(b)	1	C-H…O	2.28	0.0142	0.0431	0.0109	-0.0110	-0.0001
	2	C-H…π	2.71	0.0083	0.0283	0.0057	-0.0042	0.0015
	3	π…π	3.26	0.0073	0.0228	0.0047	-0.0037	0.0010
	4	π…π	3.33	0.0061	0.0198	0.0043	-0.0036	0.0007
	5	π…π	3.33	0.0061	0.0196	0.0043	-0.0036	0.0007
	6	C-H…π	3.42	0.0020	0.0063	0.0012	-0.0008	0.0004
	7	C-H…π	2.93	0.0054	0.0178	0.0035	-0.0025	0.0010
	8	N-H…O	1.48	0.0805	0.1438	0.0591	-0.0822	-0.0231
	9	lp…π	3.29	0.0064	0.0233	0.0047	-0.0036	0.0011
IMI-1(c)	1	C-H…π	3.03	0.0055	0.0171	0.0034	-0.0025	0.0009
	2	C-H…π	3.05	0.0053	0.0177	0.0035	-0.0025	0.0010
	3	π…π	3.15	0.0093	0.0306	0.0062	-0.0048	0.0014
	4	C-H…π	2.65	0.0095	0.0344	0.0068	-0.0050	0.0018

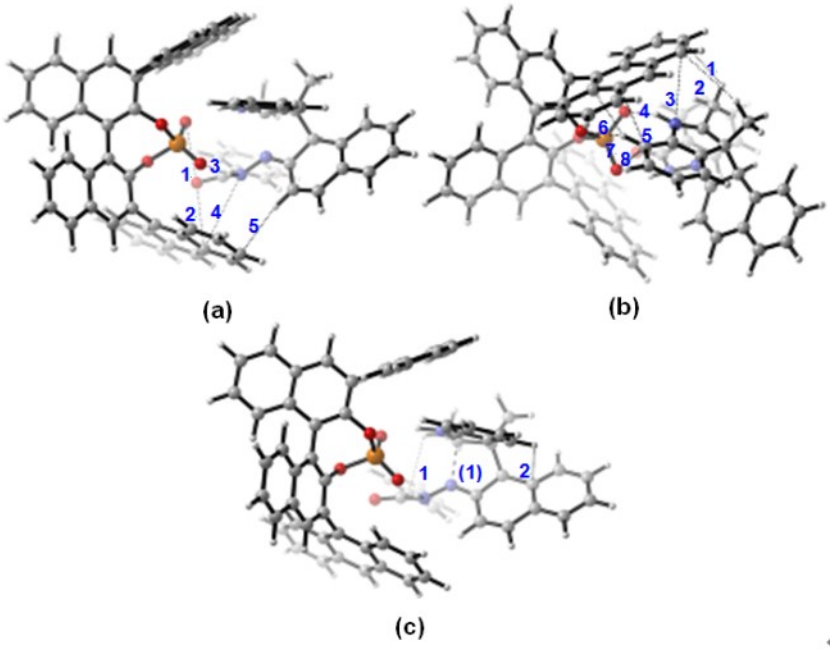

Figure S4 Intermolecular interactions in**TSI-2** and numbers of bond critical points (BCPs No.)

Table S4 Numbersof 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(a)	1	π…π	3.09	0.0089	0.0337	0.0074	-0.0064	0.0010
	2	lp…π	3.06	0.0082	0.0293	0.0064	-0.0055	0.0009
	3	N-H…O	1.77	0.0387	0.1181	0.0301	-0.0307	-0.0006
	4	lp…π	3.77	0.0025	0.0091	0.0018	-0.0014	0.0004
	5	C-H…π	2.80	0.0064	0.0177	0.0037	-0.0029	0.0008
TSI-2(b)	1	C-H…π	2.91	0.0052	0.0163	0.0032	-0.0023	0.0009
	2	C-H…π	3.17	0.0031	0.0095	0.0018	-0.0012	0.0006
	3	π…π	3.50	0.0050	0.0153	0.0033	-0.0029	0.0004
	4	N-H…O	1.66	0.0505	0.1463	0.0392	-0.0419	-0.0027
	5	π…π	3.30	0.0071	0.0221	0.0045	-0.0035	0.0010
	6	C-H…π	2.68	0.0086	0.0286	0.0059	-0.0045	0.0014
	7	C-H…O	2.35	0.0126	0.0391	0.0096	-0.0095	0.0001
	8	lp…π	3.24	0.0069	0.0238	0.0050	-0.0040	0.0010
TSI-2(c)	(1)	C…N	2.00	0.0789	0.0926	0.0432	-0.0632	-0.0200
	1	C-H…π	2.81	0.0075	0.0244	0.0048	-0.0036	0.0012
	2	C-H…π	2.71	0.0089	0.0313	0.0062	-0.0046	0.0016

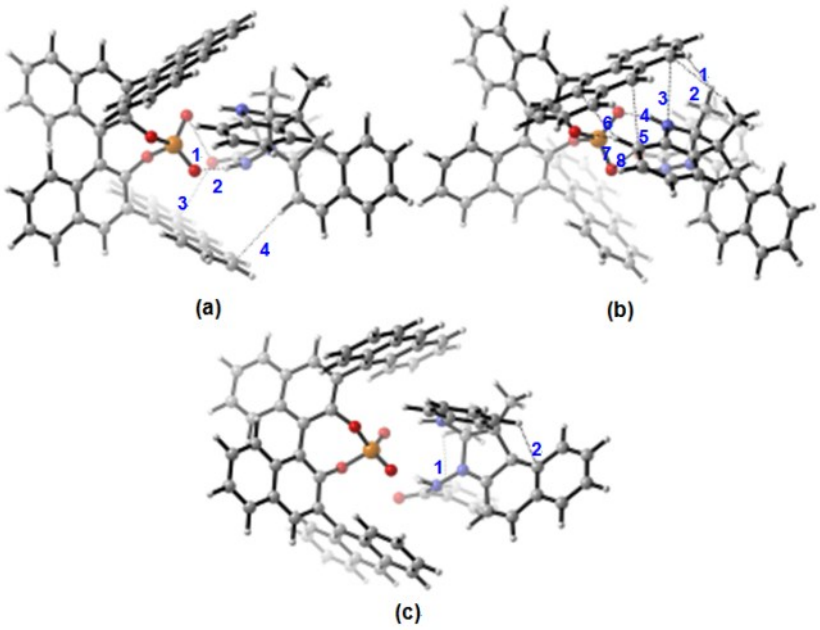

Figure S5 Intermolecular interactions in **IMI-2** and numbers of bond critical points (BCPs No.).

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-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMI-2(a)	1	π…π	3.16	0.0074	0.0273	0.0061	-0.0053	0.0008
	2	N-H…O	1.61	0.0575	0.1521	0.0437	-0.0493	-0.0056
	3	lp…π	3.35	0.0049	0.0175	0.0037	-0.0030	0.0007
	4	C-H…π	3.15	0.0035	0.0099	0.0019	-0.0014	0.0005
IMI-2(b)	1	C-H…π	2.93	0.0047	0.0150	0.0029	-0.0021	0.0008
	2	C-H…π	3.03	0.0043	0.0122	0.0024	-0.0018	0.0006
	3	lp…π	3.55	0.0050	0.0154	0.0034	-0.0028	0.0006
	4	N-H…O	1.81	0.0357	0.1109	0.0282	-0.0287	-0.0005
	5	π…π	3.30	0.0072	0.0211	0.0044	-0.0036	0.0008
	6	C-H…π	2.76	0.0072	0.0238	0.0048	-0.0037	0.0011
	7	C-H…O	2.54	0.0086	0.0284	0.0065	-0.0059	0.0006
	8	lp…π	3.39	0.0052	0.0186	0.0038	-0.0030	0.0008
IMI-2(c)	1	C-H…π	2.83	0.0079	0.0267	0.0053	-0.0040	0.0013
	2	C-H…π	2.78	0.0079	0.0260	0.0052	-0.0038	0.0014

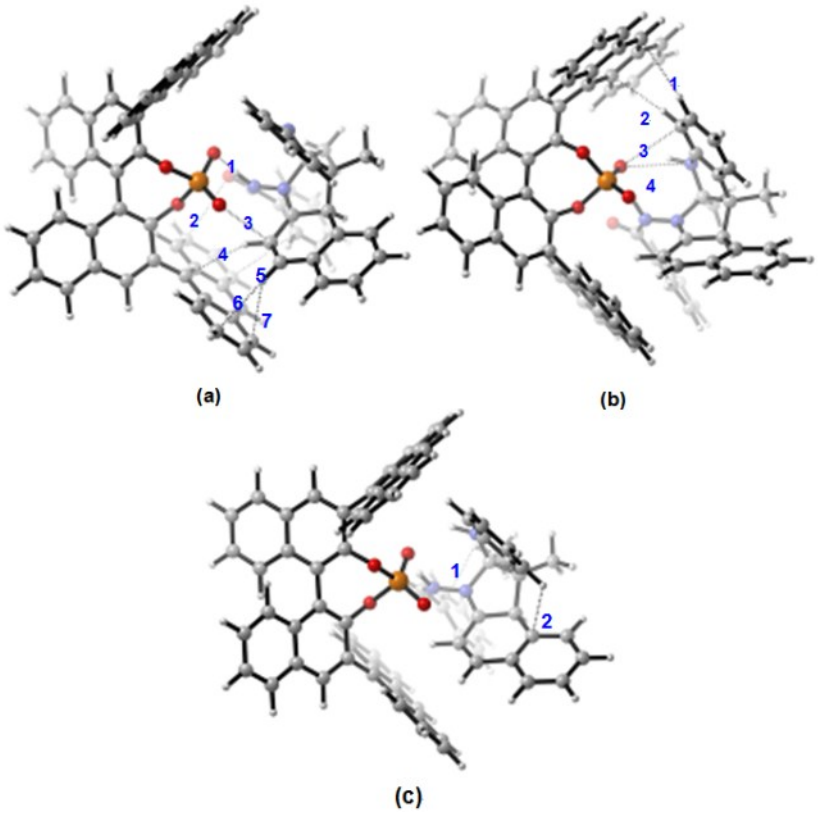

Figure S6 Intermolecular interactions in **IMI-3** and numbers of bond critical points (BCPs No.).

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-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMI-3(a)	1	N-H…O	1.66	0.0520	0.1432	0.0395	-0.0433	-0.0038
	2	π…π	3.16	0.0068	0.0223	0.0048	-0.0041	0.0007
	3	lp…π	2.99	0.0103	0.0343	0.0077	-0.0068	0.0009
	4	C-H…π	2.69	0.0082	0.0265	0.0056	-0.0045	0.0011
	5	π…π	3.24	0.0071	0.0217	0.0045	-0.0035	0.0010
	6	C-H…π	2.68	0.0087	0.0276	0.0059	-0.0050	0.0009
	7	C-H…π	2.73	0.0084	0.0299	0.0061	-0.0048	0.0013
IMI-3(b)	1	C-H…π	2.92	0.0054	0.0161	0.0032	-0.0025	0.0007
	2	C-H…π	2.53	0.0105	0.0364	0.0077	-0.0062	0.0015
	3	lp…π	3.05	0.0096	0.0330	0.0073	-0.0063	0.0010
	4	lp…lp	3.07	0.0100	0.0389	0.0086	-0.0076	0.0010
IMI-3(c)	1	C-H…π	2.86	0.0076	0.0258	0.0052	-0.0039	0.0013
	2	C-H…π	2.75	0.0084	0.0283	0.0056	-0.0041	0.0015

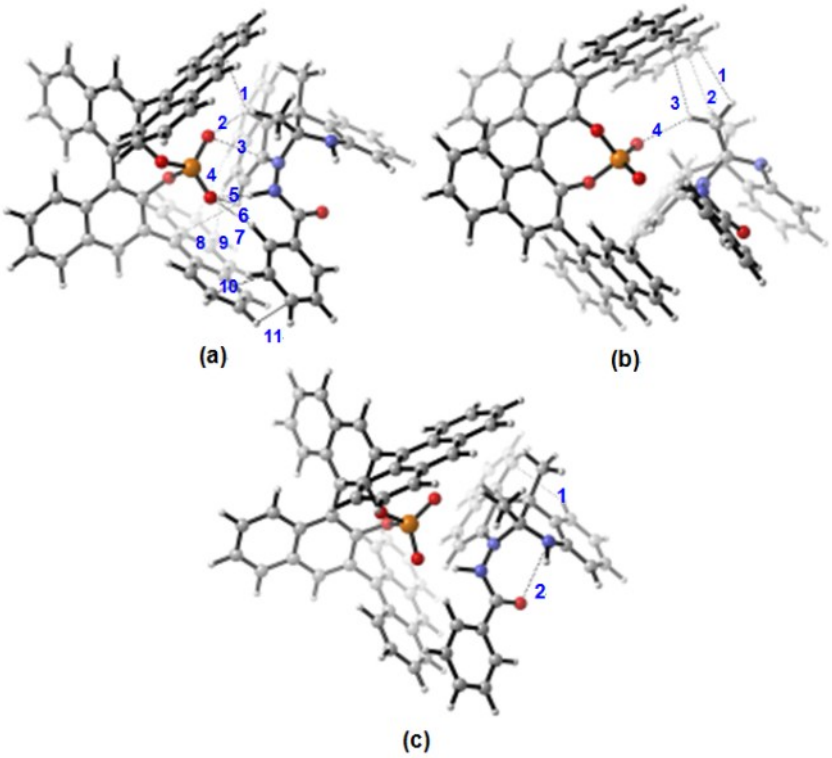

Figure S7 Intermolecular interactions in **IMI-4** and numbers of bond critical points (BCPs No.).

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-4**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMI-4(a)	1	C-H…π	3.41	0.0022	0.0068	0.0013	-0.0008	0.0005
	2	C-H…O	2.28	0.0146	0.0516	0.0121	-0.0113	0.0008
	3	lp…π	2.77	0.0140	0.0495	0.0115	-0.0106	0.0009
	4	C-H…π	3.09	0.0036	0.0107	0.0021	-0.0015	0.0006
	5	N-H…O	1.59	0.0589	0.1569	0.0453	-0.0513	-0.0060
	6	C-H…π	2.84	0.0064	0.0248	0.0049	-0.0037	-0.0013
	7	C-H…O	2.51	0.0091	0.0342	0.0075	-0.0064	-0.0013
	8	C-H…π	3.04	0.0047	0.0169	0.0034	-0.0025	0.0009
	9	C-H…π	2.54	0.0108	0.0356	0.0077	-0.0065	0.0012
	10	π…π	3.39	0.0063	0.0182	0.0037	-0.0029	-0.0013
	11	C-H…π	2.90	0.0064	0.0203	0.0040	-0.0030	-0.0013
IMI-4(b)	1	C-H…π	3.06	0.0047	0.0144	0.0029	-0.0021	0.0008
	2	C-H…π	2.66	0.0081	0.0257	0.0053	-0.0042	0.0011
	3	C-H…π	3.07	0.0043	0.0146	0.0029	-0.0021	0.0008
	4	C-H…O	2.35	0.0130	0.0415	0.0101	-0.0097	0.0004
IMI-4(c)	1	C-H…π	2.71	0.0078	0.0245	0.0050	-0.0038	0.0012
	2	lp…π	3.03	0.0099	0.0353	0.0082	-0.0077	0.0005

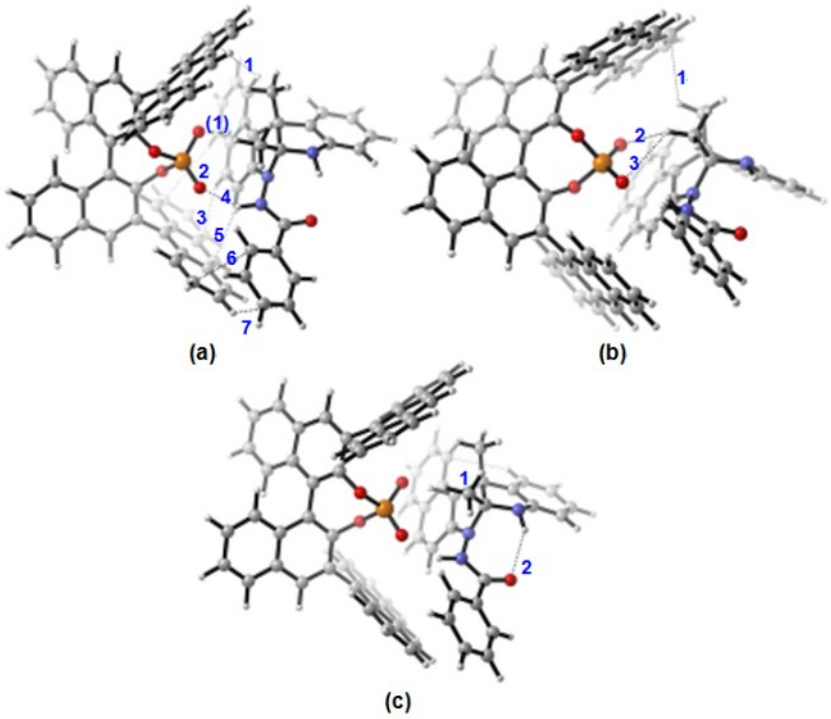

Figure S8 Intermolecular interactions in **TSI-3** and numbers of bond critical points (BCPs No.)

Table S8 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **TSI-3**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSI-3(a)	(1)	O…H	1.39	0.1041	0.0962	0.0704	-0.1168	-0.0464
	1	C-H…π	3.31	0.0027	0.0087	0.0017	-0.0012	0.0005
	2	C-H…π	3.19	0.0031	0.0094	0.0018	-0.0013	0.0005
	3	C-H…π	2.58	0.0101	0.0337	0.0072	-0.0060	0.0012
	4	N-H…O	1.85	0.0303	0.1045	0.0256	-0.0250	0.0006
	5	C-H…π	2.74	0.0076	0.0234	0.0049	-0.0039	0.0010
	6	π…π	3.32	0.0067	0.0201	0.0041	-0.0032	0.0009
	7	C-H…π	2.88	0.0063	0.0199	0.0040	-0.0031	0.0009
TSI-3(b)	1	C-H…π	2.80	0.0078	0.0263	0.0053	-0.0040	0.0013
	2	C-H…π	2.51	0.0102	0.0339	0.0078	-0.0071	0.0007
	3	C-H…π	2.71	0.0076	0.0288	0.0060	-0.0048	0.0012
TSI-3(c)	1	C-H…π	2.73	0.0072	0.0237	0.0047	-0.0036	0.0011
	2	N-H…O	2.28	0.0145	0.0511	0.0122	-0.0116	0.0006

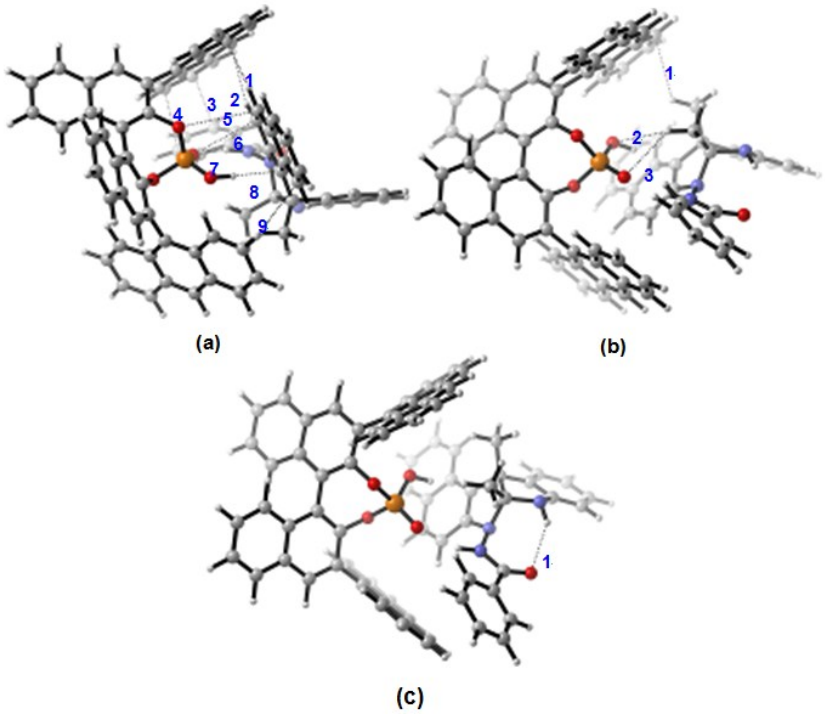

Figure S9 Intermolecular interactions in **IMI-5** and numbers of bond critical points (BCPs No.).

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-5**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMI-5(a)	1	C-H…π	2.65	0.0089	0.0328	0.0067	-0.0052	0.0015
	2	C-H…π	2.74	0.0074	0.0225	0.0047	-0.0037	0.0010
	3	C-H…π	2.89	0.0059	0.0185	0.0037	-0.0028	0.0009
	4	π…π	3.31	0.0070	0.0228	0.0045	-0.0033	0.0012
	5	lp…π	3.37	0.0051	0.0168	0.0036	-0.0029	0.0007
	6	π…π	3.24	0.0077	0.0242	0.0052	-0.0044	0.0008
	7	N-H…O	1.91	0.0258	0.0883	0.0217	-0.0213	0.0004
	8	O-H…π	2.10	0.0228	0.0513	0.0135	-0.0142	-0.0007
	9	C-H…π	3.19	0.0041	0.0122	0.0024	-0.0018	0.0006
IMI-5(b)	1	C-H…π	2.83	0.0074	0.0241	0.0049	-0.0037	0.0012
	2	C-H…O	2.76	0.0059	0.0221	0.0045	-0.0035	0.0010
	3	C-H…O	2.64	0.0080	0.0277	0.0060	-0.0051	0.0009
IMI-5(c)	1	N-H…O	2.20	0.0163	0.0528	0.0132	-0.0133	-0.0001

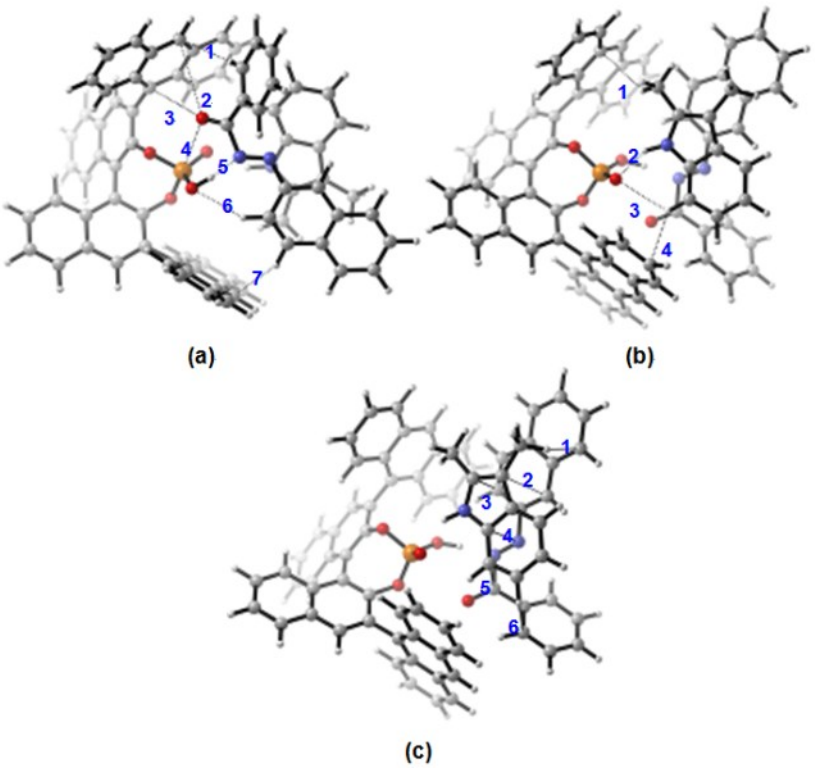

Figure S10 Intermolecular interactions in **COMII** and numbers of bond critical points (BCPs No.).

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 **COMII**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COMII(a)	1	C-H…π	2.55	0.0099	0.0319	0.0068	-0.0055	0.0013
	2	lp…π	3.53	0.0040	0.0154	0.0032	-0.0025	0.0007
	3	lp…π	3.46	0.0039	0.0155	0.0032	-0.0025	0.0007
	4	lp…π	3.13	0.0091	0.0340	0.0075	-0.0066	0.0009
	5	O-H…N	1.64	0.0597	0.1046	0.0366	-0.0471	-0.0105
	6	C-H…O	2.52	0.0086	0.0351	0.0074	-0.0060	0.0014
	7	C-H…π	2.60	0.0092	0.0291	0.0062	-0.0050	0.0012
COMII(b)	1	C-H…π	2.91	0.0053	0.0167	0.0033	-0.0024	0.0009
	2	N-H…O	1.88	0.0288	0.0949	0.0237	-0.0237	0.0000
	3	C-H…O	2.74	0.0057	0.0218	0.0045	-0.0035	0.0010
	4	C-H…π	2.96	0.0056	0.0183	0.0036	-0.0027	0.0009
COMII(c)	1	C-H…π	2.84	0.0067	0.0212	0.0042	-0.0032	0.0010
	2	π…π	3.31	0.0076	0.0214	0.0045	-0.0037	0.0008
	3	π…π	3.34	0.0066	0.0203	0.0043	-0.0035	0.0008
	4	π…π	3.17	0.0073	0.0233	0.0050	-0.0041	0.0009
	5	π…π	3.34	0.0053	0.0184	0.0035	-0.0025	0.0010
	6	C-H…π	3.06	0.0044	0.0141	0.0027	-0.0019	0.0008

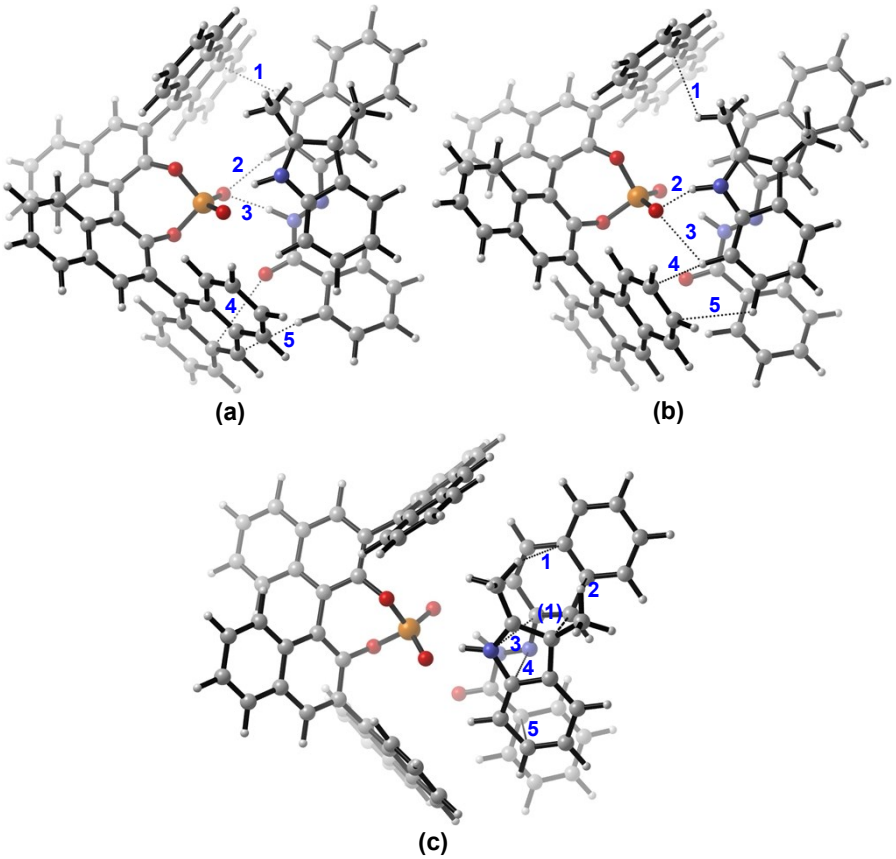

Figure S11 Intermolecular interactions in**TSII-1** and numbers of bond critical points (BCPs No.).

Table S11 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of**TSII-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSII-1(a)	1	C-H…π	2.53	0.0102	0.0324	0.0069	-0.0057	0.0012
	2	C-H…O	2.16	0.0186	0.0563	0.0145	-0.0150	-0.0005
	3	N-H…O	1.81	0.0356	0.1050	0.0271	-0.0279	-0.0008
	4	lp…π	3.44	0.0039	0.0150	0.0031	-0.0024	0.0007
	5	C-H…π	2.52	0.0099	0.0305	0.0066	-0.0056	0.0010
TSII-1(b)	1	C-H…π	2.97	0.0051	0.0172	0.0034	-0.0025	0.0009
	2	N-H…O	1.64	0.0512	0.1557	0.0410	-0.0431	-0.0021
	3	C-H…O	2.72	0.0060	0.0235	0.0048	-0.0038	0.0010
	4	C-H…π	2.85	0.0066	0.0224	0.0045	-0.0033	0.0012
	5	C-H…π	3.06	0.0051	0.0159	0.0031	-0.0023	0.0008
TSII-1(c)	(1)	C…C	2.35	0.0446	0.0466	0.0180	-0.0243	-0.0063
	1	C-H…π	2.73	0.0076	0.0252	0.0050	-0.0038	0.0012
	2	C-H…π	2.75	0.0098	0.0362	0.0071	-0.0052	0.0019
	3	π…π	2.93	0.0132	0.0457	0.0101	-0.0089	0.0012
	4	π…π	2.82	0.0146	0.0454	0.0100	-0.0086	0.0014
	5	π…π	3.43	0.0064	0.0179	0.0037	-0.0029	0.0008

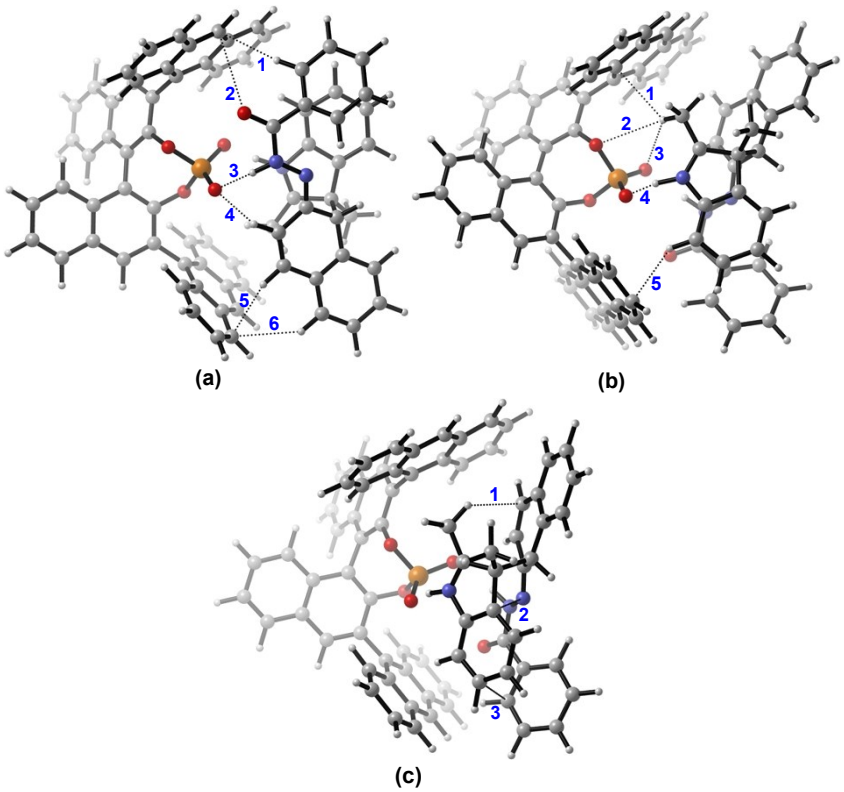

Figure S12 Intermolecular interactions in **IMII-1** and numbers of bond critical points (BCPs No.).

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 **IMII-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMII-1(a)	1	C-H…π	2.59	0.0088	0.0275	0.0058	-0.0048	0.0010
	2	lp…π	3.49	0.0043	0.0159	0.0033	-0.0026	0.0007
	3	N-H…O	1.93	0.0264	0.0785	0.0205	0.0785	0.0990
	4	C-H…O	2.29	0.0140	0.0525	0.0120	-0.0108	0.0012
	5	C-H…π	2.64	0.0094	0.0292	0.0062	-0.0051	0.0011
	6	C-H…π	2.78	0.0068	0.0227	0.0044	-0.0032	0.0012
IMII-1(b)	1	C-H…π	2.81	0.0070	0.0238	0.0047	-0.0035	0.0012
	2	N-H…O	1.40	0.0995	0.1073	0.0728	-0.1188	-0.0460
	3	C-H…O	2.86	0.0046	0.0181	0.0036	-0.0026	0.0010
	4	C-H…π	2.72	0.0079	0.0259	0.0053	-0.0041	0.0012
	5	C-H…π	2.83	0.0056	0.0199	0.0040	-0.0030	0.0010
IMII-1(c)	1	C-H…π	2.76	0.0080	0.0273	0.0054	-0.0040	0.0014
	2	π…π	3.31	0.0068	0.0197	0.0041	-0.0032	0.0009
	3	lp…π	2.89	0.0139	0.0463	0.0101	-0.0085	0.0016

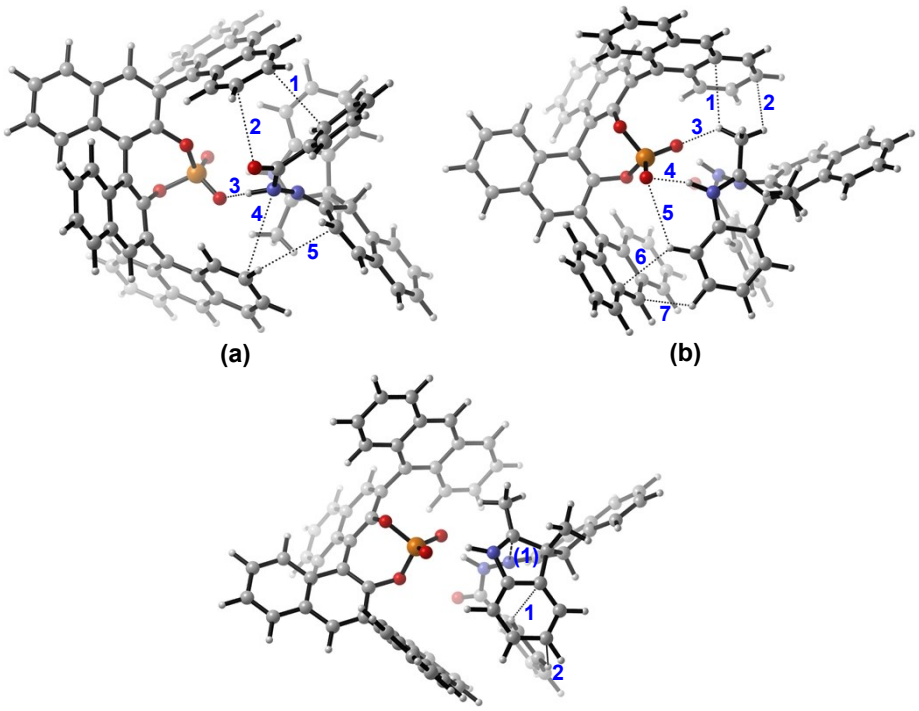

Figure S13 Intermolecular interactions in**TSII-2** and numbers of bond critical points (BCPs No.)

Table S13 Numbers of bond critical point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSII-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSII-2(a)	1	π…π	3.35	0.0065	0.0187	0.0039	-0.0031	0.0008
	2	π…π	3.22	0.0066	0.0243	0.0050	-0.0040	0.0010
	3	N-H…O	1.71	0.0419	0.1412	0.0350	-0.0347	0.0003
	4	lp…π	3.61	0.0038	0.0116	0.0024	-0.0020	0.0004
	5	C-H…π	3.46	0.0020	0.0065	0.0012	-0.0009	0.0003
TSII-2(b)	1	C-H…π	2.90	0.0056	0.0195	0.0039	-0.0028	0.0011
	2	C-H…π	2.93	0.0063	0.0193	0.0039	-0.0029	0.0010
	3	C-H…O	2.19	0.0178	0.0554	0.0140	-0.0142	-0.0002
	4	N-H…O	1.75	0.0405	0.1196	0.0309	-0.0318	-0.0009
	5	C-H…O	2.99	0.0036	0.0153	0.0029	-0.0020	0.0009
	6	C-H…π	2.85	0.0059	0.0193	0.0038	-0.0028	0.0010
	7	C-H…π	2.80	0.0070	0.0247	0.0048	-0.0034	0.0014
TSII-2(c)	(1)	C…N	2.18	0.0516	0.1108	0.0335	-0.0392	-0.0057
	1	C-H…π	2.73	0.0077	0.0244	0.0051	-0.0040	0.0011
	2	C-H…π	3.01	0.0044	0.0135	0.0026	-0.0019	0.0007

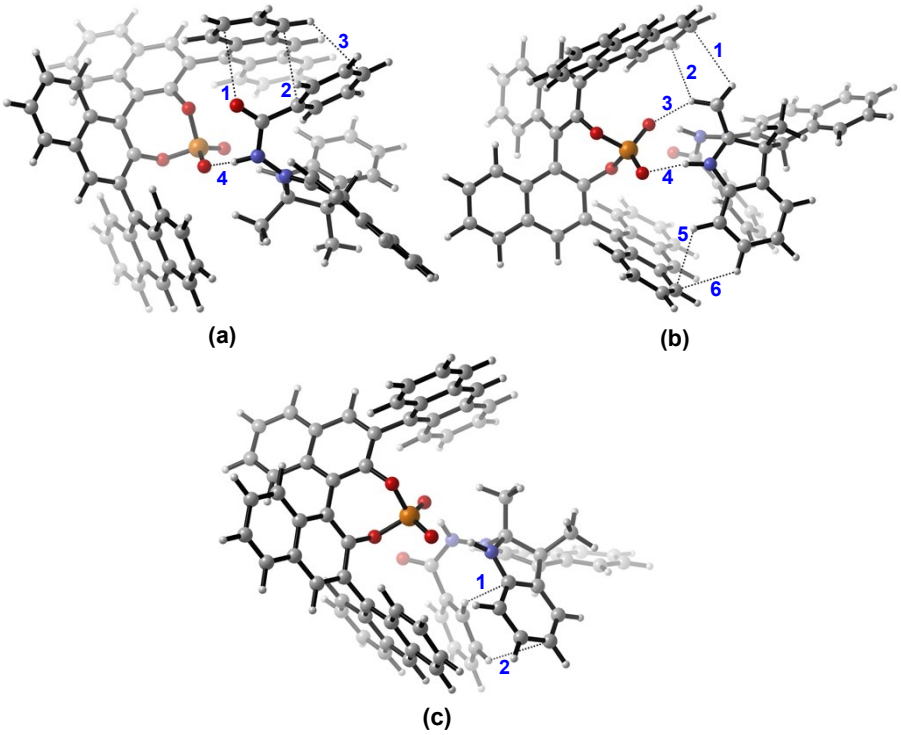

Figure S14 Intermolecular interactions in **IMII-2** and numbers of bond critical points (BCPs No.).

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(a)	1	lp…π	3.32	0.0051	0.0178	0.0038	-0.0031	0.0007
	2	π…π	3.38	0.0063	0.0184	0.0039	-0.0031	0.0008
	3	C-H…π	2.98	0.0053	0.0166	0.0033	-0.0025	0.0008
	4	N-H…O	1.57	0.0610	0.1641	0.0478	-0.0545	-0.0067
IMII-2(b)	1	C-H…π	3.16	0.0042	0.0127	0.0025	-0.0019	0.0006
	2	C-H…π	3.19	0.0036	0.0123	0.0024	-0.0018	0.0006
	3	C-H…O	2.25	0.0159	0.0492	0.0124	-0.0125	-0.0001
	4	N-H…O	1.82	0.0342	0.1068	0.0270	-0.0272	-0.0002
	5	C-H…π	2.83	0.0069	0.0226	0.0045	-0.0034	0.0011
	6	C-H…π	2.97	0.0053	0.0173	0.0034	-0.0024	0.0010
IMII-2(c)	1	C-H…π	2.43	0.0116	0.0424	0.0091	-0.0077	0.0014
	2	C-H…π	3.22	0.0033	0.0100	0.0020	-0.0015	0.0005

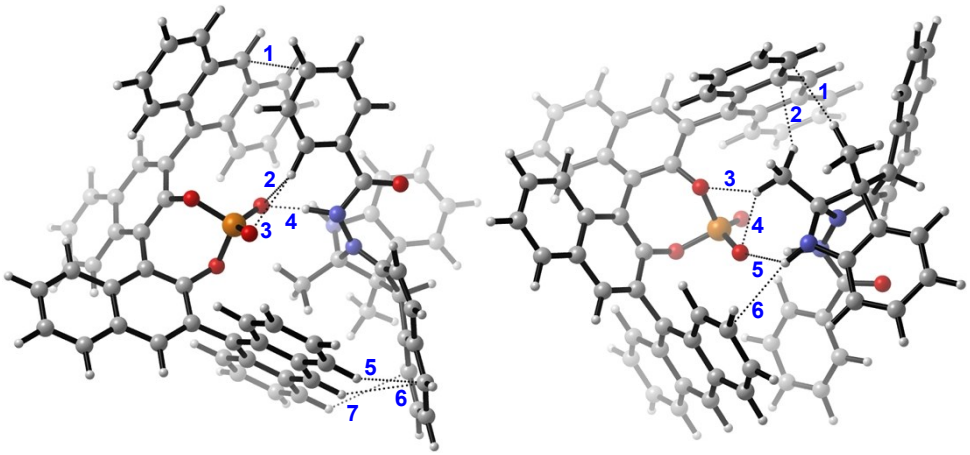

Figure S15 Intermolecular interactions in **IMII-3** and numbers of bond critical points (BCPs No.).

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(a)	1	π…π	3.28	0.0068	0.0197	0.0041	-0.0033	0.0008
	2	C-H…π	2.71	0.0085	0.0339	0.0070	-0.0055	0.0015
	3	C-H…O	2.33	0.0140	0.0402	0.0102	-0.0104	-0.0002
	4	N-H…O	1.54	0.0681	0.1603	0.0519	-0.0637	-0.0118
	5	C-H…π	2.89	0.0053	0.0168	0.0033	-0.0024	0.0009
	6	C-H…π	2.78	0.0071	0.0224	0.0046	-0.0036	0.0010
	7	C-H…π	2.95	0.0052	0.0154	0.0030	-0.0022	0.0008
IMII-3(b)	1	C-H…π	3.04	0.0044	0.0119	0.0024	-0.0018	0.0006
	2	C-H…π	2.49	0.0111	0.0358	0.0077	-0.0065	0.0012
	3	C-H…O	2.30	0.0129	0.0444	0.0106	-0.0102	0.0004
	4	C-H…O	2.27	0.0163	0.0505	0.0127	-0.0128	-0.0001
	5	N-H…O	2.62	0.0063	0.0266	0.0056	-0.0045	0.0011
	6	N-H…π	2.86	0.0048	0.0155	0.0031	-0.0023	0.0008

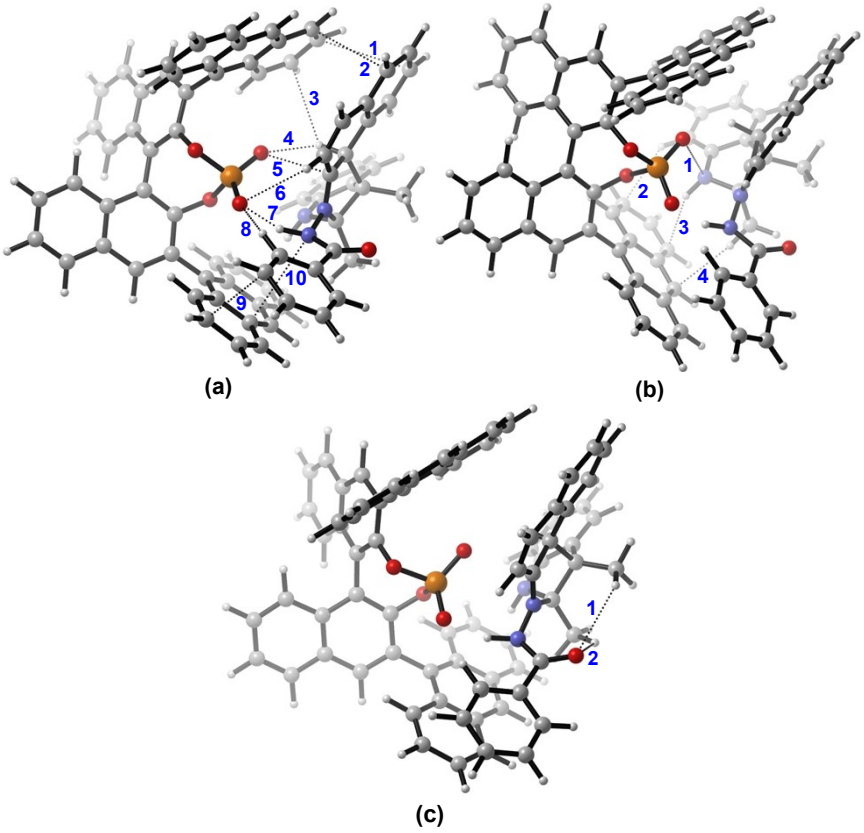

Figure S16 Intermolecular interactions in **IMII-4** and numbers of bond critical points (BCPs No.).

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 **IMII-4**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMII-4(a)	1	π…π	3.50	0.0060	0.0186	0.0037	-0.0028	0.0009
	2	π…π	3.32	0.0070	0.0213	0.0043	-0.0033	0.0010
	3	C-H…π	3.31	0.0026	0.0079	0.0015	-0.0010	0.0005
	4	C-H…O	2.26	0.0149	0.0542	0.0126	-0.0116	0.0010
	5	lp…π	2.70	0.0153	0.0547	0.0128	-0.0118	0.0010
	6	C-H…O	2.84	0.0058	0.0231	0.0046	-0.0035	0.0011
	7	N-H…O	1.65	0.0509	0.1486	0.0398	-0.0425	-0.0027
	8	C-H…O	2.25	0.0140	0.0469	0.0114	-0.0110	0.0004
	9	π…π	3.27	0.0073	0.0215	0.0044	-0.0035	0.0009
	10	lp…π	3.73	0.0031	0.0102	0.0021	-0.0016	0.0005
IMII-4(b)	1	lp…lp	3.23	0.0075	0.0236	0.0056	-0.0053	0.0003
	2	C-H…π	2.66	0.0077	0.0253	0.0051	-0.0040	0.0011
	3	N-H…π	2.65	0.0084	0.0284	0.0060	-0.0049	0.0011
	4	C-H…π	2.67	0.0081	0.0247	0.0052	-0.0041	0.0011
IMII-4(c)	1	C-H…O	2.96	0.0038	0.0156	0.0030	-0.0021	0.0009
	2	C-H…O	2.43	0.0118	0.0407	0.0093	-0.0084	0.0009

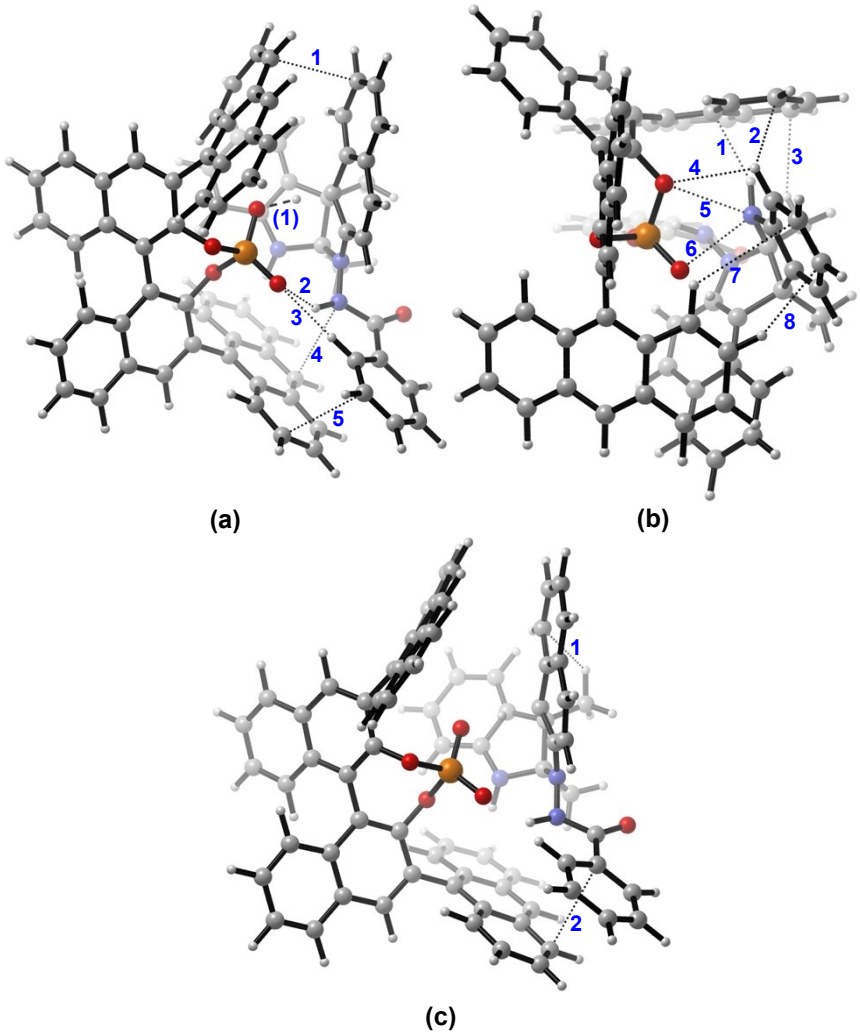

Figure S17 Intermolecular interactions in**TSII-3** and numbers of bond critical points (BCPs No.)

Table S17 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSII-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSII-3(a)	(1)	O…H	1.39	0.1029	0.0862	0.0672	-0.1128	-0.0456
	1	π…π	3.24	0.0079	0.0225	0.0047	-0.0037	0.0010
	2	N-H…O	1.89	0.0297	0.0941	0.0241	-0.0246	-0.0005
	3	C-H…O	2.46	0.0094	0.0323	0.0074	-0.0067	0.0007
	4	lp…π	3.62	0.0043	0.0131	0.0028	-0.0023	0.0005
	5	π…π	3.26	0.0076	0.0222	0.0046	-0.0036	0.0010
TSII-3(b)	1	N-H…π	2.41	0.0118	0.0405	0.0089	-0.0076	0.0013
	2	C-H…π	2.77	0.0077	0.0246	0.0049	-0.0037	0.0012
	3	C-H…π	2.76	0.0071	0.0234	0.0047	-0.0035	0.0012
	4	C-H…O	2.99	0.0042	0.0173	0.0035	-0.0026	0.0009
	5	lp…lp	2.95	0.0109	0.0350	0.0085	-0.0082	0.0003
	6	lp…π	2.95	0.0127	0.0422	0.0101	-0.0097	0.0004
	7	C-H…π	3.53	0.0017	0.0058	0.0011	-0.0008	0.0003
	8	C-H…π	2.96	0.0047	0.0143	0.0028	-0.0021	0.0007
TSII-3(c)	1	C-H…π	2.73	0.0082	0.0309	0.0060	-0.0042	0.0018
	2	π…π	3.33	0.0070	0.0196	0.0041	-0.0033	0.0008

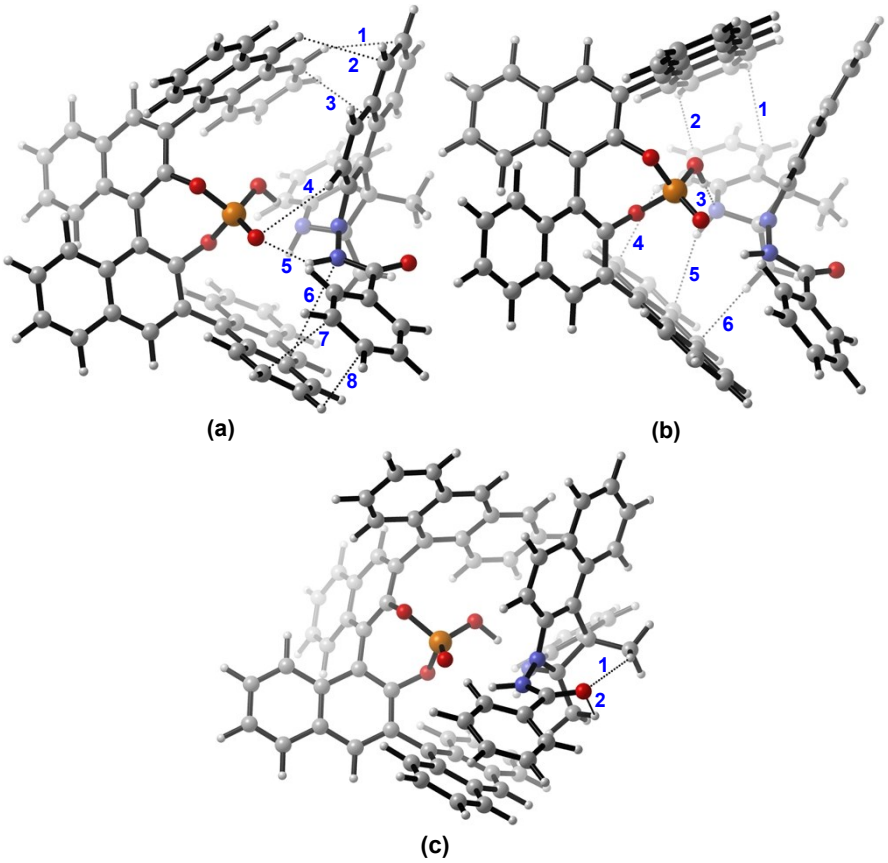

Figure S18 Intermolecular interactions in **IMII-5** and numbers of bond critical points (BCPs No.).

Table S18 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-5**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMII-5(a)	1	C-H…π	2.73	0.0080	0.0254	0.0054	-0.0044	0.0010
	2	C-H…π	2.93	0.0051	0.0160	0.0032	-0.0023	0.0009
	3	π…π	3.28	0.0071	0.0225	0.0046	-0.0036	0.0010
	4	C-H…O	2.97	0.0042	0.0168	0.0033	-0.0024	0.0009
	5	N-H…O	1.93	0.0268	0.0876	0.0223	-0.0227	-0.0004
	6	lp…π	3.90	0.0022	0.0079	0.0016	-0.0011	0.0005
	7	π…π	3.33	0.0067	0.0192	0.0040	-0.0031	0.0009
	8	C-H…π	2.98	0.0055	0.0176	0.0035	-0.0026	0.0009
IMII-5(b)	1	C-H…π	3.22	0.0034	0.0105	0.0020	-0.0015	0.0005
	2	C-H…π	2.83	0.0067	0.0205	0.0041	-0.0031	0.0010
	3	O-H…N	1.53	0.0825	0.0706	0.0475	-0.0774	-0.0299
	4	C-H…π	2.96	0.0044	0.0137	0.0027	-0.0019	0.0008
	5	N-H…π	2.85	0.0058	0.0192	0.0039	-0.0031	0.0008
	6	C-H…π	2.54	0.0104	0.0318	0.0068	-0.0057	0.0011
IMII-5(c)	1	C-H…O	2.79	0.0052	0.0196	0.0040	-0.0031	0.0009
	2	C-H…π	2.50	0.0103	0.0358	0.0080	-0.0071	0.0009

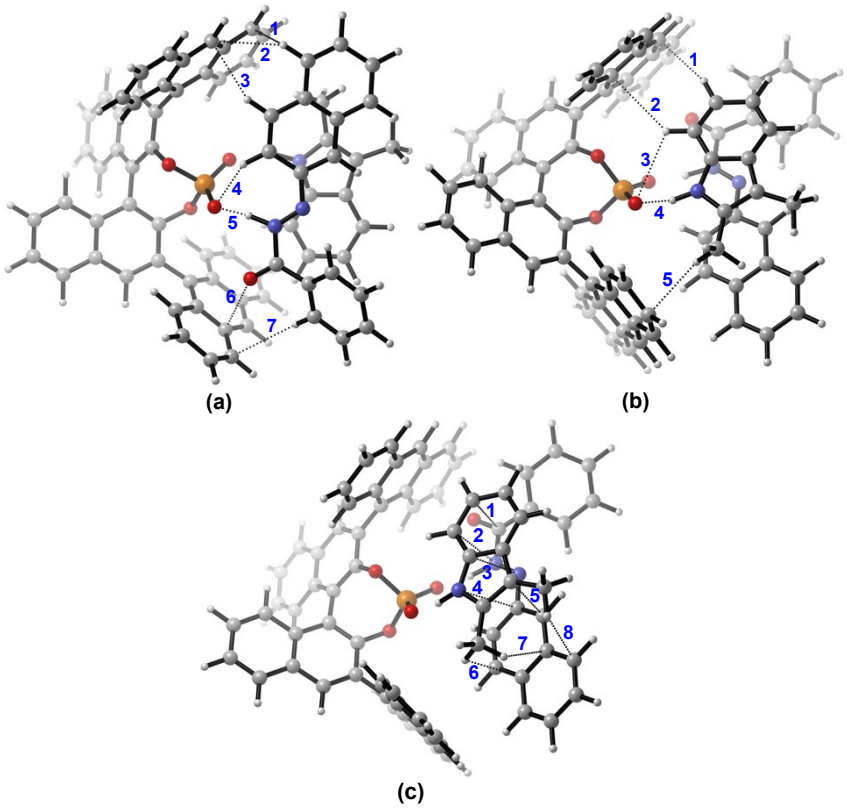

Figure S19 Intermolecular interactions in **COMIII** and numbers of bond critical points (BCPs No.).

Table S19 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 **COMIII**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COMIII(a)	1	C-H…π	2.94	0.0053	0.0187	0.0036	-0.0025	0.0011
	2	C-H…π	2.82	0.0062	0.0205	0.0040	-0.0030	0.0010
	3	C-H…π	2.65	0.0086	0.0259	0.0055	-0.0045	0.0010
	4	C-H…O	2.24	0.0171	0.0531	0.0134	-0.0135	-0.0001
	5	N-H…O	1.44	0.0855	0.1350	0.0625	-0.0913	-0.0288
	6	lp…π	2.97	0.0095	0.0354	0.0077	-0.0065	0.0012
	7	C-H…π	2.80	0.0058	0.0190	0.0038	-0.0028	0.0010
COMIII(b)	1	C-H…π	2.66	0.0086	0.0257	0.0054	-0.0044	0.0010
	2	C-H…π	3.15	0.0032	0.0102	0.0020	-0.0014	0.0006
	3	C-H…O	2.95	0.0050	0.0191	0.0037	-0.0026	0.0011
	4	N-H…O	1.78	0.0340	0.1214	0.0291	-0.0278	0.0013
	5	C-H…π	2.83	0.0067	0.0212	0.0043	-0.0032	0.0011
COMIII(c)	1	π…π	3.09	0.0086	0.0272	0.0056	-0.0043	0.0013
	2	π…π	3.07	0.0098	0.0288	0.0064	-0.0056	0.0008
	3	π…π	3.12	0.0086	0.0262	0.0056	-0.0047	0.0009
	4	π…π	3.24	0.0076	0.0241	0.0054	-0.0048	0.0006
	5	π…π	2.99	0.0127	0.0335	0.0072	-0.0060	0.0012
	6	C-H…π	2.85	0.0070	0.0239	0.0047	-0.0035	0.0012
	7	C-H…π	2.88	0.0069	0.0243	0.0048	-0.0036	0.0012
	8	C-H…π	2.85	0.0062	0.0209	0.0041	-0.0029	0.0012

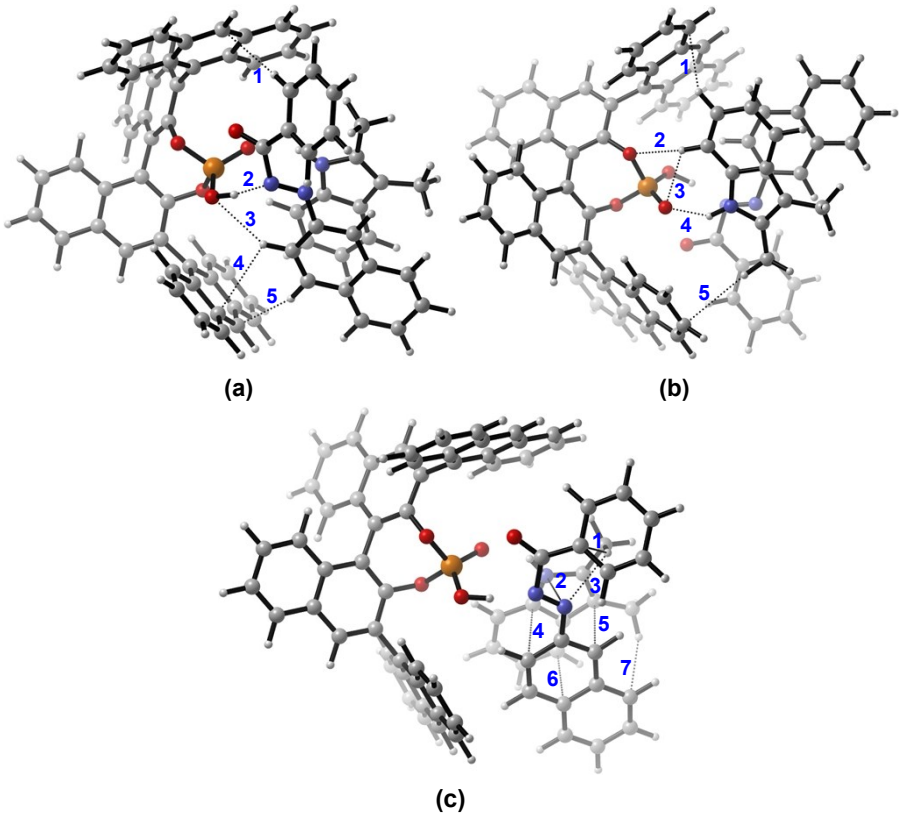

Figure S20 Intermolecular interactions in **COMIV** and numbers of bond critical points (BCPs No.).

Table S20 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 **COMIV**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COMIV(a)	1	C-H…π	2.62	0.0089	0.0278	0.0058	-0.0047	0.0011
	2	O-H…N	1.65	0.0595	0.1047	0.0366	-0.0470	-0.0104
	3	C-H…O	2.54	0.0087	0.0340	0.0072	-0.0059	0.0013
	4	C-H…π	3.22	0.0033	0.0109	0.0021	-0.0015	0.0006
	5	C-H…π	2.49	0.0109	0.0329	0.0072	-0.0062	0.0010
COMIV(b)	1	C-H…π	2.73	0.0082	0.0256	0.0054	-0.0043	0.0011
	2	C-H…O	2.55	0.0078	0.0271	0.0061	-0.0055	0.0006
	3	C-H…O	2.60	0.0088	0.0312	0.0068	-0.0057	0.0011
	4	N-H…O	1.90	0.0264	0.0934	0.0227	-0.0221	0.0006
	5	C-H…π	3.03	0.0039	0.0114	0.0022	-0.0016	0.0006
COMIV(c)	1	C-H…π	2.97	0.0046	0.0144	0.0028	-0.0021	0.0007
	2	π…π	3.10	0.0087	0.0272	0.0061	-0.0054	0.0007
	3	C-H…N	2.73	0.0073	0.0236	0.0051	-0.0042	0.0009
	4	π…π	3.30	0.0073	0.0213	0.0044	-0.0036	0.0008
	5	π…π	3.17	0.0092	0.0250	0.0054	-0.0045	0.0009
	6	π…π	3.34	0.0066	0.0192	0.0040	-0.0032	0.0008
	7	C-H…π	2.69	0.0075	0.0238	0.0048	-0.0037	0.0011

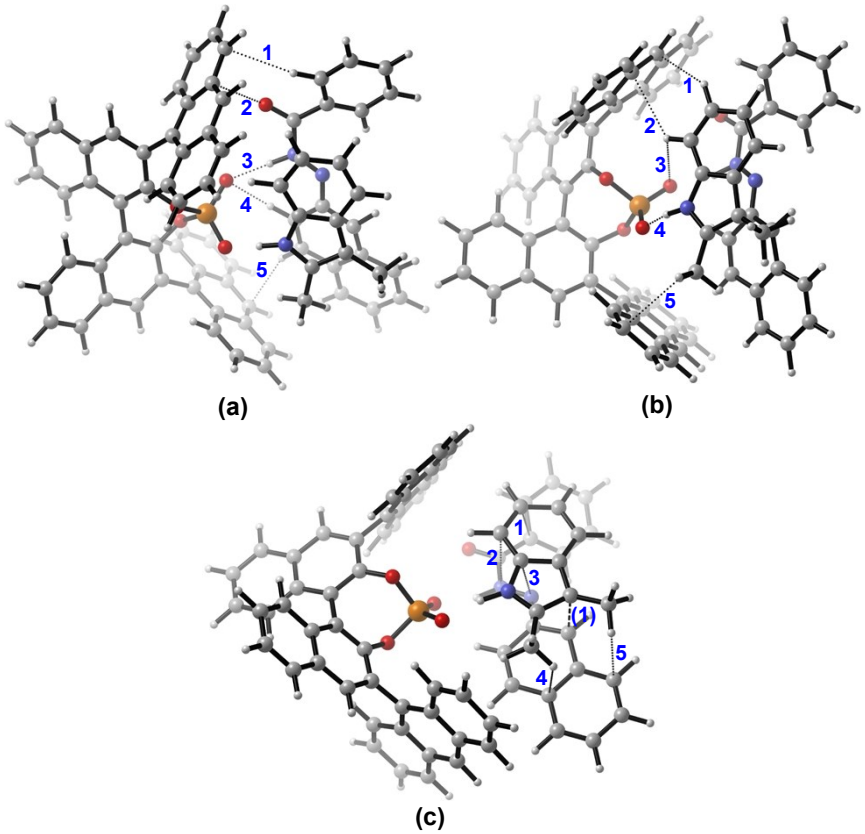

Figure S21 Intermolecular interactions in **TSIII-1** and numbers of bond critical points (BCPs No.).

Table S21 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 **TSIII-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIII-1(a)	1	C-H…π	2.69	0.0070	0.0227	0.0046	-0.0036	0.0010
	2	lp…π	3.11	0.0074	0.0270	0.0058	-0.0049	0.0009
	4	C-H…O	2.27	0.0162	0.0490	0.0124	-0.0126	-0.0002
	5	C-H…π	2.65	0.0085	0.0255	0.0054	-0.0044	0.0010
TSIII-1(b)	1	C-H…π	2.72	0.0074	0.0229	0.0047	-0.0037	0.0010
	2	C-H…π	2.85	0.0062	0.0200	0.0040	-0.0030	0.0010
	3	C-H…O	3.25	0.0026	0.0101	0.0019	-0.0012	0.0007
	4	N-H…O	1.58	0.0593	0.1651	0.0470	-0.0527	-0.0057
	5	C-H…π	2.79	0.0072	0.0236	0.0048	-0.0036	0.0012
TSIII-1(c)	(1)	C…C	2.32	0.0469	0.0480	0.0192	-0.0264	-0.0072
	1	π…π	3.32	0.0071	0.0208	0.0043	-0.0034	0.0009
	2	lp…π	3.18	0.0085	0.0266	0.0059	-0.0052	0.0007
	3	π…π	2.90	0.0133	0.0416	0.0089	-0.0074	0.0015
	4	C-H…π	2.63	0.0102	0.0352	0.0071	-0.0053	0.0018
	5	C-H…π	2.61	0.0098	0.0335	0.0067	-0.0051	0.0016

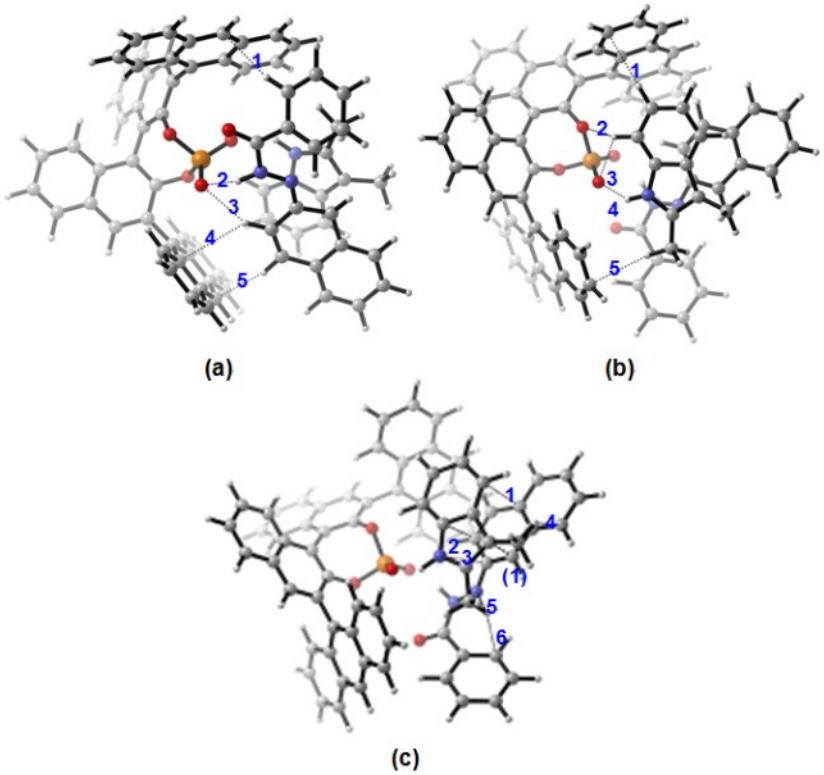

Figure S22 Intermolecular interactions in**TSIV-1** and numbers of bond critical points (BCPs No.).

Table S22 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **TSIV-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSIV-1(a)	1	C-H…π	2.60	0.0092	0.0286	0.0061	-0.0050	0.0011
	2	N-H…O	1.71	0.0446	0.1298	0.0340	-0.0355	-0.0015
	3	C-H…O	2.36	0.0132	0.0393	0.0098	-0.0098	0.0000
	4	C-H…π	3.23	0.0027	0.0090	0.0017	-0.0012	0.0005
	5	C-H…π	2.47	0.0116	0.0344	0.0076	-0.0067	0.0009
TSIV-1(b)	1	C-H…π	2.67	0.0087	0.0269	0.0058	-0.0048	0.0010
	2	C-H…O	2.35	0.0117	0.0391	0.0094	-0.0090	0.0004
	3	C-H…O	2.48	0.0113	0.0401	0.0090	-0.0080	0.0010
	4	N-H…O	1.80	0.0330	0.1187	0.0284	-0.0272	0.0012
	5	C-H…π	2.78	0.0062	0.0189	0.0038	-0.0029	0.0009
TSIV-1(c)	(1)	C…C	2.32	0.0472	0.0455	0.0189	-0.0264	-0.0075
	1	π…π	3.06	0.0103	0.0316	0.0066	-0.0053	0.0013
	2	π…π	3.16	0.0092	0.0296	0.0061	-0.0049	0.0012
	3	π…π	2.97	0.0126	0.0420	0.0092	-0.0079	0.0013
	4	C-H…π	2.55	0.0106	0.0361	0.0073	-0.0057	0.0016
	5	C-H…N	2.67	0.0094	0.0319	0.0067	-0.0055	0.0012
	6	C-H…π	2.92	0.0053	0.0167	0.0033	-0.0024	0.0009

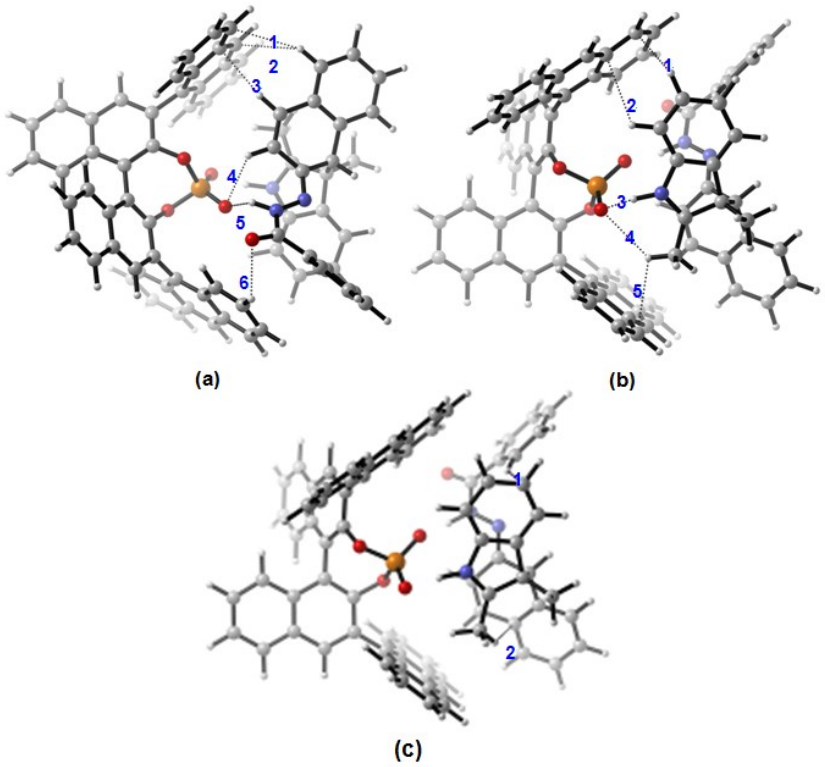

Figure S23 Intermolecular interactions in **IMIII-1** and numbers of bond critical points (BCPs No.).

Table S23 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 **IMIII-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIII-1(a)	1	C-H…π	2.99	0.0043	0.0140	0.0027	-0.0019	0.0008
	2	C-H…π	3.05	0.0042	0.0141	0.0027	-0.0019	0.0008
	3	C-H…π	2.51	0.0105	0.0329	0.0071	-0.0060	0.0011
	4	C-H…O	2.40	0.0133	0.0456	0.0106	-0.0098	0.0008
	5	N-H…O	1.98	0.0235	0.0801	0.0200	-0.0200	0.0000
	6	C-H…π	2.42	0.0118	0.0429	0.0096	-0.0085	0.0011
IMIII-1(b)	1	C-H…π	2.66	0.0080	0.0263	0.0053	-0.0041	0.0012
	2	C-H…π	3.07	0.0043	0.0139	0.0027	-0.0020	0.0007
	3	N-H…O	1.48	0.0818	0.1484	0.0610	-0.0848	-0.0238
	4	C-H…O	2.62	0.0079	0.0293	0.0063	-0.0053	0.0010
	5	C-H…π	2.95	0.0063	0.0217	0.0043	-0.0032	0.0011
IMIII-1(c)	1	C-H…π	2.63	0.0088	0.0271	0.0057	-0.0046	0.0011
	2	C-H…π	2.50	0.0112	0.0378	0.0080	-0.0065	0.0015

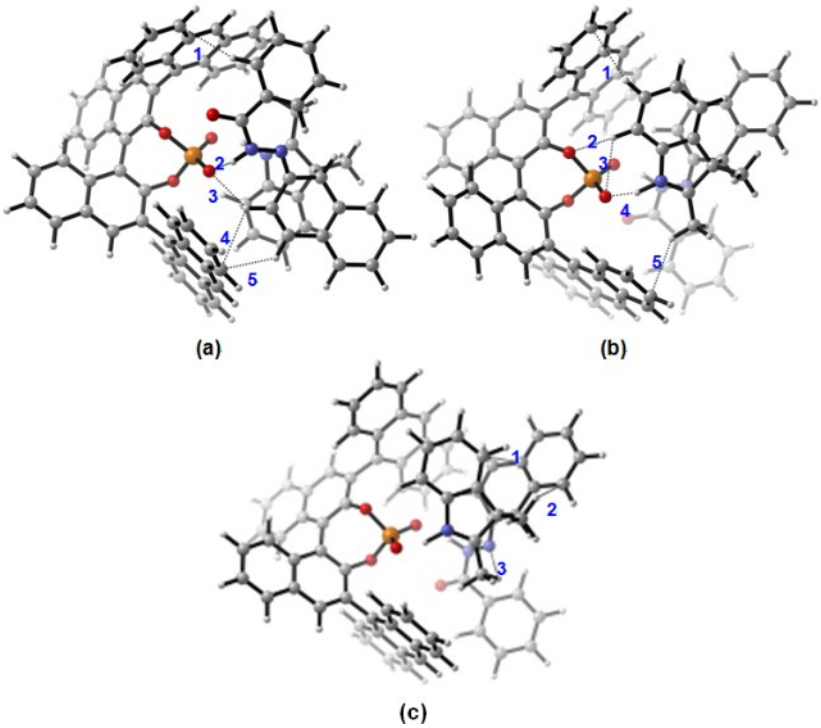

Figure S24 Intermolecular interactions in **IMIV-1** and numbers of bond critical points (BCPs No.).

Table S24 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 **IMIV-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV-1(a)	1	C-H…π	2.66	0.0078	0.0254	0.0053	-0.0042	0.0011
	2	N-H…O	1.85	0.0304	0.1047	0.0256	-0.0251	0.0005
	3	C-H…O	2.42	0.0107	0.0393	0.0088	-0.0078	0.0010
	4	C-H…π	2.97	0.0055	0.0186	0.0037	-0.0027	0.0010
	5	C-H…π	2.71	0.0074	0.0254	0.0051	-0.0038	0.0013
IMIV-1(b)	1	C-H…π	2.70	0.0085	0.0269	0.0056	-0.0045	0.0011
	2	C-H…O	2.51	0.0085	0.0306	0.0068	-0.0060	0.0008
	3	C-H…O	2.71	0.0076	0.0294	0.0060	-0.0047	0.0013
	4	N-H…O	1.39	0.1011	0.1039	0.0740	-0.1221	-0.0481
	5	C-H…π	2.99	0.0050	0.0155	0.0031	-0.0023	0.0008
IMIV-1(c)	1	π…π	3.11	0.0096	0.0321	0.0065	-0.0050	0.0015
	2	C-H…π	2.64	0.0095	0.0340	0.0068	-0.0050	0.0018
	3	C-H…N	2.54	0.0114	0.0382	0.0083	-0.0070	0.0013

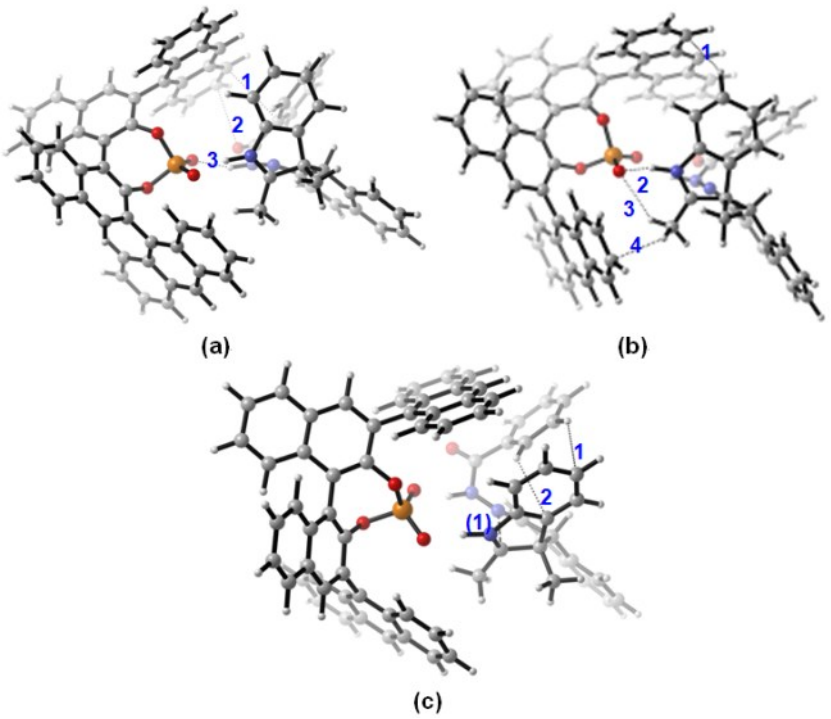

Figure S25 Intermolecular interactions in **TSIII-2** and numbers of bond critical points (BCPs No.).

Table S25 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 **TSIII-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIII-2(a)	1	π…π	3.35	0.0066	0.0190	0.0040	-0.0032	0.0008
	2	lp…π	3.09	0.0085	0.0282	0.0062	-0.0053	0.0009
	3	N-H…O	1.78	0.0353	0.1173	0.0287	-0.0281	0.0006
TSIII-2(b)	1	C-H…π	2.70	0.0079	0.0269	0.0053	-0.0039	0.0014
	2	N-H…O	1.54	0.0680	0.1663	0.0529	-0.0642	-0.0113
	3	C-H…O	2.51	0.0103	0.0358	0.0081	-0.0072	0.0009
	4	C-H…π	2.85	0.0068	0.0194	0.0040	-0.0031	0.0009
TSIII-2(c)	(1)	C…N	2.17	0.0534	0.1128	0.0347	-0.0412	-0.0065
	1	C-H…π	3.07	0.0038	0.0117	0.0023	-0.0016	0.0007
	2	C-H…π	2.90	0.0061	0.0190	0.0039	-0.0030	0.0009

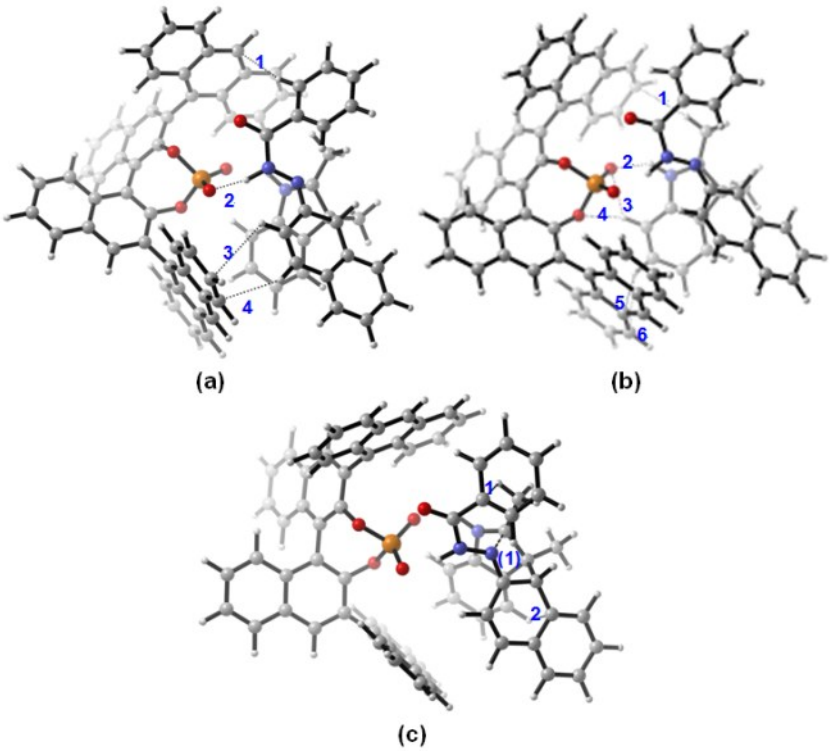

Figure S26 Intermolecular interactions in **TSIV-2** and numbers of bond critical points (BCPs No.).

Table S26 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **TSIV-2**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSIV-2(a)	1	C-H…π	2.53	0.0098	0.0300	0.0065	-0.0055	0.0010
	2	N-H…O	1.67	0.0487	0.1438	0.0379	-0.0398	-0.0019
	3	C-H…π	3.22	0.0032	0.0105	0.0020	-0.0015	0.0005
	4	C-H…π	2.67	0.0083	0.0258	0.0053	-0.0041	0.0012
TSIV-2(b)	1	C-H…π	3.44	0.0021	0.0065	0.0012	-0.0008	0.0004
	2	N-H…O	1.81	0.0344	0.1163	0.0287	-0.0284	0.0003
	3	C-H…O	2.44	0.0124	0.0438	0.0099	-0.0089	0.0010
	4	C-H…O	2.55	0.0080	0.0311	0.0067	-0.0057	0.0010
	5	C-H…π	2.77	0.0080	0.0300	0.0059	-0.0043	0.0016
	6	C-H…π	2.74	0.0081	0.0281	0.0058	-0.0045	0.0013
TSIV-2(c)	(1)	C…N	2.02	0.0742	0.0948	0.0410	-0.0583	-0.0173
	1	C-H…π	2.77	0.0080	0.0262	0.0052	-0.0039	0.0013
	2	C-H…π	2.73	0.0087	0.0309	0.0061	-0.0045	0.0016

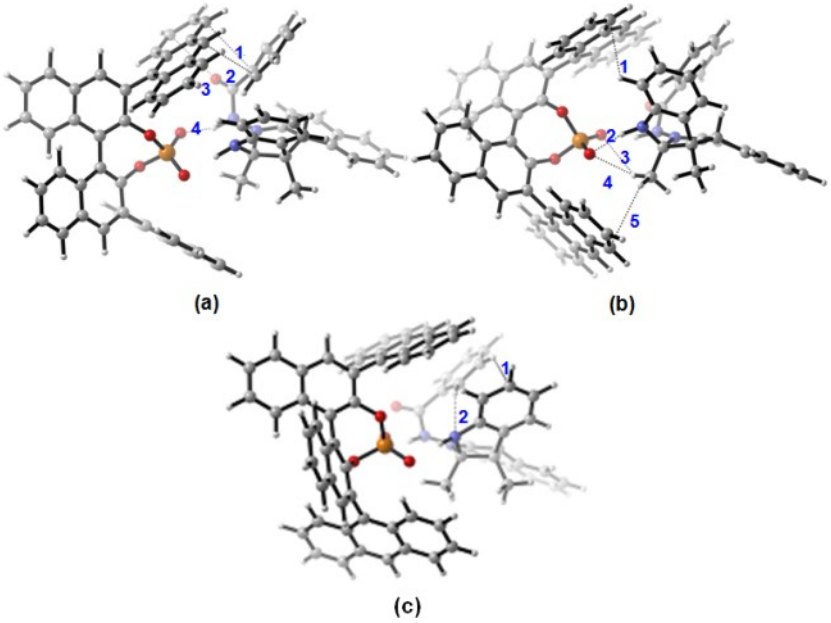

Figure S27 Intermolecular interactions in **IMIII-2** and numbers of bond critical points (BCPs No.).

Table S27 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 **IMIII-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIII-2(a)	1	π…π	3.33	0.0066	0.0194	0.0040	-0.0032	0.0008
	2	π…π	3.39	0.0060	0.0174	0.0036	-0.0028	0.0008
	3	lp…π	3.17	0.0069	0.0234	0.0051	-0.0043	0.0008
	4	N-H…O	1.67	0.0465	0.1439	0.0367	-0.0374	-0.0007
IMIII-2(b)	1	C-H…π	2.79	0.0076	0.0246	0.0049	-0.0037	0.0012
	2	N-H…O	1.79	0.0373	0.1155	0.0296	-0.0303	-0.0007
	3	C-H…π	2.75	0.0069	0.0254	0.0053	-0.0042	0.0011
	4	C-H…π	2.59	0.0103	0.0389	0.0084	-0.0071	0.0013
	5	C-H…π	3.27	0.0029	0.0090	0.0017	-0.0012	0.0005
IMIII-2(c)	1	C-H…π	3.36	0.0024	0.0077	0.0015	-0.0011	0.0004
	2	C-H…N	2.46	0.0121	0.0385	0.0089	-0.0083	0.0006

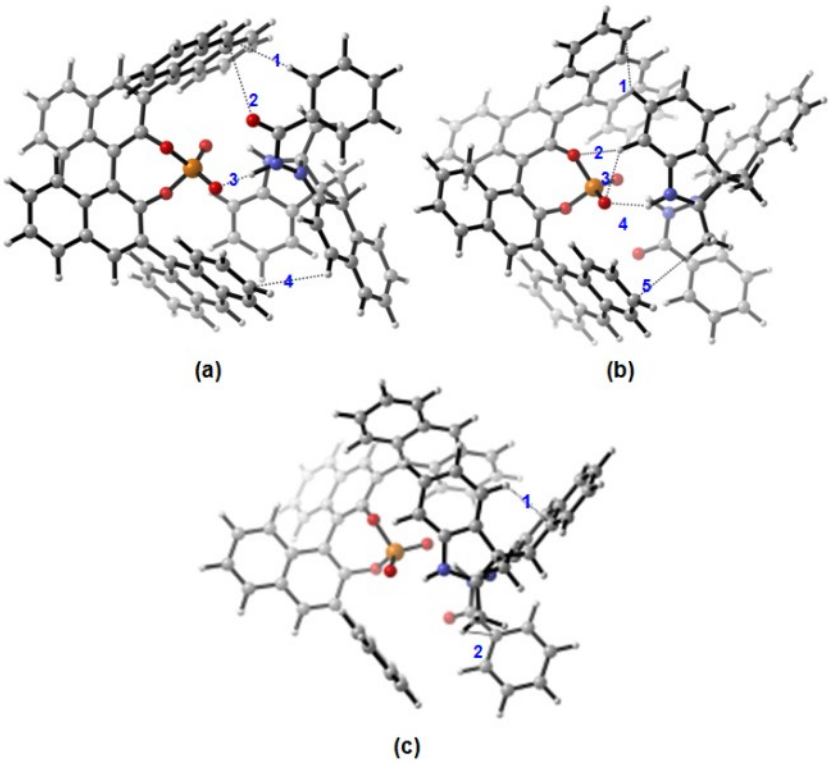

Figure S28 Intermolecular interactions in **IMIV-2** and numbers of bond critical points (BCPs No.).

Table S28 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 **IMIV-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV-2(a)	1	C-H…π	2.75	0.0065	0.0205	0.0042	-0.0032	0.0010
	2	lp…π	3.47	0.0041	0.0151	0.0031	-0.0025	0.0006
	3	N-H…O	1.54	0.0665	0.1609	0.0509	-0.0615	-0.0106
	4	C-H…π	3.19	0.0036	0.0110	0.0022	-0.0016	0.0006
IMIV-2(b)	1	C-H…π	2.75	0.0080	0.0279	0.0057	-0.0043	0.0014
	2	C-H…O	2.63	0.0069	0.0279	0.0059	-0.0047	0.0012
	3	C-H…π	2.47	0.0116	0.0405	0.0092	-0.0082	0.0010
	4	N-H…O	1.84	0.0324	0.1041	0.0264	-0.0267	-0.0003
	5	C-H…π	3.45	0.0021	0.0064	0.0012	-0.0008	0.0004
IMIV-2(c)	1	C-H…π	2.77	0.0081	0.0267	0.0053	-0.0039	0.0014
	2	C-H…π	2.77	0.0087	0.0296	0.0059	-0.0044	0.0015

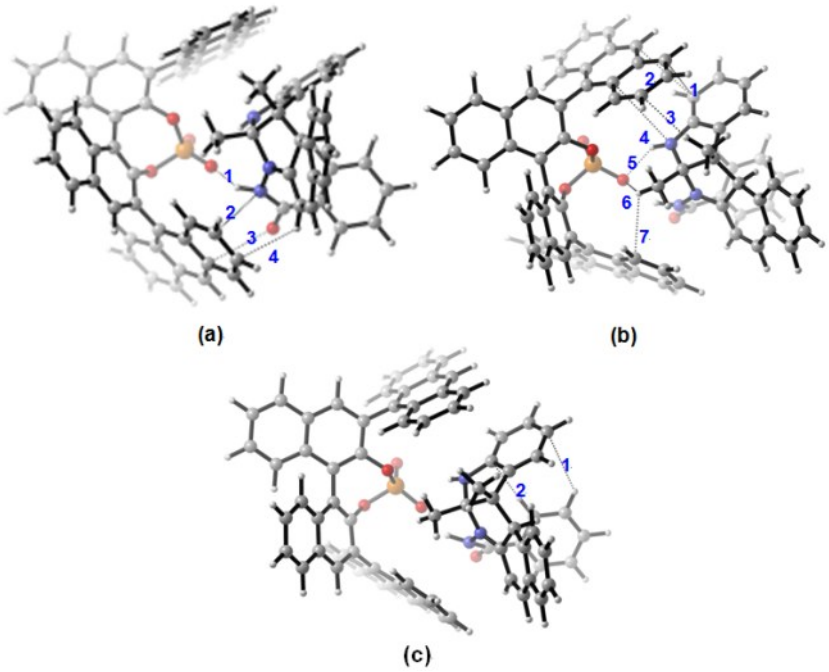

Figure S29 Intermolecular interactions in **IMIII-3** and numbers of bond critical points (BCPs No.).

Table S29 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 **IMIII-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIII-3(a)	1	N-H…O	1.77	0.0345	0.1286	0.0302	-0.0283	0.0019
	2	lp…π	3.33	0.0069	0.0201	0.0045	-0.0041	0.0004
	3	π…π	3.29	0.0060	0.0209	0.0044	-0.0036	0.0008
	4	C-H…π	2.68	0.0084	0.0300	0.0058	-0.0041	0.0017
IMIII-3(b)	1	π…π	3.38	0.0063	0.0183	0.0038	-0.0030	0.0008
	2	π…π	3.42	0.0061	0.0187	0.0038	-0.0029	0.0009
	3	C-H…π	2.60	0.0089	0.0284	0.0059	-0.0047	0.0012
	4	lp…π	3.85	0.0024	0.0089	0.0018	-0.0013	0.0005
	5	N-H…O	2.04	0.0232	0.0673	0.0181	-0.0194	-0.0013
	6	C-H…O	2.34	0.0144	0.0448	0.0110	-0.0109	0.0001
	7	C-H…π	2.89	0.0061	0.0212	0.0040	-0.0028	0.0012
IMIII-3(c)	1	C-H…π	3.43	0.0021	0.0067	0.0013	-0.0009	0.0004
	2	C-H…π	2.44	0.0117	0.0370	0.0082	-0.0071	0.0011

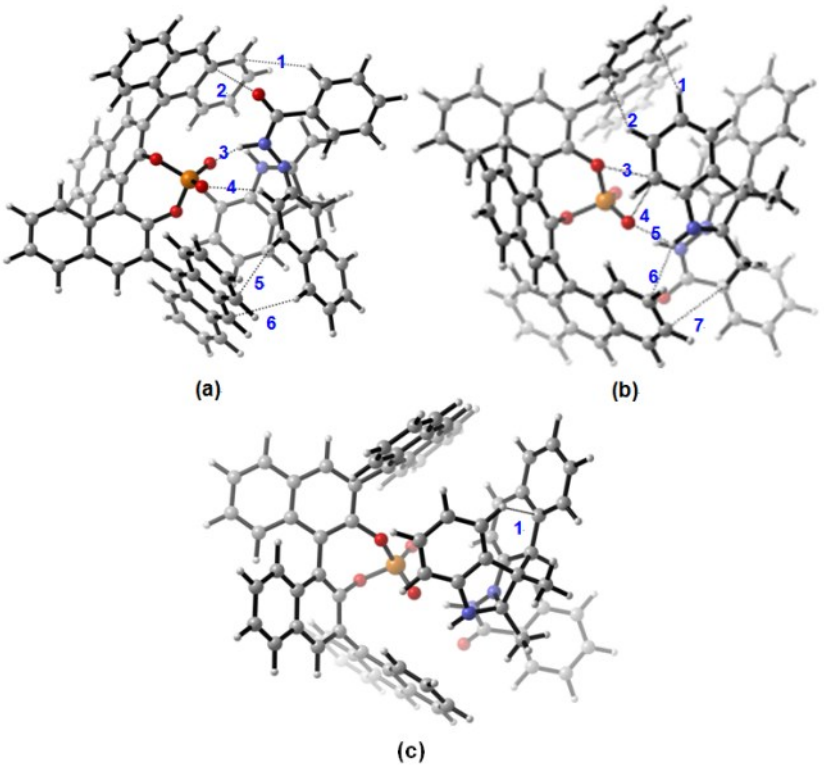

Figure S30 Intermolecular interactions in **IMIV-3** and numbers of bond critical points (BCPs No.).

Table S30 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 **IMIV-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV-3(a)	1	C-H…π	3.33	0.0023	0.0074	0.0014	-0.0009	0.0005
	2	lp…π	3.09	0.0081	0.0281	0.0061	-0.0052	0.0009
	3	N-H…O	1.57	0.0633	0.1637	0.0492	-0.0574	-0.0082
	4	C-H…O	2.41	0.0112	0.0374	0.0087	-0.0081	0.0006
	5	C-H…π	2.66	0.0085	0.0250	0.0053	-0.0043	0.0010
	6	C-H…π	3.08	0.0048	0.0161	0.0031	-0.0022	0.0009
IMIV-3(b)	1	C-H…π	2.67	0.0085	0.0265	0.0056	-0.0046	0.0010
	2	C-H…π	2.96	0.0054	0.0170	0.0033	-0.0024	0.0009
	3	lp…π	3.24	0.0062	0.0207	0.0045	-0.0038	0.0007
	4	lp…π	3.05	0.0098	0.0348	0.0076	-0.0066	0.0010
	5	N-H…O	2.35	0.0126	0.0488	0.0111	-0.0099	0.0012
	6	N-H…π	2.47	0.0111	0.0342	0.0075	-0.0065	0.0010
	7	C-H…π	2.99	0.0043	0.0127	0.0025	-0.0018	0.0007
IMIV-3(c)	1	C-H…π	2.74	0.0087	0.0294	0.0058	-0.0043	0.0015

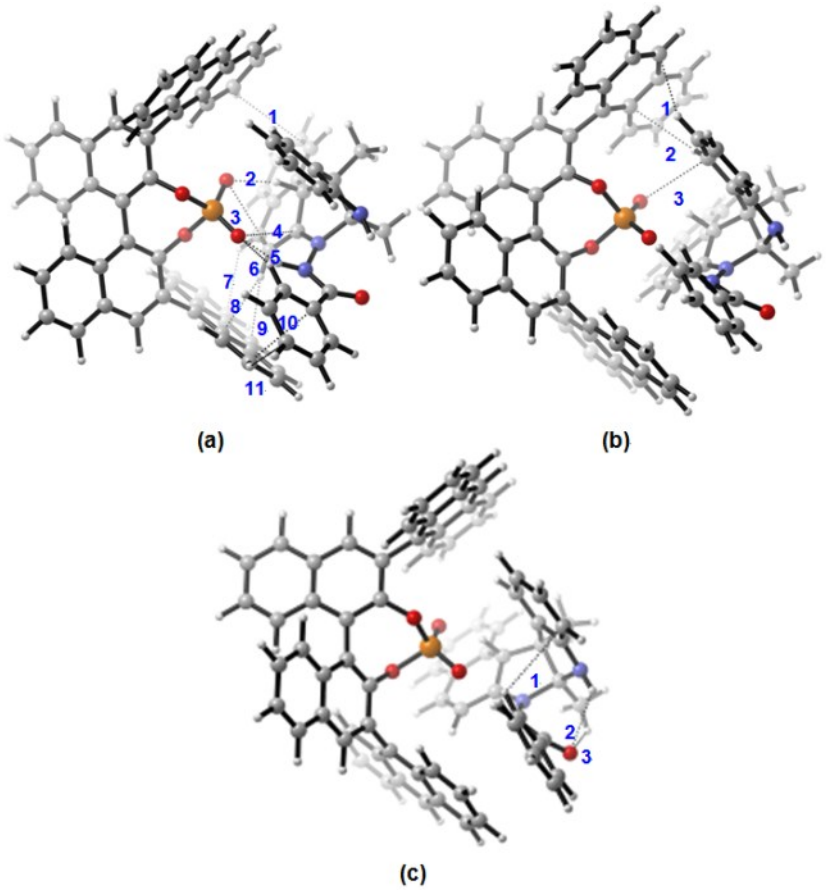

Figure S31 Intermolecular interactions in **IMIII-4** and numbers of bond critical points (BCPs No.).

Table S31 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 **IMIII-4**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMIII-4(a)	1	C-H…π	3.50	0.0018	0.0060	0.0011	-0.0008	0.0003
	2	C-H…O	1.85	0.0349	0.1020	0.0268	-0.0281	-0.0013
	3	π…π	3.25	0.0081	0.0287	0.0060	-0.0049	0.0011
	4	lp…π	3.06	0.0095	0.0332	0.0073	-0.0062	0.0011
	5	N-H…O	1.73	0.0389	0.1331	0.0323	-0.0313	0.0010
	6	C-H…O	2.46	0.0097	0.0338	0.0077	-0.0069	0.0008
	7	C-H…π	2.73	0.0079	0.0255	0.0053	-0.0043	0.0010
	8	C-H…π	2.70	0.0079	0.0269	0.0057	-0.0047	0.0010
	9	C-H…π	2.71	0.0082	0.0284	0.0059	-0.0047	0.0012
	10	π…π	3.18	0.0083	0.0263	0.0055	-0.0044	0.0011
	11	C-H…π	2.87	0.0062	0.0203	0.0042	-0.0033	0.0009
IMIII-4(b)	1	C-H…π	2.57	0.0105	0.0341	0.0073	-0.0061	0.0012
	2	C-H…π	2.82	0.0064	0.0225	0.0046	-0.0035	0.0011
	3	lp…π	3.12	0.0088	0.0328	0.0069	-0.0056	0.0013
IMIII-4(c)	1	C-H…π	3.22	0.0032	0.0097	0.0019	-0.0013	0.0006
	2	N-H…π	2.36	0.0132	0.0518	0.0114	-0.0099	0.0015
	3	C-H…O	2.35	0.0137	0.0469	0.0109	-0.0101	0.0008

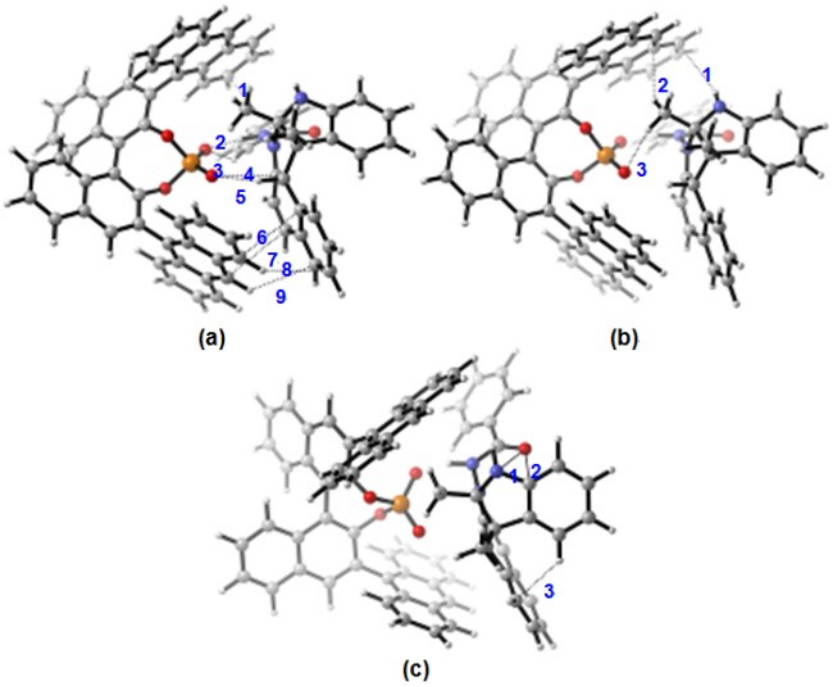

Figure S32 Intermolecular interactions in **IMIV-4** and numbers of bond critical points (BCPs No.).

Table S32 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 **IMIV-4**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV-4(a)	1	π…π	3.21	0.0081	0.0261	0.0053	-0.0041	0.0012
	2	N-H…O	1.56	0.0629	0.1662	0.0494	-0.0573	-0.0079
	3	C-H…O	2.32	0.0130	0.0439	0.0105	-0.0100	0.0005
	4	π…π	2.79	0.0133	0.0476	0.0109	-0.0100	0.0009
	5	C-H…O	2.29	0.0142	0.0508	0.0118	-0.0109	0.0009
	6	π…π	3.37	0.0064	0.0193	0.0040	-0.0032	0.0008
	7	π…π	3.37	0.0054	0.0162	0.0033	-0.0026	0.0007
	8	C-H…π	2.81	0.0070	0.0223	0.0046	-0.0036	0.0010
	9	C-H…π	2.97	0.0049	0.0156	0.0031	-0.0022	0.0009
IMIV-4(b)	1	N-H…π	3.14	0.0026	0.0088	0.0016	-0.0011	0.0005
	2	C-H…π	2.69	0.0083	0.0284	0.0059	-0.0047	0.0012
	3	C-H…O	2.32	0.0150	0.0477	0.0116	-0.0113	0.0003
IMIV-4(c)	1	lp…π	3.14	0.0084	0.0302	0.0070	-0.0064	0.0006
	2	lp…π	3.08	0.0083	0.0309	0.0068	-0.0059	0.0009
	3	C-H…π	2.64	0.0086	0.0277	0.0057	-0.0044	0.0013

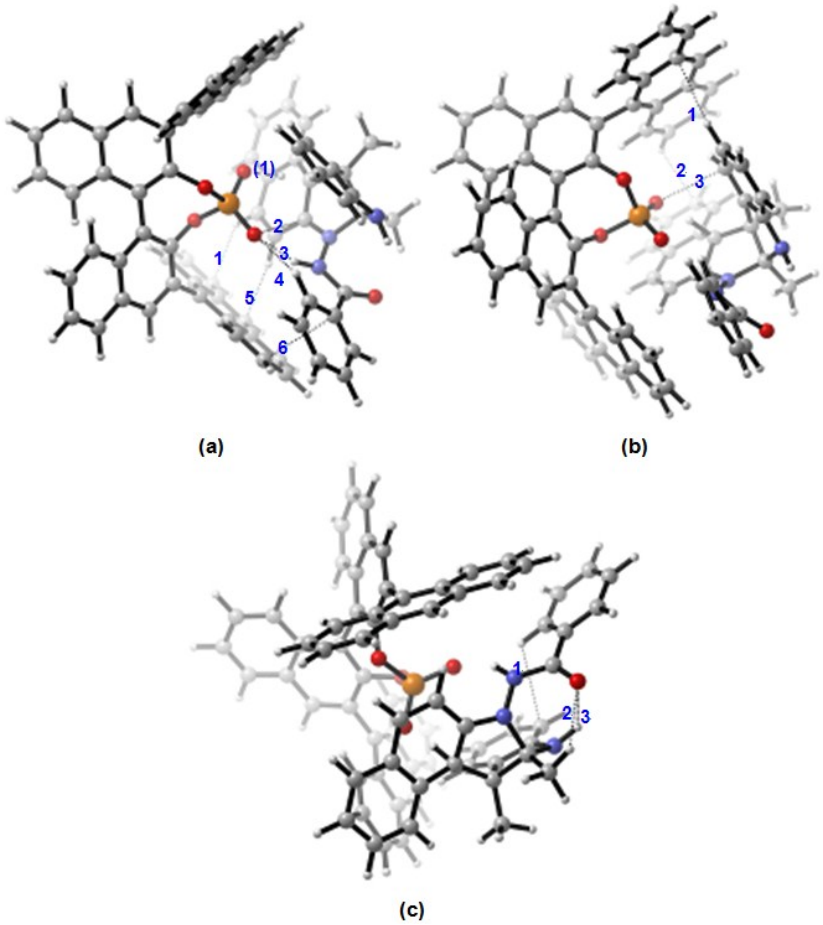

Figure S33 Intermolecular interactions in **TSIII-3** and numbers of bond critical points (BCPs No.).

Table S33 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSIII-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIII-3(a)	(1)	O…H	1.45	0.0900	0.1299	0.0611	-0.0897	-0.0286
	1	C-H…π	2.73	0.0079	0.0254	0.0054	-0.0043	0.0011
	2	π…π	3.17	0.0078	0.0275	0.0060	-0.0051	0.0009
	3	N-H…O	1.79	0.0343	0.1173	0.0284	-0.0275	0.0009
	4	C-H…O	2.49	0.0091	0.0321	0.0072	-0.0064	0.0008
	5	C-H…π	2.62	0.0095	0.0311	0.0066	-0.0055	0.0011
	6	π…π	3.14	0.0088	0.0285	0.0059	-0.0047	0.0012
TSIII-3(b)	1	C-H…π	2.61	0.0094	0.0310	0.0065	-0.0053	0.0012
	2	C-H…π	2.85	0.0063	0.0196	0.0039	-0.0029	0.0010
	3	lp…π	3.00	0.0105	0.0388	0.0084	-0.0072	0.0012
TSIII-3(c)	1	C-H…π	3.16	0.0035	0.0106	0.0021	-0.0015	0.0006
	2	C-H…O	2.35	0.0135	0.0460	0.0107	-0.0100	0.0007
	3	N-H…π	2.41	0.0125	0.0508	0.0109	-0.0090	0.0019

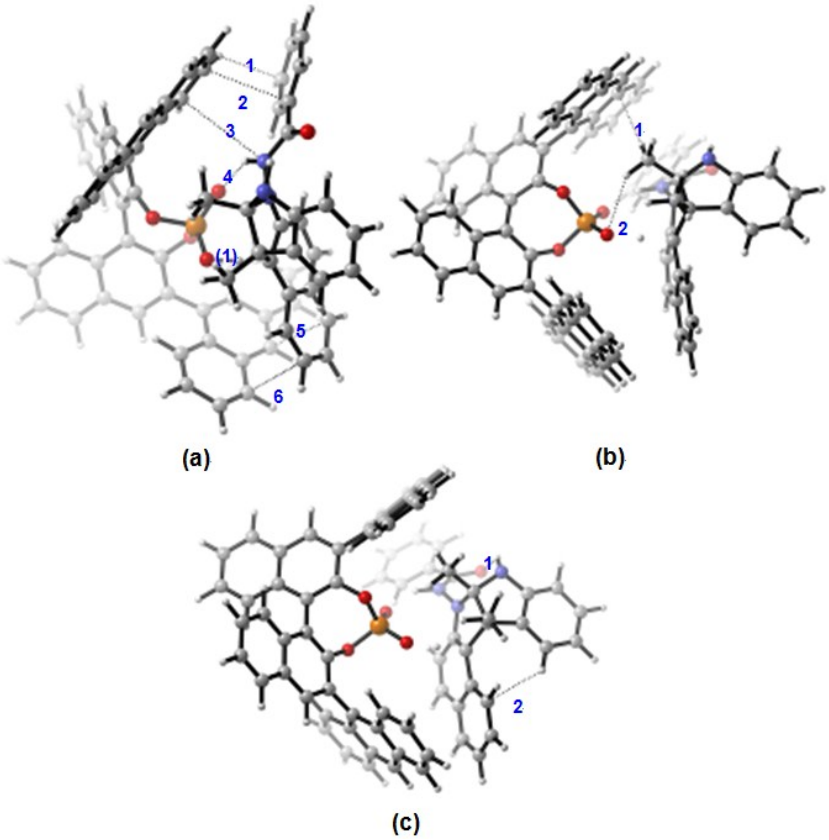

Figure S34 Intermolecular interactions in **TSIV-3** and numbers of bond critical points (BCPs No.).

Table S34 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSIV-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIV-3(a)	(1)	O…H	1.35	0.1161	0.0282	0.0734	-0.1397	-0.0663
	1	C-H…π	2.80	0.0071	0.0232	0.0047	-0.0037	0.0010
	2	π…π	3.28	0.0073	0.0224	0.0046	-0.0037	0.0009
	3	lp…π	3.88	0.0026	0.0091	0.0017	-0.0012	0.0005
	4	N-H…O	1.82	0.0324	0.1151	0.0280	-0.0273	0.0007
	5	π…π	3.27	0.0070	0.0204	0.0042	-0.0033	0.0009
	6	π…π	3.36	0.0063	0.0184	0.0038	-0.0029	0.0009
TSIV-3(b)	1	C-H…π	2.66	0.0086	0.0285	0.0060	-0.0048	0.0012
	2	C-H…π	2.47	0.0114	0.0388	0.0089	-0.0080	0.0009
TSIV-3(c)	1	N-H…O	2.28	0.0145	0.0478	0.0117	-0.0115	0.0002
	2	C-H…π	2.64	0.0084	0.0276	0.0056	-0.0043	0.0013

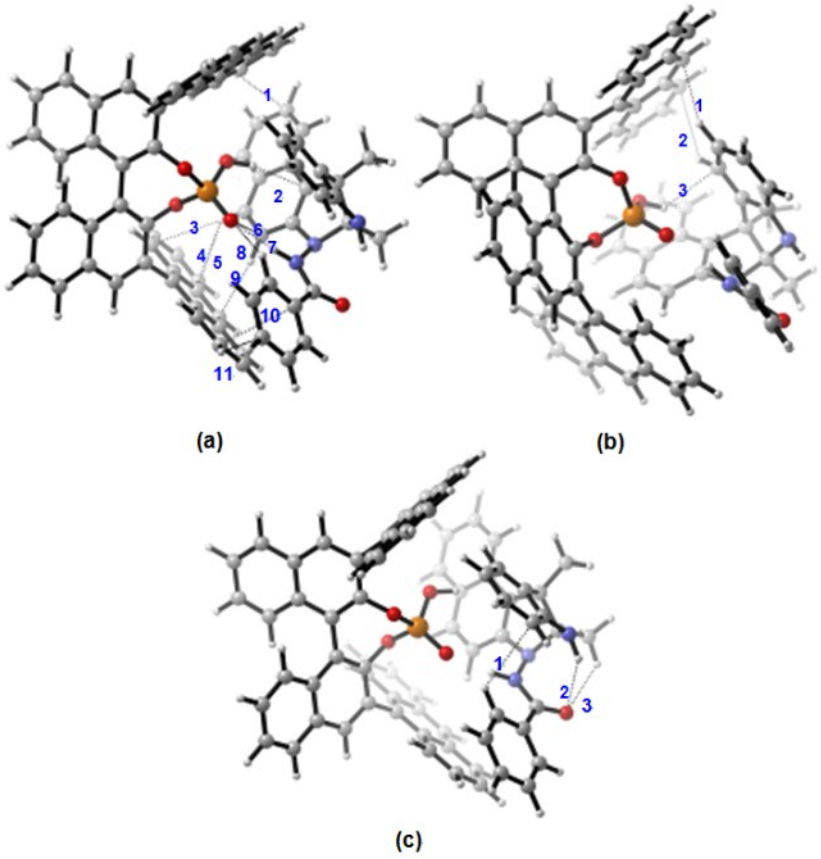

Figure S35 Intermolecular interactions in **IMIII-5** and numbers of bond critical points (BCPs No.).

Table S35 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 **IMIII-5**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIII-5(a)	1	C-H…π	2.72	0.0076	0.0251	0.0050	-0.0038	0.0012
	2	O-H…π	2.38	0.0131	0.0374	0.0087	-0.0081	0.0006
	3	C-H…π	2.82	0.0068	0.0228	0.0048	-0.0038	0.0010
	4	C-H…π	2.80	0.0070	0.0238	0.0049	-0.0039	0.0010
	5	C-H…π	2.79	0.0070	0.0258	0.0052	-0.0040	0.0012
	6	π…π	3.37	0.0063	0.0196	0.0042	-0.0034	0.0008
	7	N-H…O	1.88	0.0268	0.0934	0.0225	-0.0217	0.0008
	8	C-H…O	2.38	0.0108	0.0382	0.0087	-0.0079	0.0008
	9	C-H…π	2.62	0.0094	0.0301	0.0064	-0.0053	0.0011
	10	π…π	3.22	0.0077	0.0243	0.0051	-0.0040	0.0011
	11	C-H…π	2.83	0.0067	0.0215	0.0044	-0.0035	0.0009
IMIII-5(b)	1	C-H…π	2.57	0.0106	0.0355	0.0075	-0.0062	0.0013
	2	C-H…π	2.97	0.0052	0.0166	0.0034	-0.0026	0.0008
	3	O-H…π	2.46	0.0110	0.0429	0.0089	-0.0070	0.0019
IMIII-5(c)	1	C-H…π	3.03	0.0045	0.0138	0.0027	-0.0020	0.0007
	2	N-H…π	2.38	0.0131	0.0531	0.0115	-0.0098	0.0017
	3	C-H…O	2.54	0.0095	0.0337	0.0075	-0.0065	0.0010

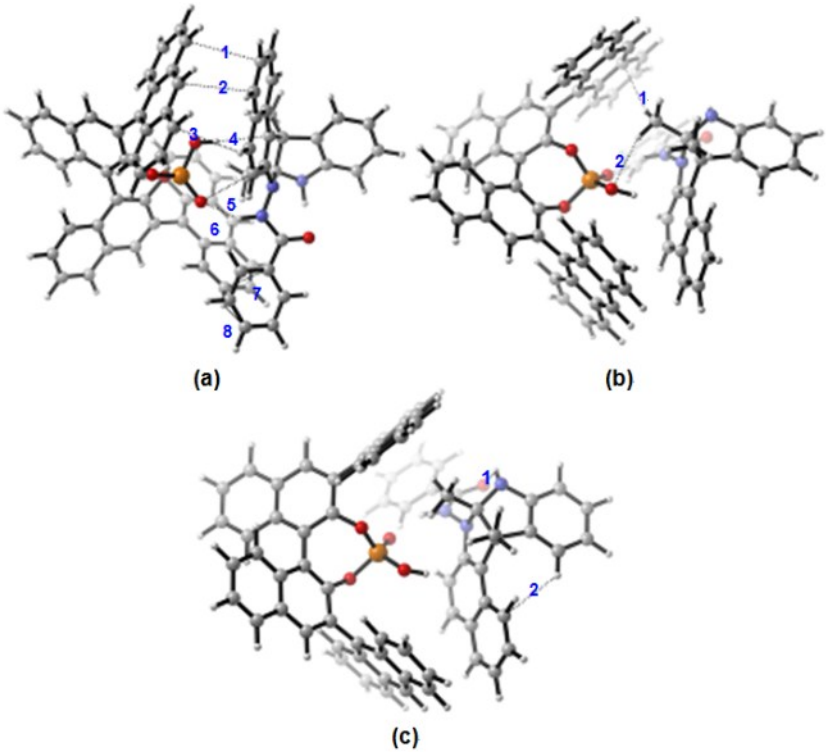

Figure S36 Intermolecular interactions in **IMIV-5** and numbers of bond critical points (BCPs No.).

Table S36 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 **IMIV-5**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV-5(a)	1	π…π	3.39	0.0059	0.0184	0.0037	-0.0027	0.0010
	2	π…π	3.23	0.0074	0.0238	0.0048	-0.0036	0.0012
	3	C-H…π	3.44	0.0019	0.0065	0.0012	-0.0008	0.0004
	4	O-H…π	2.34	0.0149	0.0369	0.0089	-0.0085	0.0004
	5	π…π	3.16	0.0078	0.0263	0.0058	-0.0049	0.0009
	6	N-H…O	1.85	0.0294	0.1063	0.0257	-0.0248	0.0009
	7	π…π	3.22	0.0079	0.0250	0.0052	-0.0041	0.0011
	8	C-H…π	2.82	0.0069	0.0224	0.0046	-0.0036	0.0010
IMIV-5(b)	1	C-H…π	2.63	0.0090	0.0295	0.0062	-0.0049	0.0013
	2	C-H…π	2.48	0.0106	0.0344	0.0080	-0.0074	0.0006
IMIV-5(c)	1	N-H…O	2.34	0.0128	0.0427	0.0103	-0.0099	0.0004
	2	C-H…π	2.82	0.0063	0.0212	0.0041	-0.0030	0.0011

2. Mechanisms of enantioselective CP3-catalyzed S_NAr reaction between the azobenzene derivative ($R1_{C2}$ (R=Bz)) and dimethylindole (R2) leading to chiral pyrroloindoline.

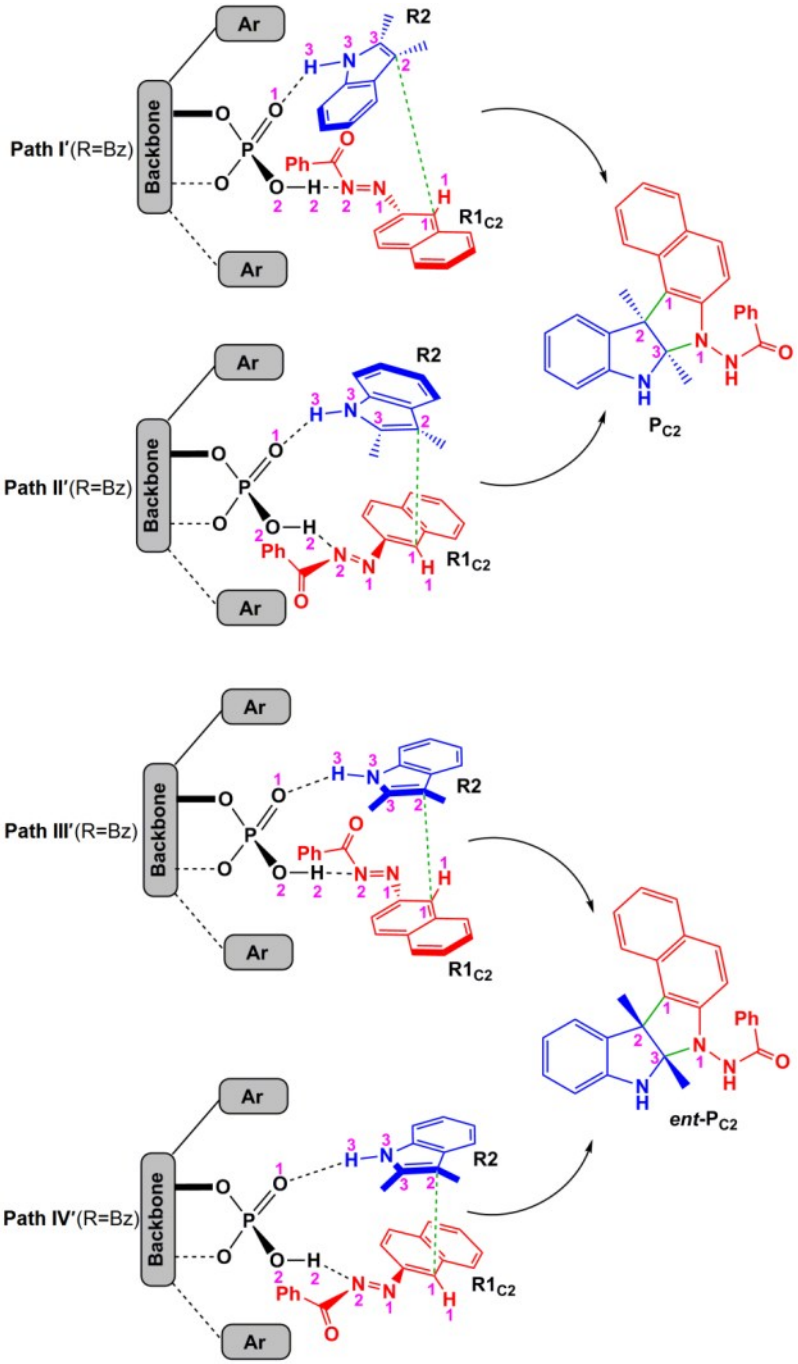

Figure S37 Four modes for the reaction between the azobenzene derivative $\mathbf{R1_{C2}}$ (R=Bz)) and dimethylindole (**R2**) catalyzed by **CP3** (Ar= 9-anthryl) and the resultant $\mathbf{P1_{C2}}$ and *ent*-$\mathbf{P1_{C2}}$ products.

The reaction between the azobenzene derivative (**R1$_{C2}$**, (R=Bz) and dimethylindole (**R2**) catalyzed by **CP3** in Scheme 1 may occur *via* four different modes which correspond to four paths (i.e., paths **I′-IV′** (R=Bz), as shown in Figure S37. The reactions between **R1$_{C2}$** (R=Bz) and **R2** in paths **I′** and **II′** (or paths **III′** and **IV′**) proceed from different directions but lead to the same products **P1$_{C2}$** (or the same products *ent*-**P1$_{C2}$**).

Paths **I′** and **II′** are the ways to yield the product **P1$_{C2}$** (R=Bz), the Gibbs free energy profile for the whole reaction processes is depicted in Figures S38 and S39, and the optimized geometries of the reactants, complex, transition states, intermediates and product are shown in Figures S40 and S41. Like the reactions in path **I** and path **II**, both the reactants **R1$_{C2}$** (R=Bz) and **R2** are activated via dual HB bonding with catalyst **CP3**, forming the trimeric complexes **COMI'** and **COMII'** respectively in path **I'** and path **II'**. From the QTAIM analyses (Figure S42 and Table S37, Figure S43 and Table S38), we found that the O2–H2···N2 HB also exists between the O2–H2 group of **CP3** and the N1=N2Bz group of **R1$_{C2}$** (R=Bz) and the O1···H3–N3 HB etween the P=O1 group of **CP3** and the N3–H3 group of **R2** in **COMI'** or **COMII'**. Not surprisingly, other interactions like C–H···π interactions between C–H groups of **R1$_{C2}$** (R=Bz), **R2** and anthryl groups of**CP3**, as well as the ···π interactions between **R1$_{C2}$** (R=Bz) and **R2** are also found in **COMI'** or **COMII'**, which contribute to the stabilization of the complex system and facilitate the subsequent C1–C2 bond formation. As shown in Table S39, in either **COMI'** or **COMII'**, the O2–H2···N2 HB is stronger than O1···H3–N3 HB in **COMI'** or **COMII'** (R=Bz), and this is related to the correspondingly shorter bond distance compared O2–H2···N2 HB with O1···H3–N3 HB. Relative to the natural atomic charge on C1

atom in $\mathbf{R1_{C2}}$ (R=Bz) (or the natural atomic charge on C2 atom in **R2**), the natural atomic charge on C1 atom (or on C2 atom) in **COMI'** or **COMII'** becomes less negative (or more negative), which indicates that the C1 atom becomes more susceptible to nucleophilic attack and the C2 atom becomes more susceptible to electrophilic attack.

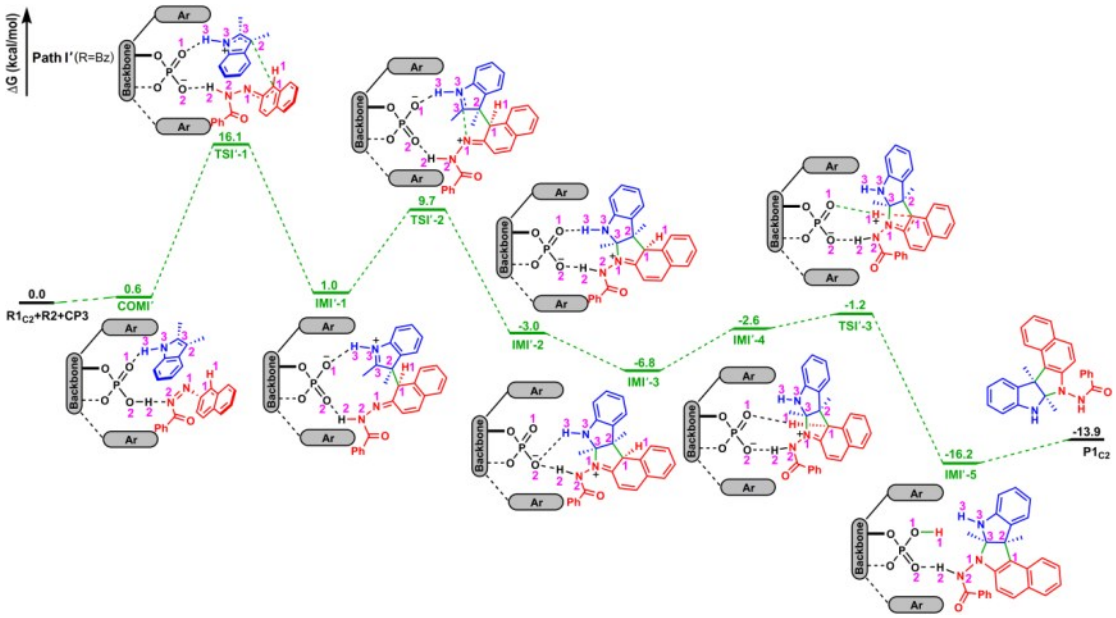

Figure S38 The path **I'** for the reaction between $\mathbf{R1_{C2}}$ (R=Bz) and **R2** catalyzed by **CP3** (Ar= 9-anthryl) and the free energy profile of the whole processes. The Gibbs free energies of [$\mathbf{R1_{C2}}$**+R2+CP3**] were set to 0.0 kcal/mol as reference.

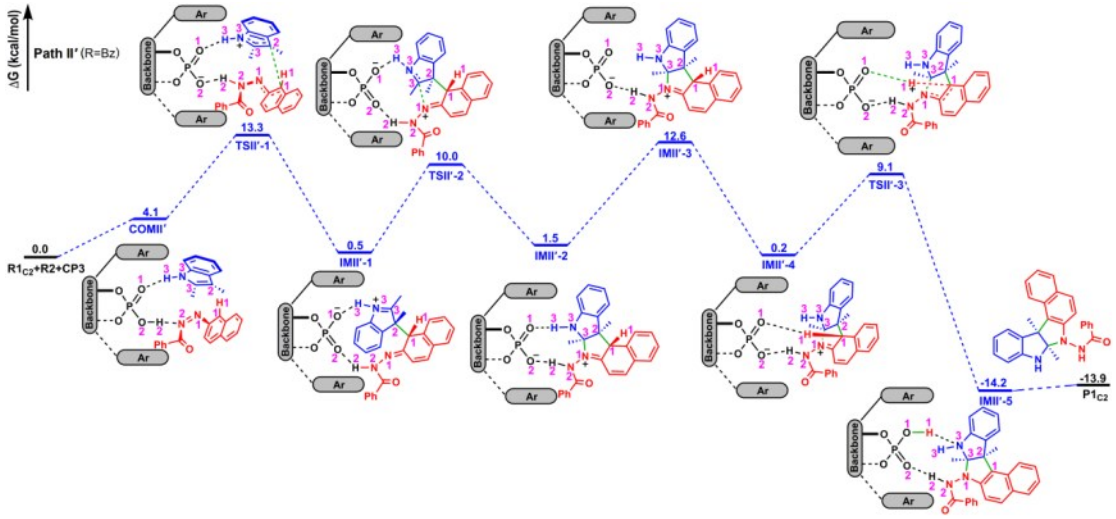

Figure S39 The path **II'** for the reaction between $\mathbf{R1_{C2}}$ (R=Bz) and **R2** catalyzed by **CP3** (Ar= 9-anthryl) and the free energy profile of the whole processes. The Gibbs free energies of [$\mathbf{R1_{C2}}$**+R2+CP3**] were set to 0.0 kcal/mol as reference.

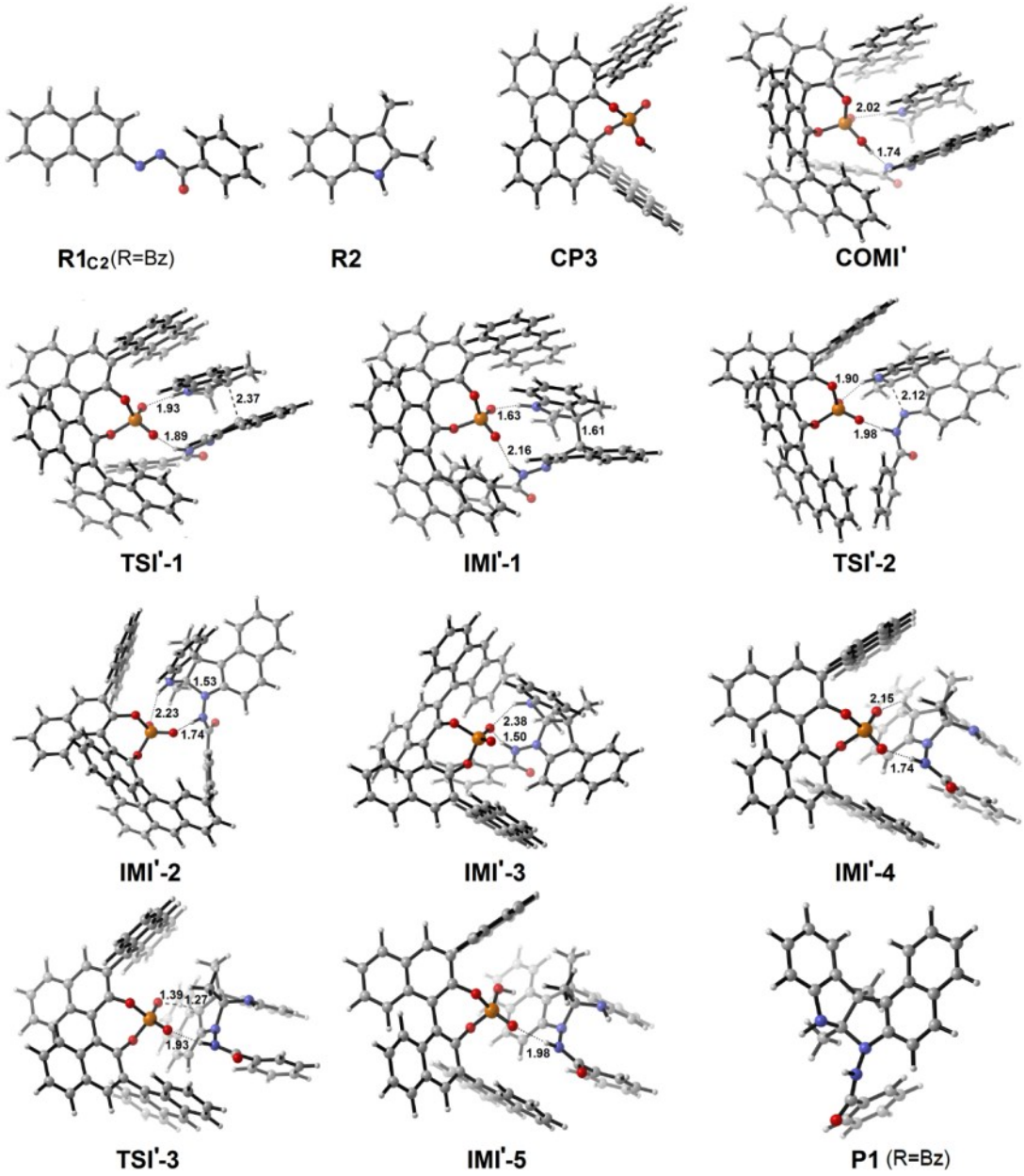

Figure S40 The optimized geometries of the complex, transition states and intermediates in path **I'** (R=Bz). The distances are in Å.

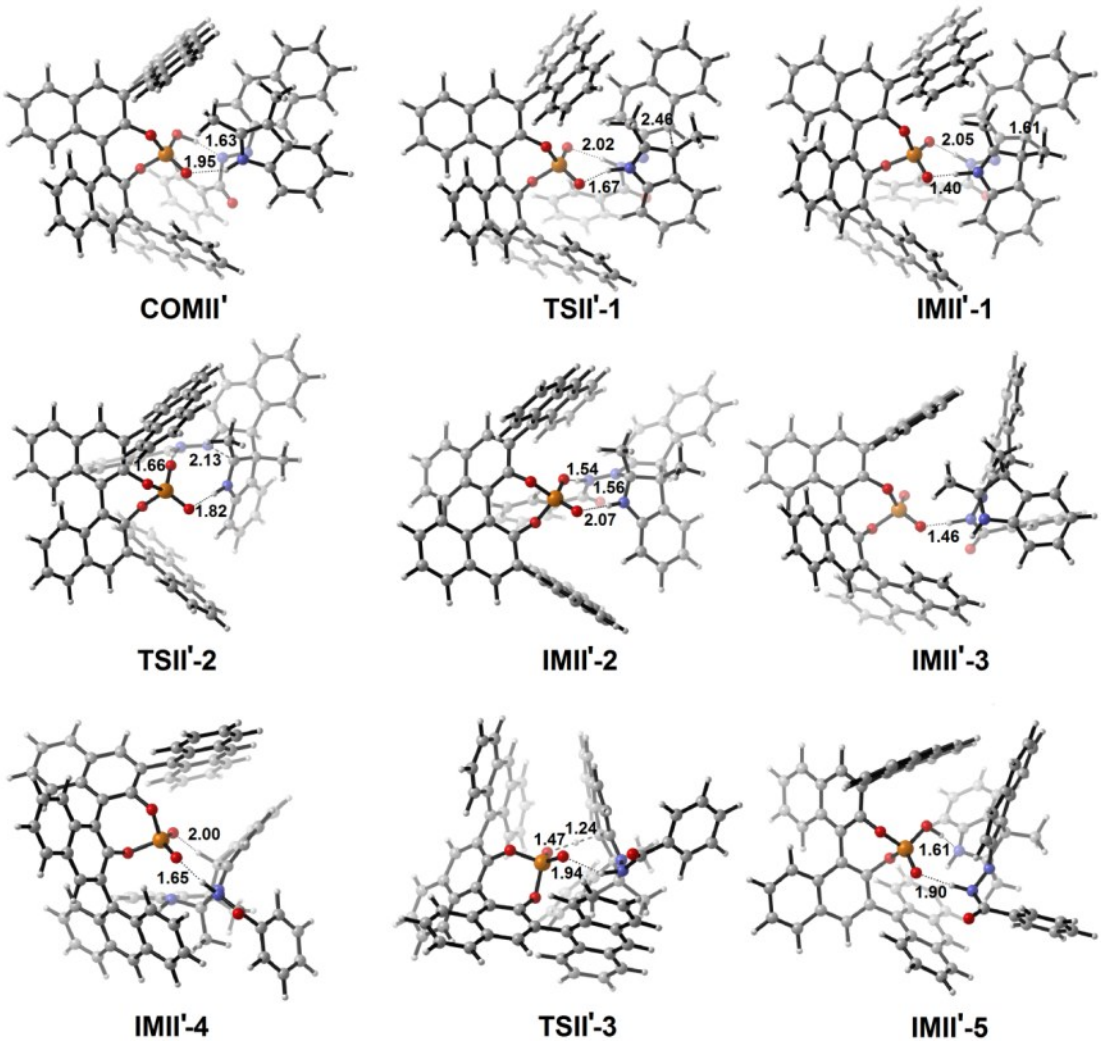

Figure S41 The optimized geometries of the complex, transition states and intermediates in path **II'** (R=Bz). The distances are in Å.

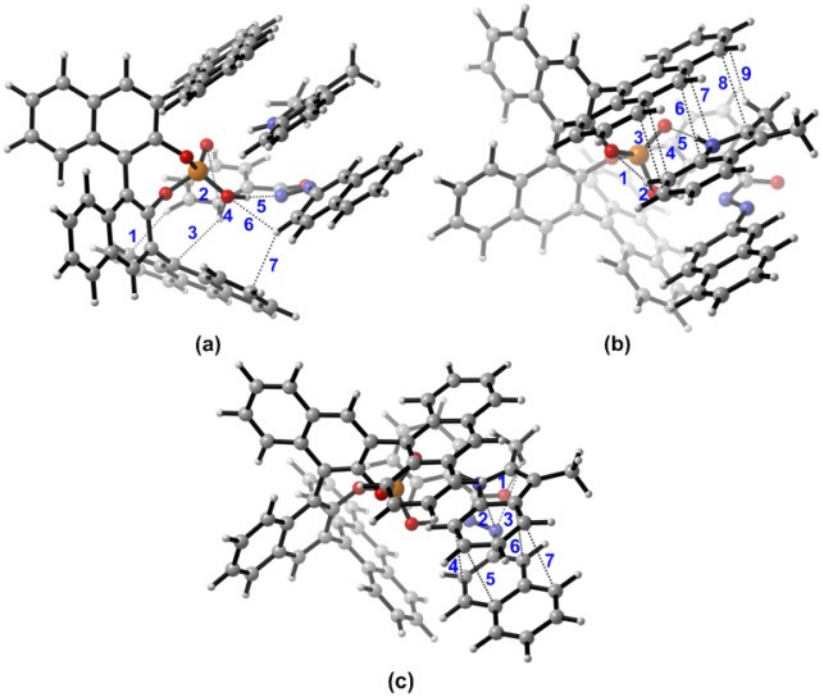

Figure S42 Intermolecular interactions in **COMI'** and numbers of bond critical points (BCPs No.).

Table S37 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'(a)	1	C-H…π	2.54	0.0107	0.0341	0.0074	-0.0063	0.0011
	2	π…π	3.07	0.0096	0.0306	0.0068	-0.0059	0.0009
	3	C-H…π	2.98	0.0052	0.0166	0.0034	-0.0027	0.0007
	4	C-H…π	2.62	0.0086	0.0345	0.0071	-0.0055	0.0016
	5	O-H…N	1.74	0.0472	0.0968	0.0285	-0.0328	-0.0043
	6	C-H…O	2.41	0.0114	0.0524	0.0106	-0.0081	0.0025
	7	C-H…π	2.59	0.0094	0.0290	0.0061	-0.0050	0.0011
COMI'(b)	1	C-H…O	2.40	0.0111	0.0368	0.0087	-0.0083	0.0004
	2	C-H…π	2.71	0.0066	0.0252	0.0053	-0.0043	0.0010
	3	π…π	3.37	0.0068	0.0199	0.0041	-0.0033	0.0008
	4	π…π	3.39	0.0068	0.0188	0.0040	-0.0032	0.0008
	5	N-H…O	2.02	0.0227	0.0659	0.0173	-0.0182	-0.0009
	6	π…π	3.34	0.0072	0.0201	0.0042	-0.0035	0.0007
	7	lp…π	3.35	0.0064	0.0194	0.0043	-0.0038	0.0005
	8	π…π	3.32	0.0069	0.0187	0.0040	-0.0033	0.0007
	9	C-H…π	2.99	0.0056	0.0180	0.0036	-0.0027	0.0009
COMI'(c)	1	C-H…π	2.66	0.0068	0.0237	0.0050	-0.0041	0.0009
	2	lp…π	3.09	0.0088	0.0282	0.0064	-0.0058	0.0006
	3	C-H…N	2.95	0.0046	0.0172	0.0035	-0.0027	0.0008
	4	π…π	3.52	0.0053	0.0146	0.0031	-0.0025	0.0006
	5	π…π	3.43	0.0057	0.0162	0.0034	-0.0027	0.0007
	6	π…π	3.21	0.0082	0.0238	0.0050	-0.0040	0.0010
	7	π…π	3.31	0.0070	0.0198	0.0041	-0.0033	0.0008

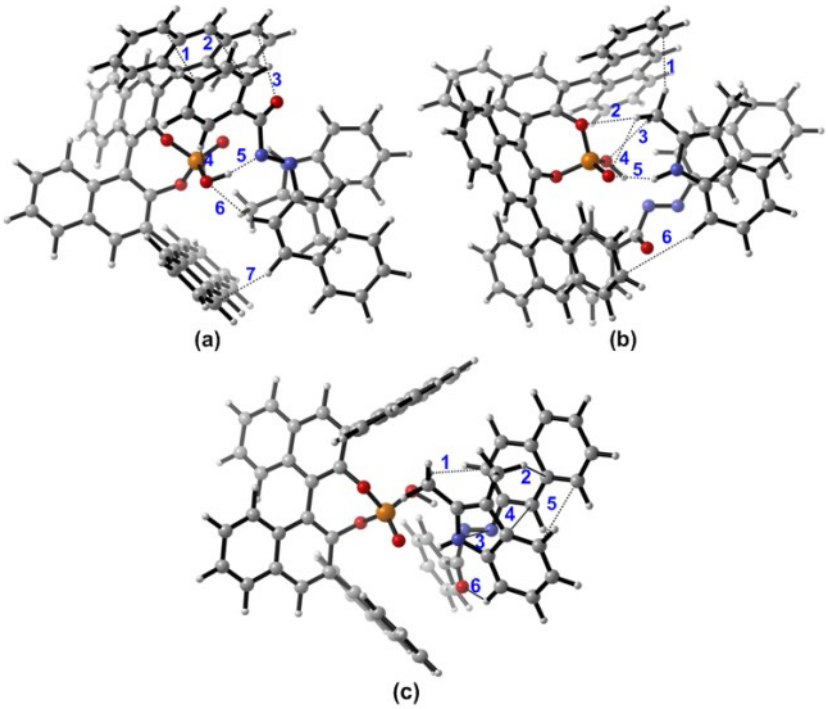

Figure S43 Intermolecular interactions in **COMII'** and numbers of bond critical points (BCPs No.).

Table S38 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'(a)	1	π…π	3.21	0.0079	0.0227	0.0047	-0.0038	0.0009
	2	π…π	3.21	0.0078	0.0222	0.0046	-0.0037	0.0009
	3	lp…π	3.33	0.0053	0.0184	0.0039	-0.0032	0.0007
	4	C-H…O	2.32	0.0136	0.0437	0.0106	-0.0104	0.0002
	5	O-H…N	1.63	0.0635	0.1021	0.0385	-0.0515	-0.0130
	6	C-H…O	2.43	0.0106	0.0448	0.0094	-0.0077	0.0017
	7	C-H…π	2.59	0.0089	0.0291	0.0061	-0.0049	0.0012
COMII'(b)	1	C-H…π	2.73	0.0078	0.0250	0.0052	-0.0041	0.0011
	2	C-H…O	2.62	0.0080	0.0307	0.0065	-0.0054	0.0011
	3	C-H…π	2.79	0.0062	0.0224	0.0046	-0.0036	0.0010
	4	C-H…π	2.74	0.0078	0.0290	0.0060	-0.0048	0.0012
	5	N-H…O	1.95	0.0239	0.0789	0.0198	-0.0199	-0.0001
	6	C-H…π	3.61	0.0012	0.0042	0.0008	-0.0005	0.0003
COMII'(c)	1	C-H…π	2.86	0.0059	0.0183	0.0037	-0.0027	0.0010
	2	C-H…π	2.92	0.0059	0.0210	0.0042	-0.0032	0.0010
	3	π…π	3.05	0.0091	0.0297	0.0067	-0.0060	0.0007
	4	π…π	3.07	0.0099	0.0310	0.0065	-0.0053	0.0012
	5	π…π	3.37	0.0060	0.0190	0.0038	-0.0028	0.0010
	6	C-H…O	2.55	0.0079	0.0288	0.0063	-0.0053	0.0010

Table S39 The intermolecular distances (d, in Å) for the HBs, the HB strengths (E_{HB}, in kcal/mol) and the natural atomic charges (q, in electrons) in the complexes **COMI'-IV'** (R=Bz) formed in paths **I'-IV'** (R=Bz).[a]

Complex	HB[b]		Natural atomic charge[c]	
	O1···H3-N3	O2-H2···N2	q_{C1}	q_{C2}
COMI'	$d_{(O1\cdots H1)}$=2.02	$d_{(H2\cdots N2)}$=1.74	–0.12878	–0.12884
	E_{HB}=–4.7	E_{HB}=–7.7		
COMII'	$d_{(O1\cdots H1)}$=1.95	$d_{(H2\cdots N2)}$=1.63	–0.13024	–0.12370
	E_{HB}=–5.3	E_{HB}=–10.4		
COMIII'	$d_{(O1\cdots H1)}$=2.23	$d_{(H2\cdots N2)}$=1.75	–0.15576	–0.12614
	E_{HB}=–3.3	E_{HB}=–7.7		
COMIV'	$d_{(O1\cdots H1)}$=2.15	$d_{(H2\cdots N2)}$=1.67	–0.14795	–0.12519
	E_{HB}=–4.1	E_{HB}=–9.4		

[a] The atomic number is shown in Figure 1.

[b] The HB strength is calculated as E_{HB}=–0.429•G_{BCP}, herein G_{BCP} is the local electronic kinetic energy density at the bond critical point (BCP) of HB.

[c]The natural atomic charge on C1 atom in $\mathbf{R1_{C2}}$ (R=Bz) (q_{C1}) is –0.17463 electrons, and that on C2 atom in **R2** (q_{C2}) is –0.12070 electrons.

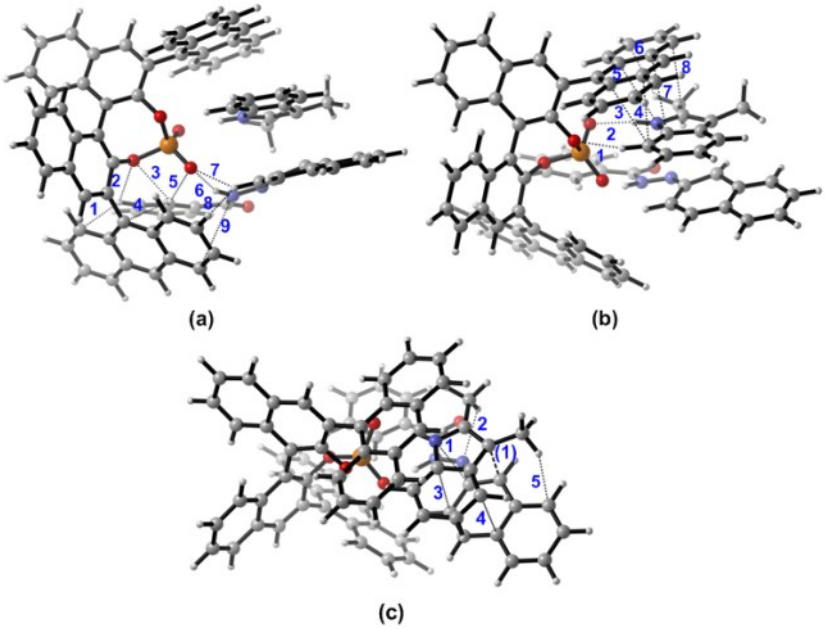

Figure S44 Intermolecular interactions in **TSI'-1** and numbers of bond critical points (BCPs No.).

Table S40 Numbers of bond critical point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSI'-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSI'-1(a)	1	C-H…π	2.54	0.0108	0.0362	0.0076	-0.0061	0.0015
	2	C-H…O	2.76	0.0064	0.0262	0.0054	-0.0042	0.0012
	3	C-H…O	2.53	0.0099	0.0395	0.0085	-0.0071	0.0014
	4	C-H…π	2.98	0.0053	0.0164	0.0034	-0.0026	0.0008
	5	C-H…π	2.47	0.0118	0.0397	0.0091	-0.0082	0.0009
	6	N-H…O	1.89	0.0294	0.0847	0.0221	-0.0231	-0.0010
	7	C-H…O	2.18	0.0165	0.0589	0.0140	-0.0132	0.0008
	8	C-H…π	2.72	0.0069	0.0221	0.0045	-0.0035	0.0010
	9	lp…π	4.23	0.0011	0.0047	0.0009	-0.0005	0.0004
TSI'-1(b)	1	C-H…O	2.13	0.0188	0.0580	0.0149	-0.0154	-0.0005
	2	N-H…O	1.93	0.0273	0.0767	0.0201	-0.0211	-0.0010
	3	π…π	3.23	0.0077	0.0239	0.0049	-0.0039	0.0010
	4	π…π	3.27	0.0077	0.0234	0.0048	-0.0038	0.0010
	5	π…π	3.24	0.0074	0.0228	0.0050	-0.0043	0.0007
	6	C-H…π	2.84	0.0063	0.0201	0.0040	-0.0029	0.0011
	7	π…π	3.30	0.0069	0.0212	0.0044	-0.0035	0.0009
	8	π…π	3.38	0.0064	0.0181	0.0038	-0.0030	0.0008
TSI'-1(c)	(1)	C…C	2.37	0.0436	0.0451	0.0173	-0.0232	-0.0059
	1	π…π	2.98	0.0121	0.0434	0.0094	-0.0080	0.0014
	2	C-H…N	2.43	0.0132	0.0417	0.0093	-0.0082	0.0011
	3	π…π	3.11	0.0096	0.0297	0.0062	-0.0051	0.0011
	4	π…π	3.07	0.0104	0.0319	0.0066	-0.0053	0.0013
	5	C-H…π	2.59	0.0097	0.0332	0.0067	-0.0050	0.0017

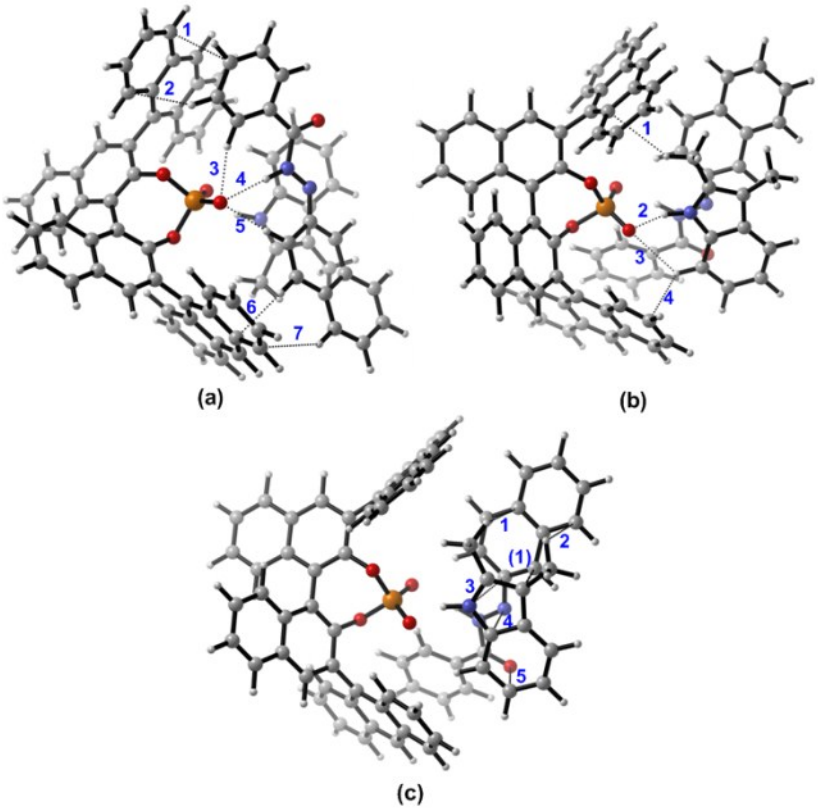

Figure S45 Intermolecular interactions in**TSII'-1** and numbers of bond critical points (BCPs No.).

Table S41 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSII'-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSII'-1(a)	1	π…π	3.20	0.0080	0.0239	0.0049	-0.0039	0.0010
	2	C-H…π	3.02	0.0053	0.0162	0.0032	-0.0024	0.0008
	3	C-H…O	2.15	0.0201	0.0563	0.0151	-0.0162	-0.0011
	4	N-H…O	2.02	0.0229	0.0627	0.0170	-0.0183	-0.0013
	5	C-H…O	2.07	0.0217	0.0670	0.0173	-0.0179	-0.0006
	6	C-H…π	2.46	0.0113	0.0361	0.0079	-0.0067	0.0012
	7	C-H…π	3.09	0.0037	0.0123	0.0023	-0.0016	0.0007
TSII'-1(b)	1	C-H…π	2.94	0.0049	0.0164	0.0033	-0.0024	0.0009
	2	N-H…O	1.67	0.0474	0.1493	0.0383	-0.0393	-0.0010
	3	C-H…O	2.69	0.0065	0.0247	0.0051	-0.0041	0.0010
	4	C-H…π	2.79	0.0073	0.0249	0.0049	-0.0036	0.0013
TSII'-1(c)	(1)	C…C	2.46	0.0358	0.0509	0.0155	-0.0183	-0.0028
	1	C-H…π	2.65	0.0084	0.0271	0.0055	-0.0043	0.0012
	2	C-H…π	2.67	0.0096	0.0333	0.0066	-0.0049	0.0017
	3	π…π	2.93	0.0129	0.0441	0.0098	-0.0087	0.0011
	4	π…π	2.83	0.0143	0.0437	0.0095	-0.0081	0.0014
	5	π…π	3.39	0.0049	0.0163	0.0035	-0.0028	0.0007

Then H2 atom is shifted to N2 atom from the O2–H2 of **CP3**, and $\mathbf{R1_{C2}}$ is protonated and further activated. The vanishment of O2–H2 bond leads to the generation of new O2···H2–N2 HB in **TSI'-1** or **TSII'-1** (Figure S44 and Table S40, or Figure S45 and Table S41). For the process of **COMI'→TSI'-1** or **COMII'→TSII'-1**, energy of 15.6 kcal/mol or 9.2 kcal/mol is needed to overcome the barrier. As the consequence of charge transfer, the O2···H2 distance of newly formed O2···H2–N2 HB becomes longer than the H2···N2 distance of newly formed O2–H2···N2 HB, while the distance of O1···H3 in O1···H3–N3 becomes also a little longer in **TSI'-1** or shorter in **TSII'-1** (Figure S40 or Figure S41). Through the QTAIM analyses, the intermolecular π···π interaction with the distance of 2.37 Å between the C1 and C2 atoms is found in **TSI'-1** (Figure S44 and Table S40) or 2.46

Å in **TSII'-1** (Figure S45 and Table S41). The π···π interaction between C1 and C2 lead to the formation of C1–C2 with the bond length of 1.61 Å either in **IMI'-1** or **IMII'-1** (Figure S40 or Figure S41). Followed by the absorption of 8.7 kcal/mol energy or 9.5 kcal/mol (Figure S38 or Figure S39), the **IMI'-1** is converted to **TSI'-2** or the **IMII'-1** is converted to **TSII'-2**, accompanied with increasing of HB bond length of O1···H3–N3 HB and decreasing of HB bond length of O2···H2–N2 HB (Figures S40 and S46, Table S42; or Figures S41 and S47, Table S43). The approaching of N1 atom to C3 atom produces the N1···C3 interaction with the 2.12 Å in **TSI'-2** or 2.13 Å in **TSII'-2** (Figure S40 or Figure S41). Similar to **IMI-1** or **IMII-1**, no such interaction between N1 atom and C3 atom was found due to the long distance between N1 atom and C3 atom in **IMI'-1** or **IMII'-1** (2.95 Å in **IMI'-1** and 3.37 Å in **IMII'-1**) (Figure S40 or Figure S41). But the lp···π interaction is found between N1 atom and C3 in **TSI'-2** or **TSII'-2** (Figure S48 and Table S44, or Figure S49 and Table S45), leads to the following N1–C3 bond formation reaction. In **IMI'-2** or **IMII'-2**, the newly formed N1–C3 bond with the length of 1.53 Å or 1.56 Å is found (Figures S40 and S50, Table S46; or Figures S41 and S51, Table S47). During the process of **IMI'-1→TSI'-2→IMI'-2** or **IMII'-1→TSII'-2→IMII'-2**, the distance of O2···H2 is decreased while the distance of O1···H3 is increased as the result of positive charge transfers from **R2** part to $\mathbf{R1_{C2}}$ part. Then followed by the breakage of O1···H3–N3 HB in **IMI'-2** or **IMII'-2**, the intermediate **IMI'-3** or **IMII'-3** is then generated. What's more, due to the close contact of O2 and H3, a new HB O2···H3–N3 is formed in **IMI'-3**, while it is not happened in **IMII'-3** (Figure S52 and Table S48; or Figure S53 and Table S49).The molecular rotation occurs via rotating the N1–N2 bond and contributes to the approach of O1 to the C1–H1 bond in **IMI'-4** or **IMII'-4**. For the process **IMI'-3→IMI'-4**, an energy of 4.2 kcal/mol is absorbed,

whlie an energy of 12.4 kcal/mol is releasedthe process **IMII'-3→IMII'-4** (Figure S38 or Figure S39). After overcoming the energy barrier of 1.4 kcal/mol or 8.9 kcal/mol, the **IMI'-4** is converted to **TSI'-3** or the **IMII'-4** is converted to**TSII'-3**. The H1 is once abstracted form C1-H1 bond to O1, forming the new O1···H1 interaction either in **TSI'-3** or in **TSII'-3**. The H1 atom is located between C1 and O1 atoms and the distances of O1···H1 and C1···H1 in **TSI'-3** or **TSII'-3** are shown in Figure S40 or Figure S41, respectively. In **IMI'-5** or **IMII'-5**, the H1 is shifted to O1 atom, forming the new O1–H1 bond and the catalyst **CP3** is recovered. Notably, a new HB O1–H1···N3 is found because of the short distance of H1···N3 in **IMI'-5**. Accompanied with a large amount of energy released (15.0 kcal/mol of **IMI'-5** and 23.3 kcal/mol of **IMII'-5**), the O2···H2–N2 HB and the O1–H1···N3 HB of **IMI'-5** or the O2···H2–N2 HB of **IMII'-5** breaks, then the catalyzed reaction is finished and the major product $\mathbf{P1_{C2}}$ is produced. QTAIM analyses of the transition states and intermediates are shown in Figures S54-S59 and Tables S50-S55.

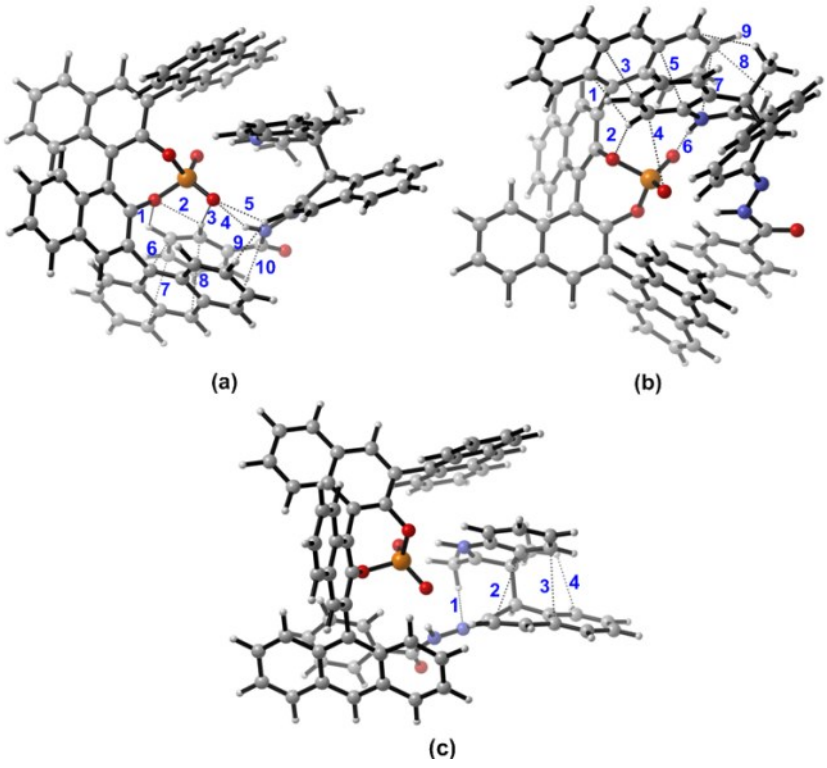

Figure S46 Intermolecular interactions in **IMI'-1** and numbers of bond critical points (BCPs No.).

Table S42 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(a)	1	C-H…O	2.54	0.0090	0.0340	0.0074	-0.0064	0.0010
	2	C-H…O	2.37	0.0129	0.0478	0.0109	-0.0098	0.0011
	3	C-H…π	2.49	0.0123	0.0432	0.0097	-0.0086	0.0011
	4	N-H…O	2.16	0.0169	0.0475	0.0127	-0.0135	-0.0008
	5	C-H…O	2.34	0.0122	0.0447	0.0102	-0.0091	0.0011
	6	π…π	3.09	0.0094	0.0302	0.0063	-0.0050	0.0013
	7	π…π	3.35	0.0066	0.0191	0.0040	-0.0032	0.0008
	8	π…π	3.45	0.0061	0.0172	0.0036	-0.0029	0.0007
	9	C-H…π	2.62	0.0081	0.0257	0.0053	-0.0042	0.0011
	10	lp…π	3.68	0.0036	0.0107	0.0023	-0.0019	0.0004
IMI'-1(b)	1	C-H…π	2.75	0.0083	0.0283	0.0056	-0.0041	0.0015
	2	C-H…O	2.21	0.0163	0.0492	0.0126	-0.0129	-0.0003
	3	π…π	3.26	0.0075	0.0230	0.0048	-0.0038	0.0010
	4	lp…π	3.32	0.0061	0.0226	0.0046	-0.0035	0.0011
	5	π…π	3.34	0.0065	0.0194	0.0040	-0.0032	0.0008
	6	N-H…O	1.63	0.0555	0.1404	0.0407	-0.0463	-0.0056
	7	π…π	3.54	0.0054	0.0160	0.0034	-0.0029	0.0005
	8	C-H…π	2.93	0.0054	0.0179	0.0035	-0.0026	0.0009
	9	C-H…π	3.08	0.0038	0.0117	0.0023	-0.0016	0.0007
IMI'-1(c)	1	C-H…N	2.53	0.0118	0.0399	0.0086	-0.0072	0.0014
	2	π…π	3.22	0.0091	0.0280	0.0059	-0.0048	0.0011
	3	π…π	3.07	0.0105	0.0356	0.0073	-0.0056	0.0017
	4	C-H…π	2.69	0.0086	0.0309	0.0061	-0.0044	0.0017

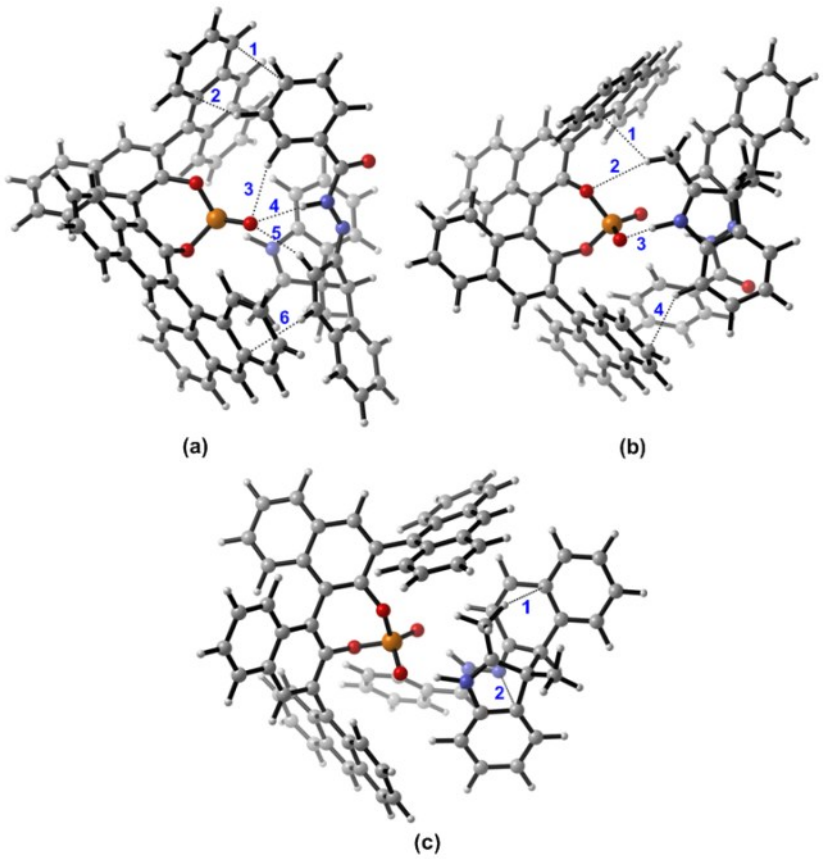

Figure S47 Intermolecular interactions in **IMII'-1** and numbers of bond critical points (BCPs No.).

Table S43 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(a)	1	π…π	3.40	0.0064	0.0184	0.0038	-0.0030	0.0008
	2	C-H…π	2.75	0.0077	0.0234	0.0048	-0.0038	0.0010
	3	C-H…O	2.28	0.0155	0.0448	0.0116	-0.0119	-0.0003
	4	N-H…O	2.05	0.0201	0.0611	0.0159	-0.0165	-0.0006
	5	C-H…O	2.28	0.0142	0.0533	0.0121	-0.0109	0.0012
	6	C-H…π	2.55	0.0102	0.0347	0.0073	-0.0059	0.0014
IMII'-1(b)	1	C-H…π	2.84	0.0059	0.0193	0.0038	-0.0028	0.0010
	2	C-H…O	2.89	0.0040	0.0155	0.0030	-0.0022	0.0008
	3	N-H…O	1.40	0.0977	0.1147	0.0720	-0.1154	-0.0434
	4	C-H…π	2.72	0.0080	0.0270	0.0055	-0.0042	0.0013
IMII'-1(c)	1	C-H…π	2.62	0.0090	0.0309	0.0063	-0.0049	0.0014
	2	π…π	2.89	0.0138	0.0462	0.0101	-0.0087	0.0014

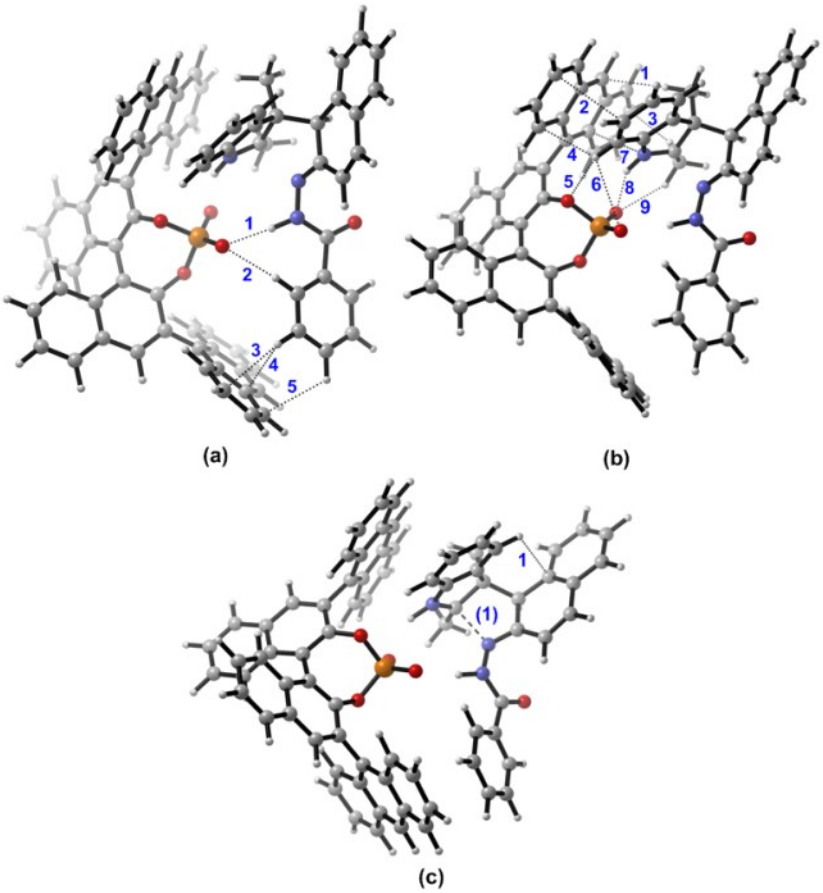

Figure S48 Intermolecular interactions in **TSI'-2** and numbers of bond critical points (BCPs No.)

Table S44 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(a)	1	N-H…O	1.98	0.0239	0.0670	0.0178	-0.0188	-0.0010
	2	C-H…O	2.41	0.0107	0.0371	0.0086	-0.0078	0.0008
	3	C-H…π	2.73	0.0080	0.0254	0.0054	-0.0044	0.0010
	4	C-H…π	2.83	0.0075	0.0275	0.0054	-0.0040	0.0014
	5	C-H…π	2.71	0.0076	0.0261	0.0052	-0.0039	0.0013
TSI'-2(b)	1	C-H…π	2.55	0.0100	0.0316	0.0068	-0.0056	0.0012
	2	π…π	3.43	0.0060	0.0163	0.0034	-0.0027	0.0007
	3	C-H…π	2.71	0.0081	0.0238	0.0050	-0.0041	0.0009
	4	C-H…π	2.75	0.0077	0.0260	0.0051	-0.0038	0.0013
	5	C-H…O	2.61	0.0072	0.0255	0.0056	-0.0048	0.0008
	6	C-H…π	3.10	0.0037	0.0142	0.0027	-0.0019	0.0008
	7	π…π	3.29	0.0071	0.0235	0.0048	-0.0038	0.0010
	8	N-H…O	1.90	0.0307	0.0888	0.0233	-0.0245	-0.0012
	9	C-H…O	2.47	0.0096	0.0337	0.0076	-0.0068	0.0008
TSI'-2(c)	(1)	C…N	2.12	0.0602	0.1075	0.0365	-0.0462	-0.0097
	1	C-H…π	2.79	0.0074	0.0248	0.0049	-0.0036	0.0013

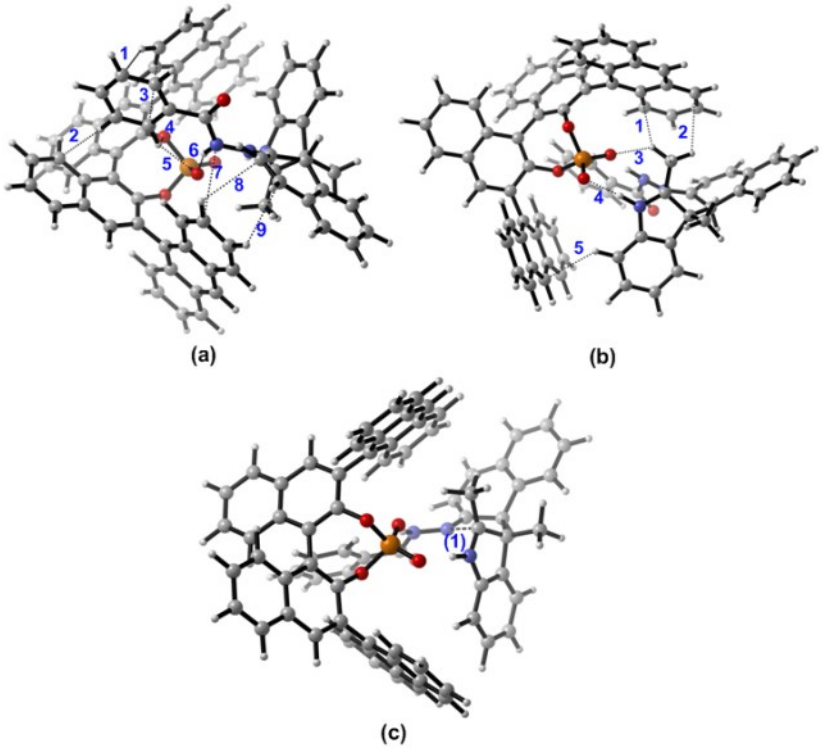

Figure S49 Intermolecular interactions in **TSII'-2** and numbers of bond critical points (BCPs No.)

Table S45 Numbers of bond critical point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSII'-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSII'-2(a)	1	C-H…π	2.78	0.0073	0.0223	0.0046	-0.0037	0.0009
	2	C-H…π	2.66	0.0087	0.0267	0.0056	-0.0045	0.0011
	3	π…π	3.62	0.0045	0.0139	0.0029	-0.0022	0.0007
	4	C-H…O	2.56	0.0086	0.0323	0.0071	-0.0062	0.0009
	5	C-H…O	2.30	0.0153	0.0443	0.0115	-0.0119	-0.0004
	6	N-H…O	1.66	0.0472	0.1607	0.0401	-0.0401	0.0000
	7	lp…π	3.26	0.0073	0.0232	0.0050	-0.0042	0.0008
	8	C-H…π	2.95	0.0051	0.0157	0.0031	-0.0022	0.0009
	9	C-H…π	2.98	0.0046	0.0150	0.0029	-0.0021	0.0008
TSII'-2(b)	1	C-H…π	2.79	0.0063	0.0214	0.0043	-0.0032	0.0011
	2	C-H…π	2.84	0.0076	0.0230	0.0047	-0.0036	0.0011
	3	C-H…O	2.23	0.0166	0.0516	0.0130	-0.0131	-0.0001
	4	N-H…O	1.82	0.0342	0.1009	0.0258	-0.0264	-0.0006
	5	C-H…π	2.76	0.0072	0.0227	0.0046	-0.0036	0.0010
TSII'-2(c)	(1)	C…N	2.13	0.0594	0.1100	0.0365	-0.0454	-0.0089

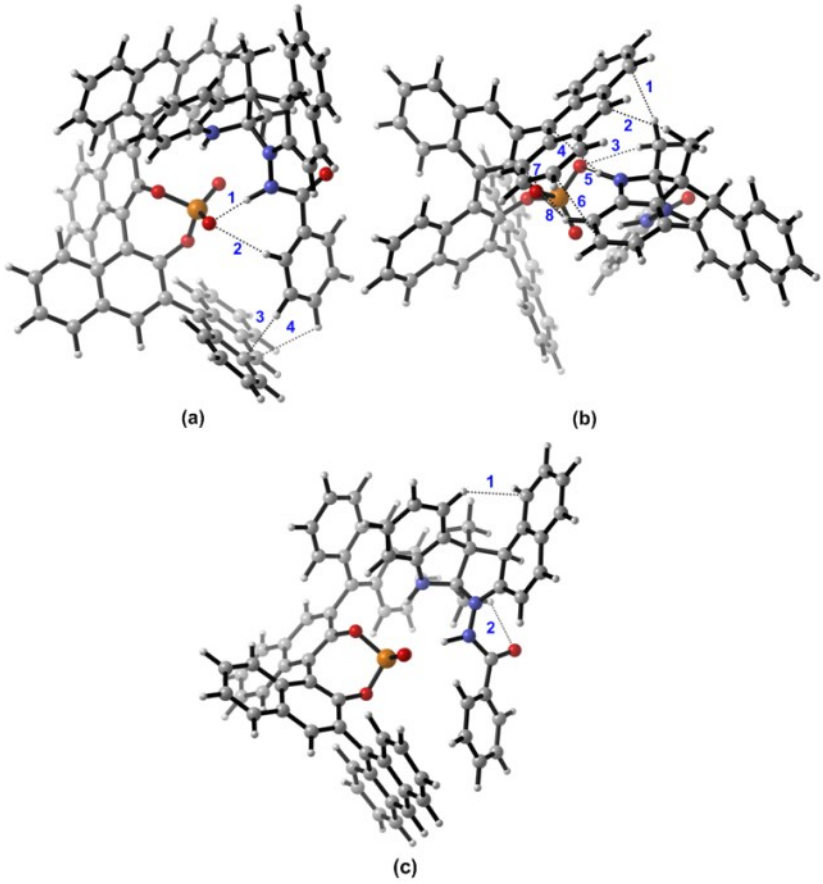

Figure S50 Intermolecular interactions in **IMI'-2** and numbers of bond critical points (BCPs No.).

Table S46 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(a)	1	N-H…O	1.74	0.0412	0.1198	0.0309	-0.0319	-0.0010
	2	C-H…O	2.56	0.0093	0.0354	0.0076	-0.0063	0.0013
	3	C-H…π	2.61	0.0096	0.0359	0.0073	-0.0056	0.0017
	4	C-H…π	2.88	0.0062	0.0198	0.0039	-0.0029	0.0010
IMI'-2(b)	1	C-H…π	2.70	0.0084	0.0246	0.0052	-0.0043	0.0009
	2	C-H…π	2.55	0.0099	0.0312	0.0067	-0.0055	0.0012
	3	C-H…O	2.44	0.0103	0.0346	0.0080	-0.0074	0.0006
	4	N-H…π	2.79	0.0071	0.0235	0.0048	-0.0037	0.0011
	5	N-H…O	2.23	0.0163	0.0504	0.0127	-0.0128	-0.0001
	6	π…π	3.40	0.0061	0.0170	0.0036	-0.0029	0.0007
	7	C-H…π	2.74	0.0081	0.0269	0.0053	-0.0039	0.0014
	8	C-H…O	2.70	0.0060	0.0223	0.0047	-0.0038	0.0009
IMI'-2(c)	1	C-H…π	2.72	0.0079	0.0252	0.0051	-0.0038	0.0013
	2	C-H…O	2.79	0.0067	0.0258	0.0054	-0.0043	0.0011

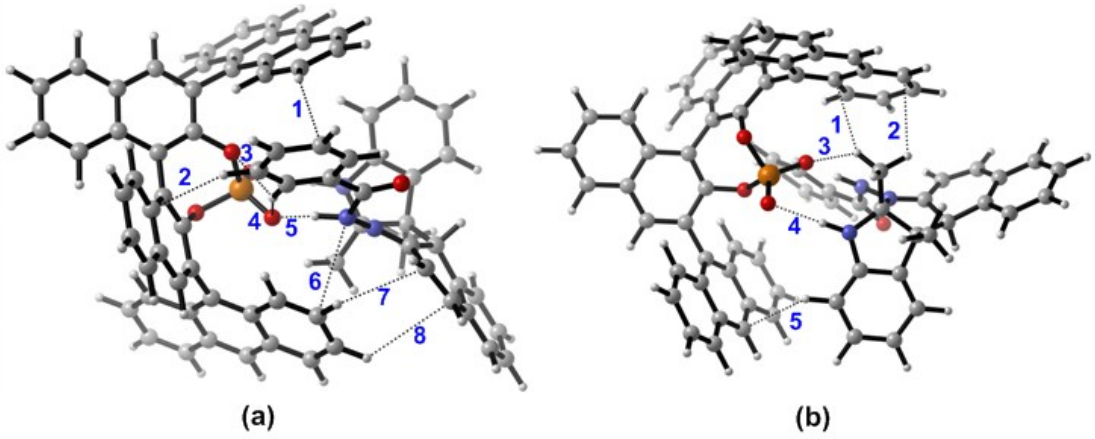

Figure S51 Intermolecular interactions in **IMII'-2** and numbers of bond critical points (BCPs No.).

Table S47 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(a)	1	C-H…π	2.74	0.0077	0.0238	0.0049	-0.0039	0.0010
	2	C-H…π	2.73	0.0075	0.0232	0.0048	-0.0038	0.0010
	3	C-H…O	2.54	0.0091	0.0352	0.0078	-0.0067	0.0011
	4	C-H…O	2.16	0.0194	0.0555	0.0148	-0.0158	-0.0010
	5	N-H…O	1.54	0.0643	0.1755	0.0521	-0.0603	-0.0082
	6	lp…π	3.28	0.0071	0.0204	0.0046	-0.0040	0.0006
	7	C-H…π	3.15	0.0037	0.0117	0.0022	-0.0016	0.0006
	8	C-H…π	3.26	0.0029	0.0090	0.0017	-0.0012	0.0005
IMII'-2(b)	1	C-H…π	2.81	0.0062	0.0209	0.0042	-0.0032	0.0010
	2	C-H…π	2.88	0.0069	0.0206	0.0042	-0.0032	0.0010
	3	C-H…O	2.21	0.0177	0.0562	0.0141	-0.0142	-0.0001
	4	N-H…O	2.07	0.0203	0.0568	0.0151	-0.0161	-0.0010
	5	C-H…π	2.68	0.0079	0.0238	0.0050	-0.0040	0.0010

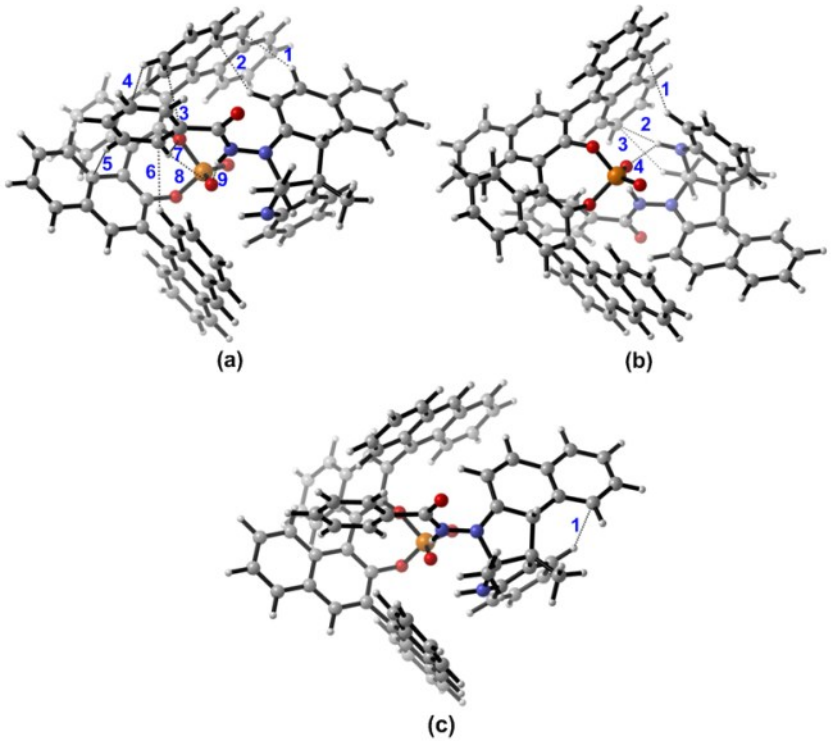

Figure S52 Intermolecular interactions in **IMI'-3** and numbers of bond critical points (BCPs No.).

Table S48 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(a)	1	C-H…π	2.57	0.0096	0.0298	0.0063	-0.0052	0.0011
	2	C-H…π	2.71	0.0072	0.0235	0.0048	-0.0036	0.0012
	3	π…π	3.31	0.0070	0.0215	0.0044	-0.0035	0.0009
	4	C-H…π	2.90	0.0060	0.0194	0.0040	-0.0031	0.0009
	5	C-H…π	2.62	0.0088	0.0282	0.0060	-0.0049	0.0011
	6	C-H…π	2.72	0.0073	0.0251	0.0049	-0.0035	0.0014
	7	C-H…O	2.41	0.0114	0.0380	0.0090	-0.0086	0.0004
	8	C-H…O	2.43	0.0121	0.0382	0.0093	-0.0090	0.0003
	9	N-H…O	1.50	0.0753	0.1687	0.0590	-0.0758	-0.0168
IMI'-3(b)	1	C-H…π	2.79	0.0070	0.0224	0.0046	-0.0036	0.0010
	2	N-H…π	2.62	0.0090	0.0286	0.0062	-0.0052	0.0010
	3	C-H…π	2.99	0.0045	0.0142	0.0028	-0.0020	0.0008
	4	N-H…O	2.38	0.0122	0.0472	0.0107	-0.0095	0.0012
IMI'-3(c)	1	C-H…π	2.69	0.0084	0.0272	0.0055	-0.0041	0.0014

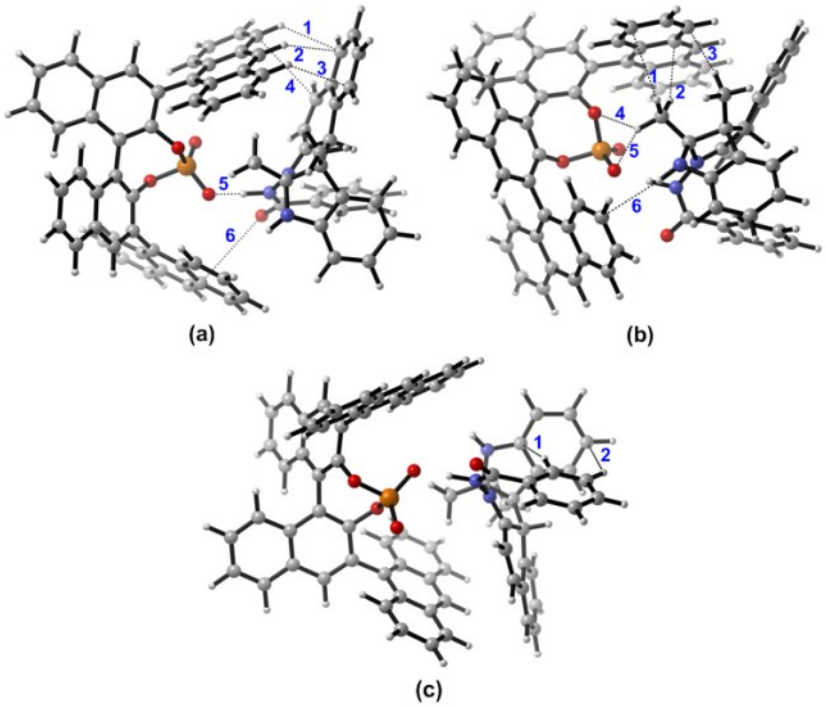

Figure S53 Intermolecular interactions in **IMII'-3** and numbers of bond critical points (BCPs No.).

Table S49 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'(a)	1	C-H…π	2.77	0.0068	0.0232	0.0045	-0.0032	0.0013
	2	C-H…π	2.77	0.0073	0.0237	0.0049	-0.0038	0.0011
	4	π…π	3.59	0.0037	0.0118	0.0023	-0.0018	0.0005
	5	C-H…π	3.00	0.0045	0.0137	0.0027	-0.0019	0.0008
	5	N-H…O	1.46	0.0823	0.1516	0.0624	-0.0869	-0.0245
	6	lp…π	4.00	0.0011	0.0060	0.0011	-0.0006	0.0005
IMII'-3(b)	1	C-H…π	3.10	0.0044	0.0138	0.0028	-0.0021	0.0007
	2	C-H…π	2.68	0.0080	0.0256	0.0053	-0.0042	0.0011
	3	C-H…π	2.70	0.0080	0.0226	0.0048	-0.0039	0.0009
	4	C-H…O	2.55	0.0081	0.0318	0.0069	-0.0059	0.0010
	5	C-H…O	2.23	0.0173	0.0511	0.0132	-0.0137	-0.0005
	6	N-H…π	2.67	0.0066	0.0212	0.0043	-0.0034	0.0009
IMII'-3(c)	1	C-H…π	2.47	0.0120	0.0378	0.0083	-0.0072	0.0011
	2	C-H…π	3.16	0.0036	0.0109	0.0021	-0.0015	0.0006

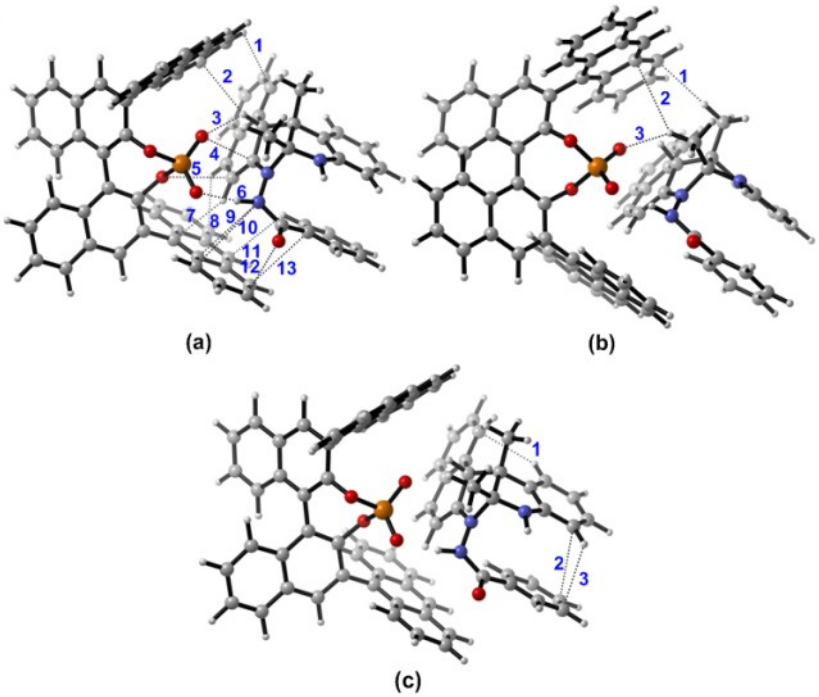

Figure S54 Intermolecular interactions in **IMI'-4** and numbers of bond critical points (BCPs No.).

Table S50 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(a)	1	C-H…π	2.97	0.0055	0.0184	0.0036	-0.0025	0.0011
	2	C-H…π	3.01	0.0045	0.0143	0.0029	-0.0021	0.0008
	3	C-H…O	2.15	0.0187	0.0678	0.0161	-0.0153	0.0008
	4	π…π	2.69	0.0162	0.0579	0.0136	-0.0127	0.0009
	5	lp…π	3.20	0.0068	0.0246	0.0052	-0.0042	0.0010
	6	N-H…O	1.74	0.0409	0.1265	0.0322	-0.0327	-0.0005
	7	C-H…π	2.65	0.0090	0.0308	0.0065	-0.0052	0.0013
	8	C-H…π	2.70	0.0084	0.0271	0.0057	-0.0046	0.0011
	9	lp…π	3.72	0.0034	0.0113	0.0023	-0.0018	0.0005
	10	lp…π	3.70	0.0032	0.0114	0.0023	-0.0018	0.0005
	11	C-H…π	3.18	0.0037	0.0115	0.0023	-0.0017	0.0006
	12	π…π	3.02	0.0092	0.0309	0.0068	-0.0059	0.0009
	13	π…π	3.43	0.0060	0.0169	0.0035	-0.0028	0.0007
IMI'-4(b)	1	C-H…π	2.73	0.0072	0.0215	0.0044	-0.0034	0.0010
	2	C-H…π	3.60	0.0013	0.0048	0.0009	-0.0005	0.0004
	3	C-H…O	2.36	0.0132	0.0404	0.0099	-0.0098	0.0001
IMI'-4(c)	1	C-H…π	2.70	0.0078	0.0249	0.0050	-0.0038	0.0012
	2	π…π	3.47	0.0059	0.0167	0.0035	-0.0028	0.0007
	3	C-H…π	2.93	0.0068	0.0214	0.0042	-0.0031	0.0011

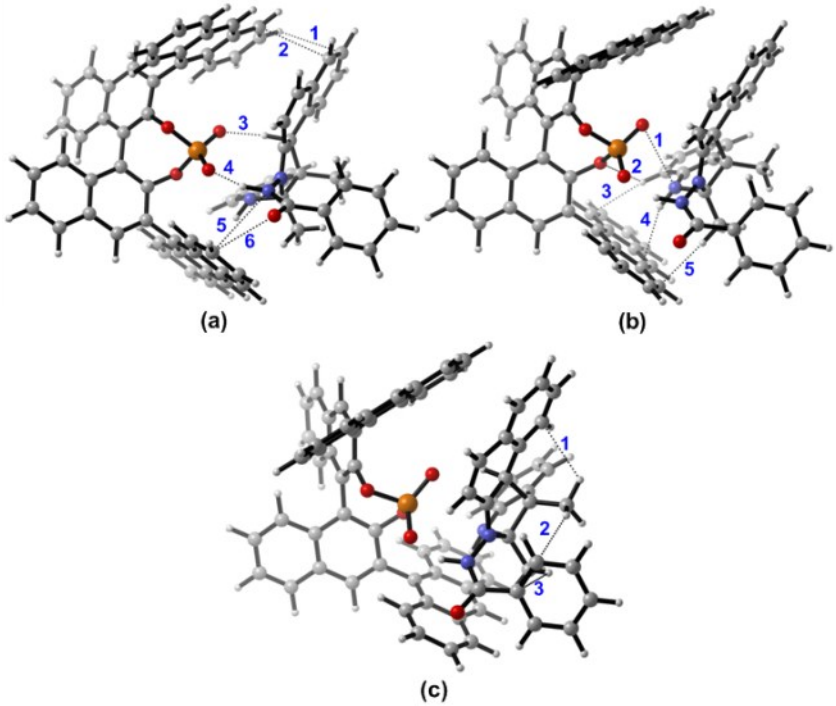

Figure S55 Intermolecular interactions in **IMII'-4** and numbers of bond critical points (BCPs No.).

Table S51 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(a)	1	C-H…π	3.11	0.0049	0.0153	0.0030	-0.0022	0.0008
	2	π…π	3.27	0.0072	0.0224	0.0045	-0.0035	0.0010
	3	C-H…O	2.00	0.0247	0.0782	0.0199	-0.0204	-0.0005
	4	N-H…O	1.65	0.0483	0.1552	0.0396	-0.0404	-0.0008
	5	lp…π	3.54	0.0044	0.0145	0.0030	-0.0023	0.0007
	6	π…π	3.01	0.0096	0.0345	0.0075	-0.0064	0.0011
IMII'-4(b)	1	lp…π	3.14	0.0096	0.0306	0.0071	-0.0066	0.0005
	2	C-H…O	3.30	0.0020	0.0094	0.0018	-0.0012	0.0006
	3	C-H…π	2.58	0.0100	0.0306	0.0067	-0.0057	0.0010
	4	N-H…π	2.65	0.0080	0.0275	0.0058	-0.0047	0.0011
	5	C-H…π	2.56	0.0096	0.0290	0.0062	-0.0052	0.0010
IMII'-4(c)	1	C-H…π	2.67	0.0089	0.0320	0.0063	-0.0047	0.0016
	2	C-H…π	2.82	0.0064	0.0185	0.0037	-0.0029	0.0008
	3	C-H…π	2.70	0.0090	0.0305	0.0061	-0.0046	0.0015

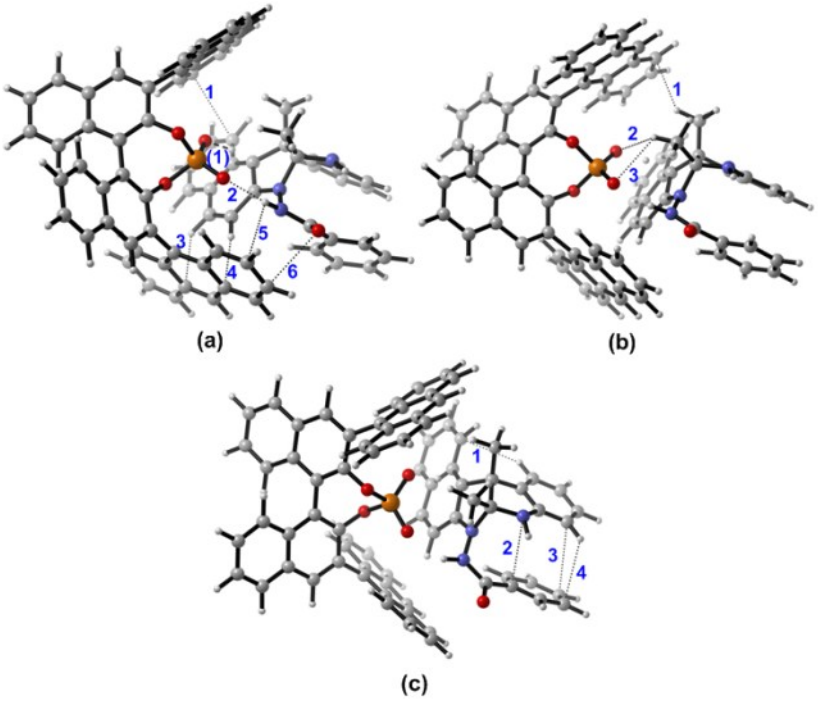

Figure S56 Intermolecular interactions in **TSI'-3** and numbers of bond critical points (BCPs No.)

Table S52 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSI'-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSI'-3(a)	(1)	O…H	1.39	0.1031	0.0959	0.0692	-0.1145	-0.0453
	1	π…π	3.49	0.0047	0.0139	0.0028	-0.0021	0.0007
	2	N-H…O	1.93	0.0258	0.0903	0.0223	-0.0220	0.0003
	3	C-H…π	2.68	0.0084	0.0303	0.0062	-0.0049	0.0013
	4	C-H…π	2.54	0.0105	0.0342	0.0073	-0.0061	0.0012
	5	N-H…π	3.08	0.0044	0.0148	0.0029	-0.0022	0.0007
	6	π…π	3.01	0.0090	0.0306	0.0068	-0.0059	0.0009
TSI'-3(b)	1	C-H…π	2.74	0.0076	0.0244	0.0050	-0.0038	0.0012
	2	C-H…π	2.55	0.0095	0.0327	0.0073	-0.0065	0.0008
	3	C-H…π	2.63	0.0092	0.0342	0.0073	-0.0060	0.0013
TSI'-3(c)	1	C-H…π	2.77	0.0067	0.0214	0.0043	-0.0032	0.0011
	2	lp…π	3.24	0.0082	0.0266	0.0057	-0.0047	0.0010
	3	π…π	3.50	0.0053	0.0155	0.0032	-0.0026	0.0006
	4	C-H…π	2.94	0.0059	0.0185	0.0037	-0.0027	0.0010

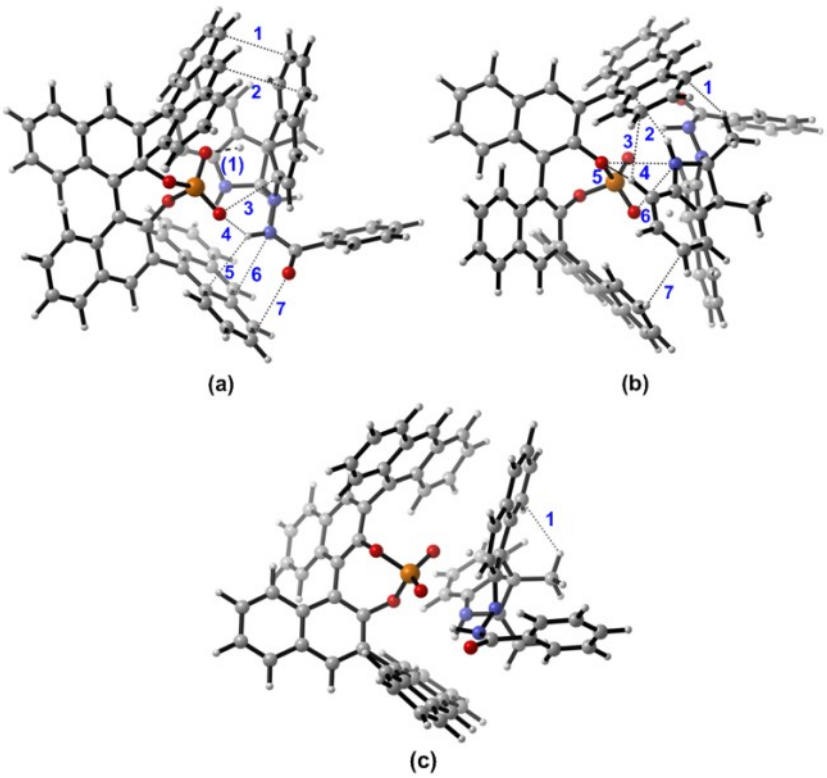

Figure S57 Intermolecular interactions in**TSII'-3** and numbers of bond critical points (BCPs No.)

Table S53 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **TSII'-3**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSII'-3(a)	(1)	O…H	1.47	0.0851	0.1370	0.0581	-0.0820	-0.0239
	1	π…π	3.16	0.0082	0.0246	0.0051	-0.0041	0.0010
	2	π…π	3.77	0.0033	0.0094	0.0019	-0.0015	0.0004
	3	lp…π	3.00	0.0103	0.0370	0.0080	-0.0068	0.0012
	4	N-H…O	1.94	0.0270	0.0834	0.0216	-0.0224	-0.0008
	5	N-H…π	2.84	0.0054	0.0191	0.0038	-0.0028	0.0010
	6	lp…π	3.36	0.0058	0.0174	0.0038	-0.0032	0.0006
	7	lp…π	3.13	0.0080	0.0264	0.0058	-0.0050	0.0008
TSII'-3(b)	1	C-H…π	2.85	0.0061	0.0199	0.0039	-0.0029	0.0010
	2	N-H…π	2.41	0.0117	0.0388	0.0086	-0.0075	0.0011
	3	C-H…π	2.76	0.0077	0.0241	0.0048	-0.0036	0.0012
	4	lp…lp	3.00	0.0099	0.0334	0.0079	-0.0074	0.0005
	5	C-H…O	2.95	0.0043	0.0176	0.0035	-0.0026	0.0009
	6	lp…π	2.93	0.0133	0.0447	0.0107	-0.0102	0.0005
	7	C-H…π	2.94	0.0049	0.0150	0.0029	-0.0022	0.0007
TSII'-3(c)	1	C-H…π	2.73	0.0080	0.0298	0.0058	-0.0042	0.0016

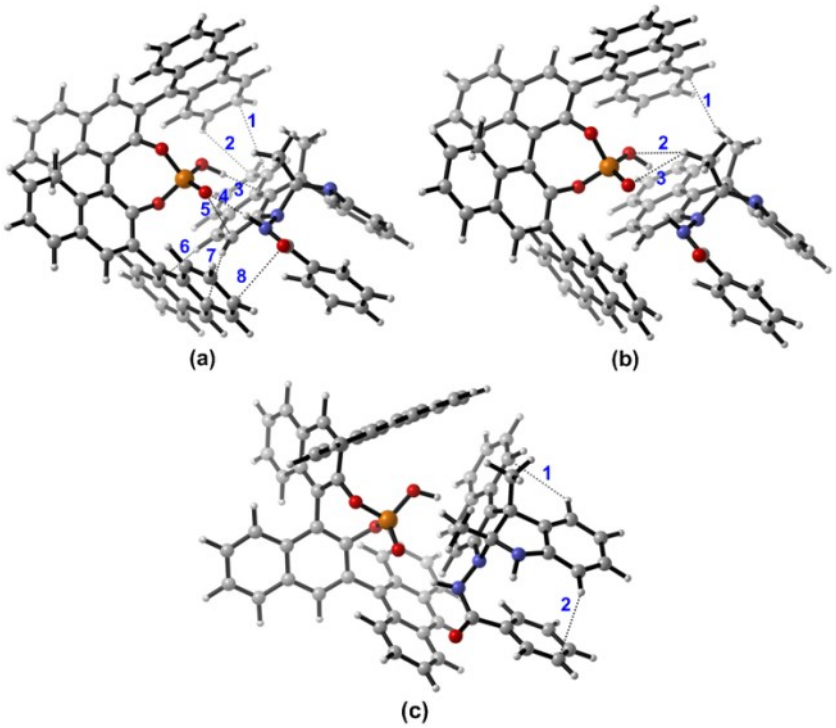

Figure S58 Intermolecular interactions in **IMI'-5** and numbers of bond critical points (BCPs No.).

Table S54 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'-5**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMI'-5(a)	1	π…π	3.46	0.0052	0.0151	0.0031	-0.0024	0.0007
	2	C-H…π	2.95	0.0054	0.0175	0.0034	-0.0025	0.0009
	3	O-H…π	2.23	0.0181	0.0447	0.0110	-0.0109	0.0001
	4	N-H…O	1.98	0.0224	0.0796	0.0195	-0.0191	0.0004
	5	π…π	3.24	0.0079	0.0258	0.0054	-0.0044	0.0010
	6	C-H…π	2.71	0.0079	0.0288	0.0058	-0.0045	0.0013
	7	C-H…π	2.58	0.0096	0.0323	0.0069	-0.0057	0.0012
	8	π…π	3.00	0.0095	0.0326	0.0072	-0.0062	0.0010
IMI'-5(b)	1	C-H…π	2.84	0.0059	0.0174	0.0035	-0.0027	0.0008
	2	C-H…π	2.74	0.0060	0.0224	0.0046	-0.0036	0.0010
	3	C-H…π	2.64	0.0084	0.0299	0.0065	-0.0054	0.0011
IMI'-5(c)	1	C-H…π	3.01	0.0043	0.0142	0.0028	-0.0020	0.0008
	2	C-H…π	3.08	0.0049	0.0150	0.0030	-0.0022	0.0008

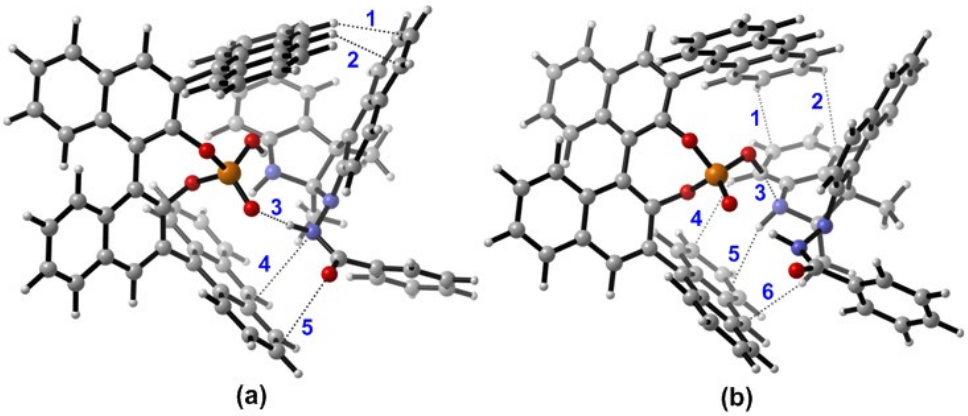

Figure S59 Intermolecular interactions in **IMII'-5** and numbers of bond critical points (BCPs No.).

Table S55 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'-5**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMII'-5(a)	1	C-H…π	2.63	0.0095	0.0302	0.0064	-0.0053	0.0011
	2	C-H…π	2.92	0.0050	0.0156	0.0031	-0.0022	0.0009
	3	N-H…O	1.90	0.0285	0.0871	0.0224	-0.0230	-0.0006
	4	lp…π	3.50	0.0047	0.0142	0.0030	-0.0025	0.0005
	5	π…π	3.23	0.0062	0.0209	0.0045	-0.0038	0.0007
IMII'-5(b)	1	C-H…π	2.72	0.0075	0.0237	0.0048	-0.0037	0.0011
	2	C-H…π	3.19	0.0037	0.0112	0.0022	-0.0016	0.0006
	3	O-H…N	1.61	0.0676	0.0964	0.0404	-0.0567	-0.0163
	4	C-H…π	2.84	0.0057	0.0174	0.0034	-0.0025	0.0009
	5	N-H…π	2.78	0.0061	0.0203	0.0041	-0.0032	0.0009
	6	C-H…π	2.57	0.0097	0.0301	0.0064	-0.0053	0.0011

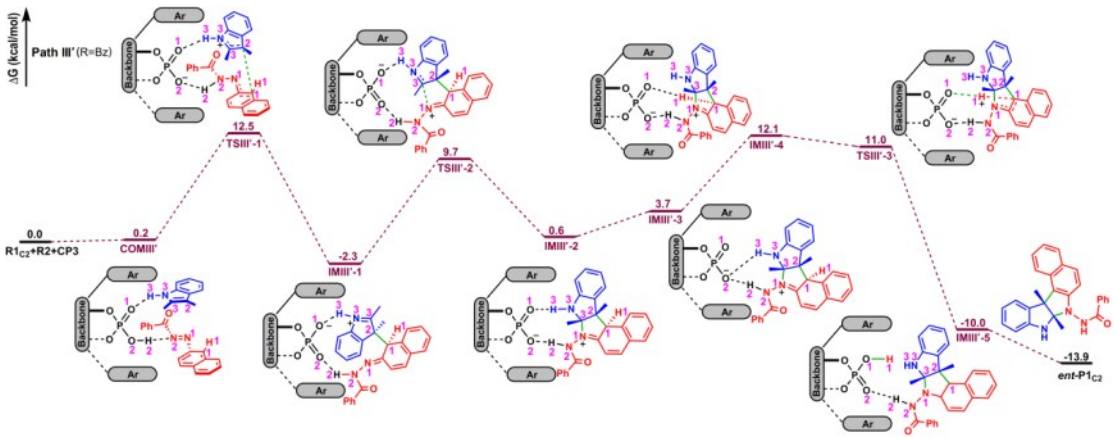

Figure S60 The path **III'** for the reaction between $\mathbf{R1_{C2}}$ (R=Bz) and **R2** catalyzed by **CP3** (Ar= 9-anthryl) and the free energy profile of the whole processes. The Gibbs free energies of [$\mathbf{R1_{C2}}$**+R2+CP3**] were set to 0.0 kcal/mol as reference.

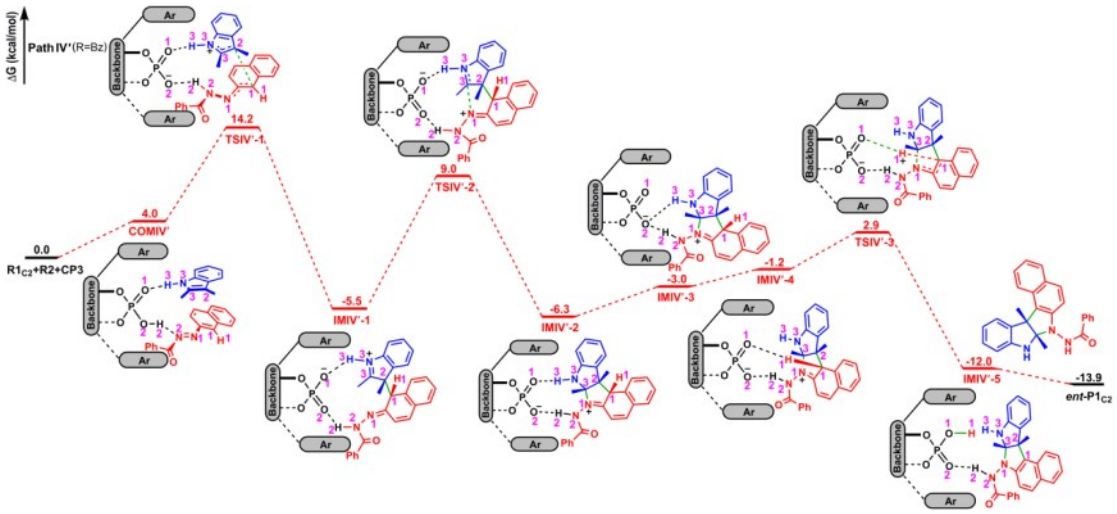

Figure S61 The path **IV'** for the reaction between $\mathbf{R1_{C2}}$ (R=Bz) and **R2** catalyzed by **CP3** (Ar= 9-anthryl) and the free energy profile of the whole processes. The Gibbs free energies of [$\mathbf{R1_{C2}}$**+R2+CP3**] were set to 0.0 kcal/mol as reference.

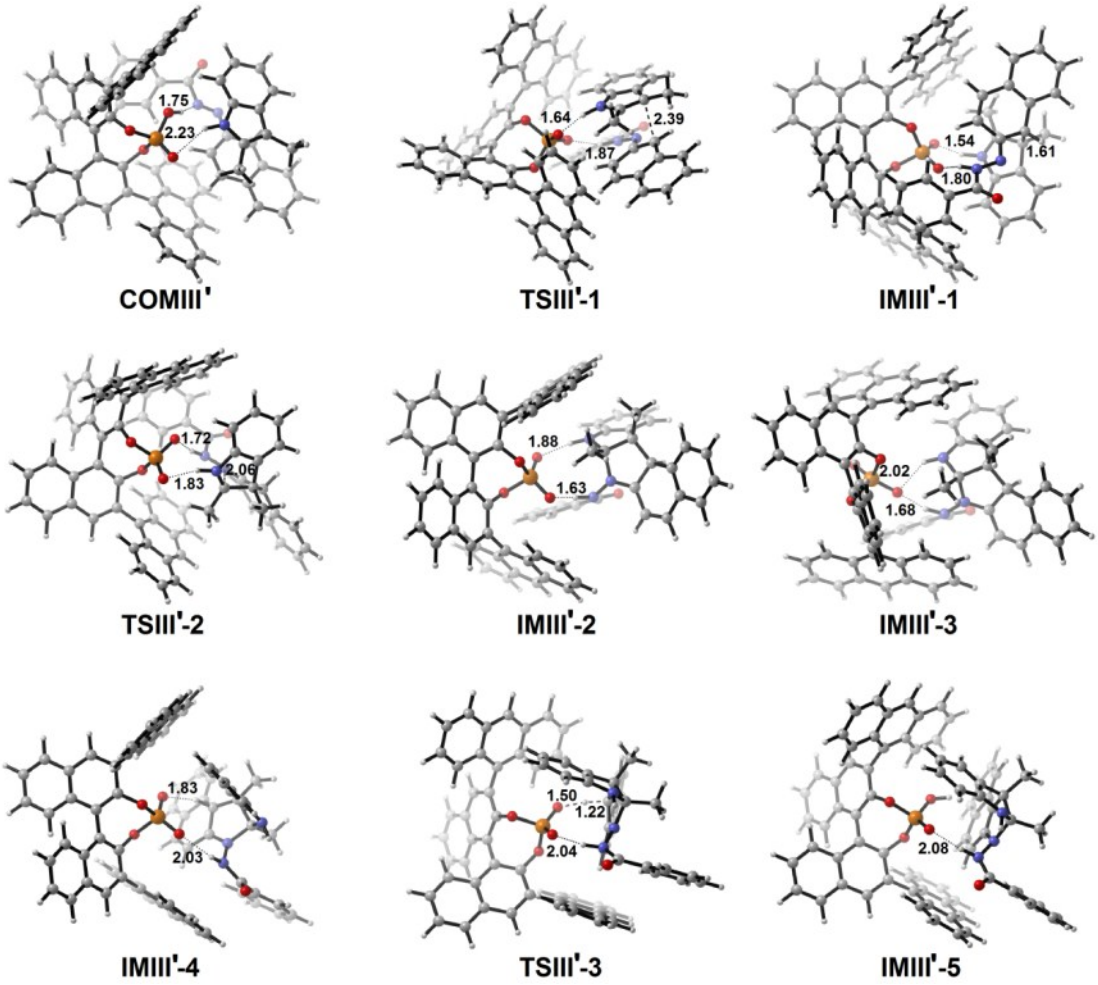

Figure S62 The optimized geometries of the complex, transition states and intermediates in path **III'** (R=Bz). The distances are in Å.

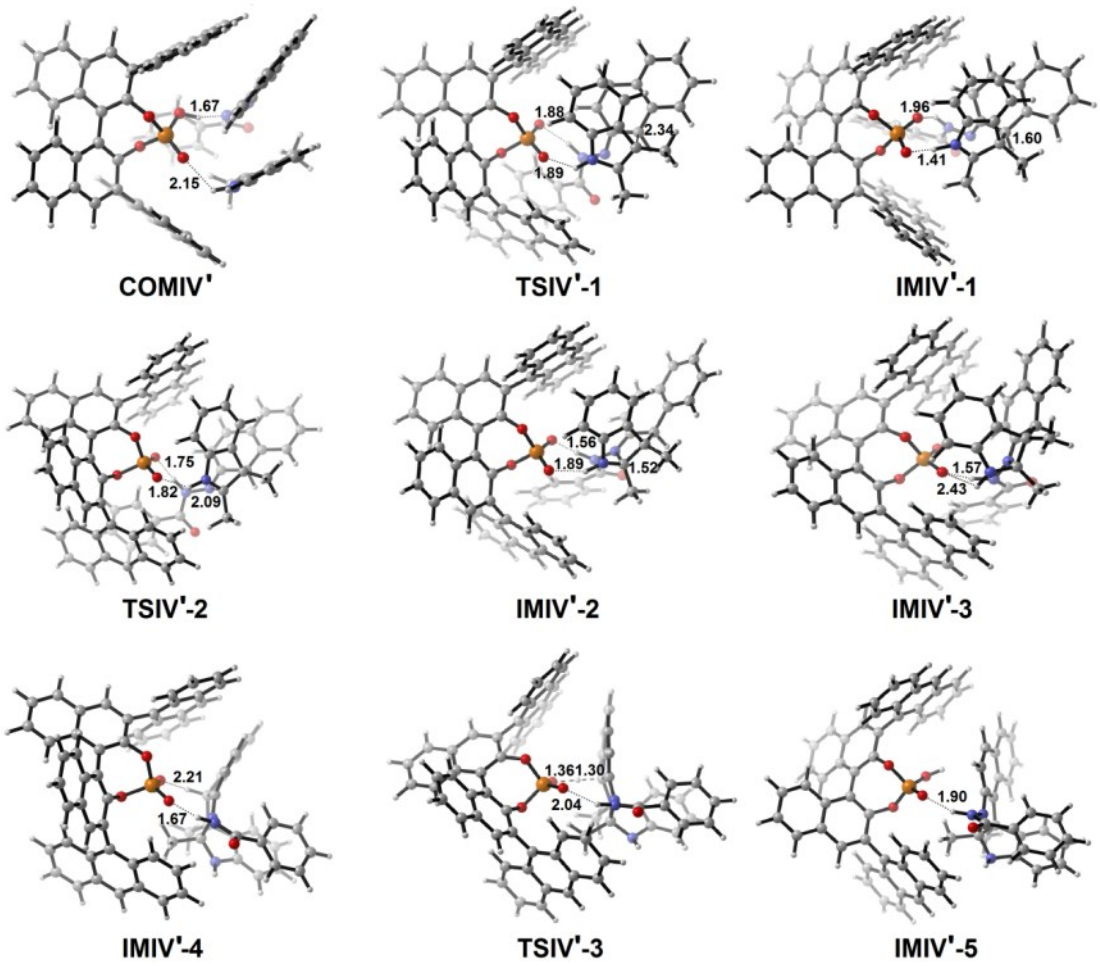

Figure S63 The optimized geometries of the complex, transition states and intermediates in path **IV'** (R=Bz). The distances are in Å.

The last two paths **III'** and **IV'** of $\mathbf{R1_{C2}}$ reacting with **R2** lead to the experiment undesired product *ent*-$\mathbf{P1_{C2}}$, and the Gibbs free energy profiles for their whole reaction processes are displayed in Figures S60 and S61, respectively. The optimized structures of complexes, transition states, intermediates and products of paths **III'** and **IV'** are displayed in Figures S62 and S63, respectively. Like the trimeric complexes **COMI'** and **COMII'** formed in path **I'** and path **II'**, the formation of **COMIII'** and **COMIV'** are also energetically unfavorable. As revealed by QTAIM analyses, the O2–H2···N2 HB between the O2–H2 group of **CP3** and N1=N2Bz group of $\mathbf{R1_{C2}}$ (R=Bz),

and the O1···H3–N3 HB between the P=O1 group of **CP3** and N3–H3 group of **R2** are found both in **COMIII'** and **COMIV'** (Figure S64 and Table S56, or Figures S65 and Table S57). Other interactions like C–H···π, π···π and C–H···O are also found between $\mathbf{R1_{C2}}$, **R2** and **CP3** in **COMIII'** and **COMIV'**, which stabilize the trimeric complexes and are able to promote the subsequent C-C bond formation. As shown in Table S39, the O2–H2···N2 HB is stronger than the O1···H3–N3 HB in **COMIII'** or **COMIV'**. Compared with $\mathbf{R1_{C2}}$ (or **R2**), the less (or more) negative natural atomic charge on C1 (or C2) atom in **COMIII'** and **COMIV'** indicates that it becomes more susceptible to be nucleophilic attack (or to be electrophilic attack) (Table S39). These results show us that both of the substrates $\mathbf{R1_{C2}}$ and **R2** are activated via dual HB activation modes and other weak intermolecular interactions.

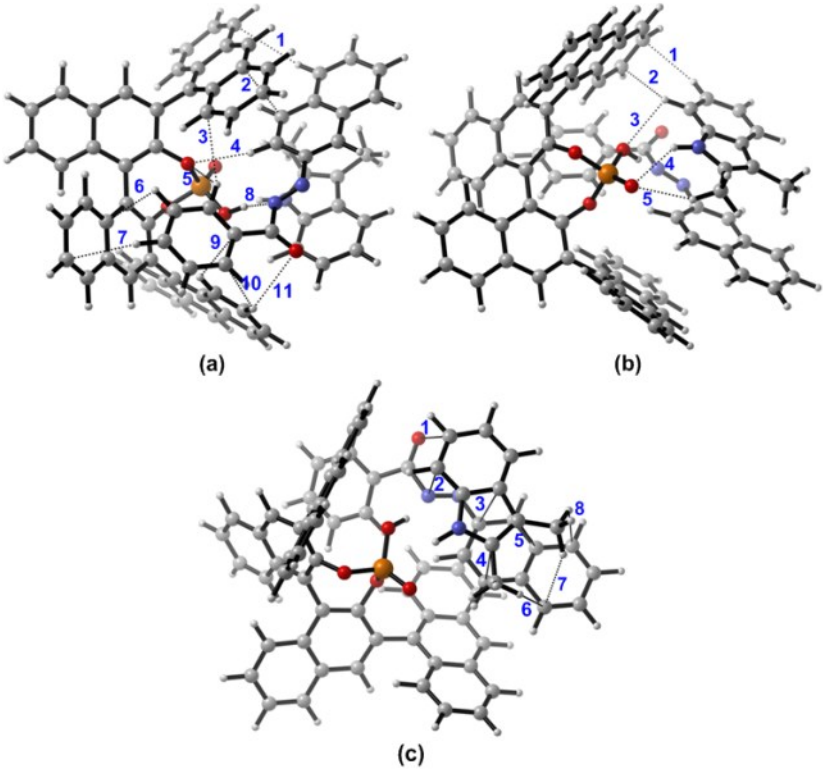

Figure S64 Intermolecular interactions in **COMIII'** and numbers of bond critical points (BCPs

No.).

Table S56 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 **COMIII'**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COMIII'(a)	1	C-H…π	2.99	0.0042	0.0134	0.0026	-0.0019	0.0007
	2	π…π	3.13	0.0091	0.0290	0.0060	-0.0047	0.0013
	3	C-H…π	2.77	0.0069	0.0216	0.0044	-0.0034	0.0010
	4	C-H…O	2.46	0.0104	0.0358	0.0083	-0.0076	0.0007
	5	C-H…O	2.39	0.0120	0.0413	0.0097	-0.0090	0.0007
	6	C-H…π	2.77	0.0081	0.0289	0.0057	-0.0041	0.0016
	7	C-H…π	2.86	0.0062	0.0198	0.0040	-0.0031	0.0009
	8	O-H…N	1.75	0.0466	0.0975	0.0285	-0.0326	-0.0041
	9	C-H…π	2.81	0.0070	0.0231	0.0046	-0.0035	0.0011
	10	C-H…π	2.75	0.0071	0.0252	0.0049	-0.0035	0.0014
	11	C-H…O	2.85	0.0049	0.0189	0.0038	-0.0029	0.0009
COMIII'(b)	1	C-H…π	2.71	0.0074	0.0249	0.0050	-0.0037	0.0013
	2	C-H…π	2.85	0.0067	0.0218	0.0045	-0.0035	0.0010
	3	C-H…O	2.57	0.0088	0.0333	0.0071	-0.0059	0.0012
	4	N-H…O	2.23	0.0152	0.0486	0.0122	-0.0122	0.0000
	5	C-H…O	2.55	0.0078	0.0282	0.0062	-0.0053	0.0009
COMIII'(c)	1	π…π	3.15	0.0072	0.0246	0.0053	-0.0045	0.0008
	2	π…π	3.13	0.0088	0.0255	0.0057	-0.0049	0.0008
	3	π…π	3.38	0.0066	0.0190	0.0040	-0.0032	0.0008
	4	π…π	3.23	0.0078	0.0227	0.0048	-0.0039	0.0009
	5	π…π	3.42	0.0060	0.0190	0.0040	-0.0032	0.0008
	6	C-H…π	2.94	0.0050	0.0159	0.0031	-0.0023	0.0008
	7	C-H…π	2.93	0.0058	0.0187	0.0038	-0.0030	0.0008
	8	C-H…π	2.89	0.0066	0.0220	0.0044	-0.0032	0.0012

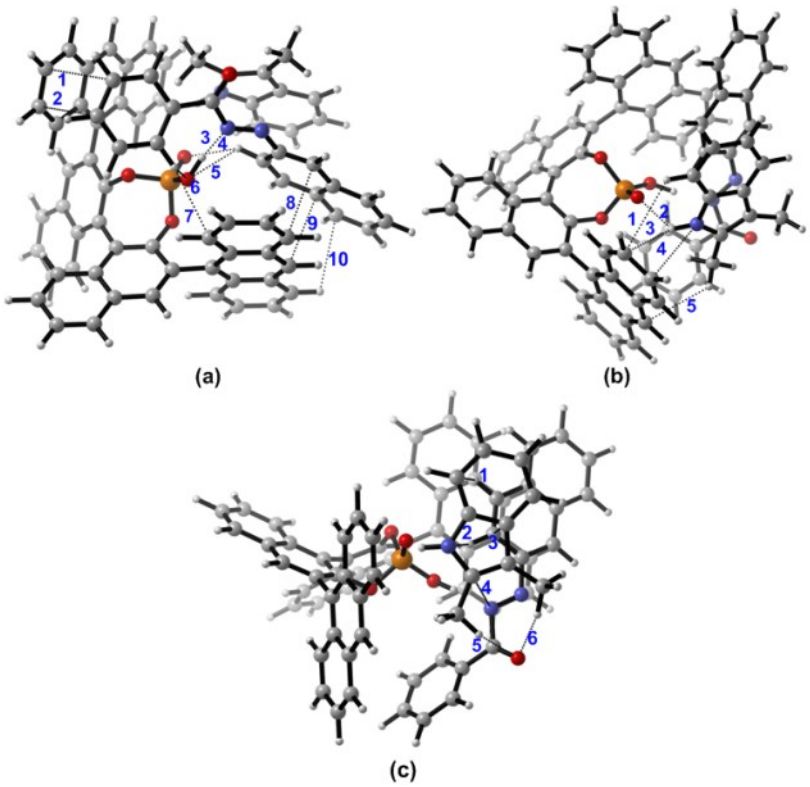

Figure S65 Intermolecular interactions in **COMIV'** and numbers of bond critical points (BCPs No.).

Table S57 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 **COMIV'**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COMIV'(a)	1	π…π	3.46	0.0052	0.0149	0.0031	-0.0024	0.0007
	2	π…π	3.43	0.0052	0.0158	0.0032	-0.0024	0.0008
	3	O-H…N	1.67	0.0572	0.1046	0.0351	-0.0441	-0.0090
	4	C-H…π	2.38	0.0126	0.0397	0.0096	-0.0093	0.0003
	5	C-H…π	2.56	0.0109	0.0485	0.0098	-0.0074	0.0024
	6	C-H…O	2.34	0.0132	0.0509	0.0113	-0.0098	0.0015
	7	C-H…π	2.86	0.0059	0.0173	0.0036	-0.0028	0.0008
	8	π…π	3.22	0.0074	0.0216	0.0045	-0.0036	0.0009
	9	π…π	3.22	0.0076	0.0234	0.0048	-0.0038	0.0010
	10	C-H…π	2.96	0.0060	0.0188	0.0037	-0.0027	0.0010
COMIV'(b)	1	lp…π	3.40	0.0062	0.0196	0.0041	-0.0033	0.0008
	2	C-H…π	2.91	0.0057	0.0180	0.0036	-0.0027	0.0009
	3	N-H…O	2.15	0.0172	0.0643	0.0152	-0.0143	0.0009
	4	N-H…π	2.81	0.0062	0.0218	0.0044	-0.0034	0.0010
	5	C-H…π	3.25	0.0027	0.0085	0.0016	-0.0011	0.0005
COMIV'(c)	1	C-H…π	2.95	0.0062	0.0193	0.0039	-0.0029	0.0010
	2	C-H…N	2.67	0.0081	0.0296	0.0065	-0.0055	0.0010
	3	π…π	3.11	0.0094	0.0302	0.0063	-0.0050	0.0013
	4	π…π	3.38	0.0056	0.0172	0.0037	-0.0032	0.0005
	5	C-H…π	2.58	0.0085	0.0308	0.0065	-0.0052	0.0013
	6	C-H…O	2.46	0.0099	0.0321	0.0075	-0.0070	0.0005

Followed by the subsequent protonation process, the complex **COMIII'** or **COMIV'** transforms into **TSIII'-1** or **TSIV'-1**. For the process of **COMIII'→TSIII'-1** or **COMIV'→TSIV'-1**, the Gibbs free energy of 12.3 kcal/mol or 10.2 kcal/mol is needed to cross the barrier. As revealed by QTAIM study, the O2···H2–N2 and O1···H3–N3 HBs are found in the transition state **TSIII'-1** or **TSIV'-1** (Figure S66 and Table S58, or Figure S67 and Table S59). The intermolecular π···π interaction between C1 atom of $\mathbf{R1_{C2}}$ and C2 atom of **R2** with the distance of 2.39 or 2.34 Å in **TSIII'-1** or **TSIV'-1**, respectively. After the nucleophilic attack between $\mathbf{R1_{C2}}$ and **R2**, the intermediate **IMIII'-1** or **IMIV'-1** is generated with an energy release of 14.8 kcal/mol or 19.7 kcal/mol. In **IMIII'-1** or **IMIV'-1**, the bond length of newly formed C1–C2 bond is measured to be 1.61 or 1.60 Å (Figure S68 and Table S60, or Figure S69 and Table S61). During the process of **COMIII'→TSIII'-1→IMIII'-1** or **COMIV'→TSIV'-1→IMIV'-1**, the distance of HB between $\mathbf{R1_{C2}}$ and **CP3** is generally increased while the distance of HB O1···H3–N3 is continuously decreased. Like the steps in path **III** and **IV**, the rotation of C1–C2 bond in **IMIII'-1** or **IMIV'-1** makes N1 atom of $\mathbf{R1_{C2}}$ approaches C3 atom of **R2**. In **TSIII'-2** or **TSIV'-2**, we found the N1···C3 interaction exists between $\mathbf{R1_{C2}}$ segment and **R2** segment through QTAIM analyses (Figure S70 and Table S62, or Figure S71 and Table S63). From **IMIII'-1** to **TSIII'-2** or from **IMIV'-1** to **TSIV'-2**, free energy of 12.0 kcal/mol or 14.5 kcal/mol is absorbed to overcome the barrier. And the interaction distance of N1 and C3 in **TSIII'-2** or **TSIV'-2** is 2.06 Å or 2.09 Å (Figure S70 and Table S62, or Figure S71 and Table S63). Then the intermediate **IMIII'-2** or **IMIV'-2** with the N1–C3 bond length of 1.55 Å or 1.52 Å is produced (Figure S72 and Table S64, or Figure S73 and Table S65). Like the case in formal steps, the O1···H3–N3 HB breaks and a new O2···H3–N3 HB is temporarily generated in **IMIII'-3** or **IMIV'-3** (Figure S74

and Table S66, or Figure S75 and Table S67). Then the following rotation of N1–N2 bond leads to the breakage of O2···H3–N3 HB and the subsequent approaching of O2 to C1–H1 bond. Due to the steric effect between indole ring and the anthryl group in **IMIII'-4,** the energy of **IMIII'-4** is even higher than the following transition state **TSIII'-3**. In path **IV'**, an energy of 1.7 kcal/mol is needed to cross the energy barrier of **IMIV'-4→TSIV'-3**. In **TSIII'-3**, the C1···H1 and O1···H1 distance in **TSIII'-3** (or **TSIV'-3**) is 1.22 and 1.50Å (or 1.30 and 1.36Å). And the HB O2···H2–N2 is increased in either **TSIII'-3** or **TSIV'-3**. After an energy release of 21.0 kcal/mol for the process of **TSIII'-3→IMIII'-5** or of 14.9 kcal/mol for the process **TSIV'-3→IMIV'-5**, the O2···H2–N2 HB is broken and the regenerated catalyst **CP3** removes from **IMIII'-5** or **IMIV'-5**, generating the product *ent*-$\mathbf{P1_{C2}}$ (R=Bz). QTAIM analyses of the transition states and intermediates are shown in Figures S76-S81 and Tables S68-S73.

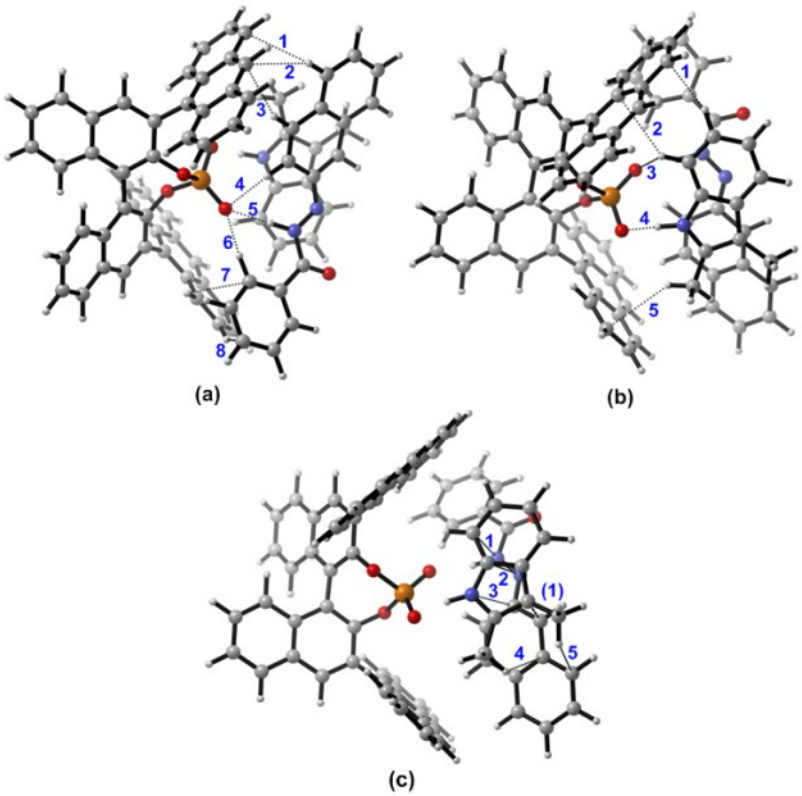

Figure S66 Intermolecular interactions in **TSIII'-1** and numbers of bond critical points (BCPs No.).

Table S58 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 **TSIII'-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIII'-1(a)	1	C-H…π	2.87	0.0059	0.0212	0.0041	-0.0029	0.0012
	2	C-H…π	2.76	0.0069	0.0230	0.0046	-0.0034	0.0012
	3	C-H…π	2.65	0.0087	0.0266	0.0056	-0.0046	0.0010
	4	C-H…O	2.33	0.0148	0.0475	0.0115	-0.0112	0.0003
	5	N-H…O	1.87	0.0285	0.0949	0.0233	-0.0228	0.0005
	6	C-H…O	2.20	0.0161	0.0517	0.0128	-0.0128	0.0000
	7	C-H…π	2.99	0.0061	0.0195	0.0038	-0.0028	0.0010
	8	C-H…π	2.73	0.0080	0.0249	0.0052	-0.0041	0.0011
TSIII'-1(b)	1	C-H…π	2.56	0.0099	0.0297	0.0064	-0.0054	0.0010
	2	C-H…π	2.95	0.0049	0.0154	0.0031	-0.0023	0.0008
	3	C-H…π	2.59	0.0092	0.0333	0.0072	-0.0060	0.0012
	4	N-H…O	1.64	0.0522	0.1529	0.0411	-0.0441	-0.0030
	5	C-H…π	3.01	0.0044	0.0136	0.0027	-0.0020	0.0007
TSIII'-1(c)	(1)	C…C	2.39	0.0414	0.0507	0.0175	-0.0224	-0.0049
	1	lp…π	3.14	0.0091	0.0262	0.0059	-0.0053	0.0006
	2	π…π	2.98	0.0124	0.0388	0.0082	-0.0067	0.0015
	3	π…π	3.03	0.0106	0.0388	0.0085	-0.0073	0.0012
	4	C-H…π	2.64	0.0101	0.0354	0.0071	-0.0053	0.0018
	5	C-H…π	2.63	0.0093	0.0317	0.0064	-0.0048	0.0016

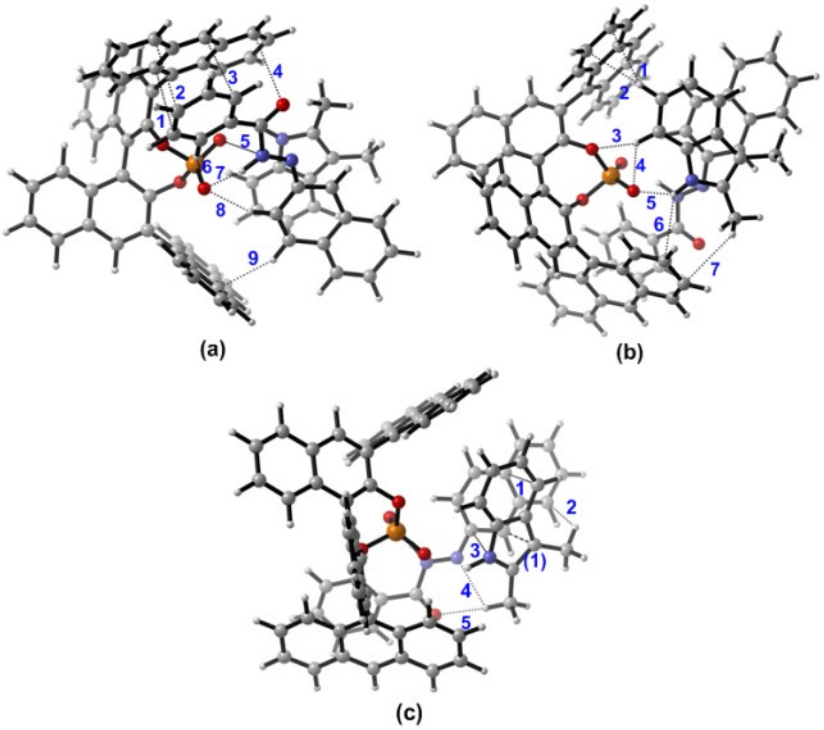

Figure S67 Intermolecular interactions in **TSIV'-1** and numbers of bond critical points (BCPs No.).

Table S59 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **TSIV'-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSIV'-1(a)	1	π…π	3.67	0.0041	0.0118	0.0024	-0.0019	0.0005
	2	π…π	3.23	0.0080	0.0228	0.0048	-0.0038	0.0010
	3	π…π	3.36	0.0062	0.0171	0.0036	-0.0029	0.0007
	4	lp…π	3.45	0.0038	0.0138	0.0028	-0.0022	0.0006
	5	lp…π	3.14	0.0082	0.0287	0.0064	-0.0057	0.0007
	6	C-H…O	2.11	0.0214	0.0610	0.0164	-0.0175	-0.0011
	7	N-H…O	1.88	0.0310	0.0891	0.0235	-0.0246	-0.0011
	8	C-H…O	2.15	0.0190	0.0548	0.0145	-0.0152	-0.0007
	9	C-H…π	2.61	0.0096	0.0297	0.0063	-0.0051	0.0012
TSIV'-1(b)	1	C-H…π	2.72	0.0081	0.0275	0.0057	-0.0046	0.0011
	2	C-H…π	2.72	0.0081	0.0262	0.0056	-0.0046	0.0010
	3	C-H…O	2.39	0.0107	0.0372	0.0087	-0.0081	0.0006
	4	C-H…O	2.45	0.0119	0.0425	0.0096	-0.0086	0.0010
	5	N-H…O	1.89	0.0270	0.0964	0.0233	-0.0226	0.0007
	6	N-H…π	2.95	0.0045	0.0148	0.0029	-0.0022	0.0007
	7	C-H…π	2.95	0.0053	0.0184	0.0035	-0.0025	0.0010
TSIV'-1(c)	(1)	C…C	2.34	0.0449	0.0477	0.0183	-0.0247	-0.0064
	1	π…π	3.11	0.0095	0.0286	0.0059	-0.0047	0.0012
	2	C-H…π	2.52	0.0111	0.0375	0.0077	-0.0061	0.0016
	3	π…π	2.97	0.0126	0.0415	0.0092	-0.0079	0.0013
	4	C-H…N	2.62	0.0095	0.0321	0.0068	-0.0056	0.0012
	5	C-H…O	2.46	0.0098	0.0306	0.0072	-0.0068	0.0004

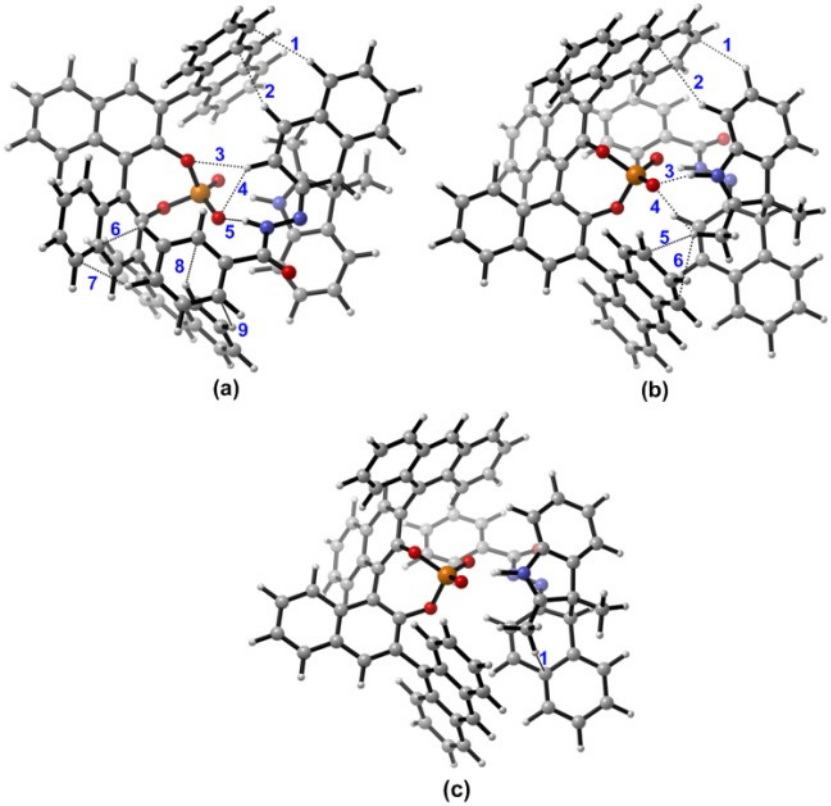

Figure S68 Intermolecular interactions in **IMIII'-1** and numbers of bond critical points (BCPs No.).

Table S60 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 **IMIII'-1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMIII'-1(a)	1	C-H…π	2.75	0.0065	0.0210	0.0043	-0.0033	0.0010
	2	C-H…π	2.57	0.0096	0.0307	0.0065	-0.0054	0.0011
	3	C-H…O	2.56	0.0077	0.0286	0.0063	-0.0054	0.0009
	4	C-H…π	2.50	0.0110	0.0383	0.0087	-0.0077	0.0010
	5	N-H…O	1.80	0.0329	0.1132	0.0274	-0.0265	0.0009
	6	C-H…π	2.72	0.0085	0.0304	0.0060	-0.0044	0.0016
	7	C-H…π	2.92	0.0055	0.0179	0.0035	-0.0025	0.0010
	8	C-H…π	2.80	0.0069	0.0217	0.0044	-0.0035	0.0009
	9	C-H…π	2.64	0.0082	0.0266	0.0054	-0.0042	0.0012
IMIII'-1(b)	1	C-H…π	2.63	0.0088	0.0272	0.0056	-0.0045	0.0011
	2	C-H…π	3.09	0.0035	0.0115	0.0023	-0.0016	0.0007
	3	N-H…O	1.54	0.0693	0.1570	0.0522	-0.0651	-0.0129
	4	C-H…O	2.49	0.0101	0.0351	0.0080	-0.0072	0.0008
	5	C-H…π	2.86	0.0062	0.0208	0.0042	-0.0033	0.0009
	6	C-H…π	2.97	0.0065	0.0219	0.0044	-0.0033	0.0011
IMIII'-1(c)	1	C-H…π	2.53	0.0107	0.0360	0.0075	-0.0061	0.0014

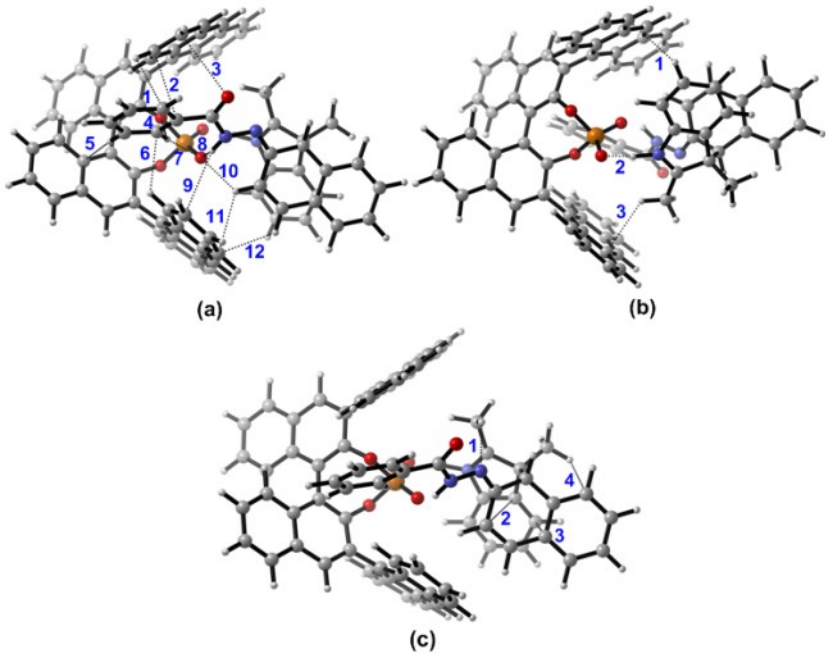

Figure S69 Intermolecular interactions in **IMIV'-1** and numbers of bond critical points (BCPs No.).

Table S61 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 **IMIV'-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV'-1(a)	1	C-H…π	2.99	0.0056	0.0185	0.0037	-0.0028	0.0009
	2	π…π	3.33	0.0065	0.0197	0.0041	-0.0033	0.0008
	3	π…π	3.53	0.0034	0.0125	0.0025	-0.0019	0.0006
	4	C-H…O	2.34	0.0128	0.0447	0.0105	-0.0099	0.0006
	5	C-H…π	2.71	0.0072	0.0221	0.0046	-0.0037	0.0009
	6	C-H…π	2.72	0.0076	0.0264	0.0052	-0.0038	0.0014
	7	C-H…O	2.31	0.0147	0.0420	0.0109	-0.0113	-0.0004
	8	N-H…O	1.96	0.0242	0.0812	0.0204	-0.0205	-0.0001
	9	N-H…π	3.19	0.0036	0.0117	0.0023	-0.0016	0.0007
	10	C-H…O	2.39	0.0113	0.0428	0.0095	-0.0083	0.0012
	11	C-H…π	2.90	0.0063	0.0219	0.0044	-0.0033	0.0011
	12	C-H…π	2.72	0.0073	0.0249	0.0049	-0.0036	0.0013
IMIV'-1(b)	1	C-H…π	2.96	0.0047	0.0149	0.0029	-0.0020	0.0009
	2	N-H…O	1.41	0.0953	0.1208	0.0703	-0.1104	-0.0401
	3	C-H…π	2.74	0.0073	0.0241	0.0048	-0.0036	0.0012
IMIV'-1(c)	1	C-H…N	2.45	0.0123	0.0387	0.0086	-0.0076	0.0010
	2	π…π	3.22	0.0091	0.0269	0.0057	-0.0047	0.0010
	3	π…π	3.05	0.0106	0.0358	0.0073	-0.0057	0.0016
	4	C-H…π	2.68	0.0088	0.0312	0.0062	-0.0046	0.0016

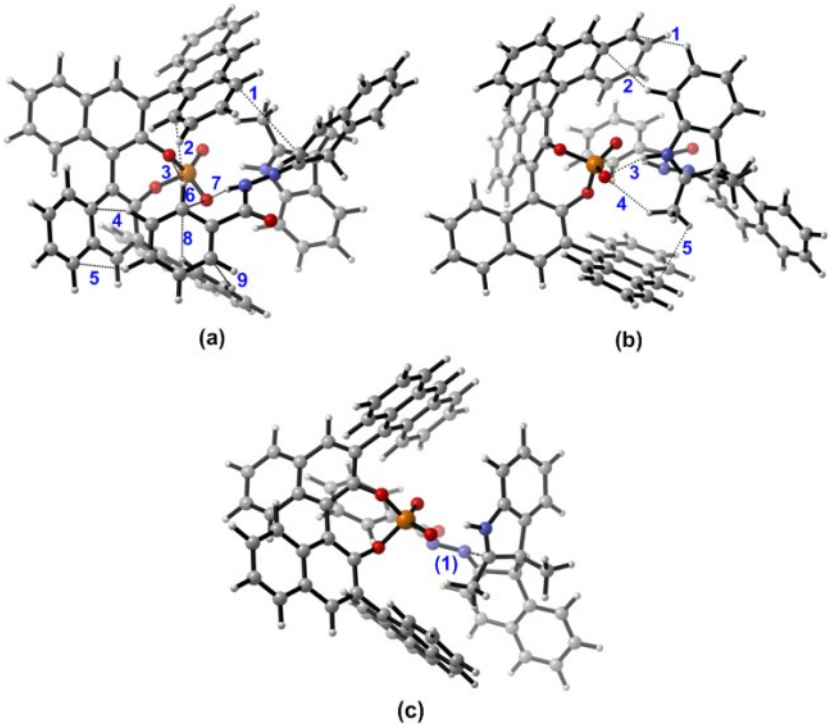

Figure S70 Intermolecular interactions in **TSIII'-2** and numbers of bond critical points (BCPs No.).

Table 62 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 **TSIII'-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIII'-2(a)	1	π…π	3.73	0.0039	0.0104	0.0021	-0.0017	0.0004
	2	C-H…π	2.80	0.0063	0.0195	0.0039	-0.0030	0.0009
	3	C-H…O	2.33	0.0129	0.0411	0.0101	-0.0099	0.0002
	4	C-H…π	2.55	0.0101	0.0334	0.0070	-0.0057	0.0013
	5	C-H…π	3.03	0.0043	0.0134	0.0026	-0.0019	0.0007
	6	π…π	3.20	0.0075	0.0279	0.0058	-0.0047	0.0011
	7	N-H…O	1.72	0.0428	0.1305	0.0335	-0.0343	-0.0008
	8	C-H…π	2.93	0.0053	0.0170	0.0035	-0.0027	0.0008
	9	C-H…π	2.71	0.0071	0.0225	0.0045	-0.0035	0.0010
TSIII'-2(b)	1	C-H…π	3.03	0.0046	0.0146	0.0028	-0.0020	0.0008
	2	C-H…π	3.09	0.0037	0.0121	0.0024	-0.0017	0.0007
	3	N-H…O	1.83	0.0338	0.1015	-0.0267	0.0260	-0.0007
	4	C-H…π	2.63	0.0085	0.0301	0.0065	-0.0055	0.0010
	5	C-H…π	2.82	0.0076	0.0256	0.0051	-0.0038	0.0013
TSIII'-2(c)	(1)	C…N	2.06	0.0679	0.1098	-0.0539	0.0407	-0.0132

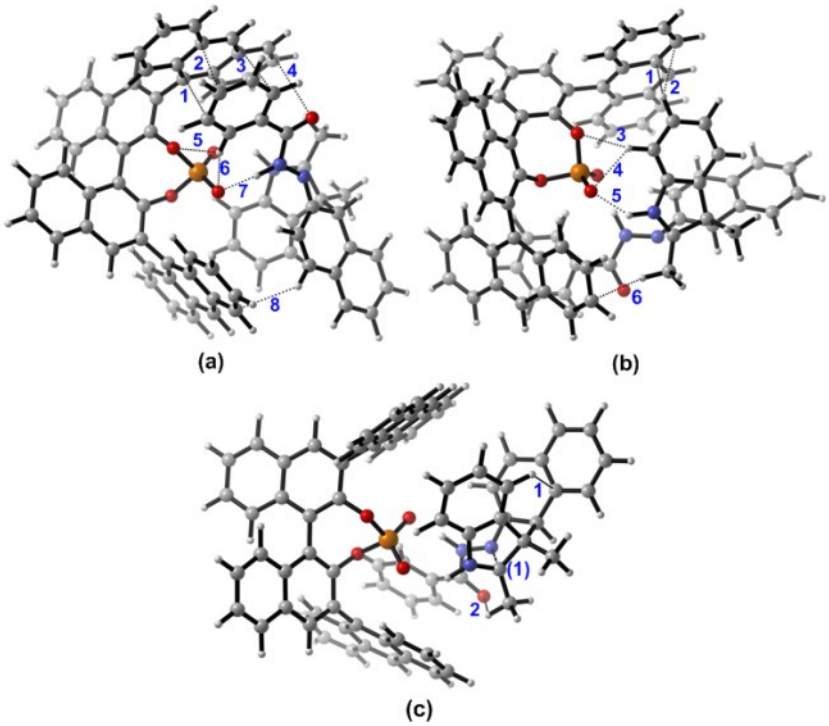

Figure S71 Intermolecular interactions in **TSIV'-2** and numbers of bond critical points (BCPs No.).

Table S63 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (G, in a.u.), the electronic potential energy density (V, in a.u.) and the electronic energy density (H, in a.u.) at the BCPs of **TSIV'-2**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
TSIV'-2(a)	1	π…π	3.49	0.0052	0.0151	0.0031	-0.0025	0.0006
	2	π…π	3.16	0.0086	0.0256	0.0054	-0.0043	0.0011
	3	π…π	3.49	0.0051	0.0140	0.0029	-0.0023	0.0006
	4	π…π	3.93	0.0014	0.0065	0.0012	-0.0007	0.0005
	5	C-H…O	2.49	0.0094	0.0365	0.0080	-0.0069	0.0011
	6	C-H…O	2.20	0.0182	0.0515	0.0137	-0.0145	-0.0008
	7	N-H…O	1.75	0.0391	0.1221	0.0308	-0.0311	-0.0003
	8	C-H…π	2.68	0.0082	0.0253	0.0052	-0.0040	0.0012
TSIV'-2(b)	1	C-H…π	2.79	0.0077	0.0287	0.0057	-0.0041	0.0016
	2	C-H…π	2.76	0.0079	0.0271	0.0056	-0.0043	0.0013
	3	C-H…O	2.56	0.0081	0.0327	0.0070	-0.0057	0.0013
	4	C-H…O	2.37	0.0141	0.0505	0.0116	-0.0105	0.0011
	5	N-H…O	1.82	0.0337	0.1140	0.0283	-0.0282	0.0001
	6	C-H…π	2.80	0.0061	0.0189	0.0038	-0.0028	0.0010
TSIV'-2(c)	(1)	C…N	2.09	0.0645	0.1009	0.0372	-0.0491	-0.0119
	1	C-H…π	2.70	0.0091	0.0324	0.0064	-0.0048	0.0016
	2	C-H…O	2.62	0.0082	0.0309	0.0066	-0.0054	0.0012

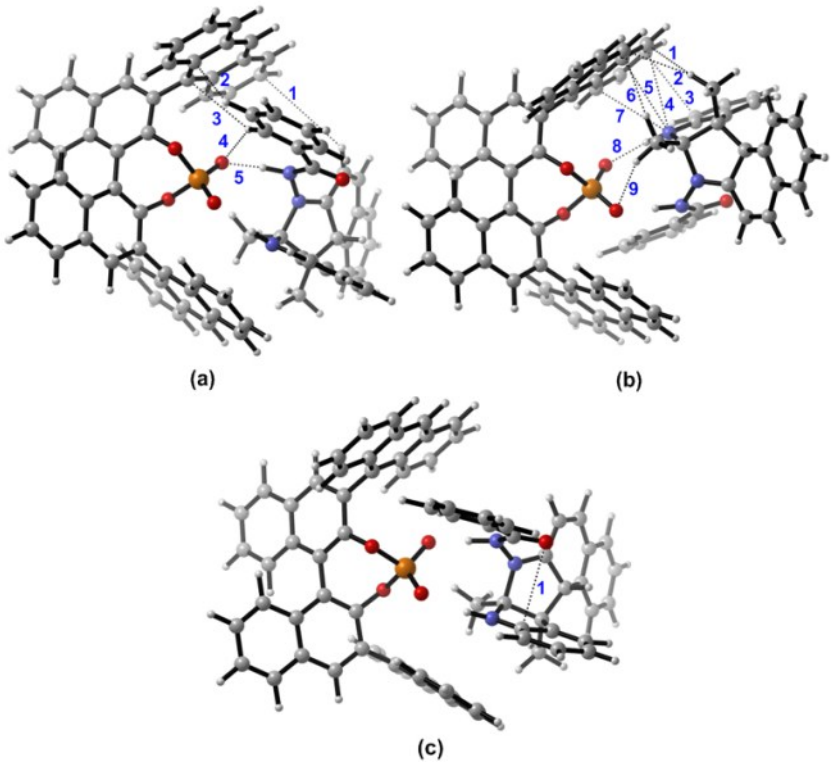

Figure S72 Intermolecular interactions in **IMIII'-2** and numbers of bond critical points (BCPs No.).

Table S64 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 **IMIII'-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIII'-2(a)	1	C-H…π	4.41	0.0002	0.0011	0.0002	-0.0001	0.0001
	2	C-H…π	2.61	0.0092	0.0329	0.0068	-0.0054	0.0014
	3	C-H…π	3.14	0.0039	0.0122	0.0025	-0.0019	0.0006
	4	C-H…π	2.38	0.0137	0.0430	0.0104	-0.0101	0.0003
	5	N-H…O	1.63	0.0533	0.1504	0.0413	-0.0450	-0.0037
IMIII'-2(b)	1	C-H…π	2.73	0.0069	0.0226	0.0046	-0.0036	0.0010
	2	C-H…π	2.80	0.0067	0.0218	0.0044	-0.0034	0.0010
	3	π…π	3.34	0.0064	0.0184	0.0038	-0.0030	0.0008
	4	lp…π	3.56	0.0050	0.0160	0.0035	-0.0030	0.0005
	5	lp…π	3.52	0.0050	0.0160	0.0034	-0.0029	0.0005
	6	C-H…π	2.66	0.0088	0.0269	0.0057	-0.0047	0.0010
	7	lp…π	3.52	0.0050	0.0167	0.0035	-0.0027	0.0008
	8	N-H…O	1.88	0.0291	0.0900	0.0228	-0.0231	-0.0003
	9	C-H…π	2.29	0.0156	0.0470	0.0118	-0.0119	-0.0001
IMIII'-2(c)	1	π…π	3.35	0.0054	0.0188	0.0040	-0.0032	0.0008

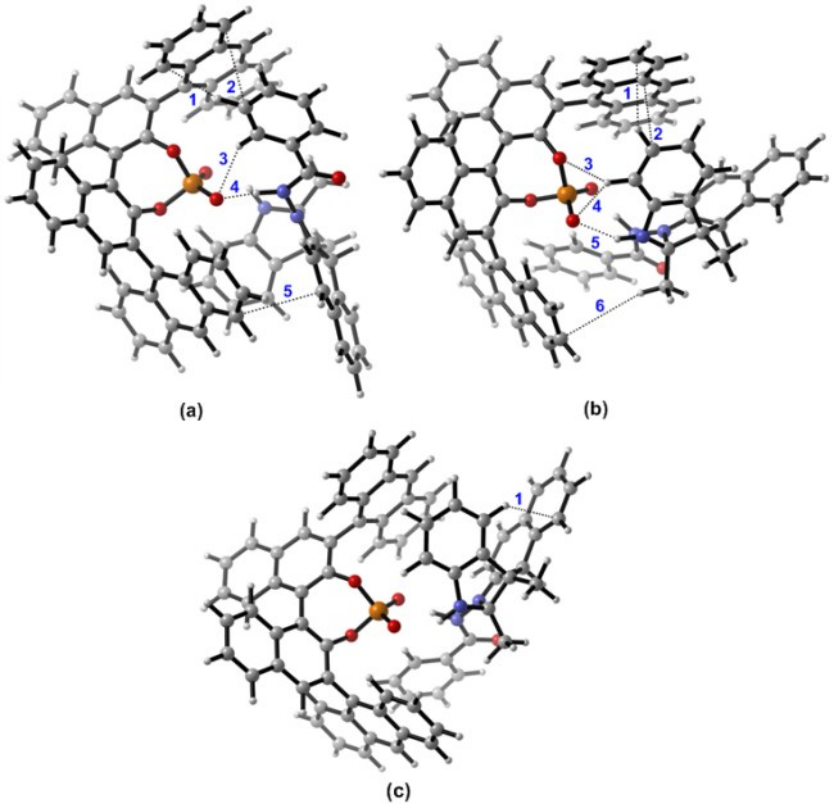

Figure S73 Intermolecular interactions in **IMIV'-2** and numbers of bond critical points (BCPs No.).

Table S65 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 **IMIV'-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV'-2(a)	1	C-H…π	2.75	0.0078	0.0239	0.0050	0.0239	0.0289
	2	π…π	3.36	0.0068	0.0230	0.0046	-0.0035	0.0011
	3	C-H…π	2.32	0.0149	0.0459	0.0114	-0.0114	0.0000
	4	N-H…O	1.56	0.0635	0.1607	0.0489	-0.0576	-0.0087
	5	π…π	3.52	0.0049	0.0139	0.0028	-0.0022	0.0006
IMIV'-2(b)	1	C-H…π	2.79	0.0074	0.0242	0.0050	-0.0039	0.0011
	2	π…π	3.31	0.0067	0.0224	0.0045	-0.0034	0.0011
	3	C-H…O	2.73	0.0059	0.0241	0.0049	-0.0038	0.0011
	4	C-H…π	2.49	0.0110	0.0380	0.0086	-0.0077	0.0009
	5	N-H…O	1.89	0.0296	0.0929	0.0238	-0.0244	-0.0006
	6	C-H…π	4.05	0.0005	0.0021	0.0004	-0.0002	0.0002
IMIV'-2(c)	1	C-H…π	2.68	0.0084	0.0268	0.0054	-0.0041	0.0013

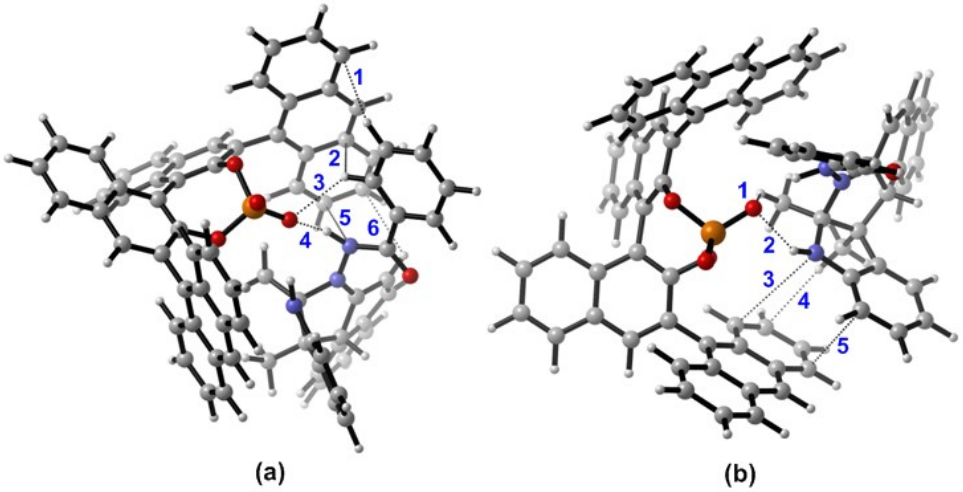

Figure S74 Intermolecular interactions in **IMIII'-3** and numbers of bond critical points (BCPs No.).

Table S66 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 **IMIII'-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIII'-3(a)	1	C-H…π	2.85	0.0060	0.0194	0.0038	-0.0028	0.0010
	2	C-H…π	2.77	0.0076	0.0262	0.0052	-0.0038	0.0014
	3	C-H…O	2.37	0.0136	0.0469	0.0110	-0.0102	0.0008
	4	N-H…O	1.68	0.0424	0.1557	0.0371	-0.0352	0.0019
	5	lp…π	3.37	0.0064	0.0187	0.0042	-0.0037	0.0005
	6	C-H…π	2.84	0.0071	0.0249	0.0048	-0.0033	0.0015
IMIII'-3(b)	1	C-H…O	2.34	0.0144	0.0453	0.0111	-0.0109	0.0002
	2	N-H…O	2.02	0.0240	0.0709	0.0190	-0.0202	-0.0012
	3	lp…π	3.97	0.0022	0.0085	0.0017	-0.0012	0.0005
	4	C-H…π	2.61	0.0086	0.0276	0.0057	-0.0046	0.0011
	5	π…π	3.40	0.0058	0.0166	0.0035	-0.0028	0.0007

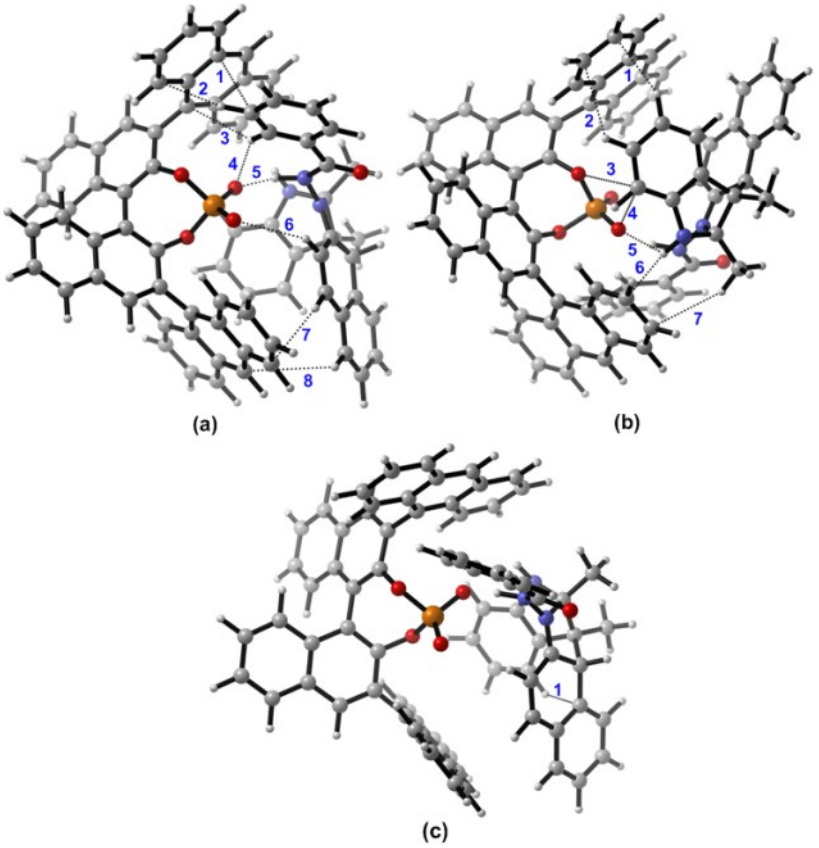

Figure S75 Intermolecular interactions in **IMIV'-3** and numbers of bond critical points (BCPs No.).

Table S67 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 **IMIV'-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV'-3(a)	1	π…π	3.23	0.0078	0.0282	0.0056	-0.0041	0.0015
	2	C-H…π	2.69	0.0085	0.0269	0.0057	-0.0047	0.0010
	3	C-H…π	3.02	0.0047	0.0146	0.0030	-0.0023	0.0007
	4	C-H…π	2.50	0.0112	0.0372	0.0085	-0.0078	0.0007
	5	N-H…O	1.57	0.0647	0.1616	0.0498	-0.0593	-0.0095
	6	C-H…O	2.63	0.0072	0.0259	0.0055	-0.0046	0.0009
	7	C-H…π	2.62	0.0093	0.0273	0.0058	-0.0048	0.0010
	8	C-H…π	3.26	0.0036	0.0118	0.0023	-0.0016	0.0007
IMIV'-3(b)	1	C-H…π	2.68	0.0083	0.0248	0.0052	-0.0041	0.0011
	2	C-H…π	3.11	0.0046	0.0137	0.0027	-0.0020	0.0007
	3	lp…π	3.57	0.0031	0.0121	0.0024	-0.0018	0.0006
	4	lp…π	3.09	0.0088	0.0307	0.0067	-0.0058	0.0009
	5	N-H…O	2.43	0.0108	0.0419	0.0094	-0.0083	0.0011
	6	N-H…π	2.42	0.0119	0.0389	0.0086	-0.0074	0.0012
	7	C-H…π	3.34	0.0025	0.0076	0.0015	-0.0010	0.0005
IMIV'-3(c)	1	C-H…π	2.75	0.0087	0.0286	0.0057	-0.0042	0.0015

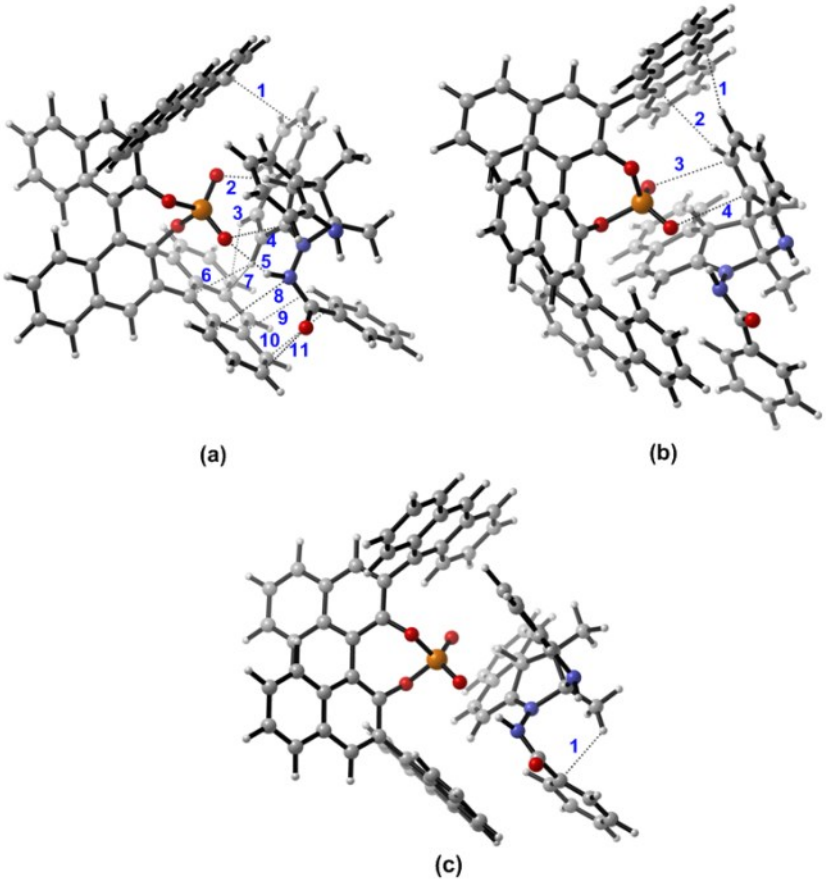

Figure S76 Intermolecular interactions in **IMIII'-4** and numbers of bond critical points (BCPs No.).

Table S68 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 **IMIII'-4**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IMIII'-4(a)	1	C-H…π	3.68	0.0013	0.0045	0.0008	-0.0006	0.0002
	2	C-H…O	1.83	0.0364	0.1041	0.0275	-0.0291	-0.0016
	3	C-H…π	2.77	0.0074	0.0237	0.0050	-0.0040	0.0010
	4	π…π	2.90	0.0119	0.0417	0.0094	-0.0083	0.0011
	5	N-H…O	2.03	0.0209	0.0733	0.0180	-0.0176	0.0004
	6	C-H…π	2.65	0.0091	0.0316	0.0067	-0.0054	0.0013
	7	C-H…π	2.67	0.0088	0.0332	0.0068	-0.0053	0.0015
	8	lp…π	3.67	0.0035	0.0116	0.0025	-0.0020	0.0005
	9	C-H…π	3.10	0.0046	0.0144	0.0029	-0.0021	0.0008
	10	π…π	3.35	0.0063	0.0182	0.0037	-0.0029	0.0008
	11	π…π	3.03	0.0092	0.0311	0.0068	-0.0058	0.0010
IMIII'-4(b)	1	C-H…π	2.54	0.0111	0.0358	0.0077	-0.0065	0.0012
	2	C-H…π	2.92	0.0054	0.0189	0.0038	-0.0028	0.0010
	3	π…π	3.19	0.0078	0.0282	0.0059	-0.0048	0.0011
	4	π…π	3.49	0.0049	0.0163	0.0034	-0.0028	0.0006
IMIII'-4(c)	1	C-H…π	2.56	0.0107	0.0350	0.0073	-0.0059	0.0014

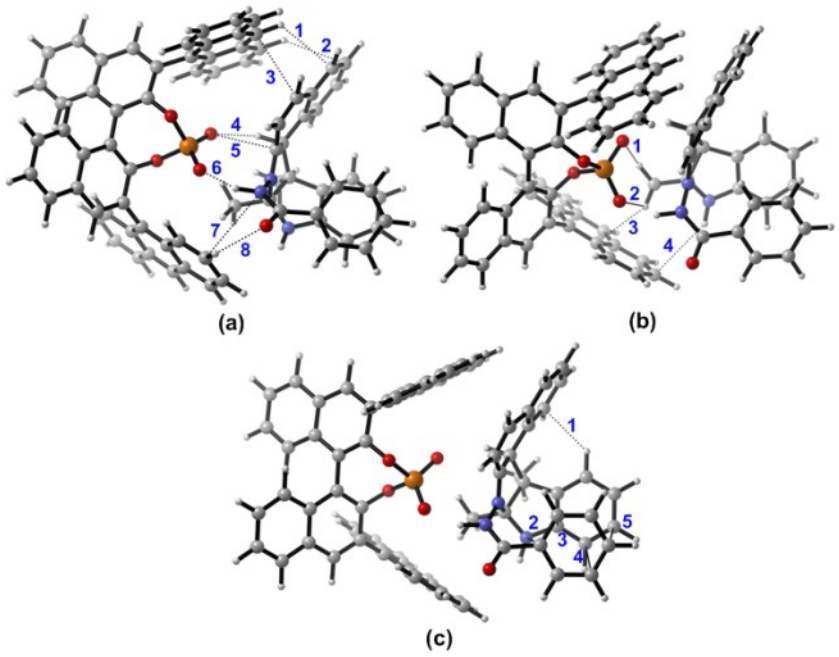

Figure S77 Intermolecular interactions in **IMIV'-4** and numbers of bond critical points (BCPs No.).

Table S69 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 **IMIV'-4**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV'-4(a)	1	C-H…π	2.88	0.0058	0.0192	0.0038	-0.0027	0.0011
	2	C-H…π	2.77	0.0076	0.0238	0.0049	-0.0038	0.0011
	3	π…π	3.19	0.0075	0.0232	0.0048	-0.0037	0.0011
	4	C-H…O	2.21	0.0163	0.0553	0.0133	-0.0128	0.0005
	5	π…π	2.91	0.0109	0.0401	0.0089	-0.0078	0.0011
	6	N-H…O	1.67	0.0460	0.1488	0.0376	-0.0380	-0.0004
	7	lp…π	3.50	0.0046	0.0146	0.0030	-0.0024	0.0006
	8	C-H…O	2.36	0.0128	0.0450	0.0103	-0.0093	0.0010
IMIV'-4(b)	1	C-H…O	2.28	0.0160	0.0489	0.0122	-0.0122	0.0000
	2	C-H…O	2.83	0.0065	0.0238	0.0049	-0.0038	0.0011
	3	C-H…π	2.63	0.0091	0.0323	0.0066	-0.0051	0.0015
	4	N-H…π	3.08	0.0033	0.0107	0.0020	-0.0014	0.0006
IMIV'-4(c)	1	C-H…π	2.57	0.0097	0.0312	0.0065	-0.0052	0.0013
	2	lp…π	3.31	0.0071	0.0217	0.0048	-0.0043	0.0005
	3	π…π	3.28	0.0077	0.0223	0.0046	-0.0037	0.0009
	4	π…π	3.44	0.0059	0.0180	0.0037	-0.0030	0.0007
	5	π…π	3.37	0.0069	0.0194	0.0040	-0.0032	0.0008

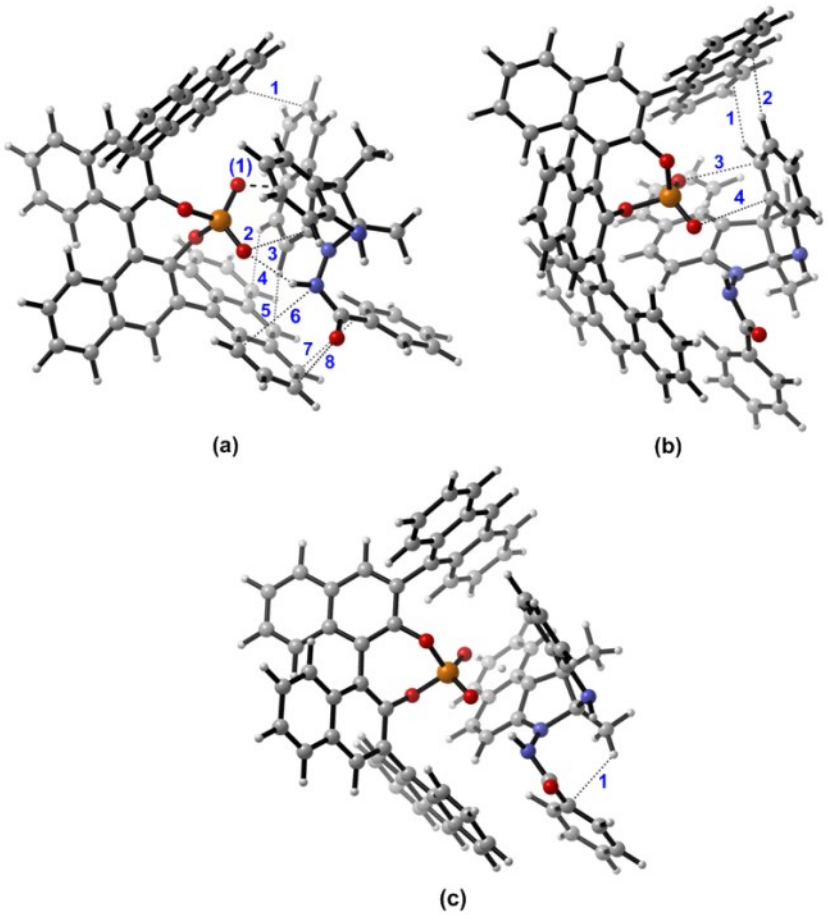

Figure S78 Intermolecular interactions in **TSIII'-3** and numbers of bond critical points (BCPs No.).

Table S70 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSIII'-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIII'-3(a)	(1)	O…H	1.50	0.0794	0.1464	0.0550	-0.0734	-0.0184
	1	C-H…π	2.89	0.0057	0.0179	0.0035	-0.0026	0.0009
	2	C-H…π	2.78	0.0073	0.0231	0.0048	-0.0039	0.0009
	3	lp…π	3.07	0.0090	0.0314	0.0069	-0.0060	0.0009
	4	N-H…O	2.04	0.0205	0.0697	0.0173	-0.0172	0.0001
	5	C-H…π	2.62	0.0095	0.0328	0.0069	-0.0057	0.0012
	6	lp…π	3.60	0.0040	0.0126	0.0027	-0.0023	0.0004
	7	π…π	3.36	0.0061	0.0175	0.0036	-0.0029	0.0007
	8	π…π	3.03	0.0094	0.0322	0.0070	-0.0060	0.0010
TSIII'-3(b)	1	C-H…π	2.82	0.0066	0.0235	0.0047	-0.0035	0.0012
	2	C-H…π	2.59	0.0104	0.0338	0.0072	-0.0059	0.0013
	3	π…π	3.05	0.0096	0.0342	0.0075	-0.0064	0.0011
	4	π…π	3.52	0.0047	0.0155	0.0032	-0.0026	0.0006
TSIII'-3(c)	1	C-H…π	2.58	0.0103	0.0332	0.0069	-0.0055	0.0014

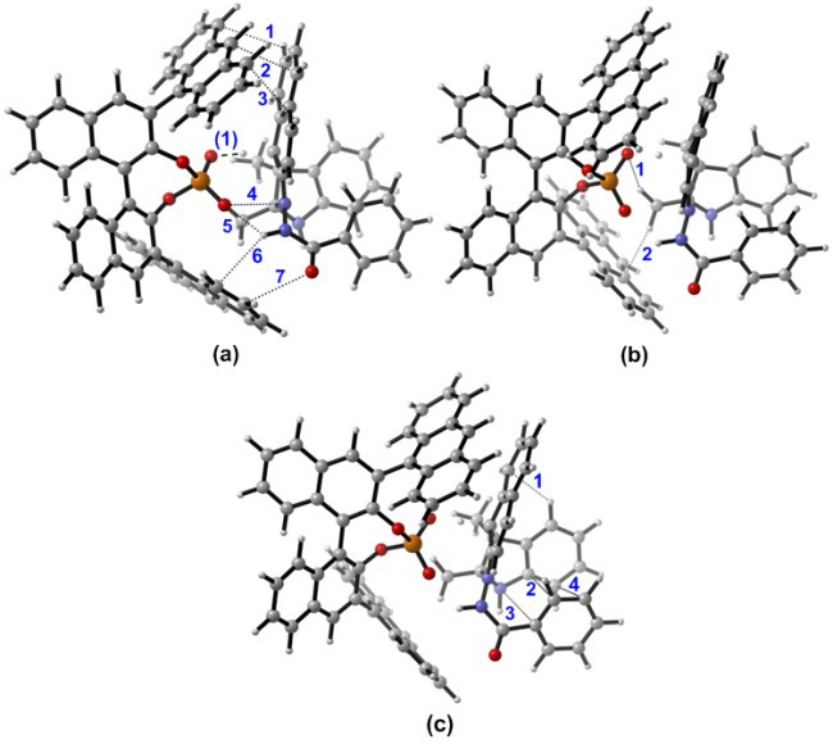

Figure S79 Intermolecular interactions in **TSIV'-3** and numbers of bond critical points (BCPs No.).

Table S71 Numbers of Bond Critical Point (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TSIV'-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TSIV'-3(a)	(1)	O…H	1.36	0.1121	0.0488	0.0715	-0.1308	-0.0593
	1	π…π	3.38	0.0061	0.0179	0.0037	-0.0029	0.0008
	2	π…π	3.15	0.0084	0.0252	0.0052	-0.0042	0.0010
	3	C-H…π	3.37	0.0022	0.0073	0.0014	-0.0009	0.0005
	4	lp…π	2.93	0.0121	0.0439	0.0101	-0.0093	0.0008
	5	N-H…O	2.04	0.0207	0.0734	0.0180	-0.0176	0.0004
	6	N-H…π	2.87	0.0055	0.0172	0.0035	-0.0026	0.0009
	7	lp…π	3.03	0.0095	0.0336	0.0073	-0.0062	0.0011
TSIV'-3(b)	1	C-H…π	2.40	0.0130	0.0435	0.0102	-0.0095	0.0007
	2	C-H…π	2.56	0.0101	0.0330	0.0070	-0.0058	0.0012
TSIV'-3(c)	1	C-H…π	2.67	0.0081	0.0257	0.0053	-0.0041	0.0012
	2	π…π	3.36	0.0065	0.0184	0.0038	-0.0031	0.0007
	3	lp…π	3.36	0.0064	0.0204	0.0045	-0.0038	0.0007
	4	π…π	3.42	0.0067	0.0189	0.0040	-0.0032	0.0008

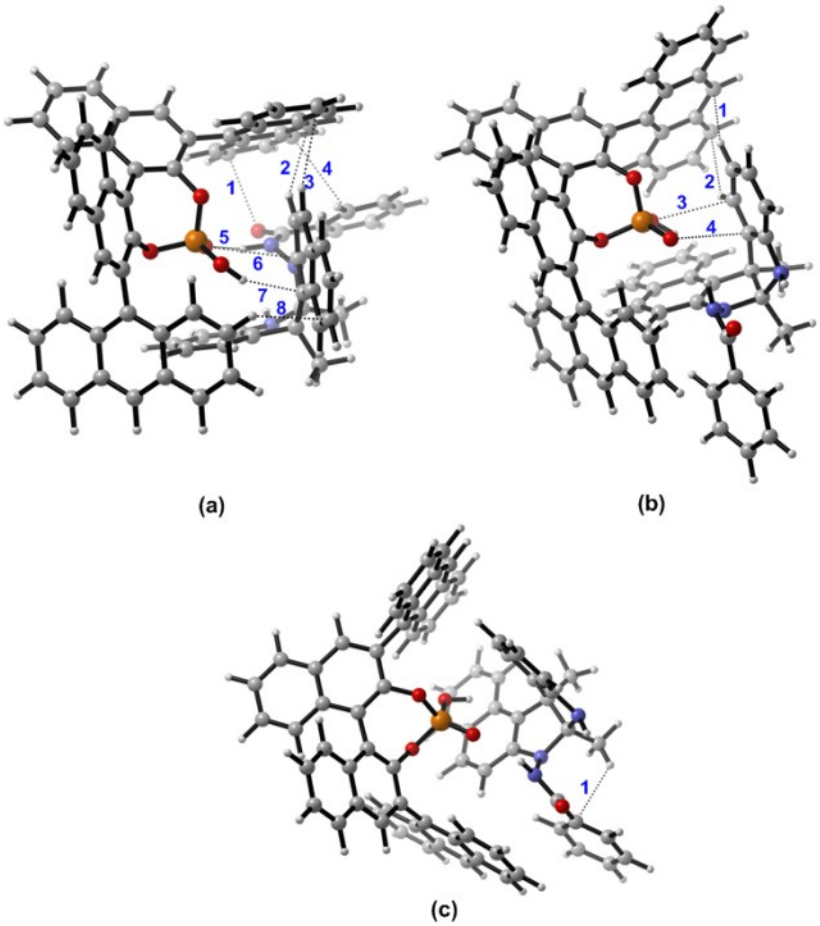

Figure S80 Intermolecular interactions in **IMIII'-5** and numbers of bond critical points (BCPs No.).

Table S72 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 **IMIII'-5**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIII'-5(a)	1	π…π	3.04	0.0091	0.0311	0.0067	-0.0057	0.0010
	2	C-H…π	2.67	0.0088	0.0300	0.0062	-0.0050	0.0012
	3	C-H…π	2.82	0.0067	0.0217	0.0045	-0.0036	0.0009
	4	π…π	3.31	0.0067	0.0194	0.0040	-0.0032	0.0008
	5	N-H…O	2.08	0.0183	0.0645	0.0157	-0.0153	0.0004
	6	π…π	3.24	0.0069	0.0226	0.0048	-0.0040	0.0008
	7	O-H…π	2.32	0.0147	0.0407	0.0097	-0.0092	0.0005
	8	C-H…π	2.76	0.0073	0.0240	0.0048	-0.0036	0.0012
IMIII'-5(b)	1	C-H…π	2.53	0.0113	0.0373	0.0081	-0.0068	0.0013
	2	C-H…π	3.06	0.0045	0.0138	0.0028	-0.0022	0.0006
	3	π…π	3.06	0.0107	0.0405	0.0085	-0.0068	0.0017
	4	π…π	3.47	0.0050	0.0172	0.0036	-0.0030	0.0006
IMIII'-5(c)	1	C-H…π	2.70	0.0081	0.0258	0.0053	-0.0041	0.0012

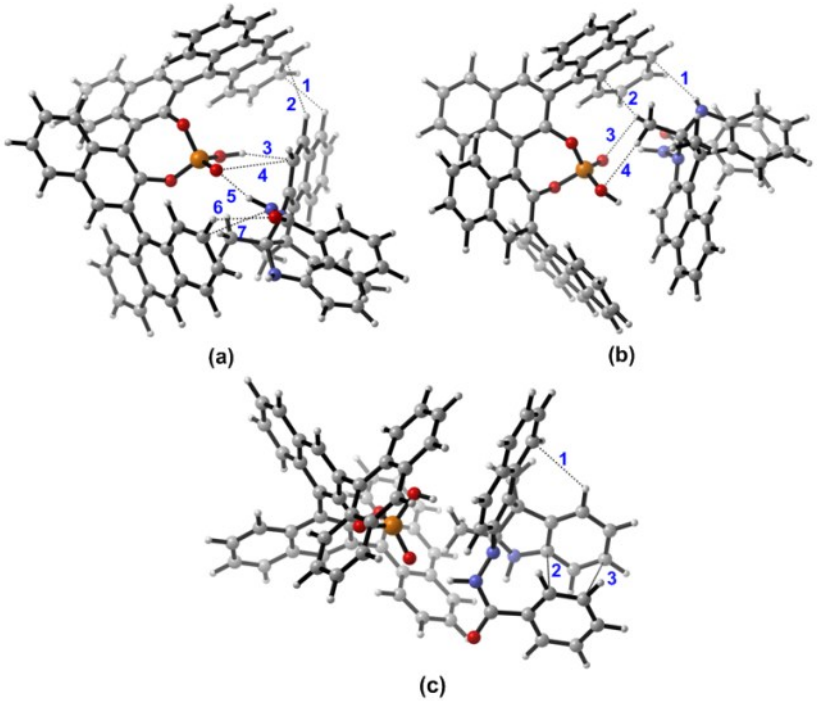

Figure S81 Intermolecular interactions in **IMIV'-5** and numbers of bond critical points (BCPs No.).

Table S73 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 **IMIV'-5**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IMIV'-5(a)	1	C-H…π	2.65	0.0089	0.0293	0.0059	-0.0045	0.0014
	2	C-H…π	3.20	0.0033	0.0103	0.0020	-0.0014	0.0006
	3	O-H…π	2.36	0.0129	0.0335	0.0079	-0.0074	0.0005
	4	π…π	3.54	0.0041	0.0145	0.0030	-0.0023	0.0007
	5	N-H…O	1.90	0.0265	0.0929	0.0227	-0.0222	0.0005
	6	C-H…O	2.49	0.0107	0.0405	0.0088	-0.0074	0.0014
	7	lp…π	3.41	0.0057	0.0191	0.0039	-0.0030	0.0009
IMIV'-5(b)	1	N-H…π	2.79	0.0064	0.0200	0.0041	-0.0031	0.0010
	2	C-H…π	2.48	0.0117	0.0408	0.0087	-0.0072	0.0015
	3	C-H…π	2.72	0.0076	0.0272	0.0058	-0.0048	0.0010
	4	C-H…O	2.60	0.0084	0.0285	0.0063	-0.0055	0.0008
IMIV'-5(c)	1	C-H…π	3.05	0.0041	0.0139	0.0027	-0.0018	0.0009
	2	π…π	3.35	0.0067	0.0191	0.0040	-0.0032	0.0008
	3	π…π	3.42	0.0067	0.0184	0.0038	-0.0031	0.0007

3. Origin of enantioselectivity

In the four reaction paths **I'-IV'**, the processes from [**R1$_{C2}$+R2+CP3**] to the transition states (i.e., **TSI'-1**, **TSII'-1**, **TSIII'-1**, **TSIV'-1**) are also the enantioselectivity-determining steps, so the distortion/interaction analyses of these transition states were carried out to reveal the origin of enantioselectivity of paths **I'-IV'**, as summarized in Table S74. As shown in Table S74, **TSIII'-1** has the relative lower total distortion energy among the **TSX'-1** (**X=I**, **IV**), and it has the relative stronger interaction energy, leading to a lowest activation energy (-44.6 kcal/mol). Thus even the activation energy of **TSIII'-1** is the lowest, which is in accordance with the fact that the Gibbs free energy of **TSIII'-1** is the lowest, we still cannot tell which factor determinates the origin of enantioselectivity. Herein, from the distortion/interaction analyses of **TSX'-1** (**X=I**, **II**, **III**,**IV**), we cannot figure out the origin of enantioselectivity.

Table S74 Distortion/interaction analyses, the distortion energy (ΔE_{dist} and ΔE_{dist}(total), in kcal/mol), the activation energy (ΔE_{act}, in kcal/mol), the interaction energy (ΔE_{int}, in kcal/mol), the activation Gibbs free energies (ΔG_{act}, in kcal/mol) and the relative activation Gibbs free energies ($\Delta\Delta G_{act}$, in kcal/mol) of **TSI'-1**, **TSII'-1**, **TSIII'-1** and **TSIV'-1**. The energies and Gibbs free energies of the optimized **R1$_{C2}$** cation, **R2** and **CP3** (anion) are set to 0.0 kcal/mol as reference.

	TSI'-1	**TSII'-1**	**TSIII'-1**	**TSIV'-1**
ΔE_{dist}(**R1$_{C2}$** cation) [a]	13.2	8.4	11.4	11.1
ΔE_{dist}(**R2**) [b]	6.4	5.1	5.8	5.3
ΔE_{dist}(**CP3** anion) [c]	4.4	2.1	1.7	2.9
ΔE_{dist}(total) [d]	24.0	15.7	18.9	19.3
ΔE_{int} [e]	-66.0	-58.6	-63.5	-62.4
ΔE_{act} [f]	-42.0	-42.9	-44.6	-43.0
ΔG_{act}	16.1	13.3	12.5	14.2
$\Delta\Delta G_{act}$ [g]	3.6	0.8	0	1.7

[a]ΔE_{dist}(**R1$_{C2}$** cation) is the energy difference between the **R1$_{C2}$** cation in the transition state **TSX'-1** (**X=I**, **II**, **III**, **IV**)and the optimized **R1$_{C2}$** cation.

[b]ΔE_{dist}(**R2**) is the energy difference between the **R2** in the transition state **TSX'-1** (**X=I**, **II**, **III**, **IV**)andthe optimized **R2**.

[c]ΔE_{dist}(**CP3** anion) is the energy difference between the **CP3** anion in the transition state **TSX'-1** (**X=I**, **II**, **III**, **IV**)andthe optimized **CP3** anion.

[d]ΔE_{dist}(total) is the sum of ΔE_{dist}(**R1$_{C2}$** cation), ΔE_{dist}(**R2**) and ΔE_{dist}(**CP3** anion).

[e]ΔE_{int} is the interaction energy of **TSX'-1** (**X=I**, **II**, **III**, **IV**).

[f]ΔE_{act} is the sum ofΔE_{dist}(total) andΔE_{int}.

[g]$\Delta\Delta G_{act}$ is the energy difference between the activation Gibbs free energy of **TSX'-1** (**X=I**, **II**, **III**, **IV**) and the activation Gibbs free energy of **TSIII'-1**.

Actually, the enantioselectivity is firstly dependent upon the complex formed between **CP3**, **R1$_{C2}$** and **R2** in which the interaction between **R1$_{C2}$** and **R2** can occur from different directions, so the stability of the complex will determine the enantioselectivity. A more stable complex will result in preferential product formation like path **I-IV**. Accordingly, the complexes (**COMI**,' **COMII'**, **COMIII'**, **COMIV'**) and transition states (**TSI'-1**, **TSII'-1**, **TSIII'-1**, **TSIV'-1**) will be analyzed. The calculated interaction energies for **COMI'**, **COMII'**, **COMIII'** and **COMIV'** are -26.0, -25.2, -29.9 and -25.7 kcal/mol, suggesting that the intermolecular interactions in **COMIII'** are strongest. As reflected by NCI analyses in Figure S82, besides the dual HBs between **CP3** and the reactants **R1$_{C2}$** (R=Bz) and **R2**, the large intermolecular green clouds for the π···π interactions between **R1$_{C2}$** (R=Bz) and **R2** in **COMIII'** are also observed. Obviously, the interactions between **R1$_{C2}$** (R=Bz) and **R2** in this mode are more favorable. On the other hand, it is noted that **COMIII'** also has the lowest Gibbs free energy. Furthermore, the interaction

energy of **TSIII'-1** is also very strong relative to **TSII'-1**, **TSIII'-1** and **TSIV'-1** (Table 74), as can be seen from the large intermolecular green clouds for the π···π interactions between $\mathbf{R1_{C2}}$ cation and **R2** (Figure 82). After a comparison of the relative activation Gibbs free energies ($\Delta\Delta G_{act}$) of **TSI'-1**, **TSII'-1**, **TSIII'-1** and **TSIV'-1**, it can be found that the $\Delta\Delta G_{act}$ value of **TSIII'-1** is the smallest one. Therefore, it can be concluded that the enantioselectivity is determined by the most favorable complex and transition state with the strongest interaction energies and the lowest Gibbs free energies, so path **III'** is the most competitive among the paths **I'-IV'** and is responsible for the experiment undesired product *ent*-**P1**.

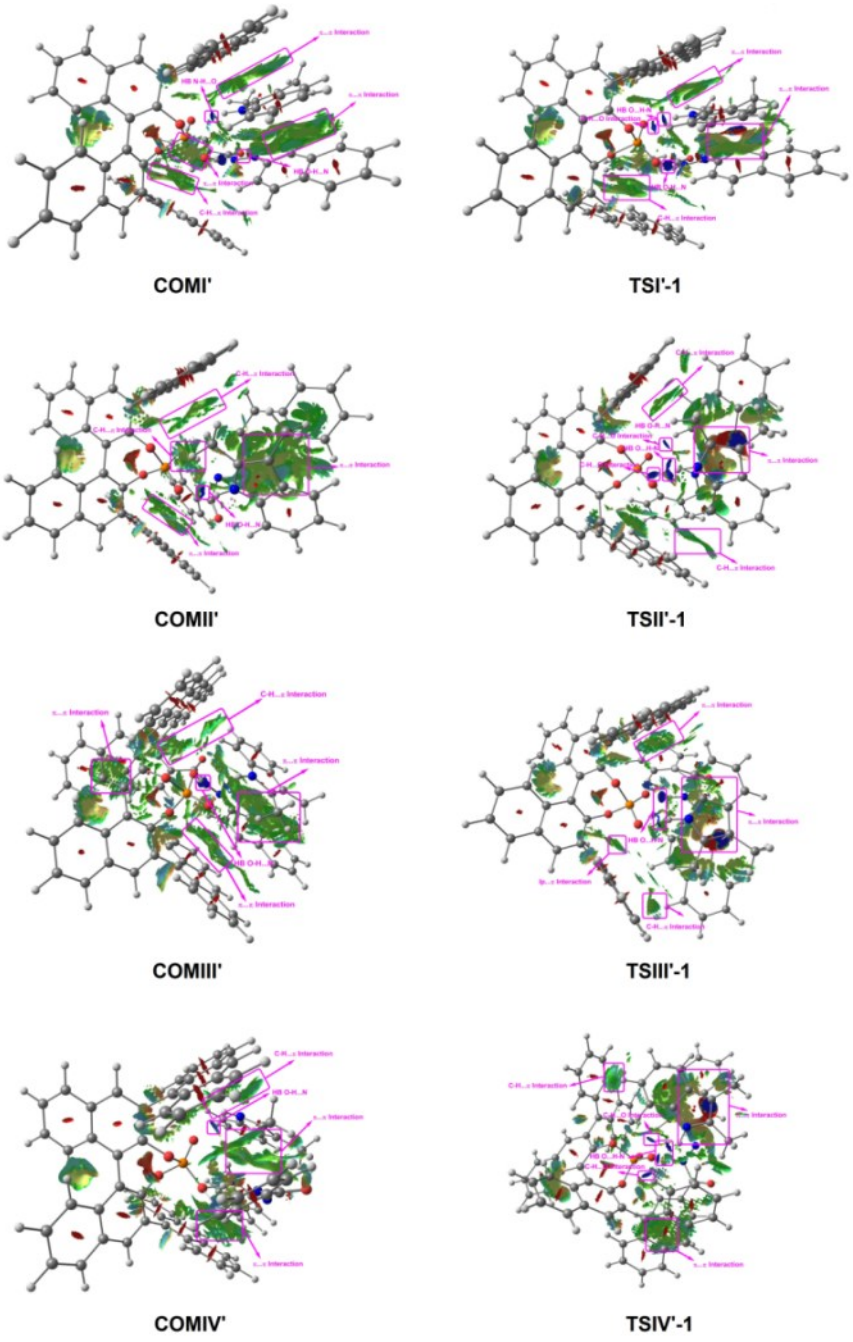

Figure S82 NCI analyses results of the complexes (**COMI'**, **COMII'**, **COMIII'**, **COMIV'**) and transition states (**TSI'-1**, **TSII'-1**, **TSIII'-1**, **TSIV'-1**). The blue, green and red regions represent strong attractions, weak interactions and steric repulsions, respectively.

4. Cartesian Coordinates

R1$_{C1}$

C	5.78077900	0.62787500	0.20218800
C	4.99138000	-0.32040200	0.80527400
C	3.61122600	-0.41069300	0.49657600
C	3.05624400	0.49675500	-0.45023900
C	3.89528000	1.46697600	-1.05770300
C	5.22818000	1.53100900	-0.73787700
H	3.20180000	-2.07440600	1.82215700
H	6.83667900	0.68902900	0.44471000
H	5.41291300	-1.01428800	1.52677700
C	2.76641500	-1.38520600	1.10433700
C	1.67644600	0.39823000	-0.76149700
H	3.46388000	2.15496600	-1.77896400
H	5.86582100	2.27398000	-1.20531000
C	0.89188200	-0.55050200	-0.15182900
C	1.43838100	-1.46068500	0.79477800
H	1.22664700	1.07309300	-1.48415500
H	0.78968800	-2.20055600	1.24858000
N	-0.47918900	-0.54829700	-0.53964200
N	-1.19145900	-1.36658300	0.07001500
O	-2.95852800	-2.34752200	-0.97402500
C	-3.40791900	-0.19999000	-0.03937500
C	-4.74027600	-0.22630600	-0.46684500
C	-2.92968500	0.88664200	0.69922300
C	-5.58611100	0.83291800	-0.16843100
H	-5.08961200	-1.08353200	-1.03272200
C	-3.78274000	1.94481000	0.99790500
H	-1.90223900	0.90920400	1.04326300
C	-5.10599000	1.91948000	0.56370200
H	-6.61783200	0.81468200	-0.50294600
H	-3.41439900	2.78883600	1.57102500
H	-5.76693100	2.74759600	0.79877400
C	-2.55743400	-1.36662100	-0.39212100

R1$_{C2}$

C	-5.98001000	0.62926700	0.23970500
C	-4.92678600	1.33548700	-0.28864800
C	-3.61740500	0.79482200	-0.27225000
C	-3.41135500	-0.49270700	0.29992700
C	-4.51768700	-1.20066100	0.83760000
C	-5.77450200	-0.65068100	0.80862700
H	-2.67211800	2.48361500	-1.24642500

H	-6.97935400	1.05182600	0.22241100
H	-5.08260700	2.31728200	-0.72632800
C	-2.50247900	1.50307700	-0.81083600
C	-2.09999800	-1.02919600	0.31656300
H	-4.35091200	-2.18218200	1.27179500
H	-6.61737400	-1.19480800	1.22161200
C	-1.04741100	-0.31806100	-0.20964300
C	-1.24595300	0.96899800	-0.78444700
H	-1.91233100	-2.00849200	0.74731600
H	-0.39393900	1.50117700	-1.19085700
N	0.21401800	-0.96544600	-0.13226200
N	1.16997500	-0.29875200	-0.56978200
O	2.47562400	-2.19639300	-0.85312500
C	3.58323100	-0.22455500	-0.09705800
C	4.82226100	-0.86500800	0.01133400
C	3.46540500	1.13501100	0.20938500
C	5.93789300	-0.14983200	0.42465600
H	4.88806400	-1.92074800	-0.23007500
C	4.58654400	1.84699200	0.62417800
H	2.50401300	1.62737200	0.11489000
C	5.81939000	1.20676400	0.73097700
H	6.89960800	-0.64439400	0.51028600
H	4.49913500	2.90198300	0.86087100
H	6.69219200	1.76602200	1.05259400
C	2.41431000	-1.03607100	-0.51819900

R2

C	0.53140200	-0.86909400	-0.00007900
C	0.30953200	0.52923900	0.00003100
C	1.41479700	1.39375700	0.00008300
C	2.69113400	0.85267500	0.00002500
C	2.88797800	-0.54193400	-0.00008500
C	1.81543100	-1.42103300	-0.00013900
C	-1.69397700	-0.50622900	-0.00001300
C	-1.11554100	0.73835300	0.00007000
H	1.26943800	2.47068800	0.00016800
H	3.55504600	1.50961500	0.00006500
H	3.89906200	-0.93661600	-0.00012800
H	1.96554600	-2.49611700	-0.00022400
H	-0.86869800	-2.46592100	-0.00017600
N	-0.70210400	-1.47195300	-0.00010500
C	-3.12936100	-0.91605500	-0.00001000
H	-3.77832200	-0.03996200	0.00016300
H	-3.36859000	-1.51577300	-0.88379100

H	-3.36850000	-1.51605400	0.88360500
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H	-1.51246200	2.66086800	-0.88076600
H	-2.87996600	1.97418300	0.00016100
H	-1.51248200	2.66071200	0.88124500

CP3

C	-1.10697600	4.98649600	2.19642100
C	-0.52172200	3.98314000	1.46625000
C	-1.29109200	2.88638000	0.99117400
C	-2.67430300	2.83542100	1.32260500
C	-3.25422400	3.89753500	2.06672700
C	-2.49096800	4.95325100	2.49127500
H	-0.50185700	5.81245800	2.55552200
C	-0.72028900	1.81587000	0.22646700
C	-3.44883100	1.71265800	0.93505900
H	-4.31353200	3.84755200	2.30153700
H	-2.94027000	5.75822500	3.06319900
C	-2.89216000	0.64640200	0.27212300
C	-1.51531700	0.72701200	-0.06203900
H	-4.50331500	1.68442600	1.19734800
C	0.70042700	1.82360200	-0.21594600
C	1.25277900	2.87616500	-1.01863000
C	1.51203000	0.75840400	0.10535700
C	2.63344800	2.82750000	-1.36237700
C	0.46786400	3.94845100	-1.52223000
C	2.88307900	0.67287400	-0.25147100
C	3.19539200	3.87093700	-2.14525000
C	3.42301000	1.72195800	-0.95366600
C	1.03624800	4.93401100	-2.28943400
H	-0.59367300	3.97732200	-1.30318100
C	2.41765700	4.90542700	-2.59564200
H	4.25277300	3.82363400	-2.38916600
H	4.47282700	1.69258100	-1.23408900
H	0.41916800	5.74143300	-2.66969900
H	2.85330400	5.69595600	-3.19748000
O	0.97826500	-0.30190200	0.83220900
H	0.54143000	4.01637500	1.25567600
O	-0.96891100	-0.34627500	-0.76137200
P	0.02523200	-1.32956100	0.03351400
O	0.84704900	-1.83715500	-1.22644600
O	-0.54606600	-2.33418600	0.93619700
H	1.42709600	-2.59102500	-1.04102400
C	-3.69130200	-0.56401800	-0.07198100

C	-4.12638400	-1.42325400	0.95603200
C	-4.01605800	-0.83298500	-1.41596400
C	-3.79310800	-1.21382300	2.33550300
C	-4.92220100	-2.57355400	0.62391300
C	-4.79998600	-1.99265000	-1.73535900
C	-3.60397300	0.01827900	-2.49256200
C	-4.23773000	-2.06496700	3.30366600
H	-3.16891700	-0.36849600	2.60265000
C	-5.37252200	-3.43877700	1.67210100
C	-5.23804300	-2.83096700	-0.70966100
C	-5.12242000	-2.26225900	-3.10373300
H	-3.02655300	0.90923100	-2.26745600
C	-3.93286600	-0.27172800	-3.78418300
C	-5.04643000	-3.19297400	2.97160900
H	-3.96998400	-1.88934300	4.34055200
H	-5.97811800	-4.29922700	1.40174100
H	-5.83632500	-3.70504900	-0.95632100
C	-4.70132000	-1.43205700	-4.09887300
H	-5.71211800	-3.14662200	-3.32835200
H	-3.61019800	0.38575200	-4.58498400
H	-5.39103900	-3.85527600	3.75897600
H	-4.94935800	-1.64512700	-5.13350900
C	3.68444300	-0.53259400	0.10728700
C	4.03342000	-0.77086100	1.45123600
C	4.09037500	-1.42480200	-0.90608100
C	3.64901700	0.11134500	2.51280600
C	4.81106200	-1.93070600	1.78587400
C	4.87475400	-2.57910800	-0.55800900
C	3.73163100	-1.24949800	-2.28513100
C	4.00045500	-0.14886600	3.80483100
H	3.07432600	1.00077200	2.27563600
C	5.15820100	-2.16804400	3.15407200
C	5.21551300	-2.80347800	0.77538800
C	5.28577100	-3.48332600	-1.58971900
H	3.11732800	-0.40037300	-2.56245600
C	4.13633500	-2.13961200	-3.23615600
C	4.76483900	-1.30769900	4.13471200
H	3.69831700	0.53125700	4.59458000
H	5.74335800	-3.05228500	3.39017900
H	5.80647900	-3.67907500	1.03371400
C	4.93213900	-3.27225400	-2.88821700
H	5.88378000	-4.34518400	-1.30737300
H	3.84858400	-1.98942400	-4.27164500
H	5.03075300	-1.49637400	5.16957600

H	5.24659500	-3.96409000	-3.66261900

COMI

C	-7.49949900	-1.65778100	-1.30588600
C	-6.25124800	-1.72755400	-0.74099700
C	-5.56028200	-0.54626400	-0.35617200
C	-6.17768400	0.71203700	-0.60576400
C	-7.47574200	0.75038500	-1.18148300
C	-8.12688200	-0.40701600	-1.51965400
H	-8.00967900	-2.56998700	-1.59742700
C	-4.25519800	-0.57214900	0.23433900
C	-5.48080300	1.90950600	-0.30138900
H	-7.93658800	1.71853200	-1.35520700
H	-9.11675400	-0.36843200	-1.96202600
C	-4.20542800	1.89133100	0.20763800
C	-3.61367000	0.62657500	0.45854100
H	-5.96267300	2.86410200	-0.49663900
C	-3.54090500	-1.83873900	0.54605300
C	-4.07326100	-2.82868400	1.43403100
C	-2.29238800	-2.04945000	0.00210100
C	-3.33630100	-4.02646700	1.65078000
C	-5.29156300	-2.64367900	2.14237600
C	-1.54444000	-3.23967100	0.19336200
C	-3.85756800	-5.01676300	2.52607500
C	-2.08739800	-4.20880300	1.00255000
C	-5.76386400	-3.61396400	2.98942500
H	-5.84318100	-1.71855200	2.01516900
C	-5.04705100	-4.81951100	3.17799100
H	-3.28856500	-5.93029500	2.67349400
H	-1.54257400	-5.13577900	1.16270700
H	-6.69371900	-3.45345600	3.52513000
H	-5.43657400	-5.57858600	3.84806100
O	-1.73339700	-1.06222300	-0.79978300
H	-5.77756900	-2.69181400	-0.59335200
O	-2.32676700	0.60999700	0.98263000
P	-1.13528100	0.23615800	-0.04678800
O	-0.06564300	-0.23594900	0.99582100
O	-0.78035000	1.29225100	-1.01256700
H	0.87887200	-0.31694300	0.63894000
C	-3.45915000	3.14909200	0.49791000
C	-2.93175200	3.91213500	-0.56044000
C	-3.30101800	3.56815700	1.83265100
C	-3.02545600	3.50078000	-1.93101600
C	-2.24844600	5.14266200	-0.26939600
C	-2.61076000	4.79578300	2.11137200
C	-3.81250500	2.81561400	2.93995600

C	-2.50046500	4.26504200	-2.93118100
H	-3.50726300	2.55698500	-2.16153400
C	-1.71679700	5.91756000	-1.35011800
C	-2.10728400	5.55604200	1.05500300
C	-2.45708800	5.21583600	3.47113800
H	-4.34409900	1.88949200	2.74579900
C	-3.64259400	3.24808400	4.22260300
C	-1.83981900	5.49666000	-2.63988300
H	-2.57694400	3.93283700	-3.96170800
H	-1.20662800	6.84702200	-1.11335800
H	-1.58810300	6.48737500	1.26939800
C	-2.95403900	4.46731000	4.49605800
H	-1.93313400	6.14765400	3.66491200
H	-4.03575700	2.66249600	5.04743900
H	-1.43017200	6.08895900	-3.45161400
H	-2.83145800	4.79386200	5.52355000
C	-0.23728200	-3.44961100	-0.49400200
C	-0.21249500	-3.65168500	-1.88974900
C	0.95373200	-3.49951400	0.25334600
C	-1.39157400	-3.59009800	-2.69981500
C	1.03435400	-3.93643200	-2.54080100
C	2.19187100	-3.81558400	-0.40710800
C	0.99738400	-3.22752600	1.66266200
C	-1.32894600	-3.76959500	-4.05135600
H	-2.34886600	-3.39711700	-2.22712100
C	1.05768500	-4.12563600	-3.95912400
C	2.20433200	-4.02338600	-1.78546400
C	3.39369200	-3.91175200	0.36597000
H	0.08277300	-2.93524300	2.16692500
C	2.16469700	-3.32498200	2.36229700
C	-0.08560800	-4.03612900	-4.69616800
H	-2.23482900	-3.71218700	-4.64605100
H	2.01389600	-4.33253600	-4.43322100
H	3.14508700	-4.24933700	-2.28293300
C	3.38017400	-3.69219500	1.71052800
H	4.31644400	-4.16104600	-0.15054300
H	2.17708000	-3.10827200	3.42587900
H	-0.05864800	-4.17434300	-5.77203500
H	4.29603300	-3.76219000	2.28895800
C	6.28028800	0.10475700	6.19283600
C	4.97366900	0.29678100	5.81284700
C	4.56849400	0.04075100	4.48030200
C	5.53774800	-0.41671100	3.54280500
C	6.88025800	-0.60650200	3.96206000

C	7.24299800	-0.35182600	5.26065800
H	2.48923100	0.57010800	4.77974500
H	6.58094500	0.30436900	7.21618900
H	4.23565000	0.64839700	6.52779500
C	3.21969000	0.22485600	4.05408700
C	5.12812600	-0.66899900	2.21237000
H	7.61065600	-0.95635600	3.23843300
H	8.26966500	-0.49780500	5.57904200
C	3.81887700	-0.47352300	1.83106800
C	2.84111100	-0.02489500	2.76557800
H	5.84163900	-1.01865300	1.47137900
H	1.81052600	0.11188400	2.45961400
N	3.57965800	-0.73094600	0.46656400
N	2.43505100	-0.49305600	0.03812500
O	1.09034400	-0.90197300	-1.71275100
C	3.36633100	-0.67202600	-2.35879500
C	3.08525400	-1.19571800	-3.62882000
C	4.60607100	-0.06946200	-2.11576800
C	4.04088100	-1.15155400	-4.63357000
H	2.10852500	-1.63518800	-3.80481500
C	5.55637800	-0.01947000	-3.13234800
H	4.82708200	0.38765600	-1.15906600
C	5.28252700	-0.56514500	-4.38305600
H	3.81962400	-1.56789100	-5.61093800
H	6.50920900	0.46533900	-2.94513300
H	6.03096300	-0.52225500	-5.16855700
C	2.24315200	-0.72043400	-1.38542700
C	3.01123000	2.58677200	-0.98166300
C	3.94565000	2.95376600	-1.98300600
C	5.25242400	3.29195100	-1.60017700
C	5.59596400	3.24313300	-0.25668000
C	4.65036700	2.87760000	0.72254300
C	3.34572700	2.55748500	0.37503300
C	2.02058600	2.35014300	-2.98336300
C	3.29071300	2.79875900	-3.25461300
H	5.99045400	3.56716700	-2.34966600
H	6.60767500	3.49057100	0.04958600
H	4.94558500	2.84159400	1.76733100
H	2.61450800	2.26843000	1.12535300
H	0.96504500	1.95630700	-1.19635900
N	1.85126100	2.23059300	-1.61824800
C	0.90213700	1.93987300	-3.88237200
H	0.67852800	0.87724200	-3.73475000
H	-0.01042100	2.49997900	-3.65299000

C	3.92837200	3.02373200	-4.58882200
H	4.80668000	2.37923500	-4.71301300
H	3.23727100	2.80272700	-5.40589000
H	4.26422100	4.05996500	-4.70692200
H	1.16213000	2.10424700	-4.92900100

TSI-1

Value of imaginary frequency = -265.5 cm^{-1}

C	7.26920200	-1.33726200	-1.69186700
C	6.21997900	-0.90648700	-0.91980400
C	4.97644400	-1.59527600	-0.93105400
C	4.83465700	-2.72561300	-1.78581100
C	5.94284700	-3.15182300	-2.56541100
C	7.13580300	-2.47773000	-2.51910600
H	8.20870100	-0.79437600	-1.67426100
C	3.85412000	-1.16879300	-0.15058900
C	3.59053200	-3.40821800	-1.84928400
H	5.82144200	-4.02036700	-3.20687800
H	7.97542500	-2.80743800	-3.12202700
C	2.49738900	-2.97440900	-1.14151700
C	2.64988600	-1.82305900	-0.32001400
H	3.50829600	-4.29378200	-2.47462600
C	3.90960400	-0.01191900	0.78887600
C	4.80140900	0.04734700	1.90858000
C	3.01261400	1.02013400	0.61004700
C	4.77216400	1.19430100	2.75303800
C	5.69071600	-1.01178400	2.23606900
C	2.97930900	2.18252900	1.42995500
C	5.65586100	1.26351200	3.86251900
C	3.86222400	2.25032500	2.47857400
C	6.52699500	-0.91862500	3.32017000
H	5.69744700	-1.90449400	1.61995900
C	6.51879700	0.23485000	4.14006600
H	5.62967300	2.14933800	4.49093900
H	3.87249900	3.13201300	3.11443800
H	7.19717500	-1.73919200	3.55515000
H	7.18880800	0.29643300	4.99118900
O	2.12188600	0.94433600	-0.43543800
H	6.32752400	-0.02400600	-0.29781700
O	1.54806200	-1.37517500	0.36835500
P	0.81232500	-0.00519900	-0.19737200
O	-0.02252500	0.44330100	0.96559000
O	0.21149200	-0.24338900	-1.54621100
H	-1.13265900	1.54592000	0.50475500
C	1.21047800	-3.73841500	-1.13144400
C	0.23472000	-3.55205100	-2.12872100
C	0.99495500	-4.66806400	-0.09277100
C	0.39757900	-2.61171000	-3.19771000
C	-0.98166200	-4.31861100	-2.08345000
C	-0.21043100	-5.44784500	-0.07428800

C	1.93839400	-4.86462600	0.96890000
C	-0.58109300	-2.43104800	-4.13069000
H	1.30515900	-2.02055800	-3.23216900
C	-1.98810100	-4.09249400	-3.07709300
C	-1.16865900	-5.25683200	-1.06985300
C	-0.42031200	-6.38537900	0.98591600
H	2.85484500	-4.28360500	0.97243800
C	1.69802300	-5.76275300	1.96794100
C	-1.79728800	-3.17707200	-4.06860200
H	-0.44117000	-1.70576300	-4.92605100
H	-2.90760300	-4.66890400	-3.01748300
H	-2.09151000	-5.83212300	-1.03883700
C	0.50122200	-6.53941500	1.97882200
H	-1.33959800	-6.96476100	0.98405100
H	2.42430400	-5.89199900	2.76386300
H	-2.56650000	-3.00982400	-4.81655100
H	0.33135600	-7.25047300	2.78073800
C	2.07820400	3.32157200	1.07332900
C	2.46732000	4.16990500	0.01745400
C	0.86978100	3.54924000	1.75641800
C	3.67811200	3.96489700	-0.72008500
C	1.63127700	5.27579900	-0.35518400
C	0.04004300	4.66090500	1.37467500
C	0.40539300	2.69505500	2.80971700
C	4.02014400	4.78479700	-1.75606600
H	4.32793900	3.14003000	-0.44738300
C	2.02355300	6.11053400	-1.44887700
C	0.44227100	5.50206500	0.33780400
C	-1.21209400	4.85951900	2.04156200
H	1.01376500	1.84345200	3.09217500
C	-0.79609800	2.91572700	3.41786000
C	3.17959500	5.87357000	-2.13231400
H	4.93994200	4.60761400	-2.30417600
H	1.37108900	6.93470700	-1.72512200
H	-0.19888300	6.33104000	0.04389900
C	-1.62330900	4.01159700	3.02656000
H	-1.82880600	5.69983000	1.73336200
H	-1.13577100	2.24692300	4.20278700
H	3.46635800	6.50881300	-2.96410400
H	-2.57835700	4.16428700	3.51934200
C	-2.51859000	-2.02160800	-0.12292300
C	-3.90251400	-2.27763000	-0.07898500
C	-4.42037500	-3.10343000	0.91686400
C	-3.53722300	-3.63636100	1.85536800

C	-2.16606100	-3.35229900	1.80347800
C	-1.62839400	-2.53844400	0.80915000
C	-3.42394300	-0.90105500	-1.83509300
C	-4.51353600	-1.48032000	-1.12986000
H	-5.48598400	-3.31013600	0.97337100
H	-3.91732400	-4.28211400	2.64086500
H	-1.49963700	-3.79294900	2.53875300
H	-0.56344600	-2.33528400	0.75929000
H	-1.33040800	-0.81797300	-1.46269400
N	-2.28029400	-1.18244000	-1.20877800
C	-3.45757000	0.01344100	-3.00464400
H	-4.27246700	-0.24435000	-3.68334600
H	-3.60735700	1.04338800	-2.65243300
H	-2.50934200	-0.02486700	-3.54566000
C	-5.86560000	-1.73358600	-1.72045700
H	-6.59135500	-1.97073800	-0.93840900
H	-6.23577800	-0.87097400	-2.28265600
H	-5.82890600	-2.59001100	-2.40234600
C	-7.46115800	-1.28712200	3.06186800
C	-6.11518900	-1.10919300	3.33490900
C	-5.26221100	-0.53068900	2.38231300
C	-5.79683200	-0.14130500	1.12823800
C	-7.17339400	-0.30662300	0.87814800
C	-7.99720900	-0.87506200	1.83275000
H	-3.47456400	-0.63732900	3.62665700
H	-8.10894100	-1.73591700	3.80789600
H	-5.70470200	-1.41354100	4.29340400
C	-3.86303300	-0.28321400	2.67643900
C	-4.91205700	0.42005800	0.14130500
H	-7.58156200	0.03195700	-0.06987800
H	-9.05665300	-0.99597700	1.63478900
C	-3.61363400	0.87744800	0.56663900
C	-3.06441800	0.39085500	1.82323500
H	-5.34161400	0.91372400	-0.72686200
H	-2.02614200	0.58871800	2.06803500
N	-3.05001200	1.74486900	-0.25517200
N	-1.81628200	2.13831200	-0.04174300
C	-1.20303200	2.98114300	-0.98921900
O	-0.02912900	2.80837300	-1.23619900
C	-1.99191500	4.09454300	-1.58593600
C	-1.46336000	4.68475800	-2.73761000
C	-3.13231900	4.63351100	-0.98316100
C	-2.08326500	5.79308900	-3.30019200
H	-0.55919300	4.26736600	-3.16812600

C	-3.74343700	5.75174000	-1.54382400
H	-3.52297300	4.19814700	-0.06989000
C	-3.22462100	6.32713000	-2.70245000
H	-1.67557800	6.24478200	-4.19840100
H	-4.62316800	6.17771700	-1.07294700
H	-3.70691000	7.19702100	-3.13688600

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C	-7.09185900	-1.44223100	2.08422700
C	-6.11948500	-0.93827600	1.25721000
C	-4.87032900	-1.60166600	1.11227200
C	-4.64134500	-2.78355600	1.87258900
C	-5.67188400	-3.28715300	2.70972400
C	-6.87347300	-2.63629200	2.81230900
H	-8.03636700	-0.91774200	2.18678000
C	-3.82623700	-1.10663600	0.26459400
C	-3.38559200	-3.43889000	1.79077100
H	-5.48191700	-4.19590900	3.27401500
H	-7.65367300	-3.02501700	3.45826100
C	-2.36042500	-2.93362700	1.03129400
C	-2.59740400	-1.73884900	0.29497800
H	-3.23360500	-4.35840100	2.35058500
C	-3.99537600	0.07640000	-0.62548100
C	-5.00024100	0.14214800	-1.64705100
C	-3.09292300	1.11606500	-0.52384300
C	-5.07555400	1.30634800	-2.46415800
C	-5.90354000	-0.92400400	-1.91217400
C	-3.13883500	2.27439000	-1.34693900
C	-6.07079000	1.39013800	-3.47372800
C	-4.13727700	2.35552600	-2.28426200
C	-6.84810600	-0.81794600	-2.90227500
H	-5.83585100	-1.83378500	-1.32588500
C	-6.94385400	0.35556900	-3.68727900
H	-6.11678300	2.29047000	-4.07997300
H	-4.20051000	3.23329200	-2.92259000
H	-7.52558400	-1.64475900	-3.08978800
H	-7.69923200	0.42739900	-4.46281300
O	-2.11268400	1.05213400	0.44211300
H	-6.29318600	-0.01647200	0.71239500
O	-1.56149000	-1.23010000	-0.45348800
P	-0.80493200	0.13176800	0.12189100
O	0.04077700	0.61311500	-1.00343600
O	-0.19095200	-0.18335200	1.46748500
H	1.22414400	2.11149800	-0.49208800
C	-1.05908200	-3.66241000	0.91765600
C	-0.05847400	-3.51249300	1.89658700
C	-0.85998300	-4.53549000	-0.17173400
C	-0.20849600	-2.63339100	3.01976600
C	1.16946600	-4.25243500	1.77746900
C	0.36136800	-5.28493800	-0.26846200
C	-1.83049200	-4.69339200	-1.21457500

C	0.78810500	-2.49274000	3.94032100
H	-1.12176600	-2.05627600	3.10466800
C	2.19129300	-4.07654600	2.76682900
C	1.34697800	-5.12536100	0.70632100
C	0.55891200	-6.15897500	-1.38301800
H	-2.75789400	-4.13242600	-1.15808500
C	-1.60026900	-5.52992800	-2.26856900
C	2.00777600	-3.22611800	3.81616600
H	0.65831200	-1.81399700	4.77734700
H	3.11027800	-4.64758000	2.66384800
H	2.27864900	-5.68019300	0.61910600
C	-0.38868200	-6.27825300	-2.35589500
H	1.48917700	-6.71767600	-1.43848700
H	-2.34602800	-5.63219800	-3.05020200
H	2.78266900	-3.10568200	4.56725000
H	-0.22785700	-6.94031300	-3.20049700
C	-2.12573600	3.36010100	-1.18994500
C	-2.28208500	4.31398500	-0.16880800
C	-1.02984100	3.42880300	-2.06937900
C	-3.37608800	4.27346200	0.75311500
C	-1.31542400	5.36421300	-0.02612400
C	-0.05494500	4.47094300	-1.90324800
C	-0.82921200	2.48303400	-3.12868800
C	-3.49841000	5.20592600	1.74204700
H	-4.11392700	3.48326300	0.65645700
C	-1.48211700	6.32601900	1.01861200
C	-0.22293200	5.41612200	-0.89151700
C	1.07630800	4.51436500	-2.78158000
H	-1.54716300	1.67999000	-3.25192300
C	0.25279400	2.56600500	-3.95407100
C	-2.53767900	6.25116300	1.87876200
H	-4.33312800	5.15577100	2.43390500
H	-0.74143800	7.11530500	1.11501200
H	0.51658500	6.20483800	-0.77092600
C	1.22757900	3.59457200	-3.77583800
H	1.81138600	5.30089500	-2.63429200
H	0.38776400	1.83479500	-4.74481400
H	-2.65305700	6.98409000	2.67072500
H	2.09048300	3.63442600	-4.43337200
C	2.34965200	-1.83127900	-0.33751200
C	3.72759100	-1.87545500	-0.53582100
C	4.24494500	-2.53655900	-1.63742000
C	3.34423800	-3.11056400	-2.54085300
C	1.96558700	-3.00970200	-2.34704500

C	1.43617700	-2.36293900	-1.22944700
C	3.19581500	-0.78401100	1.45459700
C	4.38277800	-1.05556600	0.54795300
H	5.31593800	-2.59388000	-1.80756500
H	3.72388100	-3.63640300	-3.41080500
H	1.28637500	-3.45843700	-3.06473600
H	0.36710700	-2.28906300	-1.06675500
H	1.09715500	-0.87813600	1.24859300
N	2.09674600	-1.17853500	0.90065200
C	3.23982900	-0.13952100	2.78746500
H	3.68259600	-0.84339200	3.50134500
H	3.85421000	0.76357000	2.75644700
H	2.23194600	0.12019700	3.11798600
C	5.51912000	-1.76021000	1.28815800
H	6.29933400	-2.05934300	0.58567800
H	5.96111000	-1.10429900	2.04440000
H	5.14034600	-2.66011300	1.78051500
C	7.64510600	-0.25345500	-3.26101800
C	6.31156000	0.02517900	-3.54125200
C	5.39656800	0.25960200	-2.51000900
C	5.83221900	0.19491500	-1.17123800
C	7.17724100	-0.05235800	-0.90339200
C	8.08225400	-0.28119800	-1.93899800
H	3.69051200	0.53363700	-3.85516800
H	8.34403000	-0.43443900	-4.07089700
H	5.96763700	0.07032500	-4.57090500
C	4.00501200	0.60072000	-2.81675600
C	4.82982800	0.36676200	-0.05324600
H	7.52395700	-0.06124900	0.12645200
H	9.12497000	-0.47650700	-1.71167100
C	3.60085900	1.15068100	-0.49247000
C	3.14442900	1.02885100	-1.87751100
H	5.29202100	0.90589200	0.78097700
H	2.12369100	1.29804200	-2.13395900
N	3.03775700	1.80772600	0.45648500
N	1.84818000	2.43297800	0.25932800
C	1.14412300	2.84783300	1.37653000
O	-0.06077000	3.01036400	1.30606900
C	1.89370300	3.09773900	2.64903900
C	1.22256400	2.80098100	3.83670800
C	3.17702900	3.64844300	2.69304600
C	1.84307900	3.01795400	5.06341000
H	0.21944400	2.39037000	3.77797200
C	3.78606200	3.88613400	3.92139100

H	3.69319700	3.89006100	1.77075500
C	3.12550000	3.56105400	5.10596400
H	1.32488900	2.76972700	5.98385800
H	4.77859500	4.32371400	3.95595300
H	3.60887200	3.73674200	6.06184800

TSI-2

Value of imaginary frequency = -158.7 cm^{-1}

C	-7.36450900	-0.99540300	1.92642600
C	-6.33401500	-0.56108100	1.13147700
C	-5.13207800	-1.31274600	1.02040100
C	-5.00940100	-2.50867500	1.78313200
C	-6.09865100	-2.93798700	2.58727500
C	-7.25392600	-2.20337600	2.65561400
H	-8.27186000	-0.40468300	2.00141300
C	-4.03337200	-0.89214000	0.20316300
C	-3.79952400	-3.25050300	1.73559900
H	-5.99259700	-3.85928300	3.15347400
H	-8.07995000	-2.53679000	3.27507500
C	-2.72163800	-2.81761700	1.00470000
C	-2.85407100	-1.61056000	0.26223100
H	-3.72806600	-4.17738000	2.29937900
C	-4.09120900	0.30669200	-0.67893000
C	-5.06227000	0.45687600	-1.72224700
C	-3.12030000	1.27773000	-0.53980300
C	-5.03946400	1.63451200	-2.52312200
C	-6.03003500	-0.54156300	-2.01982600
C	-3.07024500	2.45008200	-1.34280900
C	-6.00767900	1.79884800	-3.54960800
C	-4.03661700	2.61550800	-2.30335900
C	-6.94592200	-0.35847900	-3.02503200
H	-6.03461500	-1.46066700	-1.44432900
C	-6.94575600	0.82970600	-3.79388600
H	-5.98318200	2.70835100	-4.14344500
H	-4.02789500	3.50764900	-2.92459000
H	-7.67494900	-1.13427300	-3.23590100
H	-7.68059400	0.96399600	-4.58069300
O	-2.17357000	1.13450400	0.44424300
H	-6.42369400	0.37193100	0.58532500
O	-1.76969200	-1.17746400	-0.45964300
P	-0.92242900	0.11766000	0.14990400
O	-0.05021900	0.55110300	-0.98183400
O	-0.36057800	-0.23357100	1.49601900
H	1.35012400	1.46564500	-0.41353800
C	-1.46259300	-3.62053800	0.91801300
C	-0.46655400	-3.51277000	1.90748900
C	-1.28762400	-4.49614700	-0.17364800
C	-0.59313500	-2.63457200	3.03387100
C	0.73311800	-4.29899200	1.79681400
C	-0.09411600	-5.29079900	-0.26223900

C	-2.25256600	-4.61351000	-1.22739200
C	0.39711400	-2.53915100	3.96635200
H	-1.48207000	-2.02042600	3.11186800
C	1.75006700	-4.16898300	2.79813100
C	0.88637500	-5.17391300	0.72344200
C	0.08202300	-6.16594400	-1.37977100
H	-3.15906700	-4.01862200	-1.17812000
C	-2.04352100	-5.45371000	-2.28284700
C	1.58849400	-3.31760800	3.85003700
H	0.28519700	-1.85989200	4.80528600
H	2.64656300	-4.77629500	2.70282100
H	1.79646000	-5.76441800	0.64260300
C	-0.85950300	-6.24567800	-2.36250600
H	0.99146100	-6.75854500	-1.42861200
H	-2.78473600	-5.52463600	-3.07236500
H	2.35916600	-3.23232600	4.61038900
H	-0.71477500	-6.90887300	-3.20918700
C	-1.99183500	3.45672100	-1.11399200
C	-2.09604000	4.34687000	-0.02919200
C	-0.87865900	3.50680600	-1.97190600
C	-3.20365400	4.32031000	0.87782400
C	-1.06373000	5.31723800	0.19430800
C	0.15906900	4.46983300	-1.72723200
C	-0.72394200	2.61891700	-3.08702000
C	-3.27754800	5.19176000	1.92576800
H	-3.99090000	3.58927100	0.72322700
C	-1.18116800	6.21785600	1.29911900
C	0.04016000	5.35536000	-0.65735100
C	1.29804000	4.50350900	-2.59573200
H	-1.48916000	1.87230300	-3.26739600
C	0.37051900	2.68680000	-3.89666900
C	-2.25180200	6.15905600	2.14150600
H	-4.12360200	5.15207400	2.60440500
H	-0.39136600	6.94799300	1.45399000
H	0.82613500	6.08637100	-0.47964500
C	1.40117800	3.64406200	-3.64959400
H	2.07484700	5.23748100	-2.39739000
H	0.47013800	2.00047800	-4.73125100
H	-2.32896900	6.84410500	2.97970700
H	2.26666100	3.68130500	-4.30481900
C	2.23034900	-1.84778600	-0.30974000
C	3.58811400	-1.87064700	-0.62733700
C	4.01653100	-2.50416900	-1.78594400
C	3.05620900	-3.08350700	-2.62019400

C	1.70042000	-3.03328200	-2.29209200
C	1.26147200	-2.41324400	-1.12307400
C	3.18684000	-0.65771000	1.36100800
C	4.35739400	-1.19020000	0.49267200
H	5.07097200	-2.55639700	-2.04006100
H	3.37045900	-3.58064000	-3.53185000
H	0.96880400	-3.49491900	-2.94816300
H	0.21114700	-2.38502000	-0.85489200
H	1.11101400	-0.97260800	1.32360200
N	2.05658800	-1.21625000	0.93646000
C	3.32272700	-0.28282100	2.79980600
H	3.52069000	-1.19229200	3.37704000
H	4.13178600	0.43433300	2.94890200
H	2.38711800	0.15238000	3.15913500
C	5.16225900	-2.20881400	1.30763200
H	5.84418000	-2.75855700	0.65668000
H	5.73687700	-1.72361800	2.10282300
H	4.47664900	-2.93333500	1.75866400
C	8.00356700	-0.88922500	-3.14632300
C	6.91190000	-0.07362200	-3.41704600
C	5.99752500	0.25374000	-2.40981200
C	6.17383000	-0.26129700	-1.11095400
C	7.30390000	-1.02929400	-0.83827100
C	8.20799600	-1.35297800	-1.84890400
H	4.84807500	1.57601300	-3.70941700
H	8.70337700	-1.14186200	-3.93548100
H	6.76166600	0.32693900	-4.41541800
C	4.90533000	1.18000200	-2.69845800
C	5.15915300	0.03697700	-0.03099100
H	7.48970400	-1.37434300	0.17383500
H	9.07572700	-1.96140100	-1.61696000
C	4.06360100	0.99877500	-0.45711400
C	4.00427300	1.57521700	-1.77860500
H	5.68159100	0.48996100	0.82451600
H	3.20888400	2.27694700	-2.00881300
N	3.18826000	1.13344300	0.47747500
N	2.03991500	1.86624700	0.25477500
C	1.44018900	2.50387400	1.32643400
O	0.25584900	2.78338600	1.29096700
C	2.30146100	2.88166900	2.49373000
C	1.70115100	2.86048800	3.75416500
C	3.63547000	3.27810000	2.36472600
C	2.44156900	3.18494400	4.88601900
H	0.65743600	2.57214800	3.82817700

C	4.36830200	3.62319700	3.49688000
H	4.09483400	3.33318700	1.38340200
C	3.77746600	3.56254400	4.75787000
H	1.97763200	3.14671300	5.86615000
H	5.40087800	3.94091900	3.39496300
H	4.35567300	3.81973000	5.63959300

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C	-7.40279900	-0.56502300	2.12404100
C	-6.37282900	-0.20738500	1.29105000
C	-5.21533700	-1.02368900	1.17251100
C	-5.13580500	-2.20849700	1.95811600
C	-6.22369200	-2.55680300	2.80209900
C	-7.33474400	-1.75725900	2.88323800
H	-8.27623000	0.07397000	2.20514900
C	-4.11586100	-0.67599000	0.32341100
C	-3.97806900	-3.02889500	1.87587200
H	-6.15410200	-3.46921100	3.38795500
H	-8.15955900	-2.03042400	3.53302800
C	-2.90296500	-2.67306500	1.10091000
C	-2.97890400	-1.45688700	0.36744100
H	-3.95308400	-3.96202200	2.43312400
C	-4.13046800	0.50029300	-0.58895500
C	-5.10282600	0.65498700	-1.62965000
C	-3.11724100	1.43110700	-0.48936200
C	-5.03853100	1.80184900	-2.47126300
C	-6.11225000	-0.31361600	-1.88440400
C	-3.03344600	2.57838400	-1.32536300
C	-6.00659400	1.96828900	-3.49756900
C	-3.99854500	2.75097100	-2.28606400
C	-7.02693700	-0.12986200	-2.89049700
H	-6.14807300	-1.21157100	-1.27724800
C	-6.98442600	1.02927200	-3.70139700
H	-5.95104700	2.85473400	-4.12334500
H	-3.96386900	3.62657400	-2.92948900
H	-7.78736500	-0.88304300	-3.06996000
H	-7.71859800	1.16457100	-4.48864500
O	-2.16658500	1.27804200	0.48957000
H	-6.42794300	0.71330300	0.71961900
O	-1.88144800	-1.08115200	-0.36780700
P	-0.98249200	0.16549400	0.25173500
O	-0.06289200	0.53704300	-0.87294900
O	-0.45357200	-0.17516100	1.60642800
H	1.28617000	1.12283400	-0.22503900
C	-1.73811100	-3.58615200	0.88897500
C	-0.65322200	-3.63036600	1.78308500
C	-1.75410400	-4.41548600	-0.25325800
C	-0.58275600	-2.79817700	2.94821700
C	0.43463400	-4.53681500	1.53104000
C	-0.66615400	-5.32187600	-0.48934500
C	-2.81922500	-4.38108100	-1.21256600

C	0.48961700	-2.85904700	3.78917500
H	-1.38584900	-2.09389300	3.13125700
C	1.54080100	-4.56926400	2.43920400
C	0.39789400	-5.36639100	0.41156100
C	-0.68276600	-6.14487900	-1.65983900
H	-3.65062900	-3.70290700	-1.05171800
C	-2.79645600	-5.17814700	-2.31989400
C	1.56923900	-3.75793000	3.53395200
H	0.52850100	-2.21441500	4.66168500
H	2.35426000	-5.26025700	2.23358600
H	1.22678600	-6.04518500	0.22310000
C	-1.71246100	-6.07559900	-2.55120100
H	0.15131500	-6.82191900	-1.82361000
H	-3.61015300	-5.12995500	-3.03636500
H	2.41112200	-3.79272700	4.21948400
H	-1.71352000	-6.69954400	-3.43899700
C	-1.93573400	3.56609600	-1.10809100
C	-2.04462200	4.48220400	-0.04436200
C	-0.80317400	3.57252300	-1.94172900
C	-3.17579800	4.50300300	0.83439300
C	-0.99655000	5.43533600	0.18185000
C	0.24900600	4.51995900	-1.69467400
C	-0.63845100	2.64908100	-3.02575900
C	-3.25767400	5.40406500	1.85591800
H	-3.97516500	3.78588400	0.67807100
C	-1.12306500	6.36781100	1.25952800
C	0.12525400	5.43187300	-0.64757000
C	1.41113400	4.50468500	-2.53225900
H	-1.41644800	1.91566900	-3.20637200
C	0.48104300	2.66811400	-3.80338300
C	-2.21676200	6.35483200	2.07330700
H	-4.12232800	5.40114200	2.51175500
H	-0.32234800	7.08558700	1.41553200
H	0.92216600	6.15056400	-0.46879700
C	1.52584400	3.60901900	-3.55401200
H	2.19697300	5.22922200	-2.33462900
H	0.58981500	1.95443200	-4.61337100
H	-2.30208000	7.06478400	2.88961000
H	2.41039700	3.60662000	-4.18389100
C	2.14476400	-2.04689900	-0.35410100
C	3.51252400	-2.11302600	-0.65449300
C	3.94570600	-2.76812800	-1.79788000
C	2.99340400	-3.33293800	-2.65300600
C	1.63438500	-3.24132300	-2.35045900

C	1.18635700	-2.59410100	-1.19929700
C	3.12318800	-0.70440500	1.22003100
C	4.29049200	-1.46677700	0.48886600
H	5.00391000	-2.84336200	-2.03149300
H	3.31490400	-3.84156800	-3.55556500
H	0.90252600	-3.68668800	-3.01858800
H	0.12887100	-2.52081000	-0.96106800
H	1.04006800	-1.11808300	1.22640800
N	1.95653200	-1.41105500	0.86601000
C	3.22328100	-0.44232100	2.70574300
H	3.28865400	-1.39946600	3.22761300
H	4.08449000	0.18350200	2.95633400
H	2.31177600	0.06153800	3.04143500
C	4.92892100	-2.52228900	1.38717300
H	5.56279900	-3.19154900	0.80236500
H	5.52375700	-2.07150300	2.18786000
H	4.13465700	-3.12922300	1.83471400
C	8.21507200	-0.90854800	-3.03677400
C	7.28816100	0.11658600	-3.15371400
C	6.30979000	0.30580400	-2.16772200
C	6.25731500	-0.55773500	-1.05512500
C	7.22147800	-1.55445700	-0.92647400
C	8.18502300	-1.73791600	-1.91586300
H	5.48290600	2.05817000	-3.15644100
H	8.96703700	-1.05367400	-3.80418400
H	7.31371000	0.78526200	-4.00893000
C	5.37631600	1.41518500	-2.28612600
C	5.22242000	-0.31912100	0.01436900
H	7.22975200	-2.19084300	-0.04867600
H	8.92026400	-2.52781400	-1.80539500
C	4.21995800	0.73779800	-0.33372100
C	4.38299800	1.67051000	-1.40071100
H	5.75769900	0.06630600	0.90057600
H	3.65747900	2.46401300	-1.54118500
N	3.18182100	0.64495500	0.44448500
N	2.10571600	1.50140300	0.33066800
C	1.75801500	2.35706900	1.36795000
O	0.62326100	2.78708700	1.43281700
C	2.81266400	2.76353300	2.35262200
C	2.41962000	2.88854000	3.68678300
C	4.12868300	3.05444500	1.98521300
C	3.34763800	3.25171800	4.65603700
H	1.38650000	2.68277800	3.94894600
C	5.05217700	3.43456300	2.95517100

H	4.43000800	3.01841000	0.94281500
C	4.66663100	3.51889800	4.29143100
H	3.04282900	3.32933700	5.69433300
H	6.07129900	3.67000400	2.66672900
H	5.39121900	3.80463900	5.04717400

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C	5.52638200	-4.47674800	-1.89718700
C	4.91999700	-3.46484200	-1.19601100
C	3.50953100	-3.44685700	-1.01499400
C	2.74191300	-4.48883900	-1.60502700
C	3.39907500	-5.53031600	-2.31300000
C	4.76222300	-5.52979200	-2.45437500
H	6.60330000	-4.46751000	-2.03102500
C	2.83453400	-2.41006800	-0.29129000
C	1.33094700	-4.47046300	-1.47635100
H	2.79549200	-6.32271500	-2.74689600
H	5.25772300	-6.32644800	-2.99927800
C	0.67473000	-3.44090700	-0.84546300
C	1.45273700	-2.38369500	-0.29083900
H	0.75561500	-5.29328300	-1.89417800
C	3.58350700	-1.35152200	0.43701700
C	4.52981300	-1.66251400	1.46895700
C	3.33695300	-0.02709200	0.14143400
C	5.25883400	-0.60292300	2.07839600
C	4.74393500	-2.98587300	1.94280500
C	4.08900100	1.03807500	0.70917200
C	6.19819000	-0.89672000	3.10198200
C	5.03506000	0.73236300	1.65539500
C	5.64974200	-3.23794100	2.94264000
H	4.17128300	-3.80090700	1.51389000
C	6.39507500	-2.18551700	3.52503500
H	6.75047500	-0.07486900	3.54924000
H	5.62619900	1.53055200	2.09782200
H	5.79161400	-4.25420300	3.29600200
H	7.11103600	-2.40063300	4.31142000
O	2.36938900	0.28488300	-0.78234300
H	5.51637400	-2.65848400	-0.78295000
O	0.79839400	-1.36607700	0.34838900
P	0.79694900	0.16979100	-0.29390800
O	0.56514100	1.02999500	0.92116300
O	-0.04043600	0.23863400	-1.51639100
H	-0.82910000	0.45171900	1.60186700
C	-0.80722900	-3.48990400	-0.68971500
C	-1.63953900	-3.48993500	-1.83086600
C	-1.36953000	-3.62797800	0.59792700
C	-1.13309200	-3.28068500	-3.15709600
C	-3.05743100	-3.67771700	-1.67755200
C	-2.79232800	-3.77417000	0.73889800
C	-0.57331600	-3.65213100	1.79044300

C	-1.96263600	-3.30326600	-4.24233400
H	-0.07413100	-3.08939900	-3.28818800
C	-3.89102400	-3.70314400	-2.84167100
C	-3.60041000	-3.80611300	-0.39876800
C	-3.35674400	-3.90209300	2.04893600
H	0.50448000	-3.57110800	1.70883000
C	-1.15002900	-3.76936300	3.01990500
C	-3.36256100	-3.53140000	-4.08750300
H	-1.55566900	-3.13736600	-5.23440400
H	-4.95772100	-3.85806300	-2.70521700
H	-4.67465300	-3.93663000	-0.28518800
C	-2.56476900	-3.88739600	3.15651400
H	-4.43599700	-3.99490100	2.13621100
H	-0.52907100	-3.76564300	3.90922600
H	-4.00244900	-3.55224400	-4.96364500
H	-3.00337700	-3.96660600	4.14601600
C	3.91191100	2.44126100	0.23715400
C	4.37908500	2.80092700	-1.04385400
C	3.33963100	3.40897800	1.08230000
C	4.95022700	1.84913100	-1.95057700
C	4.29687500	4.16985800	-1.46972700
C	3.27876900	4.78026300	0.65228100
C	2.75671900	3.07218400	2.34888800
C	5.38540300	2.22749400	-3.18711400
H	5.03234000	0.81200300	-1.64269700
C	4.76760400	4.52645100	-2.77355500
C	3.76379800	5.12961000	-0.60709400
C	2.68245200	5.75605100	1.51488300
H	2.75080900	2.03289200	2.65683800
C	2.17588900	4.02839900	3.13001200
C	5.29195600	3.58656200	-3.60943400
H	5.80834500	1.48925500	-3.86066400
H	4.69475000	5.56648400	-3.07953600
H	3.71240600	6.16714900	-0.93000500
C	2.14691600	5.39456700	2.71442000
H	2.65257100	6.78871100	1.17852900
H	1.72486200	3.75127400	4.07760300
H	5.64297900	3.86590500	-4.59747600
H	1.68636900	6.13884500	3.35601500
C	-1.17484400	3.45641600	0.14625500
C	-2.24994700	3.42289200	-0.73917900
C	-2.06318600	3.76519400	-2.07357400
C	-0.78265100	4.11708400	-2.50493900
C	0.28643600	4.13335800	-1.60612000

C	0.10350000	3.80643400	-0.26536800
C	-2.87806100	2.51299700	1.37794000
C	-3.50620900	3.02964400	0.02565600
H	-2.89242700	3.75122000	-2.77460300
H	-0.61764100	4.37087300	-3.54645900
H	1.28272400	4.39507200	-1.95218400
H	0.92543800	3.79229900	0.43880300
H	-0.89348100	2.71142700	2.04787400
N	-1.59129700	3.14808200	1.45113900
C	-3.68875000	2.67440600	2.64621500
H	-3.85185300	3.73641400	2.83493700
H	-4.65158400	2.15921600	2.57634800
H	-3.13877100	2.26078100	3.49635700
C	-4.44163700	4.21877800	0.21898600
H	-4.69891000	4.65565200	-0.74793300
H	-5.36187000	3.93626900	0.73941700
H	-3.93184300	4.99405200	0.79788400
C	-5.17316200	1.45176600	-4.73991600
C	-4.34295100	0.51189500	-4.14735800
C	-4.02103500	0.60884900	-2.78654600
C	-4.52707400	1.67446800	-2.01745300
C	-5.40087900	2.58245500	-2.61053300
C	-5.71051000	2.47974700	-3.96503000
H	-2.81558800	-1.19745800	-2.82873200
H	-5.41633800	1.37818500	-5.79403800
H	-3.93858600	-0.31492800	-4.72495400
C	-3.20190600	-0.42158500	-2.17293100
C	-4.17097200	1.74956800	-0.55705100
H	-5.84940700	3.37336900	-2.01934500
H	-6.38098200	3.20437700	-4.41487100
C	-3.21049000	0.69567400	-0.10518900
C	-2.86966100	-0.45401400	-0.85732600
H	-5.09550400	1.55667400	0.01589700
H	-2.19194300	-1.19415200	-0.44621800
N	-2.70398100	1.03635800	1.05194500
N	-1.84423500	0.23119100	1.76760300
C	-2.22252700	-0.35210200	2.96779800
O	-1.36517800	-0.70181100	3.75661500
C	-3.68184300	-0.53790000	3.25388800
C	-4.08788100	-0.34969100	4.57617800
C	-4.61525300	-0.92772000	2.29009000
C	-5.42486700	-0.50486800	4.92633600
H	-3.34533400	-0.07371500	5.31844200
C	-5.94990400	-1.09851000	2.64579000

H	-4.29784100	-1.15386000	1.27632400
C	-6.35804000	-0.87408700	3.95960500
H	-5.73791000	-0.34247700	5.95230200
H	-6.66906100	-1.41736700	1.89817500
H	-7.40112300	-0.99935700	4.23142200

IMI-4

C	-7.14819400	-2.38560900	0.50359900
C	-6.12580300	-1.53438300	0.16855600
C	-4.80930100	-2.02611000	-0.05317100
C	-4.57285400	-3.41918600	0.12108800
C	-5.65488200	-4.27704700	0.45557000
C	-6.91711000	-3.77592900	0.63786300
H	-8.14379500	-1.98910000	0.67415500
C	-3.71345500	-1.17172500	-0.40407500
C	-3.25545400	-3.92684500	-0.01440000
H	-5.45614600	-5.33848200	0.57370800
H	-7.73726800	-4.43688400	0.89745800
C	-2.19187400	-3.10104000	-0.28117100
C	-2.44292900	-1.71415200	-0.46362700
H	-3.08485300	-4.99188500	0.12107100
C	-3.88519100	0.28800400	-0.63860600
C	-4.76437900	0.82120600	-1.63750300
C	-3.12279500	1.16654400	0.10234700
C	-4.88122700	2.23446600	-1.76889200
C	-5.49584000	-0.00286200	-2.53610900
C	-3.22058300	2.57918100	-0.01920700
C	-5.75542100	2.77431100	-2.74992100
C	-4.10799000	3.08529000	-0.93604400
C	-6.32291800	0.54859500	-3.48209400
H	-5.38578800	-1.07994000	-2.47331100
C	-6.46609700	1.95294600	-3.58584600
H	-5.84064300	3.85439700	-2.82903200
H	-4.21083000	4.16209600	-1.04429400
H	-6.86877000	-0.09757000	-4.16180600
H	-7.12840700	2.37400300	-4.33483100
O	-2.22558000	0.65978800	1.01585900
H	-6.31423000	-0.47011200	0.08072100
O	-1.37199400	-0.90894800	-0.76605900
P	-0.80237300	0.14511700	0.37176100
O	-0.11202500	1.22689800	-0.38186800
O	-0.11844900	-0.60408300	1.48342900
H	1.44557100	-0.35538600	1.65355500
C	-0.80647600	-3.64790500	-0.38036200
C	-0.09682000	-3.96862200	0.79165100
C	-0.24243200	-3.90031000	-1.64628100
C	-0.63232800	-3.73262100	2.10068800
C	1.21155900	-4.55732100	0.69037000
C	1.05138300	-4.51967100	-1.73639500
C	-0.91825400	-3.56868500	-2.86594000

C	0.07174100	-4.07378300	3.21601600
H	-1.60639500	-3.26524800	2.18815000
C	1.92508300	-4.88167800	1.88959000
C	1.75276700	-4.82214300	-0.56765300
C	1.59599200	-4.81188400	-3.02856300
H	-1.88962400	-3.08793000	-2.81130000
C	-0.35915900	-3.84881400	-4.07988700
C	1.37126700	-4.65613000	3.11258500
H	-0.34545300	-3.88444000	4.19976500
H	2.91723600	-5.31470700	1.79679600
H	2.73517200	-5.28282200	-0.63971800
C	0.91351400	-4.49046200	-4.16577900
H	2.56961400	-5.29091400	-3.07955300
H	-0.88530200	-3.58626300	-4.99176300
H	1.92000900	-4.89791900	4.01679800
H	1.33457100	-4.71609700	-5.14026900
C	-2.39581900	3.47068000	0.84703400
C	-2.70226700	3.57919600	2.21910800
C	-1.34469300	4.22493300	0.29167100
C	-3.76457700	2.83596500	2.83007300
C	-1.94157000	4.47095900	3.04819100
C	-0.60925600	5.13585100	1.12601400
C	-0.95528100	4.10999400	-1.08444100
C	-4.03633200	2.95974800	4.16115900
H	-4.35862300	2.16717600	2.21605800
C	-2.25837300	4.57206900	4.44053000
C	-0.91947100	5.23398100	2.48159100
C	0.43186500	5.93146100	0.54564500
H	-1.46084100	3.38174700	-1.70755200
C	0.04771400	4.87874400	-1.59737100
C	-3.27087500	3.83922200	4.98336800
H	-4.84387100	2.38565700	4.60362400
H	-1.67046000	5.25012200	5.05283900
H	-0.35655600	5.92102000	3.10926700
C	0.74354400	5.81824800	-0.77520800
H	0.96413300	6.62813500	1.18744800
H	0.32837000	4.77531200	-2.64136100
H	-3.50338000	3.92208000	6.03996100
H	1.53012100	6.42888500	-1.20785600
C	5.57460900	1.57268400	0.30985300
C	5.11719400	1.66400200	-1.00973800
C	5.96500900	1.35755700	-2.06368300
C	7.26674800	0.93082900	-1.78323500
C	7.70387400	0.83003100	-0.46311200

C	6.86479700	1.15205700	0.60430700
C	3.32336700	1.97816400	0.50864900
C	3.69650400	2.21238600	-0.99455000
H	5.62464400	1.43649300	-3.09159100
H	7.93692200	0.67467400	-2.59648800
H	8.71471000	0.49214700	-0.25765100
H	7.20228900	1.06668600	1.63169200
H	4.59672800	1.65179900	2.14767000
N	4.58131900	2.00726400	1.19874800
C	2.26095100	2.86722100	1.12362400
H	2.63016100	3.89277400	1.17887100
H	1.33722300	2.83087900	0.53651500
H	2.03695500	2.51810200	2.13613700
C	3.68439000	3.69715000	-1.35625400
H	4.16877800	3.86528400	-2.31968300
H	2.66494100	4.09050000	-1.38972300
H	4.25264600	4.25649100	-0.60689600
C	2.84073500	0.09115400	-5.84973000
C	2.41981400	-0.78498400	-4.85998500
C	2.38549200	-0.37859800	-3.51966600
C	2.78241900	0.92645800	-3.16593700
C	3.16664500	1.80806800	-4.17356500
C	3.20988000	1.39011000	-5.50228200
H	1.57157900	-2.27864500	-2.86579700
H	2.87112900	-0.22766900	-6.88563000
H	2.10925700	-1.79629600	-5.10881700
C	1.91849500	-1.31477300	-2.50771800
C	2.64050400	1.34510100	-1.72616700
H	3.43272200	2.83025400	-3.93086800
H	3.52650500	2.08795800	-6.27019800
C	2.43673500	0.20663900	-0.77839800
C	1.92092700	-1.06378900	-1.17833000
H	1.67277700	1.87734100	-1.64619200
H	1.59386400	-1.79202100	-0.44144500
N	2.77785800	0.56663800	0.42344700
N	2.47745700	-0.13768600	1.56663700
C	3.47561900	-0.91075600	2.12696800
O	4.59136300	-0.98869600	1.64140700
C	3.10248700	-1.57821500	3.41320500
C	4.05046900	-2.43593800	3.97827900
C	1.89921600	-1.33008300	4.07862700
C	3.80288200	-3.03844700	5.20522900
H	4.97894600	-2.60696900	3.44429000
C	1.65597900	-1.93598100	5.30881400

H	1.14801700	-0.67348400	3.65097600
C	2.60466200	-2.78493800	5.87394600
H	4.54221000	-3.70079300	5.64330000
H	0.72307300	-1.74002900	5.82697400
H	2.41169700	-3.24907300	6.83596100

TSI-3

Value of imaginary frequency = -891.1 cm^{-1}

C	6.81060500	2.68730700	1.36276300
C	5.88435700	1.75608000	0.96676600
C	4.64191400	2.15821900	0.40279300
C	4.36946900	3.55077400	0.29566400
C	5.35361400	4.49075600	0.70316500
C	6.55109900	4.07170400	1.22043500
H	7.75036100	2.35968700	1.79548800
C	3.64739200	1.21948200	-0.02509300
C	3.11000100	3.98004500	-0.19276900
H	5.13097600	5.54942500	0.60401500
H	7.29620200	4.79517200	1.53442200
C	2.12711000	3.08447900	-0.53626500
C	2.41534700	1.69788700	-0.42996100
H	2.91208800	5.04594700	-0.27382500
C	3.87818500	-0.25030300	0.00224000
C	4.94979900	-0.88031400	-0.71151000
C	2.98598700	-1.04614700	0.68803100
C	5.10170700	-2.29237100	-0.61443000
C	5.84538200	-0.16110500	-1.54900400
C	3.10093600	-2.45970300	0.77139900
C	6.16728100	-2.92946400	-1.30508100
C	4.16977700	-3.04923000	0.14069800
C	6.85638000	-0.80656300	-2.21561700
H	5.71650200	0.90922900	-1.66692700
C	7.03087700	-2.20501700	-2.08452700
H	6.27540400	-4.00630500	-1.20992000
H	4.29231200	-4.12811700	0.19537500
H	7.52609400	-0.23957800	-2.85406700
H	7.83946500	-2.70022700	-2.61174800
O	1.92115700	-0.44076200	1.32954900
H	6.09100700	0.69876600	1.09148000
O	1.42860600	0.80873000	-0.80398700
P	0.66213800	-0.05663400	0.36229200
O	0.20051500	-1.32611500	-0.32711700
O	-0.28716400	0.77270900	1.15455100
H	-2.06559200	1.24337200	1.30968100
C	0.79898600	3.57064200	-1.01338400
C	-0.11722100	4.10925200	-0.09164800
C	0.50079600	3.55696600	-2.38948200
C	0.13795400	4.12910700	1.31939600
C	-1.35757700	4.66313300	-0.56399100
C	-0.73127400	4.13216400	-2.85420000

C	1.38809400	2.98684200	-3.35915600
C	-0.76376300	4.67043700	2.18543600
H	1.05984800	3.69474500	1.68923500
C	-2.28596900	5.20380700	0.38414500
C	-1.63159700	4.67063200	-1.93185200
C	-1.01545900	4.13024900	-4.25761900
H	2.31950700	2.54488600	-3.02055400
C	1.07496800	2.99097500	-4.68830400
C	-1.99745000	5.21394100	1.71476400
H	-0.55690300	4.67527100	3.25061900
H	-3.22466200	5.60572000	0.01273200
H	-2.56488500	5.10122500	-2.28753500
C	-0.14305800	3.57599200	-5.14851200
H	-1.94866300	4.57312400	-4.59431400
H	1.75832300	2.54952500	-5.40651500
H	-2.70906600	5.61496000	2.42996600
H	-0.36990700	3.57509800	-6.20965000
C	2.09834200	-3.27825800	1.51150600
C	2.00229000	-3.17498700	2.91371200
C	1.29281400	-4.19759600	0.80866100
C	2.80988500	-2.26864800	3.67627800
C	1.08132900	-4.01571400	3.62590100
C	0.41739800	-5.07348800	1.53868100
C	1.29171100	-4.29293500	-0.62329700
C	2.68790800	-2.18546300	5.03204900
H	3.52948200	-1.64205500	3.15978300
C	0.98149300	-3.89565100	5.04922700
C	0.32218700	-4.95351000	2.92510500
C	-0.33688700	-6.06249300	0.82667500
H	1.88239600	-3.58451400	-1.19244600
C	0.54516900	-5.23732900	-1.26589100
C	1.75524900	-3.00650900	5.73294300
H	3.30739000	-1.48999200	5.58905400
H	0.27440800	-4.53558400	5.56987400
H	-0.34971900	-5.61089000	3.47254600
C	-0.26324900	-6.15590000	-0.53059900
H	-0.97135800	-6.73319300	1.39969500
H	0.55731600	-5.28734700	-2.35035500
H	1.67256400	-2.92238200	6.81166200
H	-0.83579600	-6.91025200	-1.06097300
C	-5.44005600	-1.97344100	-0.12644900
C	-4.55245700	-2.39812400	-1.11983700
C	-5.02973400	-2.82177000	-2.35015100
C	-6.40790500	-2.79891800	-2.58726000

C	-7.28242500	-2.35979200	-1.59455500
C	-6.81194000	-1.94267500	-0.34806900
C	-3.35835500	-1.46236400	0.71682800
C	-3.13087400	-2.32546000	-0.58087000
H	-4.34547600	-3.15183500	-3.12654400
H	-6.79567700	-3.11873000	-3.54840800
H	-8.34979100	-2.33827700	-1.79127300
H	-7.49325100	-1.59866100	0.42335100
H	-5.16378900	-0.93452700	1.62416600
N	-4.75146600	-1.66702900	1.05550900
C	-2.43543400	-1.72578400	1.89275700
H	-2.64230800	-2.71708900	2.29751700
H	-1.38909600	-1.67036800	1.58510700
H	-2.61197900	-0.98733800	2.67967500
C	-2.56894100	-3.70777800	-0.25282200
H	-2.63624900	-4.37544600	-1.11370300
H	-1.52071700	-3.64381900	0.05531700
H	-3.15143300	-4.16709500	0.55187700
C	-0.70981300	-1.85838900	-5.41184300
C	-0.80884700	-0.61559400	-4.82011100
C	-1.34173700	-0.48247000	-3.52339300
C	-1.78314200	-1.62568600	-2.81375800
C	-1.64753900	-2.88301300	-3.42196800
C	-1.13177000	-2.99268600	-4.70337600
H	-1.07414100	1.66028600	-3.50575000
H	-0.30121800	-1.96105400	-6.41094500
H	-0.47603200	0.27876900	-5.34073000
C	-1.44120900	0.82155300	-2.92183700
C	-2.21234700	-1.42544000	-1.42326400
H	-1.94215500	-3.77836800	-2.88817300
H	-1.04688700	-3.97386100	-5.15977200
C	-2.47502000	-0.07976900	-0.99116900
C	-1.98217600	1.05232900	-1.69301900
H	-1.07098300	-1.42465800	-0.87639000
H	-2.06498800	2.04905000	-1.27297400
N	-3.10607100	-0.07397400	0.18205300
N	-3.02314100	1.00421700	1.03210800
C	-4.16401500	1.57171900	1.52842700
O	-5.27829000	1.28039400	1.11672200
C	-3.95619100	2.54303800	2.64533500
C	-4.95286200	3.49956000	2.85470600
C	-2.86561900	2.46584500	3.51414000
C	-4.85078100	4.38975400	3.91605400
H	-5.80177100	3.52566500	2.17973100

C	-2.77564600	3.34930400	4.58748300
H	-2.09159900	1.71593200	3.37304500
C	-3.76171900	4.31274700	4.78577600
H	-5.62072800	5.13793400	4.07228700
H	-1.93468400	3.28176900	5.26980900
H	-3.68645700	5.00018100	5.62218100

IMI-5

C	7.18413200	1.71427800	1.34459500
C	6.12031600	0.93297100	0.97043800
C	4.97107800	1.51139100	0.36581300
C	4.93500700	2.92390200	0.19273300
C	6.05832400	3.70372400	0.57770900
C	7.16193900	3.11399000	1.13615700
H	8.05008000	1.25531400	1.81012500
C	3.83871500	0.73174300	-0.04144200
C	3.77231600	3.53773700	-0.33940300
H	6.01840300	4.77868800	0.42776000
H	8.01471800	3.71634900	1.43056200
C	2.65733100	2.80502000	-0.66261100
C	2.71825700	1.39926800	-0.48899100
H	3.75762300	4.61656900	-0.47097000
C	3.82158500	-0.75455100	0.03801900
C	4.78812900	-1.57404300	-0.63321800
C	2.80480700	-1.38010100	0.72460900
C	4.70812900	-2.98775600	-0.48639300
C	5.79849800	-1.03804400	-1.47699500
C	2.68508200	-2.78699600	0.86312900
C	5.66625900	-3.81285500	-1.13338700
C	3.65675300	-3.55962900	0.27406600
C	6.70119100	-1.86211800	-2.10052900
H	5.84546200	0.03360100	-1.63492500
C	6.64637400	-3.26446200	-1.91842200
H	5.59690100	-4.88862700	-1.00061700
H	3.60447900	-4.64136200	0.36745400
H	7.46147100	-1.43512900	-2.74626600
H	7.37197900	-3.90133000	-2.41317000
O	1.82096300	-0.59223800	1.32278100
H	6.14651300	-0.13688200	1.14542600
O	1.58701900	0.66813100	-0.84360600
P	0.70736500	0.01002000	0.33616200
O	0.11349900	-1.26932000	-0.36306800
O	-0.22329500	0.90487400	1.04824100
H	-2.02178600	1.54024000	1.07809100
C	1.41625200	3.44555400	-1.18449600
C	0.56804500	4.14295800	-0.30572700
C	1.11195300	3.35636500	-2.55602000
C	0.84359200	4.26442800	1.09621100
C	-0.62397500	4.76259800	-0.81828100
C	-0.07444800	3.98988200	-3.05994000
C	1.94501200	2.64837400	-3.48235400

C	0.00437600	4.95713500	1.91608500
H	1.73506000	3.79604100	1.49853000
C	-1.49219700	5.45728500	0.08526200
C	-0.91504400	4.67476600	-2.17978100
C	-0.37871100	3.89072500	-4.45519700
H	2.84854000	2.16942400	-3.11871000
C	1.61774600	2.57212400	-4.80595400
C	-1.18795200	5.55594900	1.40910300
H	0.23014200	5.04464500	2.97352600
H	-2.39919000	5.90236800	-0.31434300
H	-1.81809200	5.14417900	-2.56326700
C	0.43789400	3.20210700	-5.30338900
H	-1.28171400	4.37220100	-4.81983700
H	2.26056000	2.02862100	-5.49107700
H	-1.85350500	6.07509800	2.09177100
H	0.19636100	3.12880400	-6.35858800
C	1.55609700	-3.41213500	1.61175500
C	1.46592400	-3.25256800	3.00931700
C	0.62364900	-4.21614800	0.92354600
C	2.39247800	-2.45426100	3.75698000
C	0.42289000	-3.92546100	3.73239500
C	-0.38302800	-4.92491700	1.66641400
C	0.61768200	-4.35221800	-0.50507900
C	2.27133500	-2.31455200	5.10835500
H	3.20403500	-1.95827600	3.23487100
C	0.33033600	-3.75233000	5.15046700
C	-0.46550100	-4.75542000	3.04823000
C	-1.28171000	-5.79902200	0.97290700
H	1.32268100	-3.77106400	-1.08886000
C	-0.27043300	-5.17800400	-1.13099000
C	1.22146800	-2.96852400	5.81962400
H	2.98246700	-1.70288400	5.65403800
H	-0.46866400	-4.26507100	5.67857900
H	-1.23542600	-5.28520700	3.60452300
C	-1.22035100	-5.93458800	-0.38142100
H	-2.01835300	-6.34484500	1.55600500
H	-0.26195100	-5.25518500	-2.21351700
H	1.14329600	-2.84219400	6.89445300
H	-1.90640800	-6.59765700	-0.89893500
C	-5.96243600	-1.18477100	-0.11905800
C	-5.14428600	-1.78990600	-1.07769200
C	-5.67893300	-2.26481900	-2.26387300
C	-7.05091500	-2.12236900	-2.49430000
C	-7.85898900	-1.50970700	-1.53731300

C	-7.32808300	-1.03310000	-0.33712600
C	-3.81926100	-0.81757200	0.65201900
C	-3.71186500	-1.81879600	-0.56622600
H	-5.03890800	-2.72289000	-3.01387800
H	-7.48439800	-2.48125200	-3.42160000
H	-8.92180900	-1.39495300	-1.72713800
H	-7.96002500	-0.55283800	0.40309800
H	-5.52890600	0.01637700	1.48201800
N	-5.22728000	-0.83926800	1.02269100
C	-2.92243500	-1.11396800	1.84324300
H	-3.16601400	-2.08809400	2.26722400
H	-1.86813900	-1.10422200	1.54936700
H	-3.06589300	-0.35910400	2.62091800
C	-3.30138400	-3.22531900	-0.12181500
H	-3.47270000	-3.95941600	-0.91000600
H	-2.24355800	-3.26416900	0.16060900
H	-3.90721800	-3.53344300	0.73564700
C	-0.59722500	-2.30680200	-4.97126200
C	-0.49507400	-1.02691700	-4.48984400
C	-1.22344000	-0.61885000	-3.34344400
C	-2.06744700	-1.55525600	-2.66817200
C	-2.14963600	-2.87473000	-3.19457500
C	-1.43984600	-3.23344600	-4.31435000
H	-0.45043800	1.39127900	-3.39186800
H	-0.03936500	-2.61054500	-5.85050600
H	0.14514700	-0.29546300	-4.97697000
C	-1.11137700	0.71387000	-2.86186700
C	-2.74627700	-1.10475400	-1.49856800
H	-2.78398100	-3.60767000	-2.71235800
H	-1.52718600	-4.24458400	-4.70001500
C	-2.63833400	0.21899900	-1.10016400
C	-1.80528300	1.15089600	-1.76361000
H	-0.81437900	-1.19714800	-0.66900100
H	-1.70784500	2.16773200	-1.39535400
N	-3.43189500	0.48347100	0.01251200
N	-3.01566400	1.50870700	0.84779400
C	-3.94328500	2.24642600	1.51465900
O	-5.14767700	2.17132800	1.29346500
C	-3.40214500	3.13423900	2.59384000
C	-4.17767800	4.23636400	2.96377200
C	-2.22502800	2.84629100	3.28838700
C	-3.76990000	5.05899700	4.00631600
H	-5.10101500	4.42694800	2.42707000
C	-1.83036200	3.66164500	4.34691600

H	-1.61583900	1.98470100	3.02776900
C	-2.59489100	4.76975700	4.70209600
H	-4.36989700	5.91907700	4.28497500
H	-0.92265500	3.42786300	4.89373900
H	-2.28204500	5.40268900	5.52640000

COMII

C	-6.99996600	-1.26607000	-2.80926200
C	-5.98925100	-1.41993600	-1.89405700
C	-5.21415300	-0.30515500	-1.47290800
C	-5.49025100	0.96755800	-2.04715900
C	-6.55057900	1.09640100	-2.98315600
C	-7.29349400	0.00649800	-3.35474500
H	-7.57677000	-2.13001000	-3.12281700
C	-4.14229900	-0.42189700	-0.52794100
C	-4.69702700	2.08764000	-1.68799400
H	-6.75180100	2.07681400	-3.40536100
H	-8.09796300	0.11242600	-4.07478400
C	-3.62955900	1.96958800	-0.83289500
C	-3.35930400	0.68739400	-0.29002800
H	-4.93342100	3.05957800	-2.11357200
C	-3.82554500	-1.69623300	0.17183900
C	-4.78836000	-2.38252300	0.98270800
C	-2.54947600	-2.21172700	0.09469400
C	-4.42019800	-3.61352600	1.59508400
C	-6.08963300	-1.86678000	1.23270200
C	-2.16070000	-3.43608000	0.69670000
C	-5.36811000	-4.30970400	2.39180200
C	-3.10718600	-4.11968200	1.42065200
C	-6.97987400	-2.55731800	2.01571400
H	-6.37415700	-0.91208500	0.80426700
C	-6.62303100	-3.79844800	2.59478700
H	-5.07180900	-5.25227200	2.84328600
H	-2.84027600	-5.06355300	1.88938400
H	-7.96671600	-2.14438700	2.19771500
H	-7.34065800	-4.33456300	3.20673600
O	-1.59358700	-1.54278700	-0.65222000
H	-5.76696200	-2.40230700	-1.49173000
O	-2.25753900	0.56462900	0.55042000
P	-0.96890000	-0.15601300	-0.10442200
O	-0.11291400	-0.55663900	1.14069800
O	-0.31492300	0.55645800	-1.21887900
C	-2.81134800	3.15623500	-0.44941200
C	-1.87506600	3.69099100	-1.35240300
C	-3.02286900	3.75856100	0.80572200
C	-1.59455900	3.08571500	-2.62155600
C	-1.15433500	4.88233300	-0.99803200
C	-2.29576400	4.94729800	1.14949200
C	-3.95435000	3.23880900	1.76273500
C	-0.67077300	3.62432100	-3.46783500

H	-2.11262200	2.17204000	-2.89084200
C	-0.19262900	5.41570300	-1.91605400
C	-1.39555400	5.49123000	0.23339300
C	-2.51542500	5.55582400	2.42582000
H	-4.52212900	2.34745800	1.51572700
C	-4.13541000	3.84735700	2.97052500
C	0.04423400	4.80719700	-3.11267300
H	-0.46322800	3.14337800	-4.41814400
H	0.34815100	6.31514800	-1.63061900
H	-0.85766300	6.40117500	0.49350200
C	-3.40365500	5.02335200	3.31182800
H	-1.95197600	6.45165900	2.67191900
H	-4.84321800	3.43573900	3.68277000
H	0.78367500	5.21093000	-3.79673600
H	-3.56068600	5.48944800	4.27908500
C	-0.77545700	-3.96728900	0.54584700
C	-0.33688700	-4.44513700	-0.70568200
C	0.07091100	-4.02871100	1.67071900
C	-1.14813500	-4.37808600	-1.88544700
C	0.96769700	-5.03492000	-0.82025500
C	1.36551600	-4.64086900	1.54824800
C	-0.29380000	-3.47908000	2.94477200
C	-0.68481600	-4.83213800	-3.08525700
H	-2.14544800	-3.95626400	-1.81660700
C	1.41384000	-5.50721800	-2.09601100
C	1.77731900	-5.13817200	0.31124700
C	2.21665500	-4.71197700	2.69820600
H	-1.25201700	-2.98213500	3.04601100
C	0.55229900	-3.55311400	4.01174900
C	0.61833100	-5.40231600	-3.19734800
H	-1.31301800	-4.76514800	-3.96747300
H	2.40588200	-5.94536800	-2.16438200
H	2.75512400	-5.60893900	0.22313200
C	1.82538400	-4.18704300	3.89285500
H	3.18803400	-5.18751900	2.58948400
H	0.25989800	-3.12067300	4.96308100
H	0.96681600	-5.75651500	-4.16189200
H	2.48025700	-4.23921300	4.75638300
C	2.96131300	1.37638600	-1.92199500
C	4.33603600	1.20038200	-2.21967600
C	5.17587500	2.32650800	-2.21802700
C	4.63266700	3.57114200	-1.93684700
C	3.25750000	3.72182300	-1.66360500
C	2.40192400	2.63036400	-1.64819700

C	3.32245400	-0.81362900	-2.26464000
C	4.54472100	-0.20658300	-2.44046900
H	6.23618100	2.22391700	-2.43619500
H	5.27227400	4.44849200	-1.93405700
H	2.85643900	4.71051300	-1.45811900
H	1.33898400	2.73381000	-1.43974900
H	1.38294200	-0.01113900	-1.79486500
N	2.37595800	0.13845300	-1.95135500
C	2.93310700	-2.25163200	-2.37683300
H	3.80592600	-2.89583400	-2.23712100
H	2.19428400	-2.51834100	-1.61338900
H	2.49630600	-2.48011900	-3.35524500
C	5.84174400	-0.85884800	-2.80832000
H	6.68531400	-0.28368500	-2.41489700
H	5.91995200	-1.86880600	-2.39084100
H	5.97566800	-0.93534700	-3.89355200
C	7.64805500	-3.20058500	-0.04384200
C	6.30801800	-3.37592700	0.21158500
C	5.48301500	-2.26434000	0.50658500
C	6.06116100	-0.96458200	0.52669600
C	7.44741500	-0.81218000	0.26695300
C	8.22506000	-1.90887900	-0.01168800
H	3.66464700	-3.41132400	0.75070200
H	8.27241000	-4.05839400	-0.27177500
H	5.86539500	-4.36818000	0.19021900
C	4.09049300	-2.41422400	0.77360800
C	5.22043400	0.14208500	0.78527600
H	7.87720500	0.18547800	0.28561300
H	9.28429300	-1.78976200	-0.21298300
C	3.87376400	-0.03664600	1.02989400
C	3.29193600	-1.33882900	1.03301100
H	5.61475400	1.15419600	0.76668700
H	2.23200600	-1.47685300	1.22371400
N	3.18255800	1.16458900	1.23381900
N	1.94731900	1.10544500	1.40745700
C	1.32282400	2.41171100	1.50757900
O	0.15630400	2.46547200	1.19379200
H	0.71076300	0.03015000	1.26691200
C	2.10317800	3.58768000	1.97634900
C	1.78620100	4.82140400	1.40485100
C	3.06315000	3.50601200	2.98819000
C	2.43616800	5.97268200	1.83267200
H	1.04060800	4.85166200	0.61704900
C	3.69430900	4.66428600	3.42963800

H	3.30359500	2.54911100	3.43843900
C	3.38689900	5.89408900	2.84960600
H	2.20135600	6.92919800	1.37645900
H	4.43008500	4.60602500	4.22464000
H	3.89058200	6.79295600	3.19069300

TSII-1

Value of imaginary frequency = -200.0 cm^{-1}

C	6.66475100	-0.47027300	3.15879500
C	5.77100500	-0.75624100	2.15757300
C	4.97225900	0.26828800	1.57872900
C	5.09698300	1.59029300	2.09107400
C	6.04186900	1.85743000	3.11762500
C	6.81412300	0.85257900	3.63898000
H	7.25958900	-1.26781800	3.59226400
C	4.02095500	0.01726900	0.53542100
C	4.25913800	2.61765900	1.58803800
H	6.13040900	2.87497900	3.48771400
H	7.53025700	1.06294300	4.42644300
C	3.29918200	2.36728400	0.63826600
C	3.19224800	1.04370300	0.13312500
H	4.36667500	3.62409400	1.98492100
C	3.85894400	-1.32876100	-0.07660300
C	4.94880300	-2.00988600	-0.70880500
C	2.61695600	-1.93456800	-0.05294800
C	4.75085800	-3.33558100	-1.18374400
C	6.21916900	-1.40307000	-0.91081500
C	2.41036400	-3.27220900	-0.49193600
C	5.82695500	-4.02624900	-1.80340100
C	3.48052700	-3.94492100	-1.03415700
C	7.23643900	-2.09066300	-1.52273700
H	6.37462700	-0.38007200	-0.58580300
C	7.04546300	-3.42107000	-1.96696000
H	5.65901500	-5.04142600	-2.15196100
H	3.34909400	-4.97129900	-1.36794700
H	8.19667700	-1.60837100	-1.67427200
H	7.86149200	-3.95219500	-2.44558000
O	1.55105400	-1.26124800	0.49343300
H	5.65955900	-1.77636700	1.80721100
O	2.23759500	0.78782800	-0.82705700
P	0.88470300	0.01055000	-0.32248200
O	0.17686700	-0.45922900	-1.55453100
O	0.17654100	0.80530700	0.73248400
C	2.41412700	3.46339800	0.14922000
C	1.45101600	4.01952600	1.01354700
C	2.59835100	3.98769600	-1.14536900
C	1.19180400	3.49113600	2.32205700
C	0.68228000	5.15448000	0.58170700
C	1.81984600	5.11751200	-1.56813400
C	3.55828200	3.45122000	-2.06397700

C	0.26432700	4.06352000	3.14185400
H	1.73302000	2.60856900	2.64266500
C	-0.28726400	5.72168900	1.47124700
C	0.89670000	5.68524300	-0.69031500
C	2.01713100	5.65023400	-2.88121300
H	4.16366600	2.60423500	-1.75818100
C	3.71654700	3.98633300	-3.30885000
C	-0.48554400	5.20072100	2.71509100
H	0.07853100	3.64221700	4.12458900
H	-0.86087500	6.57963000	1.12775900
H	0.32813800	6.55779100	-1.00747100
C	2.93296400	5.10238000	-3.72824600
H	1.41582400	6.50250400	-3.18530500
H	4.44533100	3.56183700	-3.99174200
H	-1.22465100	5.63482100	3.38101000
H	3.07345600	5.51154300	-4.72342300
C	1.10462000	-3.97610500	-0.33176100
C	0.60035200	-4.24965200	0.95813100
C	0.43640400	-4.47053800	-1.47239300
C	1.22892400	-3.77066100	2.15524500
C	-0.57814400	-5.05994700	1.10231000
C	-0.70861800	-5.32427000	-1.31067300
C	0.84249300	-4.14318100	-2.80913900
C	0.70374000	-4.03999400	3.38533200
H	2.13624500	-3.18214200	2.07793100
C	-1.09580600	-5.32247100	2.41151200
C	-1.18853100	-5.59834300	-0.03011300
C	-1.35762800	-5.85361700	-2.47275600
H	1.67307900	-3.46087200	-2.95036000
C	0.18381100	-4.65006900	-3.89099000
C	-0.48094800	-4.82320200	3.52036000
H	1.19381700	-3.65932300	4.27551600
H	-1.99226200	-5.93107000	2.49510000
H	-2.05893800	-6.24082300	0.08849000
C	-0.92568200	-5.53100500	-3.72422600
H	-2.20997700	-6.51296400	-2.32963800
H	0.49994400	-4.37592100	-4.89204600
H	-0.88191700	-5.02323300	4.50882800
H	-1.42769700	-5.93212700	-4.59855500
C	-2.95104300	1.42427100	1.67548800
C	-4.28324100	1.10690200	1.99396400
C	-5.23386200	2.13328000	2.05679800
C	-4.81269700	3.43457900	1.81843100
C	-3.46947500	3.72440300	1.51638900

C	-2.51074000	2.72308900	1.43252300
C	-3.00980100	-0.79390000	1.96811200
C	-4.35401200	-0.33324700	2.10951100
H	-6.27272300	1.91857000	2.29113300
H	-5.53024400	4.24725200	1.86761900
H	-3.17454300	4.75147200	1.32613300
H	-1.47079200	2.92673700	1.18640700
H	-1.21121200	0.23484000	1.39560600
N	-2.21947300	0.23871000	1.67178300
C	-2.48841300	-2.17468800	2.16172400
H	-3.18167600	-2.91548100	1.75260000
H	-1.51116600	-2.30228600	1.68779100
H	-2.38152500	-2.38106600	3.23269000
C	-5.43522700	-1.10096200	2.79697200
H	-6.42494000	-0.73400400	2.51117100
H	-5.38674300	-2.16718400	2.56075800
H	-5.34295900	-0.98920300	3.88267500
C	-6.44463800	-4.58538000	-0.17708900
C	-5.12808100	-4.37933500	-0.55729000
C	-4.58897500	-3.08455300	-0.58170000
C	-5.40068800	-1.99322500	-0.18217800
C	-6.74451900	-2.21848600	0.17333800
C	-7.26194700	-3.50098700	0.17404900
H	-2.64089100	-3.68655300	-1.34626900
H	-6.85187600	-5.59103700	-0.16737400
H	-4.50550200	-5.21687800	-0.85870200
C	-3.24405100	-2.83265000	-1.05685800
C	-4.82902000	-0.67472600	-0.16488400
H	-7.37175400	-1.37138500	0.43431300
H	-8.29864500	-3.66926700	0.44419900
C	-3.58012400	-0.44320900	-0.83738100
C	-2.74882900	-1.58312900	-1.18661000
H	-5.48745900	0.18109000	-0.05556700
H	-1.74745100	-1.43331300	-1.57693000
N	-3.30499700	0.82767300	-1.05977000
N	-2.15294600	1.15931500	-1.60159600
C	-1.82320700	2.49959400	-1.83168500
O	-0.65362600	2.77096000	-2.02494100
H	-1.34357400	0.50917400	-1.67138700
C	-2.89917900	3.53541900	-1.86351400
C	-2.50172000	4.83055000	-1.52198900
C	-4.21440600	3.29607500	-2.26939600
C	-3.41889000	5.87340200	-1.54046800
H	-1.46974800	4.99140900	-1.22801000

C	-5.12690700	4.34688300	-2.30259600
H	-4.52564200	2.30189000	-2.56509700
C	-4.73655600	5.63045400	-1.92666900
H	-3.10789400	6.87391800	-1.25629400
H	-6.14672300	4.16144000	-2.62334700
H	-5.45631200	6.44278200	-1.94488600

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C	6.96198500	-0.84413400	2.63317300
C	5.94217000	-1.07395900	1.74386300
C	5.14635700	-0.00219500	1.25455400
C	5.40894900	1.30945900	1.74121100
C	6.47900300	1.51678600	2.65189300
C	7.24468700	0.46630300	3.08609000
H	7.55437700	-1.67710700	2.99777700
C	4.06788800	-0.19487500	0.32900400
C	4.58497000	2.38868500	1.33072300
H	6.67004800	2.52646000	3.00457500
H	8.05689400	0.63243800	3.78590900
C	3.51415700	2.19988700	0.49221900
C	3.27287100	0.88523300	0.01118300
H	4.79878900	3.38629600	1.70644600
C	3.73216700	-1.53424300	-0.22736900
C	4.67884900	-2.31206300	-0.96851100
C	2.46186900	-2.04260000	-0.03190500
C	4.32095400	-3.62856600	-1.37272500
C	5.95508400	-1.81245100	-1.34602500
C	2.09867200	-3.36842200	-0.39678300
C	5.25395800	-4.41575500	-2.09912600
C	3.03850100	-4.13369100	-1.04721900
C	6.83049400	-2.59160400	-2.05963600
H	6.22689500	-0.79836700	-1.07286000
C	6.48359400	-3.91261500	-2.43375000
H	4.96681300	-5.42194900	-2.39097600
H	2.79093000	-5.15453200	-1.32743300
H	7.79702700	-2.19028600	-2.34678700
H	7.18922300	-4.51727900	-2.99365600
O	1.52383900	-1.27398600	0.61781200
H	5.72944800	-2.08548500	1.41616500
O	2.19582800	0.69198000	-0.83258000
P	0.87101700	0.02512400	-0.15552500
O	-0.05333900	-0.40400900	-1.24123700
O	0.38829600	0.90017100	0.98026600
C	2.65339700	3.34490900	0.07662100
C	1.78359000	3.94948500	1.00395800
C	2.76727900	3.85408400	-1.23242200
C	1.60543100	3.44939800	2.33709400
C	1.03326400	5.11230500	0.61628800
C	2.00840100	5.01222400	-1.60929700
C	3.63608700	3.27082700	-2.21121500
C	0.77122800	4.07276800	3.21824800

H	2.13436300	2.54952700	2.62988300
C	0.15827800	5.73074500	1.56850100
C	1.17254400	5.62190000	-0.67418900
C	2.13516700	5.52845500	-2.93740100
H	4.22626700	2.40136400	-1.94078800
C	3.73005600	3.79254900	-3.46828100
C	0.03661900	5.23575200	2.83282600
H	0.64851800	3.67470500	4.22040000
H	-0.40229800	6.60910500	1.25736800
H	0.61277100	6.51044000	-0.96020500
C	2.96661600	4.93822600	-3.84153500
H	1.54935100	6.40284300	-3.20685200
H	4.39254700	3.33474900	-4.19578700
H	-0.62739700	5.71132600	3.54793400
H	3.05522300	5.33602800	-4.84718300
C	0.77954100	-3.97133300	-0.04320900
C	0.43768300	-4.18447400	1.31012000
C	-0.06398100	-4.45123900	-1.06728200
C	1.24697800	-3.71764900	2.39701400
C	-0.76282200	-4.90645900	1.63326700
C	-1.21263600	-5.24690000	-0.72985800
C	0.17734100	-4.18339400	-2.45625000
C	0.86428400	-3.90450100	3.69348000
H	2.17634000	-3.20232500	2.18228900
C	-1.12766200	-5.08415800	3.00597500
C	-1.54610000	-5.44079600	0.60930800
C	-1.98231000	-5.84407200	-1.78042800
H	0.99735100	-3.52648300	-2.72484200
C	-0.60864100	-4.73194000	-3.42797600
C	-0.34645600	-4.59007200	4.00770200
H	1.48974000	-3.53317000	4.49870000
H	-2.04406100	-5.62407800	3.22767000
H	-2.42794100	-6.02565800	0.86158000
C	-1.68751700	-5.60406900	-3.08951200
H	-2.80689900	-6.49544800	-1.50350600
H	-0.41039400	-4.51031100	-4.47143800
H	-0.63177500	-4.72625700	5.04569900
H	-2.27604000	-6.06075900	-3.87855700
C	-2.82268300	1.61275700	1.65302700
C	-4.15589800	1.21774300	1.63645400
C	-5.14736700	2.18033400	1.72960800
C	-4.75795700	3.51998100	1.84168100
C	-3.41030600	3.88724100	1.84055900
C	-2.40296200	2.92737900	1.73465000

C	-2.71712100	-0.61357200	1.45441200
C	-4.20346900	-0.28070100	1.43019800
H	-6.20008500	1.91201900	1.70750200
H	-5.51799000	4.29053300	1.91847400
H	-3.13570000	4.93517500	1.90326500
H	-1.34871000	3.18735600	1.70666300
H	-0.90040700	0.57280500	1.40434800
N	-2.00690100	0.46307900	1.54886500
C	-2.11420800	-1.97203900	1.43143800
H	-2.83556100	-2.72179400	1.10380300
H	-1.24100400	-1.99984600	0.77068100
H	-1.78374800	-2.23205400	2.44507400
C	-4.93824100	-1.01241400	2.55842000
H	-5.98279400	-0.69459900	2.59739300
H	-4.91147500	-2.09451000	2.41436700
H	-4.47450700	-0.76760000	3.51750500
C	-6.41923200	-4.53308600	-0.52591900
C	-5.17875300	-4.22028800	-1.06787000
C	-4.64410900	-2.93297500	-0.93586000
C	-5.36294200	-1.95064900	-0.23132000
C	-6.62570500	-2.26555600	0.26990000
C	-7.15150900	-3.54809900	0.13428200
H	-2.84441200	-3.37378200	-2.10100700
H	-6.82472800	-5.53336400	-0.63619400
H	-4.61657800	-4.96479900	-1.62406000
C	-3.38859400	-2.57993200	-1.59645700
C	-4.78846800	-0.56526400	-0.04453000
H	-7.20886400	-1.49592700	0.76841700
H	-8.13325500	-3.77388400	0.53725300
C	-3.68432700	-0.22370900	-1.03780800
C	-2.93125500	-1.31741500	-1.65091000
H	-5.59816800	0.16288400	-0.15290100
H	-2.01509200	-1.10509600	-2.18632500
N	-3.43783600	1.03412800	-1.16067400
N	-2.28783800	1.41439600	-1.78507800
C	-1.90078400	2.73800800	-1.78725400
O	-0.72459600	3.00796000	-1.98611200
H	-1.48640700	0.76954400	-1.79918500
C	-2.91775300	3.81934300	-1.57974200
C	-2.41518100	5.03227700	-1.10116100
C	-4.27789500	3.70577900	-1.87770800
C	-3.26314200	6.11126000	-0.88454600
H	-1.35228500	5.09614800	-0.89350100
C	-5.12443900	4.79187800	-1.67013300

H	-4.67418800	2.77685700	-2.26774000
C	-4.62359000	5.98950100	-1.16386500
H	-2.86574100	7.04515000	-0.49826400
H	-6.17999700	4.70176800	-1.90595500
H	-5.29153200	6.82901200	-0.99700300

TSII-2

Value of imaginary frequency = -75.7 cm^{-1}

C	7.92026000	-0.28395700	0.08107300
C	6.64556000	0.18177000	0.28177400
C	5.52629800	-0.68947500	0.17698200
C	5.75891600	-2.04904200	-0.17450700
C	7.09179500	-2.50448500	-0.36246500
C	8.15124000	-1.64514200	-0.23392800
H	8.76071600	0.39801600	0.15871600
C	4.18027800	-0.24472900	0.37987600
C	4.65752400	-2.92378100	-0.35101800
H	7.25069400	-3.54780600	-0.62004700
H	9.16560400	-1.99948400	-0.38373400
C	3.35947300	-2.48622100	-0.23497800
C	3.14613300	-1.12343200	0.11316300
H	4.84892100	-3.96289700	-0.60692700
C	3.85076200	1.13120900	0.84435600
C	4.33853900	1.66178600	2.08450500
C	2.96831600	1.88978900	0.10387400
C	3.95232700	2.97736500	2.46867800
C	5.15608000	0.91388800	2.97604600
C	2.53826600	3.18828800	0.49367800
C	4.43846500	3.52200800	3.68729200
C	3.05673700	3.71396800	1.65103800
C	5.59999400	1.46262100	4.15278700
H	5.42050100	-0.10642600	2.72280700
C	5.25086700	2.78679700	4.51024100
H	4.14174500	4.53154400	3.95728200
H	2.75382600	4.70866300	1.96825600
H	6.21955700	0.87278400	4.82041500
H	5.61481200	3.20872500	5.44108900
O	2.45921800	1.35591600	-1.06370100
H	6.47907200	1.22826500	0.51357200
O	1.84673300	-0.70293900	0.25604400
P	1.19027700	0.33944500	-0.83205500
O	0.09786100	1.04591700	-0.09668300
O	0.89791000	-0.32091200	-2.14417300
C	2.21951300	-3.42121900	-0.46267600
C	2.05420100	-4.01504200	-1.73274900
C	1.34346000	-3.75110100	0.59432900
C	2.83941400	-3.64034700	-2.87442800
C	1.04101100	-5.01846100	-1.92064500
C	0.31135700	-4.72772000	0.38062400
C	1.43510200	-3.15559000	1.89483100

C	2.65012700	-4.23352600	-4.08824000
H	3.57876900	-2.85519300	-2.76566000
C	0.88731000	-5.62933700	-3.20724100
C	0.20870600	-5.36257100	-0.85676700
C	-0.60229500	-5.03023800	1.43959400
H	2.22095000	-2.43541000	2.09232500
C	0.53783500	-3.46093200	2.87662900
C	1.66655100	-5.25295500	-4.25942800
H	3.24747700	-3.92247800	-4.93900800
H	0.12668000	-6.39723000	-3.32309600
H	-0.54983800	-6.12942100	-0.99809900
C	-0.50522800	-4.40611100	2.64624700
H	-1.39287400	-5.75042900	1.24597500
H	0.60014800	-2.96224300	3.83738000
H	1.53796100	-5.71633600	-5.23205500
H	-1.22939200	-4.60901200	3.43017600
C	1.55271400	3.95591400	-0.32322800
C	1.95462400	4.51765500	-1.55108300
C	0.23949600	4.14839700	0.15226100
C	3.27634400	4.34320300	-2.07802600
C	1.02454000	5.30533700	-2.31075400
C	-0.67890400	4.94836800	-0.61152900
C	-0.24635900	3.53566000	1.35564200
C	3.63805400	4.89807700	-3.27035500
H	3.99406000	3.75949700	-1.51105400
C	1.44455900	5.87205900	-3.55680700
C	-0.26537900	5.50996400	-1.81972400
C	-2.01435900	5.13811300	-0.12615900
H	0.41937600	2.88783600	1.91435100
C	-1.53387200	3.71551900	1.76855600
C	2.70873000	5.67461400	-4.02532800
H	4.64296400	4.75134800	-3.65257000
H	0.72781700	6.46394800	-4.11928600
H	-0.96441100	6.11386400	-2.39394300
C	-2.43156600	4.54072300	1.02527200
H	-2.68906100	5.75832800	-0.71011300
H	-1.88617400	3.21783700	2.66667600
H	3.01728600	6.10725700	-4.97135200
H	-3.44986200	4.67693200	1.37677500
C	-2.40792100	-1.60155500	-2.06564400
C	-3.76657800	-1.52012600	-1.75420400
C	-4.53136700	-2.67364200	-1.70562700
C	-3.89956600	-3.89801300	-1.94894000
C	-2.53538100	-3.95616600	-2.24017200

C	-1.75513400	-2.79988500	-2.30281900
C	-2.73469500	0.55617000	-1.56707200
C	-4.13538300	-0.05702600	-1.59593000
H	-5.59375900	-2.63591200	-1.47994300
H	-4.47777400	-4.81511200	-1.90978100
H	-2.06726800	-4.91665700	-2.42562900
H	-0.68983600	-2.83377500	-2.51039200
H	-0.84417800	-0.13702800	-2.17474600
N	-1.86343700	-0.30293200	-2.04737200
C	-2.48023000	2.01760600	-1.49137000
H	-3.26786300	2.51062300	-0.91837200
H	-1.50857400	2.20070000	-1.02445100
H	-2.47467500	2.42821700	-2.50707400
C	-4.73009500	0.42370500	-2.94302700
H	-5.60311300	-0.17183000	-3.21081700
H	-4.99975300	1.48117500	-2.91297900
H	-3.98406000	0.27271900	-3.72793300
C	-8.32338400	2.99709900	-0.04738000
C	-7.43734000	2.84878200	1.00951600
C	-6.35400500	1.96612200	0.92313600
C	-6.12207700	1.23160400	-0.26130700
C	-7.07470000	1.33234500	-1.27714700
C	-8.14926100	2.21481400	-1.18429800
H	-5.82229900	2.28710600	3.01253900
H	-9.15663100	3.68714800	0.02691300
H	-7.58391400	3.40576600	1.93042500
C	-5.52964200	1.75824800	2.10924500
C	-4.97320800	0.22162700	-0.29204500
H	-7.00818900	0.70805200	-2.15561200
H	-8.85686800	2.27610900	-2.00429100
C	-3.99485200	0.40976200	0.85615500
C	-4.44915800	0.96169700	2.12291700
H	-5.45879200	-0.74140000	-0.05668800
H	-3.83641200	0.85385800	3.00871400
N	-2.78807200	0.09384200	0.56695800
N	-1.81022900	0.12339500	1.54052900
C	-1.72987700	-0.73866800	2.60695900
O	-0.83582000	-0.60220600	3.43063200
H	-0.92795300	0.51118900	1.16707800
C	-2.73995200	-1.84125800	2.74188800
C	-3.15674500	-2.61094400	1.65218400
C	-3.15086700	-2.18149800	4.03201300
C	-3.99817600	-3.70075900	1.85663400
H	-2.79669500	-2.38590500	0.65193500

C	-4.00324700	-3.26284700	4.23209500
H	-2.78630400	-1.59557200	4.86989600
C	-4.42853700	-4.02272300	3.14275800
H	-4.30651500	-4.30281600	1.00748900
H	-4.32942500	-3.51775700	5.23505300
H	-5.08851900	-4.87027900	3.29807300

IMII-2

C	-7.72441300	-1.92102800	0.64831400
C	-6.64449600	-1.18446500	0.23123800
C	-5.34626100	-1.76133600	0.17401500
C	-5.18806600	-3.11219000	0.59611600
C	-6.32778100	-3.85210500	1.01032800
C	-7.57058900	-3.27457600	1.03202400
H	-8.70606900	-1.46020700	0.69108900
C	-4.19279400	-1.02670000	-0.25328600
C	-3.89456900	-3.69489400	0.61645100
H	-6.18989000	-4.88458700	1.31914700
H	-8.43508600	-3.84621200	1.35304200
C	-2.77674100	-2.97656700	0.26975700
C	-2.95432500	-1.62916400	-0.14946400
H	-3.78911600	-4.72984000	0.93265700
C	-4.26719400	0.37497900	-0.75337300
C	-5.05388900	0.75518600	-1.89009700
C	-3.49147200	1.33787700	-0.14153400
C	-5.06657200	2.12084000	-2.29470600
C	-5.79176900	-0.18339300	-2.66212100
C	-3.48836600	2.70417400	-0.53369500
C	-5.84834300	2.50983200	-3.41499700
C	-4.28519400	3.07253700	-1.58828200
C	-6.52937300	0.22160000	-3.74609100
H	-5.75867000	-1.23299600	-2.39104100
C	-6.57003600	1.58480600	-4.12364900
H	-5.85419000	3.55744100	-3.70298400
H	-4.31101400	4.11284200	-1.90310300
H	-7.08222300	-0.51172600	-4.32431200
H	-7.16170300	1.88982000	-4.98040000
O	-2.68571600	0.97335300	0.91450300
H	-6.77337100	-0.14491800	-0.05048400
O	-1.83228100	-0.92364700	-0.51179900
P	-1.27477900	0.23653300	0.51031600
O	-0.46113500	1.14764100	-0.36460200
O	-0.70939700	-0.33024600	1.76848000
C	-1.41275700	-3.57931200	0.30443500
C	-0.82195000	-3.92003900	1.53658100
C	-0.72834800	-3.82200000	-0.90474400
C	-1.44285400	-3.63576300	2.79838300
C	0.46738700	-4.55621100	1.55258300
C	0.57518100	-4.42168500	-0.87253000
C	-1.28527500	-3.49634000	-2.18445900
C	-0.84968800	-3.99427800	3.97354800

H	-2.39255100	-3.11266500	2.80549300
C	1.04476000	-4.93721400	2.80685600
C	1.13784800	-4.78292400	0.35216300
C	1.27894800	-4.63450600	-2.09982500
H	-2.27801800	-3.06137300	-2.23284800
C	-0.58382600	-3.71645300	-3.33289900
C	0.40810700	-4.67044400	3.98194200
H	-1.33474700	-3.76194800	4.91608700
H	2.01008100	-5.43687200	2.79498500
H	2.12147300	-5.24779400	0.36856600
C	0.72312500	-4.28432300	-3.29309400
H	2.27925800	-5.05792000	-2.05082800
H	-1.01858700	-3.44833900	-4.29042500
H	0.85578600	-4.95926000	4.92779300
H	1.27262600	-4.43099600	-4.21765500
C	-2.67338000	3.69956800	0.22412400
C	-3.12982700	4.13539600	1.48419200
C	-1.47932900	4.21226900	-0.31642100
C	-4.33924400	3.64180500	2.07384100
C	-2.37513000	5.11490500	2.21340900
C	-0.73158000	5.19252500	0.42236800
C	-0.95635600	3.77662700	-1.57848800
C	-4.76043900	4.08565900	3.29332700
H	-4.92468500	2.90516900	1.53342000
C	-2.85287000	5.55670000	3.48832100
C	-1.19614000	5.62198100	1.66520400
C	0.48297800	5.70991800	-0.13466300
H	-1.49053100	3.00577500	-2.12143800
C	0.20757300	4.28769400	-2.07179000
C	-4.00746600	5.05918600	4.01475000
H	-5.67881600	3.69763300	3.72191800
H	-2.27066900	6.30006200	4.02598100
H	-0.62825400	6.36625900	2.21907600
C	0.93747100	5.27631900	-1.34394800
H	1.03118700	6.45699200	0.43291500
H	0.59082900	3.93588700	-3.02434500
H	-4.36130900	5.40074900	4.98199300
H	1.85895100	5.67425300	-1.75750800
C	2.89479200	-0.66477400	2.24378900
C	4.22606900	-0.25686800	2.11394700
C	5.24809400	-1.01432100	2.65989200
C	4.92737500	-2.19235200	3.34426800
C	3.59397200	-2.58622500	3.46794500
C	2.55450000	-1.83522100	2.91618200

C	2.78005500	1.17536700	0.85230900
C	4.28471800	1.04623400	1.33333000
H	6.28597400	-0.70465500	2.55589200
H	5.71520600	-2.79774600	3.77879500
H	3.34975900	-3.50111600	3.99966500
H	1.51844100	-2.15284100	2.99385700
H	1.03273100	0.17691800	1.66141600
N	2.05386300	0.22101300	1.59389500
C	2.15209100	2.56354100	0.84203500
H	2.76278300	3.26022500	0.26202200
H	1.14917600	2.52096200	0.40603400
H	2.06204500	2.92800900	1.86617000
C	4.67470400	2.20975200	2.24704900
H	5.59647900	1.99075100	2.78564300
H	4.80135000	3.14508300	1.69551100
H	3.89563100	2.34575900	3.00118400
C	8.83750400	2.86690600	-0.99008800
C	7.89659300	2.57447400	-1.96666400
C	6.68556100	1.95800700	-1.62739600
C	6.40458300	1.64525400	-0.27916600
C	7.38185800	1.89478200	0.68069600
C	8.58103000	2.51331200	0.33271300
H	6.03158600	1.85871300	-3.70091600
H	9.77131000	3.34853400	-1.25802400
H	8.09292600	2.81356100	-3.00770900
C	5.73897400	1.62137800	-2.68143900
C	5.13564900	0.88021400	0.02066600
H	7.22492500	1.59749500	1.70989100
H	9.32069300	2.70966800	1.10159700
C	4.13447800	0.92347000	-1.08818100
C	4.52022900	1.07955400	-2.45971800
H	5.44986700	-0.18033600	-0.01047100
H	3.81037800	0.91349400	-3.26001500
N	2.92722400	0.78493900	-0.63334200
N	1.84662000	0.50220600	-1.42089800
C	1.82272900	-0.64834100	-2.21884600
O	0.94119200	-0.77727700	-3.04156100
H	0.90832600	0.85776800	-1.07120500
C	2.90336600	-1.66697800	-2.01796100
C	3.17425200	-2.14901900	-0.73756200
C	3.57803000	-2.18534100	-3.12240000
C	4.15230100	-3.12166800	-0.55257500
H	2.59340800	-1.78831300	0.10559200
C	4.56090400	-3.15339100	-2.93624400

H	3.33159400	-1.82545700	-4.11710100
C	4.85486900	-3.61401900	-1.65227900
H	4.35445700	-3.48929000	0.44979800
H	5.09770600	-3.54989200	-3.79181300
H	5.62527900	-4.36541300	-1.51159700

IMII-3

C	5.75550800	-5.06158000	-0.73794300
C	5.12302600	-3.93209500	-0.28260200
C	3.70581900	-3.82950800	-0.31222900
C	2.95712400	-4.91481500	-0.85057600
C	3.64084300	-6.07494000	-1.30190200
C	5.00846900	-6.15120800	-1.24550800
H	6.83889000	-5.11917700	-0.71388400
C	3.00976300	-2.66336400	0.14200400
C	1.54192600	-4.82362300	-0.93105900
H	3.05544700	-6.89853100	-1.70125500
H	5.52215600	-7.03993100	-1.59704500
C	0.87502700	-3.68583600	-0.55058700
C	1.64403400	-2.59991000	-0.05115700
H	0.98070900	-5.67454800	-1.30936200
C	3.67794100	-1.50969300	0.80716800
C	4.42263600	-1.65194400	2.02410000
C	3.47284100	-0.23939100	0.30597100
C	4.98262600	-0.49012900	2.62894000
C	4.59277600	-2.90035200	2.68460100
C	3.99026000	0.93306400	0.91833400
C	5.73579000	-0.61761700	3.82640400
C	4.75075100	0.78480700	2.05172400
C	5.31577000	-2.98983000	3.84754200
H	4.13585900	-3.78958200	2.26514700
C	5.90727800	-1.83972300	4.42203200
H	6.16420200	0.27922800	4.26511400
H	5.16908800	1.66437600	2.53484900
H	5.43085200	-3.95248600	4.33520500
H	6.48106600	-1.92721900	5.33871100
O	2.74869500	-0.08692200	-0.85368500
H	5.70252800	-3.09696100	0.09739200
O	0.97403200	-1.45211500	0.29703600
P	1.11151200	-0.17732500	-0.74515700
O	0.57834600	0.99325200	0.04619900
O	0.59122100	-0.49079300	-2.09914200
C	-0.61599000	-3.59396800	-0.58535500
C	-1.29921000	-3.44349400	-1.80668000
C	-1.33551500	-3.68008600	0.62415000
C	-0.61320600	-3.29909600	-3.05708800
C	-2.73745300	-3.40967500	-1.81643900
C	-2.77196900	-3.65022900	0.60059100
C	-0.68879800	-3.77487900	1.89989400
C	-1.30356000	-3.15720500	-4.22434400

H	0.47030200	-3.27577700	-3.05429800
C	-3.42255400	-3.26372000	-3.06515400
C	-3.44079000	-3.52003300	-0.61689300
C	-3.49484200	-3.71153700	1.83499200
H	0.39515300	-3.80713500	1.93905000
C	-1.41193600	-3.81546100	3.05680500
C	-2.73090500	-3.14541400	-4.23302800
H	-0.76628500	-3.04019600	-5.15980300
H	-4.50924000	-3.25469300	-3.05344200
H	-4.52935200	-3.49739300	-0.62700400
C	-2.83824500	-3.78186700	3.02819300
H	-4.58114600	-3.68822400	1.79286500
H	-0.90027900	-3.87718000	4.01188200
H	-3.25849500	-3.03500500	-5.17504700
H	-3.39404800	-3.81855600	3.95973700
C	3.71813000	2.28332000	0.34340000
C	4.39061800	2.68998000	-0.82598000
C	2.83279700	3.16214100	0.99570700
C	5.26671600	1.81618900	-1.54882700
C	4.21052100	4.02497300	-1.32103800
C	2.66387800	4.49801200	0.49266000
C	2.06487100	2.77581600	2.14470700
C	5.89351700	2.23191400	-2.68713600
H	5.42269700	0.80735200	-1.18079300
C	4.89652500	4.42675700	-2.51104100
C	3.36589300	4.90237300	-0.64113300
C	1.77870100	5.39617300	1.17178100
H	2.15114600	1.75861500	2.51043900
C	1.22698100	3.65923700	2.76152800
C	5.70668300	3.55784100	-3.17989100
H	6.54449500	1.55124500	-3.22622100
H	4.75420200	5.44325600	-2.86873000
H	3.23427900	5.91448800	-1.01737600
C	1.08978000	4.99656100	2.27656700
H	1.67417200	6.40528300	0.78274200
H	0.65559100	3.34747700	3.63133300
H	6.21826700	3.86917600	-4.08486200
H	0.43595200	5.69116200	2.79530700
C	-2.94590600	2.99815800	2.14796700
C	-4.22643900	2.44284200	2.02995800
C	-5.35070800	3.22303600	2.23452800
C	-5.18764100	4.57949000	2.53495100
C	-3.90889900	5.12536700	2.62997300
C	-2.76716100	4.34401100	2.43892700

C	-2.60203900	0.89651000	1.32009100
C	-4.10744200	0.95191900	1.72515900
H	-6.34650300	2.79277600	2.15530500
H	-6.05780900	5.20806500	2.68871400
H	-3.79302300	6.18127800	2.85291900
H	-1.77211400	4.77140500	2.50379300
H	-1.01749200	2.21892800	1.72995700
N	-1.98119700	1.99989200	1.96892800
C	-1.89616000	-0.42538900	1.50552200
H	-2.42274200	-1.20904300	0.95583900
H	-0.86877000	-0.36577800	1.15289600
H	-1.88490300	-0.68222600	2.56684300
C	-4.38263300	0.13832400	2.98778500
H	-5.39914100	0.32034300	3.34519200
H	-4.23515400	-0.93376300	2.82947900
H	-3.69304100	0.46960300	3.76981900
C	-7.33385200	-2.83171200	-0.63538600
C	-6.70345900	-2.05806600	-1.60232600
C	-5.86968900	-0.99589800	-1.23684500
C	-5.67815600	-0.68208700	0.13106800
C	-6.35259400	-1.43708600	1.08577700
C	-7.15334300	-2.51729400	0.70757800
H	-5.44721100	-0.48777400	-3.31636000
H	-7.96734200	-3.66213500	-0.92634300
H	-6.85141700	-2.27300400	-2.65707800
C	-5.20167600	-0.23137900	-2.28901900
C	-4.90199500	0.59612400	0.42237300
H	-6.27373400	-1.19720600	2.13671700
H	-7.64787500	-3.10303000	1.47555400
C	-3.90690900	0.86437200	-0.66473700
C	-4.25246700	0.69696400	-2.04979900
H	-5.65580900	1.38942100	0.28414800
H	-3.68545400	1.18021000	-2.83408300
N	-2.74589100	1.16661600	-0.18636300
N	-1.73357700	1.71301200	-0.92201200
C	-1.98679600	2.96432700	-1.47285600
O	-3.09848200	3.46367900	-1.46663300
H	-0.75695400	1.45126000	-0.57728400
C	-0.79216800	3.60848400	-2.08854200
C	0.28607400	2.86136900	-2.57359100
C	-0.79461400	5.00069300	-2.19521900
C	1.36684900	3.51892700	-3.15203200
H	0.27111400	1.77575600	-2.53165200
C	0.29112100	5.65104000	-2.77087200

H	-1.65013800	5.55497800	-1.82284800
C	1.36992400	4.90904900	-3.24969100
H	2.21126500	2.94511000	-3.52239400
H	0.29525900	6.73332900	-2.84929900
H	2.21985700	5.41468500	-3.69886200

IMII-4

C	7.34583200	-1.30504700	0.49847500
C	6.02615200	-1.57836100	0.24073700
C	5.12443900	-0.54211700	-0.12713000
C	5.61742800	0.79288600	-0.18068300
C	6.99192800	1.04190400	0.07881300
C	7.84152700	0.01768000	0.40607900
H	8.01579200	-2.11010800	0.78262000
C	3.74047900	-0.78297800	-0.40734100
C	4.72535500	1.85915400	-0.45995400
H	7.35217200	2.06536000	0.02270100
H	8.88876800	0.21727800	0.60754800
C	3.38300400	1.64246200	-0.65626100
C	2.91081400	0.30038700	-0.62788500
H	5.11416100	2.87408100	-0.49199900
C	3.13923200	-2.14543300	-0.40982100
C	3.59858100	-3.19919300	-1.26567000
C	2.03755600	-2.37682900	0.39095800
C	2.95735900	-4.46910800	-1.19801700
C	4.64079100	-3.02252100	-2.21728000
C	1.35987000	-3.62475700	0.43774400
C	3.41156700	-5.52764900	-2.02918600
C	1.84761400	-4.65047700	-0.33416000
C	5.04866200	-4.06055400	-3.01683600
H	5.10781700	-2.04859000	-2.31480400
C	4.43879100	-5.33391100	-2.91520100
H	2.91761400	-6.49243300	-1.95344200
H	1.35325200	-5.61863300	-0.31072600
H	5.84182800	-3.90288600	-3.74051500
H	4.77605100	-6.14684700	-3.54969800
O	1.56546600	-1.35612000	1.18419800
H	5.65582400	-2.59415700	0.32577300
O	1.57740200	0.08417200	-0.87414700
P	0.60183600	-0.26056200	0.41474900
O	-0.61927400	-0.90355200	-0.13214800
O	0.54736900	0.92313200	1.34270000
C	2.43601200	2.77005100	-0.89007800
C	2.22156900	3.73227200	0.11812000
C	1.78550100	2.89078200	-2.13569400
C	2.86223700	3.66960700	1.40072900
C	1.33203400	4.83439800	-0.13214800
C	0.88130400	3.98218200	-2.36502400
C	2.01648400	1.97420400	-3.21399600
C	2.68327400	4.65636900	2.32399700

H	3.49562000	2.82056300	1.62979500
C	1.15316100	5.83604200	0.87644700
C	0.67475700	4.92693900	-1.35771700
C	0.21520000	4.08695700	-3.63023400
H	2.71587100	1.15799300	-3.06930400
C	1.38311300	2.12158900	-4.41375700
C	1.82285200	5.76380700	2.05907900
H	3.18170800	4.59077200	3.28619500
H	0.47609100	6.65991300	0.66778000
H	0.00296300	5.76323800	-1.54108500
C	0.45371800	3.18478100	-4.62477300
H	-0.48168300	4.90767000	-3.77830800
H	1.58465200	1.42253500	-5.21947900
H	1.68418900	6.52770300	2.81718400
H	-0.05429200	3.27130500	-5.57975500
C	0.14209800	-3.81124100	1.27883800
C	0.25447800	-3.85684700	2.68191800
C	-1.11067900	-3.98830500	0.65864800
C	1.50446700	-3.67102500	3.35735600
C	-0.91243600	-4.11141900	3.47953100
C	-2.26369000	-4.28131700	1.46380400
C	-1.29561100	-3.86277400	-0.75856000
C	1.58458500	-3.72149600	4.71819100
H	2.39639200	-3.48445500	2.76795800
C	-0.78539300	-4.15884100	4.90460200
C	-2.14001400	-4.33024700	2.85228300
C	-3.52109100	-4.52217100	0.82139400
H	-0.44866000	-3.57266900	-1.36892300
C	-2.51649200	-4.07012900	-1.32963700
C	0.42186300	-3.96839500	5.50773000
H	2.54084500	-3.57384500	5.20952400
H	-3.01705400	-4.54979100	3.45800800
C	-3.64506600	-4.42821000	-0.53151500
H	-4.37715500	-4.77159100	1.44206300
H	-2.63757400	-3.95677900	-2.40261000
H	-4.60476600	-4.60436100	-1.00664100
C	-2.20268100	0.70623500	-3.36465600
C	-3.56415400	0.53049300	-3.07292000
C	-4.42345600	-0.00649200	-4.01623200
C	-3.90842700	-0.40897300	-5.25295300
C	-2.54775200	-0.26844600	-5.51841000
C	-1.67498600	0.29218400	-4.58281300
C	-2.55193300	1.92795800	-1.43867400
C	-3.79998500	0.99964200	-1.65905400

H	-5.48642600	-0.10037700	-3.80859900
H	-4.56906800	-0.82739500	-6.00412800
H	-2.15411800	-0.59024600	-6.47755300
H	-0.61919800	0.40963000	-4.79790600
H	-0.72750900	1.88136300	-2.51041100
N	-1.54326100	1.31700900	-2.29432100
C	-2.73982600	3.40522000	-1.71483700
H	-3.50152800	3.83488500	-1.06363100
H	-1.79500500	3.92684600	-1.54261700
H	-3.02567300	3.52764100	-2.76334200
C	-5.12725200	1.69164300	-1.38463400
H	-5.95557500	0.98616400	-1.47952500
H	-5.14137700	2.10088000	-0.36824300
H	-5.28954200	2.50566000	-2.09449600
C	-6.58832300	-2.71590500	0.93242800
C	-5.64458900	-2.16248800	1.78620500
C	-4.64786300	-1.31331200	1.28912100
C	-4.60013200	-1.01712200	-0.08753100
C	-5.52364100	-1.61421800	-0.94053200
C	-6.52096900	-2.44441200	-0.43368200
H	-3.69394800	-1.08102700	3.23274800
H	-7.36348700	-3.36578800	1.32364200
H	-5.66716700	-2.38450600	2.84964000
C	-3.65685400	-0.75388000	2.19675000
C	-3.50078700	-0.12886400	-0.60254500
H	-5.46376300	-1.43018500	-2.00828600
H	-7.24517900	-2.88485700	-1.11137600
C	-2.77842500	0.60134900	0.47149800
C	-2.73137900	0.16218300	1.82848600
H	-2.70306700	-0.77932900	-1.00836200
H	-2.01880500	0.59466100	2.52008600
N	-2.25537200	1.69805300	-0.00109000
N	-1.47572800	2.54579200	0.75903500
C	-2.16692800	3.43773400	1.55616200
O	-3.34401500	3.69630400	1.36044600
H	-0.56009200	2.10509700	1.01584600
H	0.50748500	-4.00696100	6.58885900
H	-1.67761400	-4.35486600	5.49314800
C	-1.38787300	4.05403700	2.67017300
C	-1.83329600	5.28970200	3.15006800
C	-0.32905700	3.39433600	3.29802900
C	-1.21475400	5.87264200	4.24728200
H	-2.67000700	5.77211800	2.65591200
C	0.26712600	3.97189900	4.41720700

H	0.03092600	2.43566500	2.93335700
C	-0.16789700	5.20714100	4.88813700
H	-1.55464300	6.83561100	4.61384300
H	1.08090600	3.45531100	4.91553200
H	0.30567600	5.65336600	5.75707400

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Value of imaginary frequency = -979.0 cm^{-1}

C	-0.36383900	6.96802600	1.66683600
C	0.18941200	5.79735600	1.21350500
C	-0.62765600	4.77178900	0.66240000
C	-2.03427500	4.97524400	0.62954600
C	-2.57713000	6.20400600	1.09266100
C	-1.76159500	7.18317600	1.59606100
H	0.27583900	7.73592800	2.08964200
C	-0.09393400	3.53717800	0.17022900
C	-2.87342800	3.93718000	0.15798000
H	-3.65345100	6.34471100	1.04865400
H	-2.18195700	8.11730100	1.95356700
C	-2.37530900	2.71671000	-0.23399800
C	-0.96214600	2.53262500	-0.21461300
H	-3.94737300	4.10406800	0.13006500
C	1.36851200	3.28632700	0.09587000
C	2.25053700	4.12396100	-0.66020200
C	1.87846900	2.16549900	0.71853600
C	3.64035600	3.82077300	-0.66908100
C	1.79507000	5.22261400	-1.44023900
C	3.25692300	1.82455800	0.68615500
C	4.53368600	4.64793500	-1.40183300
C	4.10811200	2.67443700	0.01879500
C	2.67985000	5.99539000	-2.14899500
H	0.73384200	5.44172500	-1.47929200
C	4.06753800	5.71615500	-2.12209300
H	5.59274600	4.40618400	-1.38779500
H	5.16946800	2.44164200	-0.01468900
H	2.31277500	6.82650700	-2.74255000
H	4.75397200	6.34058500	-2.68430600
O	1.00509300	1.33845500	1.39808500
H	1.26032700	5.64109400	1.28337400
O	-0.44548600	1.33154200	-0.65972000
P	0.17368600	0.28411700	0.45323000
O	1.20618300	-0.57336300	-0.24609800
O	-0.91367800	-0.31461700	1.28189500
C	-3.31102300	1.64876800	-0.68719300
C	-4.28158400	1.13718400	0.20093700
C	-3.29704300	1.23449600	-2.03459200
C	-4.38965700	1.56353200	1.56756800
C	-5.23571900	0.17127800	-0.27477100
C	-4.21358700	0.22191100	-2.47933700
C	-2.41147200	1.80872900	-3.00568500

C	-5.41395600	1.13354800	2.35835000
H	-3.64870500	2.24643300	1.96623000
C	-6.28005900	-0.27294100	0.59933000
C	-5.15558500	-0.29251000	-1.58698800
C	-4.16094900	-0.21952700	-3.84119700
H	-1.73774200	2.60214600	-2.69838400
C	-2.40597000	1.37450300	-4.30050300
C	-6.38586300	0.21267000	1.86632700
H	-5.48178700	1.47792500	3.38564700
H	-6.99184800	-1.00060400	0.21910900
H	-5.86541400	-1.04042600	-1.93396900
C	-3.28007100	0.33042000	-4.72471300
H	-4.84602400	-1.00330200	-4.15351500
H	-1.72527600	1.82155600	-5.01781900
H	-7.18506500	-0.12296200	2.51878600
H	-3.24752600	-0.01145600	-5.75374300
C	3.80466100	0.58794400	1.31351200
C	3.82074200	0.43541000	2.71341100
C	4.41895600	-0.37495000	0.48583600
C	3.20994600	1.38232900	3.59947400
C	4.49543800	-0.69273500	3.29477100
C	5.16281000	-1.44933000	1.08207900
C	4.32387600	-0.33914600	-0.94555400
C	3.23580000	1.20154000	4.95118600
H	2.71740300	2.25291600	3.17944000
C	4.49777300	-0.84603000	4.71836500
C	5.17149700	-1.59220200	2.46969000
C	5.89776100	-2.34011500	0.23620500
H	3.66877200	0.39093400	-1.40781400
C	5.01134000	-1.22990200	-1.71726800
C	3.88421700	0.06645700	5.52317500
H	2.76170300	1.92798900	5.60334800
H	5.72213200	-2.41662900	2.91790600
C	5.84491600	-2.22092600	-1.11976500
H	6.48582500	-3.12466400	0.70521200
H	4.90930600	-1.19433700	-2.79755100
H	6.40477900	-2.90328800	-1.75223700
C	0.23073200	-1.01377000	-3.01954600
C	0.90249900	-2.24101500	-3.09028800
C	2.03490300	-2.37600900	-3.87549800
C	2.52733400	-1.26004200	-4.56057100
C	1.88838800	-0.02788600	-4.43013700
C	0.73290700	0.11492300	-3.66033700
C	-1.20288200	-2.52287500	-1.98175700

C	0.20209300	-3.21941500	-2.17273900
H	2.53007900	-3.33817800	-3.97864100
H	3.40886300	-1.35285500	-5.18621700
H	2.28905300	0.84027500	-4.94469900
H	0.24051200	1.07394700	-3.55535900
H	-1.69398600	-0.51566100	-2.45364100
N	-0.91227500	-1.11852600	-2.22672000
C	-2.36172700	-3.03855900	-2.81100100
H	-2.54257300	-4.09709300	-2.61905400
H	-3.26368800	-2.48191300	-2.53916600
H	-2.15378600	-2.87554700	-3.87200700
C	0.11447300	-4.65378000	-2.68409800
H	1.11064400	-5.09503300	-2.76087000
H	-0.47319900	-5.27359500	-1.99948300
H	-0.34720200	-4.68399800	-3.67416200
C	4.12678300	-5.22903400	0.93413000
C	3.07349800	-4.84162700	1.73847900
C	1.95534500	-4.19075500	1.18555600
C	1.91749400	-3.89887300	-0.20150800
C	3.01228700	-4.26779000	-0.99286100
C	4.08737700	-4.94171500	-0.43636100
H	0.91561400	-4.06716200	3.08407300
H	4.98204300	-5.74298900	1.35970000
H	3.08673000	-5.04705200	2.80517600
C	0.82912200	-3.85811200	2.02084700
C	0.75116000	-3.16524300	-0.71484800
H	3.02308200	-4.01216400	-2.04545600
H	4.91992700	-5.23123300	-1.06969200
C	-0.39843900	-3.11162300	0.13807900
C	-0.33029900	-3.33665300	1.53999700
H	1.01685800	-1.93051400	-0.48919800
H	-1.18043200	-3.12514100	2.17699700
N	-1.47889400	-2.74798100	-0.54699900
N	-2.57516400	-2.20239000	0.08492300
C	-3.54591400	-3.08363400	0.52518400
O	-3.74567500	-4.14590500	-0.03679700
H	-2.33456300	-1.34314700	0.58940400
H	3.89154200	-0.05942700	6.60098000
H	5.00580400	-1.70867000	5.14093800
C	-4.28770900	-2.67633000	1.75703800
C	-5.50290600	-3.31810700	2.01653000
C	-3.74572500	-1.79540300	2.69703100
C	-6.18048500	-3.07237600	3.20208000
H	-5.89249900	-4.01300200	1.27998800

C	-4.42069900	-1.56892800	3.89486300
H	-2.79778800	-1.29196900	2.51940700
C	-5.63442200	-2.20074000	4.14663000
H	-7.12676200	-3.56554200	3.39891000
H	-3.99634200	-0.89076400	4.62785400
H	-6.15628100	-2.01772800	5.08071400

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C	-7.36186800	-0.79149900	-1.46036300
C	-6.10100600	-1.17458800	-1.07754500
C	-5.21274000	-0.24625100	-0.47104300
C	-5.64694000	1.09929700	-0.30052300
C	-6.96340500	1.46040000	-0.69427900
C	-7.80501900	0.53718500	-1.25747600
H	-8.02521800	-1.51239600	-1.92689200
C	-3.89093400	-0.60659600	-0.05019700
C	-4.76142400	2.06685700	0.24204500
H	-7.28474200	2.48762100	-0.54777500
H	-8.80714400	0.82290700	-1.55905600
C	-3.46480800	1.75003300	0.56714200
C	-3.05936900	0.40107200	0.39112800
H	-5.11614100	3.08535800	0.37821400
C	-3.37957900	-2.00717000	-0.04447000
C	-4.04869100	-3.05344000	0.67783800
C	-2.17072700	-2.30288600	-0.64065500
C	-3.49132800	-4.36396300	0.67072000
C	-5.22638400	-2.83140900	1.44414000
C	-1.56545600	-3.58681100	-0.59943800
C	-4.15642300	-5.41344300	1.35948200
C	-2.25014100	-4.59808900	0.02503400
C	-5.83841600	-3.86251300	2.11138800
H	-5.63843600	-1.83146200	1.51144000
C	-5.31063700	-5.17393100	2.05788800
H	-3.72135200	-6.40833600	1.32871600
H	-1.81429200	-5.59305100	0.06541500
H	-6.73404800	-3.66738600	2.69216100
H	-5.81127000	-5.98019800	2.58344300
O	-1.49431100	-1.31219600	-1.34251700
H	-5.76638600	-2.19321400	-1.24294000
O	-1.75446500	0.08575500	0.72943300
P	-0.73767300	-0.15618900	-0.51259300
O	0.46151400	-0.82987800	0.19630600
O	-0.52976200	1.02804900	-1.37558100
C	-2.49174100	2.75083900	1.08874400
C	-2.12493400	3.85870300	0.29647100
C	-1.91844400	2.56862200	2.36732600
C	-2.62413900	4.06640300	-1.03307500
C	-1.19025500	4.82082500	0.81631000
C	-0.95820600	3.51552200	2.85619300
C	-2.25096500	1.46093000	3.21580100
C	-2.26067000	5.16277800	-1.75709900

H	-3.29046400	3.32968600	-1.46607700
C	-0.83105400	5.95530300	0.01885800
C	-0.63445500	4.63021000	2.07988300
C	-0.32144100	3.28453300	4.11909300
H	-3.01288800	0.75876500	2.89537500
C	-1.62376300	1.27192300	4.41315000
C	-1.35701600	6.13011900	-1.22403500
H	-2.64673900	5.29607100	-2.76277200
H	-0.12215600	6.66845500	0.43030300
H	0.08294900	5.35398500	2.46111200
C	-0.62641400	2.18639400	4.86819400
H	0.41947600	4.00294000	4.45966400
H	-1.88932400	0.42077200	5.03206900
H	-1.07018200	6.98467300	-1.82784800
H	-0.12950500	2.01110100	5.81671700
C	-0.19852500	-3.77800200	-1.16377200
C	-0.01854600	-3.86826900	-2.55564300
C	0.90620200	-3.81493100	-0.29144700
C	-1.11798100	-3.82798200	-3.47337700
C	1.30680300	-4.00204600	-3.09125100
C	2.22847100	-3.93257100	-0.83985600
C	0.77894300	-3.68116400	1.13086200
C	-0.91357000	-3.91558800	-4.81935900
H	-2.12515900	-3.73163600	-3.07980000
C	1.47801600	-4.09056500	-4.50964600
C	2.39740400	-4.02917500	-2.22135500
C	3.35597200	-3.91525900	0.04112600
H	-0.21111600	-3.56713400	1.55965300
C	1.87934000	-3.65791900	1.93652700
C	0.40491300	-4.04892000	-5.34924600
H	-1.75942200	-3.88427100	-5.49853000
H	3.40411600	-4.11057500	-2.62637200
C	3.19039000	-3.77305300	1.38570000
H	4.34864400	-3.98728700	-0.39558100
H	1.76533700	-3.53066500	3.00858400
H	4.05359900	-3.72831900	2.04316800
C	2.14033800	-0.18492100	3.05242600
C	3.50859100	-0.22866300	2.78117900
C	4.34106900	-0.94088200	3.63450500
C	3.78736500	-1.63330500	4.71543700
C	2.41522900	-1.58975800	4.95579200
C	1.56950000	-0.85267600	4.12492800
C	2.50134100	1.50057800	1.44477400
C	3.83243800	0.65355300	1.58723300

H	5.41773000	-0.94102900	3.49355100
H	4.43472600	-2.19210800	5.38280600
H	1.99830300	-2.12177900	5.80493600
H	0.50126100	-0.79287600	4.31025500
H	0.69492200	1.16256600	2.50672700
N	1.45898600	0.61926100	2.09539300
C	2.51785400	2.86613600	2.09392100
H	3.29961500	3.48401100	1.65137300
H	1.55644900	3.35799400	1.93517000
H	2.68802700	2.75813800	3.16923600
C	5.07984200	1.52042000	1.78941600
H	5.97736700	0.89685100	1.76963500
H	5.15189900	2.24878300	0.97641500
H	5.04776300	2.04749900	2.74691000
C	6.60203500	-2.85560100	-1.43985000
C	5.63999300	-2.26629900	-2.22175600
C	4.72909700	-1.32141500	-1.68042400
C	4.80904600	-0.98920900	-0.29141200
C	5.81046000	-1.62600500	0.49191900
C	6.68398800	-2.52631800	-0.06532500
H	3.69541300	-0.98662200	-3.54996100
H	7.29791800	-3.56965400	-1.86754500
H	5.56565400	-2.50671400	-3.27977300
C	3.75284500	-0.69549800	-2.50444100
C	3.90193700	-0.02529600	0.21632500
H	5.87751400	-1.39734700	1.54816800
H	7.44306700	-2.99402600	0.55400600
C	3.01510500	0.58793400	-0.64057800
C	2.89934500	0.25313900	-2.00634600
H	0.87859100	-0.25959300	0.98052300
H	2.14558600	0.73522100	-2.62044500
N	2.24252400	1.53797100	0.02276700
N	1.66777800	2.59592300	-0.62533300
C	2.45484600	3.59028600	-1.14334400
O	3.62183400	3.74440700	-0.81282500
H	0.71153100	2.43557600	-0.93688400
H	0.54552300	-4.11626500	-6.42314200
H	2.48730000	-4.19060500	-4.90011000
C	1.78076200	4.47616700	-2.14422400
C	2.26458200	5.77932600	-2.28508000
C	0.75701700	4.01647100	-2.97634800
C	1.72015400	6.62508300	-3.24277500
H	3.07355100	6.10776500	-1.64084700
C	0.22949700	4.86088800	-3.95073100

H	0.37741400	3.00152900	-2.88547600
C	0.70500500	6.16286900	-4.08182900
H	2.09294700	7.63888600	-3.34602600
H	-0.55549100	4.49895600	-4.60675500
H	0.28892200	6.81857400	-4.84029100

COMIII

C	6.97357900	0.60426200	2.54913900
C	6.00492000	0.08553600	1.72699600
C	5.05022700	0.93308700	1.10056200
C	5.10067100	2.32675000	1.38242500
C	6.12280800	2.83554800	2.22747800
C	7.04490300	1.99616600	2.79540900
H	7.68905500	-0.06117300	3.02134400
C	4.01843800	0.43947000	0.23541600
C	4.11356800	3.18638500	0.83950400
H	6.14931500	3.90400100	2.42190000
H	7.81957500	2.39079100	3.44438200
C	3.08119600	2.70963200	0.06774100
C	3.05537300	1.31773600	-0.21503300
H	4.16368100	4.24913800	1.06307300
C	3.92330100	-0.99921400	-0.13162300
C	5.01094800	-1.68659900	-0.76267300
C	2.75951700	-1.69622200	0.13480200
C	4.91291600	-3.09060000	-0.96601300
C	6.18117100	-1.01952400	-1.21878200
C	2.65143900	-3.10529300	-0.04417500
C	5.99159300	-3.78892500	-1.57228600
C	3.73544200	-3.76950900	-0.56873700
C	7.20159800	-1.71818300	-1.81292900
H	6.25678500	0.05618600	-1.10279600
C	7.11468500	-3.12090500	-1.98416300
H	5.90073300	-4.86272100	-1.71020800
H	3.68278200	-4.84726100	-0.70129300
H	8.08326100	-1.18962300	-2.16091700
H	7.93267100	-3.65871600	-2.45185800
O	1.68859900	-1.03848500	0.69455800
H	5.95637400	-0.98436200	1.55902600
O	2.02265600	0.82446100	-0.98797300
P	0.82997300	0.07942100	-0.14552600
O	-0.00886700	-0.59535800	-1.20381700
O	0.23408300	0.99134800	0.86557900
C	2.05388400	3.65893100	-0.45229700
C	1.22098100	4.34301300	0.45682600
C	2.00751800	3.96452300	-1.82797400
C	1.17314000	4.01469000	1.85279300
C	0.38182400	5.41123400	-0.01326400
C	1.14217700	5.01432200	-2.29136200
C	2.82398400	3.29198800	-2.79502600
C	0.38700900	4.72078300	2.71499300

H	1.75868500	3.17501400	2.20849900
C	-0.42085200	6.13467800	0.92783600
C	0.37261800	5.73005700	-1.37192100
C	1.10689900	5.32555500	-3.68829600
H	3.49956100	2.51132400	-2.46235500
C	2.76065000	3.61687300	-4.11826600
C	-0.41249800	5.80869800	2.25073300
H	0.35766700	4.44957000	3.76547700
H	-1.03413500	6.95358900	0.56056700
H	-0.24410500	6.55493900	-1.72416200
C	1.88614400	4.64674500	-4.57630500
H	0.44363600	6.11898700	-4.02134500
H	3.38312500	3.09001900	-4.83409700
H	-1.02487800	6.36235900	2.95547400
H	1.85165600	4.88862000	-5.63351800
C	1.43322200	-3.87045200	0.34891300
C	1.01968100	-3.90112000	1.69976600
C	0.75266300	-4.63748700	-0.61941800
C	1.68843900	-3.16809800	2.73498000
C	-0.09880700	-4.71721100	2.07880300
C	-0.32959700	-5.49259900	-0.21457100
C	1.07389000	-4.59106500	-2.01683300
C	1.24213800	-3.19766800	4.02394500
H	2.56324500	-2.57884800	2.48459500
C	-0.54103400	-4.71621700	3.44009100
C	-0.73182600	-5.50946400	1.11874200
C	-0.98871900	-6.30433600	-1.19276600
H	1.84872200	-3.91300000	-2.35528400
C	0.40478600	-5.36069800	-2.92183500
C	0.10056300	-3.97224900	4.38430700
H	1.76188800	-2.62863400	4.78789600
H	-1.40390100	-5.32368700	3.69964700
H	-1.56095900	-6.14808900	1.41852600
C	-0.63404500	-6.24547300	-2.50550200
H	-1.78607800	-6.96382400	-0.85880800
H	0.65995400	-5.29848900	-3.97497500
H	-0.24446600	-3.97293700	5.41306700
H	-1.14267300	-6.85985000	-3.24146000
C	-2.78168100	-0.22992800	1.93780400
C	-4.18732800	-0.11772200	2.09816200
C	-4.98095000	-1.27461700	2.00080600
C	-4.36228100	-2.49031100	1.76652200
C	-2.96033700	-2.58108100	1.64154300
C	-2.14689500	-1.45943000	1.73165700

C	-3.27229200	1.94048000	2.19444000
C	-4.48317300	1.27189700	2.27543400
H	-6.06110200	-1.21253300	2.10475500
H	-4.95987900	-3.39172000	1.66876800
H	-2.50045300	-3.54905900	1.46474000
H	-1.06578900	-1.53786700	1.63497000
H	-1.29531600	1.25178600	1.74810000
N	-2.25950900	1.03716300	2.01217300
C	-2.96692900	3.39890400	2.27865900
H	-3.83628700	3.99832900	1.99298700
H	-2.67127000	3.68751600	3.29351400
H	-2.13939200	3.65646000	1.60960400
C	-5.83478600	1.86608400	2.51352100
H	-6.20502300	1.64374000	3.52037200
H	-5.81669100	2.95343300	2.40097200
H	-6.57393800	1.46809300	1.80783300
C	-4.50107900	5.91194600	-0.57133700
C	-3.35530800	5.23470700	-0.92613900
C	-3.34258800	3.82468100	-0.97315300
C	-4.53739700	3.11692600	-0.65842200
C	-5.70948300	3.83704500	-0.31167300
C	-5.68840000	5.21030500	-0.26263000
H	-1.26422300	3.65309600	-1.58020300
H	-4.49696200	6.99636700	-0.53181600
H	-2.44465800	5.77131700	-1.17178300
C	-2.16129300	3.09532200	-1.32709100
C	-4.51275800	1.70494200	-0.68385200
H	-6.61678500	3.28550900	-0.08385500
H	-6.58289500	5.76094700	0.00707900
C	-3.35154700	1.02228000	-1.03787900
C	-2.15183900	1.73679500	-1.36451100
H	-5.40313300	1.12783600	-0.45067500
H	-1.26063500	1.20297900	-1.66954600
N	-3.51385900	-0.33954500	-1.08937800
N	-2.51816900	-1.08380200	-1.29715200
C	-2.70378300	-2.51234400	-1.43273500
O	-1.69205200	-3.16576600	-1.45352600
H	-1.43769100	-0.79124100	-1.26293100
C	-4.06587200	-3.09550700	-1.56084200
C	-4.19518700	-4.40534300	-1.08394500
C	-5.15069200	-2.46523600	-2.17688900
C	-5.41110000	-5.06723600	-1.18543500
H	-3.33055500	-4.87987100	-0.62785200
C	-6.36170300	-3.14149300	-2.29198700

H	-5.05459300	-1.46496700	-2.57934500
C	-6.49735400	-4.43296100	-1.78867200
H	-5.51315700	-6.07577400	-0.79913600
H	-7.20122000	-2.65609600	-2.77790300
H	-7.44825600	-4.94914500	-1.87327200

TSIII-1

Value of imaginary frequency = -193.5 cm^{-1}

C	7.07707800	-0.37972300	2.61183500
C	6.03447700	-0.76646800	1.80784700
C	5.22415300	0.19897100	1.14928300
C	5.49784000	1.57656100	1.37935800
C	6.59398200	1.94563100	2.20432800
C	7.37230300	0.99094800	2.80465200
H	7.67881700	-1.13297900	3.11002800
C	4.12316000	-0.15640100	0.30162800
C	4.65530400	2.56257000	0.80740800
H	6.79353200	3.00248800	2.35759400
H	8.20552100	1.28022600	3.43636900
C	3.55441700	2.22750800	0.05666300
C	3.30834000	0.84783400	-0.18040900
H	4.87328700	3.61117400	0.99464700
C	3.79816400	-1.57157400	-0.02502400
C	4.75312400	-2.44456700	-0.63966500
C	2.52933100	-2.05215300	0.24159900
C	4.40823400	-3.81005400	-0.83887900
C	6.02704000	-1.99910800	-1.08886000
C	2.16119200	-3.41098100	0.03212600
C	5.35453000	-4.69416700	-1.42408800
C	3.11651400	-4.26138600	-0.47494300
C	6.91488800	-2.87267000	-1.66384200
H	6.28846200	-0.95182400	-0.98453500
C	6.58402700	-4.24002700	-1.82313000
H	5.07666000	-5.73591400	-1.55760800
H	2.86600800	-5.30779500	-0.63008600
H	7.87877900	-2.51114100	-2.00707300
H	7.29997000	-4.92006700	-2.27265800
O	1.59962500	-1.21090600	0.80382300
H	5.81392700	-1.82016100	1.67884000
O	2.21306800	0.50400500	-0.94406000
P	0.90646200	-0.02458100	-0.10094200
O	-0.04235100	-0.60272800	-1.09879900
O	0.48913900	1.02570300	0.88644100
C	2.66768300	3.29526700	-0.49041800
C	1.95603600	4.12993500	0.39641900
C	2.62087100	3.53007600	-1.87974700
C	1.92771400	3.90619600	1.81343800
C	1.22945100	5.25815300	-0.11957200
C	1.87432600	4.64851100	-2.38578300
C	3.32443300	2.71256000	-2.82379200

C	1.26722800	4.75885100	2.64891400
H	2.42606900	3.03045600	2.21220200
C	0.54245700	6.12456500	0.79144600
C	1.21632900	5.49756000	-1.49440700
C	1.83840700	4.88593300	-3.79720900
H	3.91043800	1.87472700	-2.46185000
C	3.26515600	2.97066200	-4.16177400
C	0.56820200	5.89161100	2.13410300
H	1.25533900	4.56674200	3.71708000
H	0.00819800	6.97950000	0.38487600
H	0.68929600	6.36776900	-1.88158900
C	2.50712600	4.07148700	-4.66073300
H	1.26391500	5.73377400	-4.16008000
H	3.80159200	2.33465900	-4.85834300
H	0.04917900	6.55727300	2.81647700
H	2.47247000	4.25740800	-5.72916400
C	0.79745600	-3.93328500	0.33745000
C	0.30256900	-3.92968800	1.65983500
C	0.04585800	-4.52891100	-0.69895000
C	1.02558800	-3.36002600	2.75908500
C	-0.96642000	-4.54142600	1.94276600
C	-1.18130000	-5.20873100	-0.38622700
C	0.45203500	-4.49586600	-2.07473900
C	0.50149500	-3.34587400	4.01886600
H	2.00476400	-2.93020600	2.58136100
C	-1.48321800	-4.50259600	3.27720500
C	-1.66468700	-5.18685500	0.92028200
C	-1.87895200	-5.91168500	-1.42036000
H	1.33522500	-3.93012900	-2.34774000
C	-0.25944300	-5.14913000	-3.03697000
C	-0.77886100	-3.91479300	4.28450900
H	1.06485200	-2.89979200	4.83209000
H	-2.45283600	-4.95659100	3.46446800
H	-2.59921400	-5.69512600	1.15260200
C	-1.43016800	-5.89273600	-2.70498800
H	-2.77804200	-6.46051100	-1.15081000
H	0.06608000	-5.10346200	-4.07137900
H	-1.18021100	-3.88575300	5.29224000
H	-1.96541700	-6.42671800	-3.48351100
C	-2.85804000	-0.05471700	1.79672600
C	-4.15452300	0.46960000	1.97003900
C	-5.25391800	-0.39866200	1.94021400
C	-5.01978400	-1.75355700	1.76119400
C	-3.71219800	-2.25233900	1.61421000

C	-2.60470800	-1.41433800	1.62667900
C	-2.62017500	2.15807100	1.98673000
C	-4.02508800	1.90463700	2.03295800
H	-6.26556800	-0.01804800	2.04960700
H	-5.85574700	-2.44456500	1.71371300
H	-3.56191800	-3.31780600	1.46872100
H	-1.59706400	-1.80064900	1.48811700
H	-0.94445300	0.95749900	1.55071300
N	-1.96249100	1.00832300	1.82010500
C	-1.89298200	3.44628500	2.12841100
H	-2.48442100	4.28306900	1.74960100
H	-1.68618100	3.63659600	3.18784600
H	-0.93693400	3.40257600	1.59840700
C	-5.05176000	2.84884700	2.57212100
H	-5.14523400	2.72659200	3.65598700
H	-4.78477500	3.88972000	2.37478100
H	-6.03656900	2.65635200	2.13420100
C	-3.61189400	6.51837600	-0.66145600
C	-2.58575200	5.64286800	-0.98038300
C	-2.76635700	4.25786200	-0.86256000
C	-4.01055300	3.76180500	-0.39709800
C	-5.05050800	4.66393800	-0.10485900
C	-4.85311200	6.02817600	-0.23260900
H	-0.76456100	3.73685400	-1.55804400
H	-3.45868300	7.58830500	-0.75788300
H	-1.63009300	6.01652700	-1.33542600
C	-1.71929000	3.32813500	-1.23797000
C	-4.17583600	2.33741600	-0.24252800
H	-6.01305600	4.27677500	0.21585500
H	-5.65970200	6.71690100	-0.00631300
C	-3.21306500	1.46000400	-0.84895600
C	-1.92252500	1.99429900	-1.24819300
H	-5.17671600	1.93732800	-0.10995200
H	-1.13795600	1.32462400	-1.58086800
N	-3.62742200	0.21419500	-0.99016700
N	-2.81569600	-0.69476600	-1.46779900
C	-3.23158400	-2.01554000	-1.68770800
O	-2.37603900	-2.82409500	-1.98550800
H	-1.78448500	-0.57279800	-1.49924600
C	-4.67260500	-2.39333000	-1.55908200
C	-4.89802300	-3.71949500	-1.17548900
C	-5.75802500	-1.55639700	-1.82952800
C	-6.19317800	-4.19540300	-1.01803800
H	-4.03676100	-4.35508400	-0.99201000

C	-7.05533100	-2.04317500	-1.68863000
H	-5.59748300	-0.53553500	-2.15116100
C	-7.27572200	-3.35354500	-1.27145600
H	-6.36039600	-5.22044500	-0.70333400
H	-7.89702100	-1.39392100	-1.90633800
H	-8.28969400	-3.72227300	-1.15311300

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C	-7.59431600	-0.66131200	-0.04814500
C	-6.27263100	-0.93517100	0.19801600
C	-5.30063300	0.10343200	0.19991900
C	-5.73049300	1.42800400	-0.09477200
C	-7.10746500	1.68156700	-0.33438100
C	-8.02299900	0.66252600	-0.30754200
H	-8.31875900	-1.46935100	-0.05064500
C	-3.90907700	-0.13943700	0.44436200
C	-4.77643100	2.47452600	-0.15760200
H	-7.41607500	2.70093000	-0.54862400
H	-9.07241800	0.86323100	-0.49586900
C	-3.43520100	2.23816800	0.01703500
C	-3.01889400	0.90747900	0.29077800
H	-5.11827000	3.48708300	-0.35705300
C	-3.39544900	-1.49671100	0.78277100
C	-3.83744700	-2.24168400	1.92435100
C	-2.42314400	-2.04933600	-0.02216200
C	-3.31743900	-3.55112400	2.13165400
C	-4.74594600	-1.71507000	2.88209800
C	-1.89924500	-3.35809700	0.15719200
C	-3.74757900	-4.30201100	3.25772600
C	-2.36842000	-4.08699600	1.22243900
C	-5.13534300	-2.46194700	3.96570300
H	-5.12425300	-0.70659800	2.75307800
C	-4.63944600	-3.77391200	4.15450800
H	-3.34504500	-5.30129600	3.39715100
H	-1.99547100	-5.09488200	1.38685800
H	-5.82606700	-2.04104700	4.68913100
H	-4.95796300	-4.35273900	5.01506800
O	-1.94202900	-1.30299600	-1.07632300
H	-5.95738100	-1.95602200	0.38332400
O	-1.67022400	0.68579200	0.46462500
P	-0.84178000	-0.15972200	-0.67712600
O	0.35535300	-0.72513700	0.00423600
O	-0.67752200	0.65579200	-1.93954800
C	-2.47161300	3.38183800	-0.01441800
C	-1.99553300	3.88428600	-1.23929900
C	-2.13427400	4.02052900	1.19530200
C	-2.28328400	3.24807700	-2.49139400
C	-1.19545300	5.07987100	-1.25352000
C	-1.34716100	5.22296900	1.16964400
C	-2.55475400	3.51640300	2.46939000
C	-1.81678500	3.76530000	-3.66422500

H	-2.86259500	2.33188000	-2.48594300
C	-0.72963500	5.59181900	-2.50760900
C	-0.89970500	5.72643800	-0.05351900
C	-1.02252100	5.86892600	2.40561500
H	-3.15003800	2.60979600	2.50272200
C	-2.20938900	4.15189900	3.62622100
C	-1.03198000	4.95811500	-3.67601700
H	-2.03755900	3.26500800	-4.60142100
H	-0.12887800	6.49712100	-2.50227000
H	-0.30800200	6.63937900	-0.07110200
C	-1.43351400	5.34878600	3.59683000
H	-0.43820100	6.78492400	2.37074700
H	-2.52884900	3.74823100	4.58135900
H	-0.67425400	5.35309500	-4.62156200
H	-1.17652800	5.84278200	4.52802800
C	-0.90979700	-3.92640600	-0.80366200
C	-1.29793400	-4.16283800	-2.14075900
C	0.38091200	-4.28583800	-0.36472500
C	-2.60907200	-3.85464900	-2.63144300
C	-0.36584300	-4.75862700	-3.05635900
C	1.28144200	-4.93995600	-1.27694100
C	0.85448900	-4.02402700	0.96414000
C	-2.95076500	-4.08808400	-3.93155600
H	-3.34221100	-3.43432600	-1.95150700
C	-0.75964300	-4.98050000	-4.41447000
C	0.89655200	-5.14252200	-2.60129200
C	2.56284000	-5.37750200	-0.80804100
H	0.23025600	-3.46101100	1.64969700
C	2.08532500	-4.45234900	1.36945300
C	-2.01066600	-4.65245200	-4.84377900
H	-3.94992000	-3.84522400	-4.27853200
H	-0.03577600	-5.42389800	-5.09268300
H	1.58805300	-5.62279400	-3.29058300
C	2.95134900	-5.15197500	0.47731200
H	3.21534300	-5.89311500	-1.50855700
H	2.41293000	-4.24200500	2.38134400
H	-2.30119700	-4.82650600	-5.87472200
H	3.92432200	-5.48266800	0.82716400
C	2.81487900	-0.29791600	-2.08669700
C	4.05450300	0.28878300	-1.84522600
C	5.18931000	-0.50346200	-1.78332100
C	5.04193100	-1.87790100	-1.99084900
C	3.78271100	-2.44705100	-2.20114900
C	2.63002500	-1.66157200	-2.23943500

C	2.38322500	1.90305700	-2.00571600
C	3.84773500	1.77200400	-1.64135200
H	6.16812300	-0.07403700	-1.59100700
H	5.91877400	-2.51713500	-1.97567400
H	3.69411900	-3.51932200	-2.33484300
H	1.64602600	-2.09659800	-2.38383300
H	0.76513000	0.62191200	-2.24782100
N	1.85120300	0.73626000	-2.18032900
C	1.61019300	3.14740900	-2.23829200
H	1.96142400	3.96952800	-1.61514600
H	1.75598100	3.43844700	-3.28627200
H	0.54358400	2.96683200	-2.07573900
C	4.74348800	2.64684200	-2.51992200
H	4.63200300	2.35881400	-3.56800900
H	4.49363400	3.70462200	-2.41452000
H	5.79113100	2.50916600	-2.23839000
C	3.83940900	6.29421400	0.83664900
C	2.72062400	5.48806000	1.01237200
C	2.78238700	4.11736300	0.74187200
C	3.97994800	3.55183800	0.26489200
C	5.10102700	4.36630900	0.11459400
C	5.03465800	5.72960000	0.39553700
H	0.67322800	3.74142600	1.20168100
H	3.78505600	7.35557900	1.05465700
H	1.78727400	5.90715600	1.37944400
C	1.61929400	3.26004100	0.97247300
C	4.02949800	2.07657200	-0.07215000
H	6.03792600	3.93013300	-0.22119200
H	5.91782600	6.34800200	0.27396800
C	3.01370600	1.28725800	0.73172700
C	1.70547000	1.91951900	0.95804900
H	5.02534300	1.68392400	0.15749300
H	0.82976900	1.31877900	1.17165600
N	3.39721500	0.14493300	1.18242800
N	2.47254500	-0.61101200	1.83505900
C	2.80793600	-1.62176300	2.69155600
O	1.94974400	-2.10424100	3.42248400
H	1.47959300	-0.50256400	1.62228400
C	4.21071600	-2.14077700	2.69883300
C	4.74821500	-2.56116300	3.91574600
C	4.91505600	-2.35090300	1.51148900
C	6.00669200	-3.15347000	3.95239000
H	4.16970200	-2.42239700	4.82359400
C	6.16291100	-2.96419500	1.54891400

H	4.47509500	-2.04845000	0.56765400
C	6.71420100	-3.35576400	2.76843700
H	6.43075600	-3.46738700	4.90062100
H	6.70437100	-3.13890200	0.62411800
H	7.69188000	-3.82677900	2.79616600

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Value of imaginary frequency = -74.3 cm^{-1}

C	7.41471100	0.39589700	2.56772900
C	6.42958600	-0.04033900	1.71741100
C	5.49649700	0.87189000	1.15253300
C	5.58510000	2.24412200	1.52474600
C	6.62344300	2.66584500	2.39672000
C	7.52389100	1.76579600	2.90453400
H	8.11456300	-0.31774300	2.99036000
C	4.44873900	0.46036300	0.26366900
C	4.62245000	3.16998300	1.04281400
H	6.68162400	3.71824000	2.66020500
H	8.31195300	2.09663600	3.57283700
C	3.58458700	2.77118100	0.23895100
C	3.52174900	1.40093300	-0.13371900
H	4.70369400	4.21368200	1.33644200
C	4.27327900	-0.95024400	-0.18316900
C	5.29405100	-1.67697000	-0.87828300
C	3.06049700	-1.57363400	0.04087800
C	5.06267700	-3.04079000	-1.21646500
C	6.52089600	-1.08064700	-1.27930900
C	2.81306000	-2.93512700	-0.28665900
C	6.07435300	-3.77310100	-1.89326600
C	3.82099200	-3.64544100	-0.89042900
C	7.47359200	-1.81062800	-1.94440000
H	6.69356100	-0.03214400	-1.06126600
C	7.25660300	-3.17624700	-2.24636600
H	5.88476700	-4.81551300	-2.13372100
H	3.66195000	-4.69088800	-1.14317700
H	8.40101400	-1.33543600	-2.24762500
H	8.02220300	-3.74142500	-2.76746500
O	2.05234400	-0.88090800	0.66638500
H	6.35047200	-1.09468300	1.47600000
O	2.47980600	1.00706800	-0.94374700
P	1.23101700	0.26570900	-0.18178800
O	0.37128200	-0.32154400	-1.24665000
O	0.67358700	1.17283900	0.88072500
C	2.55778000	3.73277700	-0.25934200
C	1.59673300	4.26916100	0.61930400
C	2.57359200	4.11395400	-1.61617700
C	1.50800800	3.88247100	1.99761900
C	0.64408400	5.22658900	0.12608200
C	1.60979300	5.06154500	-2.10004700
C	3.53174600	3.59486600	-2.54727600

C	0.56721400	4.42479700	2.82219500
H	2.19036200	3.12741300	2.37034500
C	-0.32202300	5.78038600	1.02814100
C	0.67165700	5.59906000	-1.21763300
C	1.63610200	5.44237400	-3.47991900
H	4.27359900	2.88483600	-2.19679400
C	3.52375100	3.98108400	-3.85528300
C	-0.35805200	5.39818400	2.33589500
H	0.51420800	4.11301900	3.86041100
H	-1.02615600	6.51170000	0.64055500
H	-0.05209700	6.32264600	-1.58595300
C	2.56081700	4.91902000	-4.33308500
H	0.89887200	6.15978900	-3.82970800
H	4.25638700	3.57348100	-4.54423300
H	-1.09222100	5.82400900	3.01269900
H	2.57193900	5.21239600	-5.37777300
C	1.49970700	-3.55995700	0.04888600
C	1.17510600	-3.80722300	1.39851500
C	0.59919700	-3.91202400	-0.97471400
C	2.05237700	-3.45943600	2.47762300
C	-0.07216500	-4.43858700	1.72410600
C	-0.65582900	-4.52690700	-0.63420900
C	0.86849400	-3.66010600	-2.36079500
C	1.71654800	-3.72064200	3.77436900
H	3.00036500	-2.98186800	2.25214300
C	-0.37421500	-4.72146000	3.09407600
C	-0.96275000	-4.77310000	0.70300800
C	-1.57292000	-4.87262900	-1.67902800
H	1.79273900	-3.16214800	-2.63143400
C	-0.02844100	-4.01064800	-3.32467700
C	0.48582000	-4.36871500	4.09188800
H	2.39502300	-3.44477200	4.57512000
H	-1.31022900	-5.22709800	3.31726800
H	-1.91466000	-5.23726800	0.95362900
C	-1.26867500	-4.62776700	-2.98243200
H	-2.52893500	-5.31091500	-1.40089100
H	0.18594100	-3.79436800	-4.36609400
H	0.24492400	-4.58536900	5.12785500
H	-1.97978600	-4.87042100	-3.76540300
C	-2.37750600	-0.34320600	2.38728700
C	-3.75545900	-0.13693200	2.29068400
C	-4.63536200	-1.02933500	2.87935100
C	-4.10623500	-2.13595000	3.54970700
C	-2.72652700	-2.33369500	3.62319100

C	-1.82879200	-1.43800700	3.03761500
C	-2.58491300	1.42968800	1.03836900
C	-4.00654300	1.15459900	1.53685500
H	-5.71028100	-0.87703700	2.82158600
H	-4.77570400	-2.85108000	4.01597000
H	-2.33522000	-3.19932600	4.14513200
H	-0.75575800	-1.60107100	3.08090800
H	-0.67818700	0.80383800	1.50802300
N	-1.72196800	0.69927300	1.70528800
C	-2.15376900	2.66745800	0.33160900
H	-2.89949200	2.97955400	-0.40080700
H	-2.02716600	3.46748000	1.07083400
H	-1.18368800	2.50730600	-0.14553400
C	-4.26546100	2.28602900	2.56342300
H	-3.36486800	2.42503300	3.16862700
H	-4.50738000	3.22931900	2.06854600
H	-5.06979100	2.01710800	3.24682900
C	-8.41508100	3.65173600	-0.28773900
C	-7.72048400	3.09952200	-1.35407100
C	-6.63417500	2.24284200	-1.13848300
C	-6.20229000	1.95829200	0.17373700
C	-6.96670000	2.45456100	1.23051400
C	-8.04774100	3.30459700	1.00903800
H	-6.44453700	1.79217700	-3.26285900
H	-9.25286600	4.31737300	-0.46490900
H	-8.02465300	3.31082500	-2.37525600
C	-6.01949900	1.58181700	-2.28482300
C	-5.06674400	0.96339800	0.38587300
H	-6.74291100	2.16513000	2.24810400
H	-8.60885500	3.68344900	1.85688500
C	-4.32224600	0.60700000	-0.88885500
C	-4.97602600	0.74208100	-2.18073300
H	-5.58634600	0.02182800	0.63494400
H	-4.52759900	0.29625900	-3.05956900
N	-3.10888000	0.23852900	-0.69321300
N	-2.36016300	-0.23859500	-1.74549300
C	-2.67905800	-1.40538000	-2.42783700
O	-2.08202900	-1.68521400	-3.45185400
H	-1.34556300	-0.07572800	-1.64378600
C	-3.72991000	-2.31817700	-1.86534500
C	-4.52131600	-3.03294000	-2.76424900
C	-3.81140100	-2.58625500	-0.49536600
C	-5.41227400	-3.99479900	-2.29836900
H	-4.41732600	-2.83572600	-3.82685200

C	-4.69213300	-3.56018700	-0.03286600
H	-3.16815900	-2.05921500	0.20496300
C	-5.49725400	-4.25900600	-0.93172100
H	-6.03351700	-4.54375400	-2.99846800
H	-4.74232000	-3.77241400	1.03084600
H	-6.18784900	-5.01307600	-0.56745800

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C	7.39308600	-0.26200600	2.60899700
C	6.37205400	-0.56497700	1.74318700
C	5.57627500	0.46103200	1.16380200
C	5.83746800	1.80915600	1.54234300
C	6.91088500	2.09155300	2.42851800
C	7.67883100	1.08178000	2.94727400
H	7.98386400	-1.06176100	3.04397500
C	4.49959800	0.19096800	0.25351600
C	5.00336500	2.85149300	1.05962100
H	7.10277900	3.12737500	2.69453000
H	8.49434000	1.30649600	3.62671300
C	3.92911200	2.59065800	0.24720900
C	3.70170800	1.24218100	-0.14546700
H	5.20895400	3.87422900	1.36614500
C	4.16672000	-1.18755000	-0.20334500
C	5.12630400	-2.03105500	-0.85350800
C	2.88742200	-1.67517900	-0.00699900
C	4.77568400	-3.37828600	-1.15160000
C	6.41259200	-1.56793200	-1.24369700
C	2.52914500	-3.02724500	-0.27495700
C	5.72590000	-4.22540400	-1.78148700
C	3.48052000	-3.85210700	-0.82283300
C	7.30498600	-2.40597500	-1.86362700
H	6.67903100	-0.53326900	-1.05587200
C	6.96569300	-3.75476700	-2.12732800
H	5.44410900	-5.25335500	-1.99214700
H	3.23379300	-4.89129200	-1.02643400
H	8.27855300	-2.03026000	-2.16148200
H	7.68395500	-4.40753000	-2.61228200
O	1.93000800	-0.87708100	0.56205200
H	6.15806700	-1.60035300	1.50268600
O	2.63663600	0.98795100	-0.97915000
P	1.28473100	0.40668500	-0.24915400
O	0.38755000	-0.02398600	-1.36901300
O	0.80051300	1.31962500	0.82882000
C	3.00655500	3.66421900	-0.22463600
C	2.08742400	4.24942300	0.66730200
C	3.05165700	4.07312800	-1.57184500
C	1.98791500	3.85641400	2.04275300
C	1.18375500	5.25995300	0.18850600
C	2.15093700	5.08983600	-2.03671000
C	3.97799200	3.51349200	-2.51117900
C	1.07213800	4.42868500	2.87439700

H	2.64311500	3.07436500	2.40825500
C	0.23442000	5.83498200	1.09480200
C	1.23718500	5.65687500	-1.14737300
C	2.20907000	5.49972500	-3.40714900
H	4.67039100	2.74960700	-2.17227500
C	4.00289000	3.93059700	-3.80966300
C	0.17892200	5.43524700	2.39626900
H	1.00991700	4.11120900	3.91029300
H	-0.44090300	6.59705300	0.71538000
H	0.55112000	6.42169200	-1.50457200
C	3.10402400	4.93920700	-4.26849500
H	1.52032600	6.27000400	-3.74325300
H	4.71281900	3.49462300	-4.50507300
H	-0.54376000	5.87589900	3.07584500
H	3.13991600	5.25628300	-5.30570300
C	1.16947100	-3.53928100	0.06588700
C	0.77831200	-3.64482700	1.41774400
C	0.30084800	-3.96374000	-0.96054400
C	1.62379600	-3.23892600	2.50259600
C	-0.50361300	-4.20373700	1.74543000
C	-0.98337000	-4.51115900	-0.61785700
C	0.63360300	-3.86206800	-2.35273900
C	1.22446800	-3.37551500	3.80076400
H	2.60045000	-2.82062200	2.28256900
C	-0.88395100	-4.33594600	3.11967800
C	-1.35285900	-4.62150900	0.72137400
C	-1.87056500	-4.92867200	-1.66026300
H	1.58482400	-3.42506800	-2.63445700
C	-0.23512700	-4.28266800	-3.31531600
C	-0.04883200	-3.93539000	4.11982500
H	1.88298000	-3.06006500	4.60357200
H	-1.85972100	-4.76061200	3.34196200
H	-2.32599600	-5.03950500	0.97000000
C	-1.50851600	-4.82349800	-2.96844000
H	-2.85153600	-5.30408300	-1.37681800
H	0.03178100	-4.18281700	-4.36247000
H	-0.34450300	-4.03891300	5.15914600
H	-2.19299400	-5.12807700	-3.75386500
C	-2.52591000	-0.13263300	2.20979700
C	-3.80784600	0.41858700	2.26883200
C	-4.71224000	-0.01692100	3.22634900
C	-4.31812700	-1.00995000	4.12797200
C	-3.03162800	-1.54858300	4.06071500
C	-2.11763400	-1.12336200	3.09647000

C	-2.61129200	1.27052800	0.38395700
C	-3.96934200	1.46716200	1.18041700
H	-5.71496100	0.40193200	3.27861200
H	-5.01481700	-1.36323300	4.88034000
H	-2.73338700	-2.32422600	4.76015100
H	-1.12466800	-1.55748300	3.02541000
H	-0.80966900	0.64860700	1.24031700
N	-1.79683800	0.38326300	1.13631800
C	-1.87000900	2.51761200	-0.08587100
H	-2.54806900	3.18592200	-0.62138900
H	-1.42719400	3.03701900	0.76587000
H	-1.04580200	2.23351700	-0.74374700
C	-4.07469700	2.87488700	1.77157200
H	-3.12916500	3.13498600	2.25392400
H	-4.30155500	3.62528300	1.00920000
H	-4.84448900	2.91833800	2.54232900
C	-8.86650400	3.09610200	-0.45707600
C	-8.18625700	2.51554100	-1.51775200
C	-6.95162800	1.88625000	-1.31290000
C	-6.38093300	1.85393600	-0.02223400
C	-7.09856300	2.39722100	1.03985000
C	-8.32347900	3.02569200	0.82386900
H	-6.79057900	1.28571700	-3.39833600
H	-9.82052000	3.58432800	-0.62181400
H	-8.60798200	2.53699800	-2.51831900
C	-6.28227600	1.24924600	-2.43831400
C	-5.10470800	1.06860100	0.16877800
H	-6.71522300	2.32489300	2.05046200
H	-8.85724900	3.45496600	1.66514100
C	-4.38541400	0.76965300	-1.10728400
C	-5.06548200	0.66402600	-2.36405000
H	-5.44659200	0.05975200	0.46822300
H	-4.56647500	0.26564900	-3.23865000
N	-3.11708000	0.59859100	-0.89122000
N	-2.26392700	0.03099900	-1.79482100
C	-2.55333000	-1.24511700	-2.32203300
O	-1.95519500	-1.61577000	-3.30607500
H	-1.23968600	0.21218000	-1.64517800
C	-3.58868100	-2.07911800	-1.63332400
C	-4.52588700	-2.78016400	-2.39156200
C	-3.54473200	-2.23043600	-0.24671200
C	-5.44683800	-3.60500900	-1.75312100
H	-4.52588600	-2.67351000	-3.47236400
C	-4.46167200	-3.06163200	0.38911900

H	-2.76522600	-1.73031000	0.32132300
C	-5.41835700	-3.74179200	-0.36434100
H	-6.18604200	-4.14415300	-2.33618100
H	-4.41702100	-3.17865300	1.46853000
H	-6.14012400	-4.38504600	0.12889200

IMIII-3

C	-7.75742900	-0.29490900	1.71105200
C	-6.44325800	-0.64448000	1.52509200
C	-5.47793400	0.32519900	1.13878400
C	-5.91592800	1.66065200	0.91373100
C	-7.27952100	1.99459800	1.12887400
C	-8.18235200	1.04180800	1.52336500
H	-8.47982400	-1.05187000	1.99934000
C	-4.09715600	0.00107800	0.92791600
C	-4.99029900	2.63681400	0.46273800
H	-7.59301900	3.02158200	0.96283800
H	-9.22332400	1.30417300	1.68070000
C	-3.68409700	2.31499900	0.19080000
C	-3.26356500	0.97420600	0.40986200
H	-5.33427800	3.65702400	0.31059700
C	-3.51973600	-1.33902800	1.22149900
C	-3.60076600	-1.93759400	2.52189400
C	-2.80018000	-1.98720400	0.23473000
C	-3.02804300	-3.22557600	2.72540800
C	-4.20316700	-1.28896200	3.63556500
C	-2.15332100	-3.23802500	0.44902300
C	-3.13249000	-3.84688000	3.99897800
C	-2.31493800	-3.84735200	1.67001100
C	-4.27599800	-1.90792300	4.85796300
H	-4.60235100	-0.28847600	3.51365500
C	-3.74929800	-3.20873100	5.04291500
H	-2.70080000	-4.83544500	4.12888400
H	-1.84864500	-4.81306100	1.84988000
H	-4.73876900	-1.39326800	5.69386700
H	-3.82347600	-3.68849600	6.01325800
O	-2.74536800	-1.44039400	-1.02097400
H	-6.12986200	-1.67403000	1.66159600
O	-1.96096500	0.65451800	0.11045300
P	-1.74952500	-0.16071700	-1.31961500
O	-0.31433600	-0.59996000	-1.27355000
O	-2.31818900	0.58344900	-2.46691600
C	-2.71296900	3.33751800	-0.29211700
C	-2.84731900	3.88820900	-1.58139900
C	-1.67814000	3.76796400	0.56238400
C	-3.85649700	3.45523500	-2.50383400
C	-1.93442200	4.91114100	-2.01294100
C	-0.75252400	4.76577600	0.10800000
C	-1.51795600	3.25960400	1.89363900
C	-3.97430600	4.02722400	-3.73560000

H	-4.51249600	2.64281100	-2.21417400
C	-2.09600900	5.48854900	-3.31384300
C	-0.90590600	5.31897700	-1.16374600
C	0.31114500	5.18079200	0.97213500
H	-2.22462100	2.52548400	2.26684800
C	-0.50480500	3.69682600	2.69642300
C	-3.08934400	5.06882700	-4.14634700
H	-4.74077800	3.68006700	-4.42085500
H	-1.40449200	6.26921300	-3.61897200
H	-0.20421200	6.07940100	-1.50078500
C	0.43578400	4.66332800	2.22589300
H	1.02158700	5.91250800	0.59670000
H	-0.40879700	3.30649800	3.70553900
H	-3.20511300	5.51287100	-5.12981300
H	1.24589600	4.98287100	2.87433400
C	-1.27624900	-3.83044400	-0.60026700
C	-1.81678300	-4.25578000	-1.82994100
C	0.10528700	-3.97442500	-0.34328600
C	-3.21848200	-4.18246400	-2.11992100
C	-0.95242400	-4.80973200	-2.83391000
C	0.95242700	-4.55810000	-1.34666900
C	0.72442700	-3.55779400	0.88459500
C	-3.71359000	-4.60234800	-3.31897900
H	-3.89026000	-3.78751500	-1.36554600
C	-1.51001800	-5.23270900	-4.08315400
C	0.40953200	-4.94593800	-2.57002100
C	2.34130200	-4.76089900	-1.06492300
H	0.11774200	-3.07621300	1.64296400
C	2.05337500	-3.76729300	1.11651300
C	-2.84705200	-5.13072000	-4.32239000
H	-4.77848800	-4.53597900	-3.51691500
H	-0.83746400	-5.63951000	-4.83310800
H	1.06127700	-5.37111800	-3.32962000
C	2.87295400	-4.40443200	0.13761300
H	2.95504100	-5.22715100	-1.83094400
H	2.49523700	-3.45000800	2.05726700
H	-3.26132900	-5.45451800	-5.27168300
H	3.91774400	-4.60195100	0.35745200
C	2.15722700	2.61657000	-0.46349200
C	3.21921300	2.66816800	0.44637900
C	4.14467500	3.69644800	0.38727900
C	4.00803700	4.67479200	-0.60439800
C	2.95406400	4.60206800	-1.51600400
C	2.01485400	3.57081000	-1.46509400

C	2.00150000	0.63835400	0.70825100
C	3.13713100	1.48362600	1.39977800
H	4.97151800	3.74016700	1.09342900
H	4.72619200	5.48475400	-0.66846200
H	2.86071400	5.35996900	-2.28782600
H	1.19533600	3.51600200	-2.17382000
H	0.63589200	1.13986000	-0.80447800
N	1.35694300	1.51575100	-0.19443300
C	1.02941800	-0.12070400	1.59681000
H	1.56300700	-0.79061900	2.27670200
H	0.43979100	0.59924500	2.16700000
H	0.33808200	-0.69607300	0.97572900
C	2.71694900	1.93564600	2.79903900
H	1.69469200	2.31582200	2.75088900
H	2.76280300	1.12236100	3.52818600
H	3.34138600	2.76080600	3.14438000
C	7.18481100	-0.41436600	4.49090300
C	6.91698600	-1.31132200	3.46710500
C	6.00245700	-0.98693100	2.45682300
C	5.32976100	0.25487800	2.48208600
C	5.65509400	1.16693400	3.48197400
C	6.56041500	0.83039400	4.48666700
H	6.37692700	-2.83776700	1.37431400
H	7.88823400	-0.67290800	5.27452900
H	7.42032800	-2.27314400	3.43297900
C	5.78480000	-1.92617100	1.36637400
C	4.43535100	0.59662100	1.31018800
H	5.21349400	2.15465500	3.48681900
H	6.78096300	1.55250000	5.26567000
C	4.02315200	-0.60173400	0.51511300
C	4.87205700	-1.74809900	0.38408100
H	5.11276700	1.10892900	0.60037200
H	4.68275200	-2.49753300	-0.37236000
N	2.85053900	-0.42901500	-0.01356100
N	2.31865400	-1.20942400	-1.00135800
C	2.92679500	-1.39516800	-2.24427800
O	2.39998200	-2.14065600	-3.04250100
H	1.28849400	-1.28785000	-0.98843700
C	4.22372700	-0.70095800	-2.52925600
C	5.25762400	-1.45018700	-3.09258300
C	4.38633100	0.66916600	-2.31572300
C	6.46896500	-0.83694700	-3.39718200
H	5.10436800	-2.50849500	-3.28159200
C	5.59416200	1.28240700	-2.63389900

H	3.56525100	1.26330200	-1.92772500
C	6.63955400	0.52660000	-3.16234200
H	7.27810800	-1.42087800	-3.82285900
H	5.71035500	2.34928900	-2.47033600
H	7.58493400	1.00279900	-3.40107900

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C	-5.51127100	3.97729400	2.09064000
C	-4.38048200	3.64066900	1.38996500
C	-4.21807100	2.33373400	0.85084100
C	-5.24195000	1.37648800	1.09196600
C	-6.40721500	1.75832200	1.80917200
C	-6.54501900	3.03221200	2.29462200
H	-5.61225100	4.97755100	2.49936700
C	-3.05233300	1.93236500	0.11829300
C	-5.07703000	0.04944000	0.62394600
H	-7.18193800	1.01421200	1.97144600
H	-7.43517800	3.31611200	2.84610100
C	-3.93493800	-0.35740100	-0.02169100
C	-2.91206700	0.60646500	-0.24595600
H	-5.87624800	-0.66887800	0.78905400
C	-1.95851600	2.89540800	-0.18266300
C	-2.17984800	4.10462900	-0.91713100
C	-0.68467800	2.61865800	0.27221900
C	-1.11262900	5.03704700	-1.04981100
C	-3.42022100	4.40409500	-1.54377600
C	0.38195000	3.55578500	0.18082200
C	-1.32563600	6.24629600	-1.76377800
C	0.14620900	4.74474600	-0.46565800
C	-3.59257000	5.57544900	-2.23747700
H	-4.23120800	3.68667300	-1.47615500
C	-2.53857800	6.51479200	-2.34267500
H	-0.50285700	6.95101800	-1.84633700
H	0.94421800	5.47938800	-0.54196800
H	-4.54481100	5.78246200	-2.71512600
H	-2.69250600	7.43969600	-2.88857300
O	-0.44746100	1.43688100	0.92271100
H	-3.59316400	4.37340600	1.25355100
O	-1.75686200	0.21354300	-0.88560400
P	-0.42067300	0.02043600	0.06647900
O	0.74613300	0.00393100	-0.87483600
O	-0.65520800	-1.03312000	1.09278200
C	-3.86414400	-1.76284900	-0.52967000
C	-3.49305100	-2.81983300	0.32312900
C	-4.31278500	-2.02858600	-1.83885200
C	-3.01555500	-2.59761900	1.65590200
C	-3.58927700	-4.17639700	-0.14523100
C	-4.42331900	-3.38869000	-2.29027800
C	-4.68442600	-0.98442600	-2.74846600
C	-2.62879600	-3.64032200	2.44604900

H	-2.92274800	-1.57811900	2.00839500
C	-3.18040300	-5.24275600	0.71879200
C	-4.06869600	-4.42982200	-1.43065000
C	-4.88971800	-3.64614200	-3.61893700
H	-4.60933300	0.04717700	-2.42006600
C	-5.12177900	-1.27151800	-4.00835400
C	-2.70926300	-4.98455000	1.97180200
H	-2.24541600	-3.44948600	3.44361600
H	-3.25091700	-6.26101800	0.34659600
H	-4.14962300	-5.45767900	-1.77710900
C	-5.22760800	-2.62301800	-4.45357800
H	-4.96544700	-4.67976100	-3.94520800
H	-5.39272300	-0.46598700	-4.68316500
H	-2.39522000	-5.79948200	2.61666000
H	-5.57864700	-2.82872000	-5.45957900
C	1.70591000	3.28049800	0.81091900
C	1.81820500	3.24209200	2.21804200
C	2.84956500	3.12084000	0.00409100
C	0.68546500	3.37539700	3.08590300
C	3.10945200	3.06516300	2.82308200
C	4.13820400	2.95386100	0.62212300
C	2.78446700	3.09448500	-1.42944500
C	0.82470500	3.31779400	4.44297800
H	-0.29749600	3.52201600	2.65108700
C	3.21513100	3.01804500	4.25001300
C	4.23889200	2.93377300	2.01227700
C	5.29877600	2.80977000	-0.20585900
H	1.81507100	3.16703500	-1.91006100
C	3.91376500	2.96235600	-2.18108000
C	2.10832900	3.13579200	5.03869400
H	-0.04893900	3.41280300	5.07947400
H	4.19999400	2.88178800	4.68798600
H	5.21501900	2.80622700	2.47443600
C	5.19369100	2.82593200	-1.56330900
H	6.26359600	2.68950400	0.27869600
H	3.84265100	2.92565200	-3.26438700
H	2.19726700	3.09490100	6.11941000
H	6.07642300	2.71907300	-2.18601800
C	1.99628200	-3.50780500	-1.78121800
C	1.22038600	-3.58935300	-0.61941600
C	-0.16064300	-3.54309400	-0.69762100
C	-0.75356100	-3.39426300	-1.95714500
C	0.03121600	-3.31388100	-3.10514000
C	1.42540800	-3.37360700	-3.03820300

C	3.45913900	-3.16939000	-0.07462300
C	2.14571700	-3.67595600	0.59685600
H	-0.77391300	-3.56858000	0.20081500
H	-1.83086900	-3.31606300	-2.03637900
H	-0.44734200	-3.18592000	-4.07115000
H	2.04033200	-3.29060200	-3.92865400
H	4.07130000	-3.24179400	-2.07840200
N	3.35521500	-3.55380700	-1.43535600
C	4.76186800	-3.54035700	0.60165700
H	4.72296600	-3.27464100	1.66197400
H	4.91731000	-4.61701800	0.51143800
H	5.58856200	-3.00918400	0.13091400
C	2.26629300	-5.11488700	1.08887300
H	2.66623900	-5.73377700	0.28020600
H	2.92746900	-5.20043700	1.95549000
H	1.28000900	-5.50750200	1.34839000
C	0.89983700	-2.49112900	5.85044000
C	1.21669000	-1.33790400	5.14964700
C	1.55184300	-1.39883600	3.79002000
C	1.57453400	-2.64894700	3.12056400
C	1.22054400	-3.79491600	3.83080700
C	0.90179000	-3.71650000	5.18500600
H	1.79409900	0.75968500	3.65433500
H	0.64350700	-2.43986400	6.90285800
H	1.20624800	-0.36991700	5.64339800
C	1.88959100	-0.16815400	3.09375400
C	1.77709300	-2.57161800	1.63486700
H	1.18478000	-4.75735900	3.33849700
H	0.64566800	-4.62383700	5.72242200
C	2.53494800	-1.38079700	1.18465800
C	2.37406500	-0.12230500	1.82789000
H	0.76657000	-2.18641000	1.33132800
H	2.71014600	0.79136000	1.35418900
N	3.23306900	-1.64074700	0.10955400
N	3.36086000	-0.69933800	-0.88286800
C	4.38937200	-0.76924000	-1.78110600
O	5.42526900	-1.37981300	-1.54795500
H	2.44675100	-0.25178800	-1.07674900
C	4.12907200	-0.08286300	-3.08068600
C	2.83558200	0.12983200	-3.56795000
C	5.23900300	0.30975300	-3.83246200
C	2.66300900	0.75749700	-4.79910700
H	1.96170200	-0.19420600	-3.00754800
C	5.05993600	0.94666800	-5.05429800

H	6.23176900	0.11825300	-3.43805000
C	3.76992000	1.17209600	-5.53723700
H	1.66133600	0.91986400	-5.18243800
H	5.92167400	1.26272000	-5.63272900
H	3.62858000	1.66396700	-6.49429400

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Value of imaginary frequency = -669.2 cm^{-1}

C	-4.96323100	4.75281500	1.77016400
C	-3.85958200	4.21129100	1.16095400
C	-3.88045800	2.87748700	0.66546200
C	-5.06300300	2.11151400	0.85362700
C	-6.19511800	2.70360800	1.47453400
C	-6.15159700	3.99871200	1.91958400
H	-4.92244900	5.76925400	2.14812100
C	-2.75078900	2.26857700	0.02408700
C	-5.08585400	0.75971800	0.43161500
H	-7.09196500	2.10263100	1.59691500
H	-7.01768100	4.44457600	2.39723900
C	-3.98203000	0.14796300	-0.11057300
C	-2.79942400	0.92131100	-0.28296400
H	-6.00127900	0.18643700	0.55544700
C	-1.51873600	3.05593800	-0.24776200
C	-1.53522100	4.26082800	-1.02308400
C	-0.31997300	2.62517600	0.27951800
C	-0.34513800	5.03519800	-1.11524700
C	-2.68712600	4.70291600	-1.72896400
C	0.87167100	3.39706800	0.22141700
C	-0.35227000	6.24016300	-1.86768300
C	0.83018300	4.59081200	-0.45837300
C	-2.65970500	5.86420500	-2.45918400
H	-3.59008500	4.10276200	-1.69485600
C	-1.48400100	6.65034500	-2.52269600
H	0.56194700	6.82478600	-1.91842900
H	1.72488600	5.20652300	-0.50749300
H	-3.54605200	6.18117900	-2.99915100
H	-1.48047400	7.56899700	-3.09976200
O	-0.28475400	1.42425200	0.95119500
H	-2.95324100	4.79884200	1.06761000
O	-1.69734200	0.31450500	-0.84932200
P	-0.34210200	0.05653500	0.04199900
O	0.80158500	-0.01722700	-0.91475500
O	-0.58748900	-1.03357300	1.05297700
C	-4.09510800	-1.28066000	-0.53638800
C	-3.78556400	-2.31501200	0.36559200
C	-4.63496000	-1.57716100	-1.80319100
C	-3.24543900	-2.05592100	1.66630000
C	-4.01853000	-3.68230600	-0.01338700
C	-4.88819400	-2.94570700	-2.16294200
C	-4.95251700	-0.55789800	-2.76015600

C	-2.92745500	-3.07760100	2.51156400
H	-3.05915200	-1.02919500	1.95840200
C	-3.66857400	-4.72695200	0.90187500
C	-4.57544000	-3.96449800	-1.26106200
C	-5.44733100	-3.23548000	-3.44842200
H	-4.76034700	0.47888000	-2.50375300
C	-5.48120700	-0.87634600	-3.97683700
C	-3.13357100	-4.43555600	2.12234500
H	-2.49795400	-2.86059200	3.48449400
H	-3.83810300	-5.75591000	0.59691000
H	-4.76106400	-4.99912900	-1.54066500
C	-5.73702800	-2.23555600	-4.32821500
H	-5.63414400	-4.27474500	-3.70438300
H	-5.70904500	-0.09052500	-4.68981600
H	-2.86626900	-5.23411600	2.80824200
H	-6.16043700	-2.46551800	-5.30054300
C	2.12120300	2.96583800	0.91169700
C	2.16996300	2.92868100	2.32225600
C	3.27652600	2.68803900	0.15392500
C	1.02456500	3.19059200	3.14293900
C	3.41235100	2.63325900	2.98131500
C	4.51660500	2.40507400	0.82609100
C	3.27047700	2.66307600	-1.28105100
C	1.10377500	3.13525300	4.50496600
H	0.08035900	3.43713300	2.66972600
C	3.45605400	2.59200600	4.41169700
C	4.55715000	2.38891700	2.21955600
C	5.69149900	2.14348300	0.04871400
H	2.33324400	2.81992800	-1.80316200
C	4.41368600	2.42426500	-1.98342200
C	2.33656300	2.82905800	5.15402500
H	0.22092000	3.33257900	5.10424200
H	4.40461900	2.36429900	4.88998500
H	5.49682600	2.17520500	2.72361300
C	5.64631800	2.16474400	-1.31203800
H	6.61792500	1.93075200	0.57464600
H	4.38602400	2.39327100	-3.06885300
H	2.37792200	2.79234000	6.23768100
H	6.53968900	1.96637700	-1.89597200
C	1.51204400	-3.57826300	-1.83867600
C	0.71054200	-3.59193600	-0.69168200
C	-0.65544100	-3.39859800	-0.78972800
C	-1.21019500	-3.15493200	-2.05118600
C	-0.39915100	-3.12965600	-3.18441000

C	0.97813400	-3.34864500	-3.09948500
C	2.98642700	-3.54924100	-0.09585700
C	1.58661000	-3.84462500	0.53404000
H	-1.27743100	-3.39468400	0.10230400
H	-2.27358800	-2.96816400	-2.14295900
H	-0.84374900	-2.93032600	-4.15466300
H	1.61092200	-3.32240600	-3.98086100
H	3.60734300	-3.61410300	-2.10256800
N	2.84072400	-3.83898500	-1.48162700
C	4.18147000	-4.21102800	0.56052500
H	4.18220800	-3.99930100	1.63371100
H	4.13127600	-5.29100900	0.41129000
H	5.09978300	-3.81945600	0.12312700
C	1.45574700	-5.29501300	0.99372900
H	1.80227000	-5.95320300	0.19126100
H	2.04175700	-5.49812400	1.89444800
H	0.40756700	-5.53809800	1.18331000
C	-0.02928700	-2.54350000	5.63565000
C	0.62126500	-1.47302300	5.05252800
C	1.13513900	-1.57003900	3.74701600
C	0.98470100	-2.77766900	3.01171000
C	0.29416400	-3.84058300	3.60998800
C	-0.18667000	-3.72850600	4.90682700
H	1.87103100	0.47047100	3.76702200
H	-0.41993900	-2.46575000	6.64419200
H	0.74535400	-0.53787400	5.59202500
C	1.82280000	-0.43878700	3.17131900
C	1.42119400	-2.72602200	1.60267900
H	0.12788000	-4.76006700	3.06572100
H	-0.70236200	-4.57223300	5.35520500
C	2.38577300	-1.70331800	1.25664300
C	2.44919800	-0.47408800	1.96388900
H	0.48016700	-1.99564300	1.23881100
H	3.03608300	0.35194100	1.58118900
N	3.07659500	-2.03475300	0.17298700
N	3.33649300	-1.10131000	-0.80570200
C	4.37967400	-1.29428400	-1.66285200
O	5.31141700	-2.04985000	-1.40951400
H	2.50317100	-0.54367500	-1.04137600
C	4.27388000	-0.56094100	-2.96046700
C	3.04470300	-0.18083000	-3.50763000
C	5.46060200	-0.30512300	-3.65046300
C	3.01523900	0.47973300	-4.73337100
H	2.11071000	-0.39976300	-2.99583400

C	5.42642000	0.36498700	-4.86733800
H	6.39905700	-0.62973100	-3.21250200
C	4.20193100	0.76004700	-5.40816700
H	2.06290900	0.77449000	-5.16130000
H	6.34948400	0.57716600	-5.39656500
H	4.17299800	1.28060800	-6.36010600

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C	-5.95186900	3.62096700	1.69729100
C	-4.74084000	3.35417900	1.11076500
C	-4.45975300	2.06720400	0.57450000
C	-5.45138200	1.05502000	0.69861600
C	-6.70119500	1.36544500	1.29804400
C	-6.95137100	2.62222500	1.78223600
H	-6.14302900	4.60701200	2.10787600
C	-3.20750400	1.74094600	-0.04561300
C	-5.16855100	-0.25714500	0.24601800
H	-7.44835800	0.58080800	1.37449700
H	-7.90589700	2.85150000	2.24398400
C	-3.94404400	-0.59744500	-0.27481100
C	-2.96843500	0.42735700	-0.39265400
H	-5.93556100	-1.02180400	0.33707100
C	-2.16105200	2.77765000	-0.25483200
C	-2.41020100	3.98041600	-0.99331000
C	-0.90655500	2.59169400	0.28160500
C	-1.39767200	4.97946100	-1.03924900
C	-3.61802300	4.20502100	-1.70746700
C	0.11212000	3.57831400	0.26891600
C	-1.63720000	6.18336500	-1.75421300
C	-0.16296300	4.75966200	-0.37740700
C	-3.81470200	5.37275400	-2.40033400
H	-4.38361000	3.43663100	-1.70948600
C	-2.82027200	6.37988900	-2.41713100
H	-0.85797100	6.93998500	-1.77064300
H	0.59118700	5.54239300	-0.39835700
H	-4.74068300	5.52488600	-2.94506700
H	-2.99506500	7.30050800	-2.96372500
O	-0.62859900	1.38827300	0.92276500
H	-3.98217500	4.12714800	1.06614600
O	-1.73495300	0.08367400	-0.94197400
P	-0.41193100	0.10471800	-0.02411000
O	0.80350100	0.08883200	-0.85723900
O	-0.59561200	-1.03798500	1.04093200
C	-3.69820900	-2.00671800	-0.70653100
C	-3.31062000	-2.96866600	0.24369300
C	-3.96139100	-2.38167100	-2.03807200
C	-3.03642100	-2.62816400	1.60849300
C	-3.18702700	-4.34563700	-0.14967400
C	-3.85467000	-3.76382000	-2.41685400
C	-4.34320300	-1.43194400	-3.04097700
C	-2.63415400	-3.57603800	2.50121200

H	-3.13230400	-1.59388300	1.91998300
C	-2.75828800	-5.31066700	0.81861100
C	-3.47723600	-4.71265300	-1.46432800
C	-4.12415700	-4.13565200	-3.77255800
H	-4.43144600	-0.38570900	-2.76592300
C	-4.58966000	-1.82733500	-4.32321100
C	-2.48259300	-4.93827500	2.10083900
H	-2.41277300	-3.29360100	3.52491200
H	-2.65518500	-6.34470800	0.50183400
H	-3.38940100	-5.75598500	-1.75851800
C	-4.47889500	-3.19965100	-4.69780000
H	-4.03656600	-5.18371400	-4.04495200
H	-4.87320800	-1.09345500	-5.07076300
H	-2.14949200	-5.67361200	2.82691800
H	-4.67962800	-3.49093900	-5.72357700
C	1.41654800	3.36649600	0.96042600
C	1.46014500	3.30060700	2.36952300
C	2.60440300	3.30601300	0.20527700
C	0.28206500	3.34493000	3.18510000
C	2.73045700	3.19689600	3.03233800
C	3.87033100	3.21862900	0.88296300
C	2.61168400	3.31407700	-1.22939900
C	0.36207100	3.26065200	4.54558000
H	-0.68816600	3.44831200	2.71035200
C	2.77177000	3.11409900	4.46060400
C	3.90394600	3.17282400	2.27584800
C	5.07676100	3.17112000	0.11206800
H	1.66708100	3.33430400	-1.76178200
C	3.78239100	3.27290500	-1.92554500
C	1.62488800	3.13850800	5.19752000
H	-0.54420300	3.28951100	5.14176400
H	3.74196200	3.02517300	4.94125500
H	4.86291700	3.10127000	2.78381600
C	5.03671600	3.20580900	-1.24857700
H	6.02228900	3.10401100	0.64261700
H	3.76549200	3.25799800	-3.01139000
H	1.66526600	3.06981900	6.27956500
H	5.95310200	3.16616000	-1.82884100
C	2.45636000	-3.30437500	-1.61043000
C	1.68102500	-3.49143300	-0.45675700
C	0.29913100	-3.51498000	-0.53952600
C	-0.30681400	-3.29999300	-1.78449300
C	0.47393000	-3.10912100	-2.92185400
C	1.86958300	-3.11941000	-2.85600600

C	3.91408300	-2.98905000	0.11891300
C	2.61282300	-3.58768100	0.75267600
H	-0.31595100	-3.67880500	0.34755800
H	-1.38589500	-3.27003300	-1.86064400
H	-0.01093500	-2.93931500	-3.87840800
H	2.47656100	-2.95386800	-3.74080200
H	4.49313300	-2.90996200	-1.89492300
N	3.81273800	-3.33062700	-1.27341900
C	5.22950300	-3.41149900	0.74109000
H	5.22754500	-3.17307200	1.80851900
H	5.39659600	-4.48244900	0.61171900
H	6.03332700	-2.85042500	0.26076900
C	2.79629400	-5.03917500	1.19715300
H	3.31994200	-5.58851600	0.40906200
H	3.37512400	-5.11075200	2.12240300
H	1.83136900	-5.52873500	1.34218600
C	-0.20478600	-2.50989400	5.27164400
C	0.32587500	-1.34428000	4.78049000
C	1.14432800	-1.34311900	3.62191100
C	1.40959600	-2.57862500	2.94512000
C	0.81496400	-3.76425100	3.46342600
C	0.04689800	-3.72968600	4.60051100
H	1.42090700	0.80306100	3.62472700
H	-0.81896500	-2.50116300	6.16596300
H	0.13604900	-0.39479000	5.27468100
C	1.68133800	-0.12450600	3.12147700
C	2.24863600	-2.53324100	1.79438800
H	0.98283500	-4.71068400	2.96643000
H	-0.38119400	-4.65092000	4.98478700
C	2.82801200	-1.33474600	1.41463800
C	2.52132800	-0.10582700	2.03841800
H	0.15401500	-1.66073400	1.06773400
H	2.94702500	0.81639500	1.65684300
N	3.76070000	-1.48947000	0.38037400
N	3.58297400	-0.64803200	-0.71159800
C	4.60323300	-0.48726900	-1.58586000
O	5.72955900	-0.94164100	-1.38390300
H	2.62527600	-0.36429700	-0.92163000
C	4.26628600	0.22567100	-2.86217400
C	2.96483500	0.33468400	-3.36036100
C	5.33381100	0.76440300	-3.58438100
C	2.73908700	1.00122000	-4.56277800
H	2.12213000	-0.10170100	-2.83197700
C	5.10401700	1.43676800	-4.77900400

H	6.33684800	0.64953400	-3.18718600
C	3.80324900	1.55697000	-5.26963200
H	1.72840300	1.08143800	-4.94936700
H	5.93599500	1.86350100	-5.32991200
H	3.62131900	2.07592700	-6.20541800

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C	-6.21752900	-2.19395100	-3.33024300
C	-5.33611700	-2.16280600	-2.27919000
C	-4.82772000	-0.92693800	-1.79537600
C	-5.22565300	0.27406200	-2.44729700
C	-6.14892100	0.20915500	-3.52460100
C	-6.63911000	-0.99603000	-3.95509500
H	-6.59116000	-3.14656200	-3.69120700
C	-3.90097700	-0.84737000	-0.70547000
C	-4.69199900	1.51688900	-2.01820500
H	-6.45117100	1.13544800	-4.00482000
H	-7.34049600	-1.03783000	-4.78169200
C	-3.75948700	1.59360900	-1.01298700
C	-3.36374600	0.38120400	-0.39169400
H	-5.02488500	2.42932200	-2.50631100
C	-3.47643700	-2.03723300	0.07920400
C	-4.41791500	-2.85565500	0.78450400
C	-2.13266600	-2.32836900	0.19455800
C	-3.94203600	-3.99032700	1.49880100
C	-5.80836500	-2.56036700	0.83486000
C	-1.63910100	-3.45518300	0.89867100
C	-4.86349200	-4.81634500	2.19625600
C	-2.55322400	-4.26980400	1.52210900
C	-6.67265800	-3.37075500	1.52649400
H	-6.18302700	-1.67794700	0.32799100
C	-6.20064000	-4.51871300	2.20722600
H	-4.48218400	-5.68378600	2.72751200
H	-2.20208800	-5.14446900	2.06364000
H	-7.72937200	-3.12614600	1.55756500
H	-6.89828500	-5.15158700	2.74547200
O	-1.20751700	-1.51467300	-0.44421700
H	-5.01084300	-3.08731800	-1.81439600
O	-2.39309300	0.44591600	0.60459900
P	-0.92343700	-0.02392400	0.12366400
O	-0.15817400	-0.22996800	1.46950400
O	-0.30492100	0.80160300	-0.92849900
C	-3.23232200	2.90688600	-0.54234700
C	-2.32334600	3.63562200	-1.33044800
C	-3.69677200	3.42600600	0.68267300
C	-1.78068700	3.12492500	-2.55547100
C	-1.89438500	4.93459600	-0.89033900
C	-3.25186000	4.71974300	1.11769000
C	-4.61821100	2.71529200	1.51894900
C	-0.89147800	3.85462900	-3.28859900

H	-2.06956200	2.13143600	-2.87933900
C	-0.96670400	5.67203000	-1.69484900
C	-2.37324000	5.44813000	0.31525200
C	-3.73014800	5.24064200	2.36181600
H	-4.97782200	1.74209100	1.20116600
C	-5.04942400	3.24455200	2.69992800
C	-0.48079000	5.15248600	-2.85730500
H	-0.48335900	3.44556000	-4.20719200
H	-0.65506800	6.65503200	-1.35058400
H	-2.04776900	6.43420700	0.64178600
C	-4.59854700	4.52673500	3.13252600
H	-3.38149900	6.22012700	2.67711800
H	-5.74483300	2.68748300	3.31939100
H	0.22413300	5.71815000	-3.45839500
H	-4.95448200	4.92884400	4.07538800
C	-0.18653300	-3.79842600	0.96487400
C	0.40438400	-4.51911700	-0.09091400
C	0.54312300	-3.51877400	2.13541400
C	-0.28633500	-4.79095900	-1.31690300
C	1.73620700	-5.03525400	0.06281400
C	1.88267200	-4.02071400	2.27023700
C	0.00023700	-2.74480300	3.21321000
C	0.29935900	-5.52813100	-2.30514100
H	-1.29053400	-4.40151400	-1.45134700
C	2.31004700	-5.81383400	-0.99271500
C	2.43608400	-4.78747400	1.24378100
C	2.62311000	-3.72305700	3.45905200
H	-1.00286800	-2.34483700	3.11413800
C	0.73894800	-2.48063700	4.32851800
C	1.61500500	-6.05666100	-2.14017600
H	-0.23821100	-5.71967800	-3.22802300
H	3.31524400	-6.20340700	-0.85685400
H	3.43896500	-5.19354800	1.36360600
C	2.07120500	-2.97664700	4.45675300
H	3.63751000	-4.10378800	3.54223800
H	0.31529300	-1.88103300	5.12761500
H	2.05844600	-6.64591200	-2.93607900
H	2.64106100	-2.75137500	5.35227200
C	2.71724400	-0.06447200	-2.12787000
C	4.06991400	0.00680000	-2.54569200
C	4.75482500	-1.18202900	-2.83839400
C	4.08244200	-2.38984400	-2.72151500
C	2.72968700	-2.43497500	-2.32984600
C	2.02781100	-1.27793700	-2.02991200

C	3.34177800	2.09502700	-2.09935500
C	4.44628000	1.39616300	-2.52945100
H	5.80171200	-1.15612000	-3.13269400
H	4.60321100	-3.31937500	-2.93402100
H	2.22375500	-3.39317600	-2.26065800
H	0.98723200	-1.31108700	-1.72382400
H	1.36980800	1.44838200	-1.54730800
N	2.30798300	1.21703200	-1.85869500
C	3.16054200	3.54992900	-1.81237900
H	2.18985100	3.90458600	-2.17456000
H	3.19940000	3.73806000	-0.73210800
H	3.94204600	4.14143000	-2.29234800
C	5.79247900	1.93462600	-2.89695100
H	5.99926900	1.81670600	-3.96675800
H	5.88189800	2.99690800	-2.65533400
H	6.58438200	1.40147200	-2.35867600
C	7.71964200	-2.22523000	-0.26372200
C	6.42869500	-2.51237000	0.10894800
C	5.51488400	-1.47069700	0.39848600
C	5.95497200	-0.12207200	0.29364100
C	7.29719200	0.14758300	-0.08278200
C	8.16063900	-0.88301900	-0.35928000
H	3.84188400	-2.77430200	0.83001600
H	8.41197400	-3.03084800	-0.48604700
H	6.08722800	-3.54153200	0.17968300
C	4.16824100	-1.74130600	0.78078900
C	5.02625000	0.91108000	0.55013000
H	7.62593100	1.18131700	-0.14559300
H	9.18542900	-0.67413200	-0.64759100
C	3.72882000	0.61588800	0.92767100
C	3.28881700	-0.73537100	1.05514100
H	5.31584100	1.95367800	0.45027400
H	2.26476100	-0.96456600	1.33497400
N	2.94390900	1.75380700	1.12719300
N	1.75979100	1.60615000	1.50306200
C	1.02948400	2.85426500	1.60520400
O	-0.17297400	2.77506500	1.49928900
H	0.62482900	0.41577900	1.56504200
C	1.74375600	4.14330200	1.82506700
C	1.12700800	5.28636300	1.30885600
C	2.93527400	4.25732200	2.54919500
C	1.71010600	6.53502900	1.48822500
H	0.19589800	5.17242400	0.76452200
C	3.50236600	5.51212300	2.74541000

H	3.40993700	3.37812700	2.96882600
C	2.89818800	6.64796000	2.20806200
H	1.23745000	7.41851600	1.07096200
H	4.42037600	5.60280400	3.31619500
H	3.35313500	7.62241700	2.35422500

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Value of imaginary frequency = -245.7 cm^{-1}

C	6.05147800	-1.86145200	3.48366300
C	5.24681500	-1.88403300	2.37234200
C	4.69429600	-0.68303000	1.84869000
C	4.96784900	0.53791500	2.52635500
C	5.81255900	0.53019200	3.66823400
C	6.34842400	-0.64117100	4.13634400
H	6.45942100	-2.78952000	3.87098200
C	3.84216900	-0.65974800	0.69705300
C	4.38397400	1.74301800	2.05852900
H	6.01759200	1.47347000	4.16675800
H	6.98927400	-0.63939400	5.01174400
C	3.52659600	1.76068700	0.98613400
C	3.25278600	0.53139800	0.32864100
H	4.61633500	2.67358700	2.57045100
C	3.51683600	-1.88089700	-0.08539600
C	4.52756900	-2.67093000	-0.72149600
C	2.19012600	-2.23239900	-0.24774400
C	4.14379600	-3.84822300	-1.42232000
C	5.90311500	-2.30784300	-0.71611800
C	1.79564200	-3.41578600	-0.92808100
C	5.13706700	-4.64283600	-2.05476900
C	2.77283700	-4.20171500	-1.48840100
C	6.83860500	-3.08963000	-1.34519500
H	6.20771800	-1.39494800	-0.21581600
C	6.45689800	-4.27705600	-2.01511500
H	4.82530000	-5.54214200	-2.57860100
H	2.48887700	-5.11388000	-2.00730300
H	7.88226300	-2.79212600	-1.33536200
H	7.20976600	-4.88617300	-2.50431400
O	1.21168800	-1.44743900	0.31770800
H	5.01729200	-2.82688800	1.88796400
O	2.37388900	0.53523900	-0.73353700
P	0.85352000	0.01092100	-0.38259500
O	0.15041700	-0.21237900	-1.68709500
O	0.25685900	0.85165600	0.69599400
C	2.96352000	3.05074400	0.49297000
C	1.94941200	3.70906100	1.21199100
C	3.52289300	3.64140800	-0.65765500
C	1.31123800	3.12236200	2.35499800
C	1.51757100	5.01245000	0.78991500
C	3.07220600	4.93697600	-1.08044500
C	4.55076700	3.00237400	-1.42456300

C	0.32693800	3.78541400	3.02746500
H	1.60311500	2.12251600	2.65400900
C	0.49037200	5.68086800	1.53236800
C	2.09261200	5.59841000	-0.33813700
C	3.65186500	5.53133800	-2.24604200
H	4.90999100	2.02692700	-1.11381200
C	5.07818100	3.60105300	-2.53111800
C	-0.08628000	5.09040800	2.61671300
H	-0.15436600	3.31889400	3.88154400
H	0.17944100	6.66982400	1.20523700
H	1.76620900	6.58875100	-0.65069600
C	4.62210800	4.88528400	-2.95239100
H	3.29748600	6.51097300	-2.55441400
H	5.85389500	3.09822200	-3.09946100
H	-0.86750300	5.60347000	3.16914400
H	5.05425700	5.34297400	-3.83625800
C	0.36862200	-3.84979100	-1.00400600
C	-0.17973600	-4.59419500	0.05822600
C	-0.38008000	-3.61362100	-2.17131900
C	0.54574500	-4.85548100	1.26708600
C	-1.50050800	-5.14505600	-0.07032300
C	-1.69604200	-4.17805600	-2.29511500
C	0.12545500	-2.82874600	-3.25873900
C	-0.00321900	-5.60140900	2.27028800
H	1.54681300	-4.45033600	1.37520100
C	-2.04328800	-5.91357700	1.00881900
C	-2.21799300	-4.94136900	-1.24947400
C	-2.44849600	-3.93617500	-3.48896500
H	1.10469100	-2.37479800	-3.16065300
C	-0.62279500	-2.62120700	-4.37920900
C	-1.32012900	-6.13810100	2.14289700
H	0.56141300	-5.78828200	3.17795300
H	-3.04533700	-6.31935900	0.89818600
H	-3.20929900	-5.37932700	-1.35292500
C	-1.92908700	-3.18386800	-4.49978200
H	-3.44432000	-4.36444400	-3.56624500
H	-0.22916900	-2.01319600	-5.18712500
H	-1.73941500	-6.72507900	2.95360700
H	-2.50717500	-3.00213200	-5.40019300
C	-2.44132500	-0.19511700	2.10314800
C	-3.81842900	-0.30104300	2.37342500
C	-4.37213500	-1.55005100	2.65102000
C	-3.53033600	-2.66081300	2.63365800
C	-2.16222200	-2.53241800	2.35785100

C	-1.58771400	-1.29252800	2.09122300
C	-3.28885400	1.87665700	1.91618800
C	-4.38987500	1.02069900	2.17170600
H	-5.43573000	-1.65896400	2.84705300
H	-3.93884100	-3.64782400	2.83010900
H	-1.53470900	-3.41713800	2.35162700
H	-0.53382000	-1.18511900	1.86541600
H	-1.24730600	1.43910200	1.49273600
N	-2.17151700	1.14581300	1.83506300
C	-3.30003100	3.33689300	1.63350200
H	-2.28252600	3.73210300	1.57671900
H	-3.78534700	3.52833900	0.66797000
H	-3.85023400	3.87605100	2.40924700
C	-5.71690800	1.48272200	2.68612400
H	-5.65120000	1.72695000	3.75155300
H	-6.06793300	2.37504000	2.15850500
H	-6.47006800	0.69840400	2.57811100
C	-7.45513700	-2.60276300	0.16804600
C	-6.12398600	-2.79000400	-0.16407500
C	-5.25401400	-1.69473300	-0.27303100
C	-5.75348400	-0.39192900	-0.02233300
C	-7.11684900	-0.21795800	0.28925500
C	-7.95862000	-1.31078400	0.38522900
H	-3.51331100	-2.88992400	-0.81286500
H	-8.11751000	-3.45859000	0.24783000
H	-5.73628400	-3.78844600	-0.34701800
C	-3.87446300	-1.87569600	-0.68354200
C	-4.84168800	0.71680600	-0.08449000
H	-7.50119700	0.78657500	0.44067400
H	-9.00775900	-1.16958500	0.62073600
C	-3.55863900	0.51719800	-0.71951600
C	-3.05745600	-0.83124000	-0.92890200
H	-5.24284400	1.72685700	-0.11387000
H	-2.03502600	-0.98621100	-1.27026000
N	-2.97505900	1.64882400	-1.04678300
N	-1.81420000	1.69461800	-1.64676500
C	-1.23601000	2.94622000	-1.90398200
O	-0.06202900	2.98962300	-2.21034600
H	-1.16407100	0.87755600	-1.76019500
C	-2.08109900	4.17469900	-1.78246900
C	-1.42150300	5.32182700	-1.33747800
C	-3.43169200	4.24525200	-2.14259400
C	-2.11262900	6.52094500	-1.20241200
H	-0.36662400	5.25181900	-1.09670700

C	-4.11363800	5.45225900	-2.02764700
H	-3.94514200	3.36780000	-2.51738200
C	-3.46135400	6.58619400	-1.54448000
H	-1.59745600	7.40461100	-0.83885500
H	-5.15804400	5.50769800	-2.31635400
H	-4.00272200	7.52163100	-1.44517700

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C	-6.96029100	-1.49206800	-2.67031800
C	-5.92743800	-1.57226100	-1.77031400
C	-5.13844500	-0.43017300	-1.46480300
C	-5.42399000	0.79127500	-2.13779500
C	-6.50734700	0.84512900	-3.05437500
C	-7.26307700	-0.26860900	-3.31391900
H	-7.54762700	-2.37610500	-2.89638800
C	-4.04297300	-0.47403400	-0.54229300
C	-4.61897100	1.93451600	-1.89158300
H	-6.71810900	1.78775200	-3.55164600
H	-8.08661200	-0.21935000	-4.01854400
C	-3.53405600	1.88282000	-1.05240800
C	-3.25351500	0.64869000	-0.40680600
H	-4.86467400	2.86814500	-2.39158300
C	-3.69853200	-1.67909600	0.26095800
C	-4.62288400	-2.27009200	1.18172300
C	-2.41192700	-2.17871200	0.19884400
C	-4.20990500	-3.40054400	1.94234000
C	-5.92934200	-1.75142100	1.40208300
C	-1.96828700	-3.26979400	0.99034200
C	-5.12166800	-4.00593800	2.84865800
C	-2.87907700	-3.87414200	1.82295700
C	-6.78368600	-2.35181400	2.29139500
H	-6.24568600	-0.86473900	0.86434000
C	-6.38387800	-3.50005900	3.01662900
H	-4.79127700	-4.87243600	3.41458300
H	-2.56390700	-4.71448300	2.43632400
H	-7.77440600	-1.93722100	2.44715000
H	-7.07298300	-3.96448100	3.71415000
O	-1.51804300	-1.61379300	-0.68385800
H	-5.69646800	-2.51664300	-1.28895100
O	-2.12957600	0.58296700	0.39705300
P	-0.85511300	-0.15462100	-0.31727500
O	0.24736700	-0.30033400	0.66613800
O	-0.61686400	0.49285600	-1.66512100
C	-2.70964300	3.09417300	-0.76865100
C	-1.84632900	3.62318800	-1.74683100
C	-2.84509600	3.73056400	0.48234100
C	-1.64458700	2.99470300	-3.02035400
C	-1.11839400	4.83165200	-1.46848100
C	-2.12147600	4.94245600	0.74409800
C	-3.69805200	3.22216900	1.51571400
C	-0.79600300	3.53194800	-3.94338100

H	-2.16063200	2.06416500	-3.22503100
C	-0.24129000	5.36556300	-2.46782100
C	-1.27857700	5.46588800	-0.23729300
C	-2.28035000	5.59207600	2.01033500
H	-4.25875200	2.31093800	1.33589300
C	-3.81233000	3.86237300	2.71455300
C	-0.08559800	4.73993700	-3.66832700
H	-0.65278500	3.03730500	-4.89877300
H	0.29779200	6.28123600	-2.24111800
H	-0.72989700	6.38371400	-0.03489100
C	-3.09317600	5.06707800	2.96992300
H	-1.73168400	6.51395700	2.18853300
H	-4.45898600	3.45497500	3.48476700
H	0.58255500	5.15118200	-4.41838900
H	-3.20209300	5.56237100	3.92917200
C	-0.54481000	-3.72801000	0.99409700
C	-0.09257200	-4.66965100	0.05179600
C	0.30698000	-3.29043400	2.02680800
C	-0.90589200	-5.10475200	-1.04469500
C	1.21996200	-5.23789800	0.18942900
C	1.61821900	-3.86343300	2.15585000
C	-0.08329800	-2.28047800	2.96671100
C	-0.45564300	-6.04685200	-1.92444700
H	-1.89379400	-4.67079400	-1.16503200
C	1.64859600	-6.23423600	-0.74488300
C	2.04038100	-4.82890700	1.24136000
C	2.45903700	-3.44234800	3.23728300
H	-1.05702400	-1.81528100	2.85927200
C	0.75967200	-1.88212900	3.96207300
C	0.83793700	-6.63155000	-1.76732600
H	-1.08476000	-6.36104200	-2.75091500
H	2.63819100	-6.66525300	-0.61919800
H	3.02521400	-5.27783400	1.35513000
C	2.04716600	-2.48078800	4.11056900
H	3.43683600	-3.90600800	3.34087900
H	0.45186800	-1.10116200	4.64963900
H	1.17227300	-7.38777100	-2.47011700
H	2.69509500	-2.16230700	4.92073200
C	2.25744500	-0.86887700	-2.22621000
C	3.64869800	-0.89050500	-2.23047700
C	4.30772200	-2.10034300	-2.38999000
C	3.53376000	-3.26197300	-2.48481600
C	2.13812300	-3.21459200	-2.43750400
C	1.46433900	-1.99992100	-2.31771500

C	2.81997000	1.28869100	-2.03508200
C	4.13521500	0.52344900	-2.00000500
H	5.39201600	-2.15352600	-2.41799500
H	4.02613100	-4.22274400	-2.59731000
H	1.56563300	-4.13392100	-2.50470300
H	0.38102000	-1.94263500	-2.29861900
H	0.72216900	0.66263600	-1.99326800
N	1.82189300	0.47648500	-2.12575100
C	2.65930800	2.76040400	-1.95719200
H	1.60317900	3.03031400	-1.88589300
H	3.19356500	3.14458300	-1.08397400
H	3.08647500	3.21883600	-2.85581000
C	5.10612000	1.02229700	-3.07383900
H	4.62800100	0.99295600	-4.05635300
H	5.42877100	2.04739600	-2.86792600
H	5.98805100	0.37952800	-3.10663700
C	7.99025100	-2.07536400	-0.01353500
C	6.72148000	-2.38149600	0.46739300
C	5.66813000	-1.47186400	0.33394100
C	5.89573800	-0.24045000	-0.30946300
C	7.17568100	0.06775900	-0.76466200
C	8.22129800	-0.84382700	-0.62194900
H	4.17223200	-2.78997800	1.23903700
H	8.79872700	-2.79048600	0.09639900
H	6.53817400	-3.33310200	0.95878200
C	4.34189600	-1.78058000	0.87438700
C	4.73296900	0.69949300	-0.52977700
H	7.35867300	1.03237100	-1.23051400
H	9.21237700	-0.58932800	-0.98257800
C	3.65001100	0.50866400	0.51903000
C	3.36733300	-0.86018300	0.96890000
H	5.07349900	1.73887800	-0.46814100
H	2.40447100	-1.10642000	1.40836500
N	3.09017200	1.59395600	0.92235400
N	2.03963500	1.50959900	1.79009100
C	1.40968800	2.65656400	2.21931000
O	0.26459100	2.59078200	2.64266500
H	1.39733600	0.71339500	1.69524900
C	2.16158700	3.95380200	2.20823100
C	1.38495900	5.11066900	2.11690900
C	3.54696600	4.06153200	2.36277300
C	1.98359400	6.36494500	2.14002600
H	0.30974100	5.00021600	2.03145600
C	4.14241400	5.31911300	2.40610800

H	4.15411300	3.16909500	2.45728200
C	3.36578100	6.47017100	2.28444400
H	1.37278300	7.25875900	2.05622300
H	5.21664600	5.40068900	2.53686900
H	3.83741300	7.44756000	2.31132000

TSIV-2

Value of imaginary frequency = -172.9 cm^{-1}

C	6.81224500	-1.86663600	2.64382200
C	5.79774100	-1.88195900	1.72004500
C	5.14900100	-0.67809900	1.32967000
C	5.55382200	0.53819000	1.94796400
C	6.61604100	0.52344800	2.89086900
C	7.23719600	-0.65032000	3.22996100
H	7.29105000	-2.79672000	2.93289100
C	4.08075800	-0.64761800	0.37578700
C	4.87662300	1.74314300	1.62944000
H	6.91932800	1.46311900	3.34432900
H	8.04564600	-0.65359500	3.95368100
C	3.81346000	1.76671600	0.76047100
C	3.42202500	0.54412900	0.14903200
H	5.19921000	2.66781900	2.10182900
C	3.60932400	-1.86449100	-0.33750500
C	4.47501600	-2.64671500	-1.16767100
C	2.27687500	-2.22017100	-0.23362400
C	3.96097300	-3.82060800	-1.78537900
C	5.82448100	-2.28181700	-1.43229500
C	1.75277100	-3.39249300	-0.84207300
C	4.81240500	-4.61481300	-2.59943400
C	2.60272300	-4.17214400	-1.58876000
C	6.61965900	-3.06203900	-2.23294300
H	6.21917800	-1.36825200	-1.00120600
C	6.11514200	-4.24981900	-2.81568200
H	4.40430700	-5.51409100	-3.05230400
H	2.22266600	-5.08022000	-2.05043100
H	7.64491500	-2.76398700	-2.42748600
H	6.75843000	-4.85989500	-3.44111300
O	1.43481200	-1.44602300	0.52828800
H	5.47394200	-2.82148100	1.28539800
O	2.35414400	0.55255000	-0.72003100
P	0.92741200	0.00152200	-0.10193900
O	0.01369700	-0.25829200	-1.25871700
O	0.53318400	0.83543200	1.07343800
C	3.11577700	3.04954500	0.45091900
C	2.22592500	3.61488600	1.38393100
C	3.40392500	3.71759000	-0.75527600
C	1.88099700	2.96100300	2.61267400
C	1.62132400	4.88785100	1.10506900
C	2.80761200	4.99702100	-1.01577300
C	4.29436600	3.17656500	-1.73918600

C	0.99463800	3.52231200	3.48354600
H	2.31340600	1.98953500	2.82156900
C	0.69011800	5.44107700	2.04308200
C	1.94218800	5.55734800	-0.07581400
C	3.12016100	5.67749700	-2.23505800
H	4.75529700	2.21124300	-1.55635100
C	4.56502300	3.85472500	-2.89180500
C	0.38387000	4.78038700	3.19538800
H	0.73972500	3.00554500	4.40326700
H	0.23314600	6.39977600	1.81005700
H	1.49976100	6.53222000	-0.27404100
C	3.96989900	5.12595500	-3.14654700
H	2.65945600	6.64473100	-2.41615300
H	5.24012300	3.42651600	-3.62567000
H	-0.32441200	5.20557100	3.89964700
H	4.19846400	5.64838600	-4.06975100
C	0.33852700	-3.83694500	-0.65512000
C	-0.00702800	-4.56287000	0.50136600
C	-0.60032500	-3.65884000	-1.68747000
C	0.90691400	-4.74686400	1.58990700
C	-1.31063600	-5.15658700	0.60551800
C	-1.90084200	-4.25950200	-1.57458100
C	-0.30498300	-2.90041800	-2.86751200
C	0.54871300	-5.45983700	2.69775400
H	1.89540600	-4.30345900	1.52365900
C	-1.64245200	-5.90861800	1.77770300
C	-2.22505300	-4.99553400	-0.43541400
C	-2.82923900	-4.11419900	-2.65485100
H	0.65829300	-2.40880600	-2.93985600
C	-1.22188400	-2.77389900	-3.86914900
C	-0.74549500	-6.05465100	2.79481400
H	1.25322200	-5.58098500	3.51413700
H	-2.63064700	-6.35711500	1.83890100
H	-3.20765400	-5.45597200	-0.35757400
C	-2.50242900	-3.39854100	-3.76847000
H	-3.80080900	-4.59421200	-2.56401900
H	-0.98127100	-2.19178800	-4.75265600
H	-1.00843100	-6.62281300	3.68107200
H	-3.21351100	-3.29731700	-4.58275100
C	-2.31370500	-0.25933000	1.93404600
C	-3.68719100	-0.47160000	1.83417900
C	-4.20660300	-1.73998200	2.05648600
C	-3.31890400	-2.77433100	2.36279900
C	-1.94664700	-2.53747200	2.45812000

C	-1.41329000	-1.26794900	2.24493600
C	-3.13243000	1.78473000	1.36957800
C	-4.36582300	0.85455100	1.53439600
H	-5.27505600	-1.92629300	2.00044000
H	-3.69881700	-3.77676400	2.53396400
H	-1.27827900	-3.35511300	2.70733700
H	-0.35067700	-1.07014100	2.31188200
H	-1.07118800	1.42792800	1.65269300
N	-2.04830600	1.11251300	1.74406500
C	-3.17912300	3.26957000	1.51511500
H	-2.22142500	3.71025000	1.22809400
H	-3.96724500	3.70238100	0.89704800
H	-3.36528900	3.50760700	2.56774600
C	-5.21852700	1.33092500	2.71468900
H	-4.58936900	1.46282900	3.59940000
H	-5.71575800	2.27928800	2.48935400
H	-5.97413800	0.58121000	2.95618800
C	-8.10830700	-2.28027800	-0.13954300
C	-6.95132800	-2.34972300	-0.90562000
C	-5.98446100	-1.34126500	-0.83170000
C	-6.17424600	-0.25305800	0.04036800
C	-7.36190000	-0.16706200	0.76376300
C	-8.31973500	-1.17772200	0.68460700
H	-4.73098600	-2.26412200	-2.35871800
H	-8.85083200	-3.06843900	-0.20155000
H	-6.78837400	-3.18626900	-1.57942700
C	-4.81381300	-1.40383400	-1.70125200
C	-5.10517400	0.80852000	0.16348500
H	-7.55177100	0.70015200	1.38855000
H	-9.23456700	-1.09675700	1.26216700
C	-3.96215500	0.66372900	-0.82991200
C	-3.85975500	-0.45384300	-1.73646800
H	-5.56602300	1.79275900	-0.00317400
H	-2.99705300	-0.53121100	-2.39062500
N	-3.09746900	1.60065500	-0.64656900
N	-1.91436600	1.62813000	-1.33699500
C	-1.29623200	2.83685200	-1.56631600
O	-0.10720700	2.88293700	-1.83845900
H	-1.27018800	0.80075700	-1.31730600
C	-2.13332100	4.08154500	-1.51814100
C	-1.50972700	5.23490100	-1.03982600
C	-3.45822000	4.13926400	-1.95937000
C	-2.21670500	6.42906300	-0.95338900
H	-0.47300400	5.16943600	-0.72640700

C	-4.15706400	5.34171500	-1.89402500
H	-3.93647400	3.25451100	-2.36575400
C	-3.54343600	6.48241500	-1.37819500
H	-1.73288100	7.31825900	-0.56112500
H	-5.18188400	5.38893400	-2.24755300
H	-4.09661300	7.41427800	-1.31777000

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C	-7.10339800	-1.25677900	-2.60260500
C	-6.07954900	-1.38250500	-1.69724300
C	-5.30083800	-0.25555300	-1.31727600
C	-5.58878200	1.00152300	-1.92072400
C	-6.66158000	1.10114200	-2.84561600
C	-7.40669500	-0.00033600	-3.17883300
H	-7.68273000	-2.12999400	-2.88474100
C	-4.21257800	-0.34577100	-0.39012300
C	-4.79378700	2.13411900	-1.60098700
H	-6.87192800	2.06942400	-3.29137700
H	-8.22083900	0.08455100	-3.89098300
C	-3.71723800	2.04084900	-0.75510400
C	-3.43341100	0.77252700	-0.17757400
H	-5.03946300	3.09278000	-2.05149700
C	-3.84900300	-1.59855200	0.32823900
C	-4.76371800	-2.26741300	1.20395200
C	-2.55710000	-2.07979500	0.21857900
C	-4.33846300	-3.44923700	1.87367200
C	-6.07512800	-1.78097000	1.46518400
C	-2.11402400	-3.24900100	0.89487600
C	-5.24086500	-4.13018200	2.73386500
C	-3.01246900	-3.91643700	1.69113900
C	-6.92121700	-2.45572700	2.30836500
H	-6.40174500	-0.85985800	0.99503400
C	-6.50743600	-3.65118300	2.94370300
H	-4.90077500	-5.03613000	3.22801300
H	-2.69762600	-4.81891100	2.20941700
H	-7.91647100	-2.06544900	2.49550600
H	-7.18989300	-4.17616500	3.60394100
O	-1.67113000	-1.43704200	-0.61320100
H	-5.84733100	-2.35185300	-1.26863700
O	-2.32386500	0.66097100	0.63167200
P	-1.01824200	0.00034800	-0.12832100
O	0.01125400	-0.25023900	0.93332000
O	-0.70128900	0.76388700	-1.36961500
C	-2.89423000	3.23444000	-0.39929800
C	-1.99398100	3.79111800	-1.32706200
C	-3.05504800	3.81603900	0.87525900
C	-1.77620200	3.22393700	-2.62602900
C	-1.24208500	4.96285600	-0.96794700
C	-2.30846200	4.99271600	1.21746700
C	-3.96052200	3.28724400	1.85223300
C	-0.88310300	3.77747200	-3.49472300

H	-2.31076900	2.31979400	-2.89108800
C	-0.31161100	5.51188100	-1.90964300
C	-1.42597000	5.54198600	0.28695700
C	-2.48827300	5.58368700	2.50802000
H	-4.54034800	2.40309500	1.60856400
C	-4.10453200	3.87925200	3.07294200
C	-0.13579700	4.93940400	-3.13363100
H	-0.72590100	3.32592900	-4.46899000
H	0.25021000	6.39736900	-1.62193600
H	-0.86802300	6.43903700	0.54889000
C	-3.35656800	5.04574900	3.41029500
H	-1.91235400	6.47235300	2.75111400
H	-4.79566800	3.46173700	3.79802700
H	0.57314000	5.36051100	-3.83961200
H	-3.48515700	5.50034100	4.38725200
C	-0.72168100	-3.77044400	0.73791700
C	-0.41791500	-4.60726400	-0.35327700
C	0.25145100	-3.49996000	1.71723900
C	-1.36505300	-4.88202000	-1.39278800
C	0.87882300	-5.21725200	-0.44281300
C	1.55778200	-4.08874600	1.59958700
C	-0.00737500	-2.65242900	2.84415200
C	-1.04766300	-5.70364400	-2.43583400
H	-2.34670000	-4.42176600	-1.34128200
C	1.16518900	-6.08935500	-1.54113300
C	1.83771000	-4.93888400	0.53036500
C	2.54384000	-3.80407500	2.59836800
H	-0.98410100	-2.19037600	2.93504800
C	0.95596000	-2.41101600	3.77813800
C	0.23535600	-6.32504000	-2.51030300
H	-1.77714700	-5.89230200	-3.21682000
H	2.14752100	-6.55238400	-1.58780200
H	2.82386000	-5.39125000	0.45068900
C	2.25324600	-2.99519500	3.65630900
H	3.52652300	-4.25707400	2.49303600
H	0.74058000	-1.76352300	4.62193300
H	0.46440200	-6.98189200	-3.34315700
H	3.00281200	-2.79468900	4.41635800
C	2.21420500	-0.54547600	-2.05932200
C	3.57080300	-0.85859400	-1.92108600
C	4.00633300	-2.16589100	-2.09201500
C	3.06417100	-3.15802100	-2.37667900
C	1.71344700	-2.83157400	-2.50187300
C	1.26511000	-1.52190000	-2.34741500

C	3.16002700	1.41208100	-1.32432500
C	4.34353800	0.43370800	-1.68073000
H	5.05912200	-2.41863000	-2.00446200
H	3.38150100	-4.18941500	-2.49425300
H	0.99087300	-3.61310600	-2.71922900
H	0.21711700	-1.26204000	-2.43929300
H	1.06654200	1.15776300	-1.71034700
N	2.01438700	0.82945300	-1.92359200
C	3.31985100	2.88146300	-1.64912300
H	2.41487400	3.42668700	-1.36748800
H	4.17012200	3.32357100	-1.12171800
H	3.45431200	2.99341800	-2.72631700
C	5.09833200	0.86479300	-2.93496900
H	4.38048700	1.05615300	-3.73773400
H	5.69022500	1.76981300	-2.76691800
H	5.75692900	0.06424800	-3.27668800
C	8.02765800	-2.74501100	0.38745100
C	7.02542700	-2.47078000	1.30629800
C	6.09847600	-1.44760700	1.06194000
C	6.17280200	-0.70212900	-0.13153100
C	7.21403200	-0.95290700	-1.02139300
C	8.12650200	-1.97531000	-0.77133400
H	5.10046700	-1.72975300	2.97335900
H	8.74013400	-3.53986700	0.57768100
H	6.95271400	-3.04083900	2.22800500
C	5.09210600	-1.13430400	2.06371000
C	5.17891600	0.40366700	-0.37149900
H	7.32287200	-0.34788000	-1.91450000
H	8.92210400	-2.16595200	-1.48375500
C	4.09838100	0.49142100	0.66074200
C	4.14685700	-0.17254000	1.92035800
H	5.72838800	1.35946500	-0.29884700
H	3.37099200	0.00034600	2.65636000
N	3.11042900	1.21043200	0.20837800
N	1.98041500	1.46502600	0.95113900
C	1.62814200	2.74684000	1.33043400
O	0.47901100	2.98347400	1.65509300
H	1.19695200	0.73887100	0.91249500
C	2.68637600	3.80749700	1.36063100
C	2.31381000	5.07980400	0.92308300
C	3.98288800	3.58238800	1.82791200
C	3.24636600	6.11023200	0.90198600
H	1.29272300	5.23278300	0.58581000
C	4.90993800	4.62136200	1.82482100

H	4.26530200	2.61040900	2.22163000
C	4.54731700	5.87964900	1.34790700
H	2.95981900	7.09302400	0.54198700
H	5.91379600	4.44947200	2.19880600
H	5.27581900	6.68391000	1.33427600

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C	-7.42151500	-1.10174400	1.17127100
C	-6.27221700	-0.54059600	0.67503600
C	-5.04607600	-1.26261500	0.68088600
C	-5.03733700	-2.56740500	1.24611800
C	-6.24540200	-3.12651800	1.74227700
C	-7.41535800	-2.41420500	1.70206400
H	-8.34459100	-0.53118100	1.16358100
C	-3.82420200	-0.71348700	0.17353400
C	-3.81812600	-3.28678900	1.30597700
H	-6.21788100	-4.12873900	2.16099200
H	-8.33399100	-2.84529100	2.08609600
C	-2.63247700	-2.73864500	0.88119600
C	-2.64567300	-1.41966600	0.34835900
H	-3.82352300	-4.29954800	1.70152700
C	-3.78387000	0.60964800	-0.50394800
C	-4.55632900	0.90344400	-1.67568400
C	-2.92572800	1.57181900	-0.01512900
C	-4.47339900	2.20605700	-2.24352500
C	-5.37550500	-0.06186400	-2.32293900
C	-2.81518400	2.87103000	-0.58377300
C	-5.23981900	2.51648500	-3.39836600
C	-3.60501800	3.16828300	-1.66670700
C	-6.09528000	0.26390400	-3.44523600
H	-5.42166400	-1.06924300	-1.92391200
C	-6.03852500	1.57038000	-3.98622900
H	-5.17016000	3.51906800	-3.81128200
H	-3.54586000	4.15744900	-2.11438500
H	-6.71091300	-0.48938600	-3.92626900
H	-6.61788000	1.81504900	-4.87030300
O	-2.14759200	1.26187900	1.07578500
H	-6.28903200	0.47043000	0.28319800
O	-1.45577600	-0.88421300	-0.07546900
P	-0.78423300	0.39294200	0.73805700
O	0.00710500	1.13710900	-0.30446000
O	-0.18156500	-0.01428000	2.03199700
C	-1.39650300	-3.57904200	0.91561600
C	-0.60791900	-3.64101100	2.07877200
C	-1.12241900	-4.42719200	-0.17526800
C	-0.85051900	-2.79452600	3.20926100
C	0.45374400	-4.60639400	2.16658300
C	-0.03326800	-5.36032900	-0.09361100
C	-1.92277000	-4.42916300	-1.36541900
C	-0.11144800	-2.91628600	4.34905300

H	-1.61884800	-2.03400900	3.13263000
C	1.18584200	-4.72169900	3.39303200
C	0.72492300	-5.43273800	1.07547100
C	0.21170300	-6.24422800	-1.19338000
H	-2.74594900	-3.72578300	-1.44225800
C	-1.66834300	-5.29954100	-2.38549800
C	0.91402300	-3.90387800	4.45073300
H	-0.30391900	-2.25995700	5.19118800
H	1.95133600	-5.49020600	3.46881400
H	1.52337000	-6.16860000	1.14692100
C	-0.58529200	-6.22563000	-2.29951400
H	1.03962000	-6.94370100	-1.11576900
H	-2.29024300	-5.28854600	-3.27493200
H	1.47228500	-4.00215600	5.37633800
H	-0.39931800	-6.90991300	-3.12106600
C	-1.86859600	3.87805900	-0.02513900
C	-2.13846600	4.47975400	1.21929000
C	-0.72655000	4.25029400	-0.76174800
C	-3.28745600	4.13739700	2.00461100
C	-1.24807600	5.48393300	1.72987700
C	0.15749100	5.25240500	-0.23793600
C	-0.38591100	3.64869200	-2.01905600
C	-3.52409500	4.73919400	3.20589800
H	-3.97675600	3.38816000	1.62891800
C	-1.53198700	6.09098900	2.99470900
C	-0.12579900	5.85043300	0.98761800
C	1.33290600	5.60704700	-0.97559600
H	-1.03072300	2.87209800	-2.41502700
C	0.73437100	4.02603100	-2.70176200
C	-2.63227100	5.73096100	3.71337300
H	-4.39891800	4.46343900	3.78587600
H	-0.84451200	6.84488600	3.36807500
H	0.55448700	6.60069500	1.38335700
C	1.61588900	5.01785100	-2.17109200
H	1.99312000	6.36061400	-0.55444000
H	0.97290500	3.55554400	-3.65108600
H	-2.83705100	6.19501900	4.67272000
H	2.50535000	5.29717600	-2.72750800
C	1.56969200	-0.23450600	-2.50634800
C	2.55726700	-1.20406400	-2.33273700
C	2.25416400	-2.54967800	-2.49951600
C	0.94104400	-2.91015200	-2.80586200
C	-0.04305100	-1.93054100	-2.94731000
C	0.25741500	-0.57829300	-2.80839200

C	3.37754700	0.95306700	-1.70685100
C	3.87288200	-0.51885900	-1.99029400
H	3.01544500	-3.31430600	-2.37840400
H	0.67934500	-3.95738300	-2.90945200
H	-1.06598400	-2.23082600	-3.15399000
H	-0.50993400	0.18388600	-2.88788300
H	1.47501100	1.77100600	-2.02651500
N	2.10946600	1.05458400	-2.37731400
C	4.30119700	2.10656600	-2.02922500
H	3.81805000	3.04622800	-1.74175700
H	5.25113500	2.02473100	-1.49250000
H	4.48474200	2.13268000	-3.10445900
C	4.87720000	-0.60126100	-3.13416700
H	4.46964300	-0.09477000	-4.01358900
H	5.83409900	-0.13972800	-2.87207600
H	5.04879300	-1.64302500	-3.41238700
C	4.89811300	-5.15689600	0.33788800
C	4.09342100	-4.34995400	1.12855400
C	3.92949600	-2.99159000	0.82539500
C	4.57730700	-2.44321500	-0.29893800
C	5.42352000	-3.24971900	-1.05590300
C	5.57119000	-4.60054000	-0.74975800
H	2.61822100	-2.65072700	2.52843600
H	5.01735500	-6.20843700	0.57453100
H	3.58833600	-4.75623800	1.99932400
C	3.11299000	-2.15773300	1.69340500
C	4.40054200	-0.98012000	-0.59916900
H	5.97583400	-2.82660900	-1.88800000
H	6.22106700	-5.21874200	-1.35997500
C	3.44179900	-0.27790000	0.31058200
C	2.91137500	-0.82720200	1.50861900
H	5.37328000	-0.48682600	-0.42174900
H	2.21812300	-0.25263400	2.11415400
N	3.13589300	0.88222800	-0.20768200
N	2.38174000	1.82789500	0.44460500
C	2.94795000	2.92216500	1.06167800
O	2.23556600	3.79287200	1.52494100
H	1.33833900	1.73153100	0.27699100
C	4.44509700	3.02762600	1.11401400
C	4.99938200	4.23653400	0.68858800
C	5.27544200	2.01309100	1.59495700
C	6.37885700	4.41205200	0.69377400
H	4.33674300	5.02285200	0.33889200
C	6.65558900	2.19845300	1.61711500

H	4.85150400	1.09260400	1.98522900
C	7.20856200	3.39048400	1.15336900
H	6.80630100	5.34588500	0.34394600
H	7.29796600	1.41328200	2.00187600
H	8.28484200	3.52788200	1.16175700

IMIV-4

C	-7.19779900	1.54815500	-2.09985700
C	-6.20120900	0.86558100	-1.44878700
C	-5.12455300	1.55853200	-0.82946200
C	-5.08013500	2.97793400	-0.94979100
C	-6.13288700	3.65581300	-1.62088800
C	-7.17499200	2.96086700	-2.17693200
H	-8.00897600	0.99925200	-2.56728000
C	-4.06983100	0.88790700	-0.12647400
C	-3.95845700	3.69263900	-0.45317500
H	-6.08673600	4.73893200	-1.69283000
H	-7.97362100	3.48664800	-2.68958800
C	-2.91432800	3.04700100	0.15912500
C	-3.01436200	1.64103300	0.34618800
H	-3.91075500	4.76809000	-0.60502400
C	-4.00449700	-0.59450000	0.00873300
C	-5.03701500	-1.37736300	0.62073400
C	-2.87633000	-1.24409300	-0.45491400
C	-4.90993100	-2.79530700	0.64124500
C	-6.16633700	-0.79093600	1.25402000
C	-2.74448100	-2.66061500	-0.46746800
C	-5.92798400	-3.57800200	1.24762700
C	-3.76566400	-3.40720100	0.06522600
C	-7.12757600	-1.57317100	1.84351000
H	-6.25542600	0.29008800	1.27640500
C	-7.01587900	-2.98393900	1.83327100
H	-5.81994900	-4.65902200	1.24551300
H	-3.69584800	-4.49224900	0.06015100
H	-7.97893000	-1.10599200	2.32781200
H	-7.78626200	-3.58949100	2.29916700
O	-1.82371400	-0.50271500	-0.94522700
H	-6.22636400	-0.21758100	-1.40744100
O	-2.01146700	1.01824300	1.04805500
P	-0.86848600	0.17783700	0.21766400
O	-0.42104500	-0.88595000	1.18525700
O	0.09739900	1.07126000	-0.47308800
C	-1.64710700	3.73726100	0.53771300
C	-0.72157400	4.06525800	-0.47242100
C	-1.34539100	3.98278700	1.88922300
C	-0.95615800	3.78425400	-1.85886400
C	0.53487700	4.66046300	-0.11103900
C	-0.09099400	4.58779600	2.23900000
C	-2.24962800	3.64237900	2.94701300
C	-0.01870000	4.07523700	-2.80574400

H	-1.88732000	3.30897900	-2.14681300
C	1.48930900	4.95777300	-1.13588600
C	0.81691700	4.91567900	1.23140300
C	0.20442300	4.82982300	3.61867300
H	-3.20071800	3.18436800	2.69355500
C	-1.93004300	3.88505600	4.25074700
C	1.22582100	4.67115800	-2.44193300
H	-0.21368300	3.84271400	-3.84784000
H	2.43787100	5.40204800	-0.84344300
H	1.76919900	5.37222900	1.49587900
C	-0.68353300	4.48884000	4.59513000
H	1.15638900	5.29197400	3.86739900
H	-2.62719900	3.61861500	5.03859400
H	1.96474900	4.88653100	-3.20788300
H	-0.44983100	4.67487800	5.63840700
C	-1.55900700	-3.30328400	-1.10957500
C	-1.43318600	-3.25078700	-2.51498500
C	-0.60138800	-3.98803500	-0.33643500
C	-2.37396300	-2.56004100	-3.34666700
C	-0.33411900	-3.91619800	-3.15606700
C	0.49787400	-4.64728100	-0.99244700
C	-0.65825800	-4.04461500	1.09634000
C	-2.21980900	-2.51738800	-4.70183800
H	-3.22111500	-2.06470800	-2.88425400
C	-0.20887400	-3.84980700	-4.58011600
C	0.60166000	-4.60299000	-2.38150200
C	1.47751000	-5.33271400	-0.20221600
H	-1.45466700	-3.51442600	1.60635100
C	0.28500100	-4.72303900	1.81003600
C	-1.11881600	-3.16839200	-5.33227100
H	-2.94243200	-1.98362100	-5.31058700
H	0.63266300	-4.35513800	-5.04601400
H	1.43546900	-5.10169700	-2.87078000
C	1.37269000	-5.37620500	1.15518200
H	2.29932400	-5.82421100	-0.71654700
H	0.23291200	-4.74737600	2.89455900
H	-1.01392600	-3.12033600	-6.41124900
H	2.11533300	-5.89948500	1.74948600
C	5.03819300	-1.66688600	-1.20380200
C	5.07948600	-0.29017700	-1.45463400
C	6.29379500	0.38141500	-1.43051900
C	7.45796400	-0.32838400	-1.12274100
C	7.39762400	-1.69626300	-0.85926100
C	6.18683600	-2.38643300	-0.90022100

C	2.83388000	-1.04295700	-1.32749500
C	3.67739400	0.18713300	-1.81666400
H	6.34443300	1.44580700	-1.63603100
H	8.41050200	0.18900900	-1.08702000
H	8.30717400	-2.23676000	-0.61665600
H	6.13786200	-3.45022100	-0.69274800
H	3.45679600	-2.97762900	-0.83804400
N	3.73594400	-2.15901800	-1.37032800
C	1.50316500	-1.30519800	-2.00173800
H	0.92810300	-2.02009600	-1.40385800
H	0.91811700	-0.38643600	-2.07656200
H	1.67031800	-1.73530300	-2.99092600
C	3.54226300	0.40548300	-3.32386100
H	3.70116300	-0.54453400	-3.84226300
H	2.55300600	0.79038600	-3.58808400
H	4.30142800	1.10141100	-3.68530800
C	5.14747400	5.08153500	-0.18827800
C	4.49846700	4.41056300	0.83841900
C	3.85811700	3.18711900	0.59725700
C	3.88150700	2.62203100	-0.69372300
C	4.49806100	3.32802100	-1.72457700
C	5.13803800	4.53951000	-1.47365800
H	3.09980100	3.04964400	2.63564900
H	5.64642300	6.02470900	0.00484300
H	4.47949400	4.82791400	1.84159300
C	3.14740500	2.52495400	1.68426400
C	3.11906900	1.34278300	-0.93481400
H	4.48205400	2.93605700	-2.73536800
H	5.62762500	5.06346800	-2.28781500
C	2.73368700	0.63834300	0.32258600
C	2.58477900	1.30046100	1.57892600
H	2.13406100	1.63984600	-1.34576800
H	2.09936200	0.80038200	2.40814100
N	2.57594400	-0.63152400	0.10018900
N	2.09304700	-1.51873900	1.03622200
C	2.99028100	-2.06965700	1.92558600
O	4.19386100	-2.06895300	1.73100200
H	1.04932400	-1.41835200	1.18176700
C	2.36341200	-2.66741100	3.14398000
C	3.02720200	-3.72687500	3.76588500
C	1.17290600	-2.17093700	3.68125600
C	2.48537700	-4.31202800	4.90468900
H	3.95864700	-4.08538100	3.33923800
C	0.64846300	-2.74246800	4.83753600

H	0.64244500	-1.35533600	3.19856000
C	1.29660600	-3.81686700	5.44315800
H	2.99097500	-5.14680700	5.37866600
H	-0.27193200	-2.35283100	5.25937400
H	0.87871000	-4.26743500	6.33774000

TSIV-3

Value of imaginary frequency = -1081.8 cm^{-1}

C	-6.69485000	-2.52971600	-2.03220200
C	-5.46933400	-2.51605800	-1.41564300
C	-4.97771000	-1.33367000	-0.79649300
C	-5.77109300	-0.15465200	-0.87268100
C	-7.04244700	-0.20394000	-1.50530300
C	-7.50045600	-1.36615900	-2.06782800
H	-7.04874500	-3.44119900	-2.50297800
C	-3.70849200	-1.27291500	-0.13148500
C	-5.26543400	1.06150300	-0.35105800
H	-7.63790800	0.70389200	-1.54139200
H	-8.47045200	-1.39625400	-2.55295000
C	-4.01500900	1.14538300	0.21369700
C	-3.25342000	-0.04950500	0.31576100
H	-5.87287800	1.95962700	-0.43008100
C	-2.84682300	-2.47784900	0.00692500
C	-3.30384200	-3.67610800	0.64629400
C	-1.56299600	-2.44744400	-0.49946200
C	-2.46940000	-4.82785600	0.62653600
C	-4.54534800	-3.75152900	1.33446200
C	-0.72791000	-3.59679000	-0.56242300
C	-2.91281100	-6.02360400	1.25249700
C	-1.20682000	-4.76311200	-0.01377200
C	-4.94054100	-4.91602500	1.94305400
H	-5.17589800	-2.87044900	1.38470200
C	-4.12242900	-6.07039600	1.89491400
H	-2.26739800	-6.89672900	1.21990200
H	-0.59412900	-5.66009200	-0.05666700
H	-5.88736000	-4.95235200	2.47200600
H	-4.45200400	-6.98528000	2.37609000
O	-1.07614800	-1.25836200	-1.01303200
H	-4.86036600	-3.41279400	-1.40782900
O	-2.02993000	0.02064600	0.94917500
P	-0.65059700	-0.12895200	0.09352500
O	0.38667500	-0.62607100	1.03835300
O	-0.41634800	1.12185800	-0.73978300
C	-3.48582500	2.46178600	0.66957500
C	-3.27971400	3.48174600	-0.28352400
C	-3.26328000	2.71137400	2.03855900
C	-3.40950400	3.26400700	-1.69606900
C	-2.91291900	4.79854600	0.15827900
C	-2.84670500	4.01939700	2.46086400
C	-3.46044900	1.71267000	3.04765700

C	-3.23683700	4.28389600	-2.58546800
H	-3.63472100	2.26596700	-2.05448700
C	-2.76353600	5.84562600	-0.80636300
C	-2.70824000	5.03645500	1.51654200
C	-2.60108800	4.26120300	3.85047800
H	-3.80297300	0.72681000	2.75159600
C	-3.22020600	1.98270600	4.36295900
C	-2.92605900	5.60171100	-2.13681800
H	-3.33261700	4.09265400	-3.64947900
H	-2.50643000	6.83880300	-0.44816800
H	-2.42510000	6.03393500	1.84500000
C	-2.77397900	3.27418200	4.77397400
H	-2.27700400	5.25467000	4.14944900
H	-3.37003400	1.20959800	5.10952700
H	-2.80586000	6.40048400	-2.86155900
H	-2.58404200	3.46578100	5.82504800
C	0.59702700	-3.58645700	-1.24792700
C	0.66441500	-3.36802700	-2.64149700
C	1.76420400	-3.90455500	-0.52188200
C	-0.48643800	-3.04524600	-3.43321800
C	1.92577400	-3.49236100	-3.31772700
C	3.01315100	-4.05909800	-1.21873600
C	1.77300900	-4.06666600	0.90468500
C	-0.38016100	-2.82170200	-4.77512200
H	-1.45765600	-2.97686700	-2.95544100
C	1.99517200	-3.25028700	-4.72663000
C	3.06425300	-3.85183800	-2.59590000
C	4.18969900	-4.41616700	-0.48418400
H	0.85589000	-3.89180200	1.45641800
C	2.91494600	-4.41160100	1.56672900
C	0.88032100	-2.91636000	-5.43518500
H	-1.26499800	-2.57107600	-5.35107800
H	2.96138900	-3.34105400	-5.21522100
H	4.01258400	-3.96338700	-3.11665000
C	4.14198800	-4.60157100	0.86386800
H	5.11990000	-4.53605200	-1.03266700
H	2.90574400	-4.51542800	2.64755900
H	0.94196300	-2.73075400	-6.50244400
H	5.03541400	-4.87454200	1.41619700
C	5.10506300	1.84902400	-1.55011100
C	4.09137700	2.80848000	-1.63926800
C	4.41445600	4.15572800	-1.71468600
C	5.75881600	4.53699500	-1.67071200
C	6.75869500	3.57202900	-1.55932000

C	6.44594600	2.21378600	-1.50086400
C	3.16470300	0.64422100	-1.25805800
C	2.73749300	2.10729200	-1.66847400
H	3.63802500	4.91064200	-1.79084600
H	6.02271800	5.58806400	-1.71735000
H	7.79915200	3.87907300	-1.51761100
H	7.22296900	1.46097000	-1.41586200
H	5.07579300	-0.12281200	-1.00021000
N	4.57784100	0.55016100	-1.57827400
C	2.37218900	-0.50181400	-1.85437100
H	2.61916800	-1.43230800	-1.33695200
H	1.29732000	-0.32942700	-1.77693000
H	2.63412400	-0.61657900	-2.90761500
C	2.10318100	2.15360100	-3.05993800
H	2.72784600	1.60239700	-3.76865600
H	1.10114800	1.71580200	-3.05183000
H	2.03732000	3.18052000	-3.42339000
C	0.32385600	6.43217400	0.47862900
C	0.53240500	5.48722200	1.46202500
C	1.03308900	4.21288500	1.13594500
C	1.32933000	3.88866800	-0.21246200
C	1.06043000	4.84738100	-1.20166000
C	0.58146200	6.10073300	-0.85900000
H	0.98866200	3.52267900	3.19004300
H	-0.05300700	7.41721500	0.73410100
H	0.31244100	5.71191700	2.50249700
C	1.27253800	3.24727100	2.17735600
C	1.82135800	2.53404200	-0.49781500
H	1.23761600	4.61229900	-2.24400500
H	0.39605700	6.83153200	-1.63988100
C	2.24176300	1.74662700	0.61996800
C	1.85425300	2.03822500	1.95627600
H	0.70598400	1.85315000	-0.61190700
H	2.06612000	1.34058300	2.75639700
N	2.96102100	0.69498500	0.22434500
N	3.07785300	-0.41298800	1.02866700
C	4.26478500	-0.71543900	1.64105600
O	5.33710200	-0.26816900	1.26167400
H	2.18121000	-0.86093700	1.23445500
C	4.13668000	-1.63504900	2.81266800
C	5.25801400	-2.38104800	3.17959200
C	2.95814000	-1.72938700	3.55887500
C	5.19574400	-3.23760200	4.27263000
H	6.16555000	-2.28371700	2.59245300

C	2.90538700	-2.57195600	4.66568300
H	2.07959700	-1.14948300	3.28905300
C	4.02005600	-3.33076100	5.01824600
H	6.06354200	-3.82711300	4.54926800
H	1.99373500	-2.63643000	5.24992200
H	3.97539600	-3.99175600	5.87778700

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C	-7.08363500	-1.36335500	-2.11669700
C	-5.87827800	-1.56756700	-1.49362500
C	-5.20984200	-0.49901900	-0.83432700
C	-5.79975600	0.79510000	-0.88358500
C	-7.05547600	0.97166900	-1.52456400
C	-7.69046700	-0.08496600	-2.12136900
H	-7.57494800	-2.19096000	-2.61765800
C	-3.95570800	-0.66038100	-0.15526500
C	-5.10600600	1.90305000	-0.33893400
H	-7.49299800	1.96567800	-1.54053000
H	-8.64810500	0.05625000	-2.61100200
C	-3.86568800	1.77212500	0.23823300
C	-3.32776100	0.46417800	0.33386600
H	-5.55016600	2.89171000	-0.42017200
C	-3.29044000	-1.98745700	-0.05658600
C	-3.93785700	-3.12966500	0.51820600
C	-2.01073300	-2.14263600	-0.54765000
C	-3.29507800	-4.39598000	0.43854500
C	-5.18218100	-3.04061800	1.19850200
C	-1.36115800	-3.39887400	-0.66973200
C	-3.92991800	-5.53738000	0.99726900
C	-2.02924800	-4.50094800	-0.19028700
C	-5.76261300	-4.15789100	1.74361700
H	-5.66439600	-2.07398400	1.29556200
C	-5.13790700	-5.42366000	1.63377100
H	-3.43126400	-6.49896800	0.91746300
H	-1.56698000	-5.48063200	-0.28026500
H	-6.70839700	-4.07092900	2.26819900
H	-5.61390700	-6.29825300	2.06430100
O	-1.31724000	-1.01029800	-0.98808400
H	-5.42438200	-2.55154400	-1.51305800
O	-2.11413200	0.32162400	0.99983900
P	-0.78230800	-0.05695700	0.19255700
O	0.22102100	-0.63122800	1.10711500
O	-0.36934700	1.21004800	-0.65363400
C	-3.10953700	2.98217400	0.66898800
C	-2.69897100	3.90363200	-0.31813800
C	-2.86528600	3.23855200	2.03139300
C	-2.83172500	3.64942300	-1.72407300
C	-2.10267900	5.14693300	0.08264500
C	-2.23242200	4.46984700	2.41544300
C	-3.24456800	2.32515200	3.06832900
C	-2.43444400	4.57160400	-2.64738900

H	-3.23983600	2.70006000	-2.05198000
C	-1.72068600	6.09692200	-0.91732300
C	-1.89647100	5.40501400	1.43712700
C	-1.97363100	4.71976800	3.80123300
H	-3.74790700	1.40248400	2.79798500
C	-2.97961400	2.59892100	4.37805100
C	-1.88186600	5.82250800	-2.24193000
H	-2.53406300	4.35179300	-3.70546600
H	-1.28640900	7.03720200	-0.58989300
H	-1.45148000	6.35186400	1.73455400
C	-2.32711700	3.81140800	4.75385600
H	-1.48837100	5.65356300	4.07307600
H	-3.26911300	1.89067300	5.14763400
H	-1.58079200	6.54495100	-2.99366700
H	-2.12382700	4.00710700	5.80154900
C	-0.03819700	-3.55087300	-1.34176300
C	0.07789800	-3.27818800	-2.72203500
C	1.06211000	-4.05673800	-0.61977600
C	-1.01141300	-2.77907300	-3.50867400
C	1.32382800	-3.53087300	-3.39053600
C	2.29413200	-4.33134700	-1.30983000
C	1.02151100	-4.29249700	0.79519100
C	-0.85878300	-2.51363100	-4.83830200
H	-1.97569800	-2.61768800	-3.03883800
C	1.44481400	-3.23465900	-4.78558400
C	2.39477400	-4.06519400	-2.67416100
C	3.40780800	-4.85442800	-0.57719500
H	0.12032100	-4.04288900	1.34471900
C	2.10326800	-4.79737100	1.45487300
C	0.39066900	-2.73401200	-5.48930600
H	-1.69828800	-2.13395500	-5.41166700
H	2.40018000	-3.42084800	-5.26828500
H	3.33222700	-4.26529300	-3.18801300
C	3.31496200	-5.08985900	0.76106400
H	4.32845100	-5.05514000	-1.11791800
H	2.05943300	-4.95096800	2.52912700
H	0.49159200	-2.51044200	-6.54618600
H	4.16300400	-5.48273000	1.31301200
C	5.66243200	0.71914200	-1.32415100
C	4.96420800	1.92487700	-1.44238600
C	5.64395200	3.13146000	-1.48686800
C	7.03968800	3.12713600	-1.40277200
C	7.72806800	1.92120000	-1.27486200
C	7.05060500	0.70157400	-1.23424200

C	3.45475200	0.12615200	-1.06052900
C	3.47046300	1.63652600	-1.51851600
H	5.09991300	4.06934800	-1.56455700
H	7.58683700	4.06347800	-1.42702400
H	8.81119000	1.92765700	-1.20024700
H	7.58811200	-0.23540600	-1.12835000
H	5.05989500	-1.14127500	-0.74532100
N	4.78908500	-0.37958900	-1.36456000
C	2.36902400	-0.74543300	-1.66473200
H	2.32791200	-1.70496500	-1.14345500
H	1.39068100	-0.26441200	-1.58493000
H	2.57351200	-0.93783600	-2.71884300
C	2.94493300	1.81558600	-2.94625600
H	3.40704100	1.06995400	-3.59978200
H	1.85784000	1.70179900	-2.99365100
H	3.21189400	2.79626900	-3.34282500
C	1.46750500	6.35877600	0.21402800
C	1.32412800	5.42330700	1.20548100
C	1.70397500	4.07256300	1.00016100
C	2.25841600	3.67992800	-0.26037600
C	2.36327000	4.67045700	-1.27801800
C	1.98264900	5.96812000	-1.04447400
H	1.10941400	3.43722300	2.97831300
H	1.18759900	7.39294700	0.38808900
H	0.92761400	5.70134100	2.17859400
C	1.57387600	3.12026700	2.04815200
C	2.69816800	2.33438100	-0.40211400
H	2.76417000	4.39951800	-2.24679900
H	2.08465000	6.70621500	-1.83389200
C	2.63143300	1.47535400	0.68278700
C	2.03163600	1.83543900	1.91241000
H	0.46509100	1.63365200	-0.36766600
H	1.95314000	1.11016000	2.71414400
N	3.26576600	0.27254200	0.40478000
N	2.98608400	-0.82449900	1.18674900
C	3.98880100	-1.45954600	1.86198100
O	5.17256500	-1.31681700	1.58689000
H	2.00619400	-1.08558500	1.28249100
C	3.52894400	-2.34746400	2.97864400
C	4.42068000	-3.31378200	3.44784900
C	2.27208700	-2.21214900	3.57603100
C	4.05334400	-4.15510200	4.49210000
H	5.39581500	-3.39349800	2.97833300
C	1.90966800	-3.04902800	4.62768300

H	1.56932700	-1.45826600	3.23229500
C	2.79644900	-4.02287900	5.08357800
H	4.74605400	-4.90977500	4.84989200
H	0.93562500	-2.93781100	5.09229500
H	2.51113300	-4.67452000	5.90322700

$P1_{C1}$

C	1.24061600	-2.30360500	-0.85810500
C	2.19598900	-1.80914000	0.03823100
C	3.49022800	-2.30388700	0.01334700
C	3.84105600	-3.25867800	-0.94638600
C	2.89014800	-3.71521300	-1.85660800
C	1.57376900	-3.25097400	-1.81973300
C	0.00598700	-1.16522900	0.74991300
C	1.52677800	-0.80021900	0.95259000
H	4.22501300	-1.97635800	0.74402800
H	4.85189700	-3.65048700	-0.97480700
H	3.16872000	-4.45854600	-2.59721400
H	0.82731900	-3.63154400	-2.50970100
H	-0.79610100	-2.36856700	-0.77968900
N	-0.01911700	-1.73677400	-0.61368500
C	-0.60452500	-2.11732700	1.76027500
H	-0.59222800	-1.68205500	2.76045600
H	-1.64690700	-2.31657100	1.49294300
H	-0.05575800	-3.06372700	1.76178400
C	2.00157600	-0.85772200	2.40517900
H	3.03770600	-0.51477900	2.47513100
H	1.39039900	-0.20404100	3.03378600
H	1.95207200	-1.87789400	2.79525000
C	4.68424900	3.31802200	-0.54609000
C	3.37525600	3.71340400	-0.64843000
C	2.31510500	2.82861200	-0.31885700
C	2.62211200	1.50204700	0.11968700
C	3.98980000	1.12512200	0.21477700
C	4.99000400	2.00776200	-0.10699700
H	0.75435300	4.25964700	-0.75348500
H	5.48632000	4.00374400	-0.79809100
H	3.12577200	4.71756200	-0.98098400
C	0.96001400	3.24789800	-0.41525400
C	1.54009700	0.63870300	0.42887800
H	4.24065000	0.12400900	0.54171100
H	6.02724600	1.69840100	-0.02549000
C	0.24998300	1.10550600	0.34420500
C	-0.07279700	2.40890500	-0.08503700
H	-1.10958400	2.72268500	-0.14598400
N	-0.67640000	0.13791600	0.78223600
N	-1.91091500	0.17377400	0.16403200
C	-3.06588400	0.16144700	0.90165900
O	-3.08332600	0.07370100	2.11726600
H	-1.93127900	-0.01158300	-0.83441200

C	-4.31990900	0.26287200	0.08535000
C	-4.35978600	0.90672100	-1.15424400
C	-5.48817600	-0.27697300	0.62705100
C	-5.56068300	0.99360200	-1.85299600
H	-3.46662300	1.36910700	-1.56413500
C	-6.68428300	-0.19646700	-0.07671700
H	-5.43838300	-0.75413500	1.60028800
C	-6.72043800	0.43753600	-1.31811800
H	-5.59191200	1.50326700	-2.81020000
H	-7.58944500	-0.62335700	0.34230800
H	-7.65532300	0.50488100	-1.86511400

ent-**P1**$_{C1}$

C	-1.24142800	-2.30378800	-0.85812900
C	-2.19656600	-1.80891600	0.03824800
C	-3.49097800	-2.30319800	0.01353100
C	-3.84224000	-3.25797000	-0.94606700
C	-2.89157000	-3.71492600	-1.85632500
C	-1.57502500	-3.25114100	-1.81962500
C	-0.00627600	-1.16562000	0.74965700
C	-1.52693500	-0.80013900	0.95245500
H	-4.22557500	-1.97532800	0.74424700
H	-4.85322200	-3.64942300	-0.97435900
H	-3.17047100	-4.45823200	-2.59683600
H	-0.82878800	-3.63203800	-2.50964400
H	0.79530800	-2.36927200	-0.78001000
N	0.01847200	-1.73733900	-0.61388600
C	0.60409900	-2.11777900	1.76005500
H	0.59206300	-1.68231900	2.76016200
H	1.64639600	-2.31731300	1.49260000
H	0.05510100	-3.06403700	1.76177900
C	-2.00158500	-0.85739400	2.40510300
H	-3.03761700	-0.51418100	2.47516200
H	-1.39016900	-0.20381800	3.03358900
H	-1.95229100	-1.87754500	2.79525000
C	-4.68330500	3.31901400	-0.54595300
C	-3.37421200	3.71402500	-0.64839000
C	-2.31427700	2.82891400	-0.31894500
C	-2.62163500	1.50242100	0.11958100
C	-3.98942900	1.12587600	0.21474800
C	-4.98940200	2.00881100	-0.10690300
H	-0.75314200	4.25950900	-0.75363500
H	-5.48520300	4.00497800	-0.79785000
H	-3.12446900	4.71812000	-0.98094100
C	-0.95908100	3.24780700	-0.41543700
C	-1.53986300	0.63875600	0.42866500
H	-4.24052200	0.12480500	0.54163200
H	-6.02672800	1.69974700	-0.02533100
C	-0.24960700	1.10517600	0.34386000
C	0.07352000	2.40848600	-0.08535200
H	1.11038600	2.72200700	-0.14633700
N	0.67647100	0.13728100	0.78177500
N	1.91108800	0.17268500	0.16384400
C	3.06592100	0.16109400	0.90167100
O	3.08319200	0.07380600	2.11730500
H	1.93165700	-0.01214200	-0.83468600

C	4.32004000	0.26256400	0.08548300
C	4.36003600	0.90652200	-1.15403700
C	5.48822800	-0.27739800	0.62726300
C	5.56099500	0.99339700	-1.85268300
H	3.46687600	1.36896900	-1.56387600
C	6.68439100	-0.19689500	-0.07639900
H	5.43831000	-0.75461000	1.60046400
C	6.72066800	0.43721100	-1.31775300
H	5.59235100	1.50312500	-2.80984800
H	7.58951600	-0.62385400	0.34262900
H	7.65559300	0.50455900	-1.86467500

COMI'

C	5.21660700	5.00263300	0.83659700
C	4.58359000	3.93167400	0.25812000
C	3.17972400	3.75838400	0.39680000
C	2.45012300	4.70346700	1.17086400
C	3.13305300	5.80742000	1.74743200
C	4.48509700	5.95767400	1.58271100
H	6.29010200	5.11681600	0.72674600
C	2.47881400	2.64930700	-0.17723600
C	1.05462400	4.53043200	1.35914700
H	2.56051200	6.52432000	2.32887000
H	5.00021400	6.80046100	2.03138700
C	0.38428000	3.44013700	0.85993300
C	1.14146900	2.49680600	0.11903400
H	0.50289600	5.28004400	1.92047300
C	3.13314800	1.64858500	-1.06272500
C	3.76704300	2.02215500	-2.29407800
C	3.05718700	0.31008900	-0.74524400
C	4.36639200	1.01006500	-3.09557600
C	3.78663000	3.36093000	-2.77251200
C	3.63630800	-0.71506400	-1.53830700
C	5.00825800	1.36732600	-4.31106600
C	4.29410000	-0.34520100	-2.68480900
C	4.40324900	3.67348900	-3.95787000
H	3.29825100	4.13919200	-2.19704200
C	5.03320400	2.67071500	-4.73262600
H	5.47065700	0.58233300	-4.90240800
H	4.75756700	-1.10981600	-3.30301300
H	4.40324100	4.70040700	-4.30820500
H	5.52289000	2.93617200	-5.66355900
O	2.41362500	-0.07347600	0.43009300
H	5.15446700	3.19960600	-0.30309400
O	0.48795300	1.35630900	-0.35047600
P	0.80266100	0.02223700	0.50374000
O	0.21411700	-1.07801600	-0.44641000
O	0.31106200	0.01809600	1.89401500
H	-0.20242400	-1.86108100	0.04045200
C	-1.09653900	3.31574900	1.01815500
C	-1.65611100	2.85047600	2.22225100
C	-1.92410000	3.77536600	-0.02639600
C	-0.85530100	2.40529000	3.32487100
C	-3.08577800	2.82224800	2.37120400
C	-3.34869900	3.77399400	0.14807400
C	-1.40058500	4.26698800	-1.26603400

C	-1.43307500	1.96662000	4.48011800
H	0.22375900	2.40747400	3.21981300
C	-3.65108200	2.33524600	3.59341300
C	-3.89531400	3.28430200	1.33467400
C	-4.18141600	4.28200500	-0.89736700
H	-0.32634500	4.26976600	-1.42153700
C	-2.23005200	4.73968800	-2.24227900
C	-2.85331800	1.92842300	4.62069200
H	-0.80822800	1.63291900	5.30264400
H	-4.73411400	2.30008900	3.67803500
H	-4.97652200	3.26287100	1.45317700
C	-3.64290500	4.75836700	-2.05542600
H	-5.25724000	4.26946100	-0.74540600
H	-1.81136500	5.11191300	-3.17217700
H	-3.28961900	1.56327000	5.54515100
H	-4.28344000	5.14209000	-2.84290500
C	3.55289500	-2.13889300	-1.10672400
C	4.40359600	-2.58963000	-0.07978900
C	2.65307800	-3.02214500	-1.73183700
C	5.37703300	-1.73570900	0.53557700
C	4.30760600	-3.94783900	0.37442800
C	2.57156300	-4.38290000	-1.27469800
C	1.81619200	-2.62508700	-2.82733000
C	6.17621900	-2.19523200	1.54261600
H	5.47467300	-0.71266700	0.18707100
C	5.15531200	-4.38522300	1.44110100
C	3.38656200	-4.80837900	-0.22478600
C	1.66018100	-5.28083900	-1.91891700
H	1.85737600	-1.59759800	-3.17240700
C	0.99036500	-3.52287900	-3.43797900
C	6.05891200	-3.53781100	2.01088100
H	6.90861700	-1.53470700	1.99522100
H	5.06117200	-5.41112700	1.78568800
H	3.31144700	-5.83508300	0.12573400
C	0.90087200	-4.87028600	-2.97298600
H	1.60105300	-6.30221600	-1.55373900
H	0.38207000	-3.21192300	-4.28170000
H	6.69694700	-3.87946700	2.81912400
H	0.22177700	-5.56058800	-3.46250200
C	-3.23782900	0.25660100	0.07878300
C	-4.63461200	0.21085000	0.30908000
C	-5.50635700	0.68313000	-0.68368900
C	-4.97305900	1.15618700	-1.87198800
C	-3.58174400	1.16795500	-2.08976000

C	-2.69577500	0.71851000	-1.12380100
C	-3.58429100	-0.63696300	2.11308800
C	-4.83405600	-0.36929900	1.61101900
H	-6.58264000	0.65572300	-0.53022700
H	-5.63508500	1.51754700	-2.65374600
H	-3.19453200	1.54420000	-3.03221200
H	-1.62357800	0.72481800	-1.28885000
H	-1.65037600	-0.14763300	1.45140100
N	-2.62401200	-0.27337500	1.18964000
C	-3.15449700	-1.26841800	3.39644300
H	-3.88628200	-1.08683200	4.18657600
H	-3.03403900	-2.35203800	3.27835200
H	-2.19528400	-0.85170100	3.72261500
C	-6.15864200	-0.62770100	2.25675700
H	-6.74826100	-1.36200700	1.69448000
H	-6.04079900	-1.00986900	3.27392400
H	-6.75782600	0.28864300	2.31076100
C	-5.82524800	-1.56854700	-4.43856600
C	-4.46027800	-1.68867400	-4.33377300
C	-3.86596600	-2.09316100	-3.11405800
C	-4.70683100	-2.36134400	-1.99717300
C	-6.11309500	-2.22694100	-2.13297100
C	-6.66175200	-1.84459500	-3.33051200
H	-1.82876800	-2.09103100	-3.85179800
H	-6.27022000	-1.25934100	-5.37913400
H	-3.81987700	-1.47808200	-5.18559200
C	-2.45650800	-2.26638300	-2.98238600
C	-4.11341100	-2.76583200	-0.78075100
H	-6.74172600	-2.43061700	-1.27029100
H	-7.73732700	-1.74506000	-3.43260700
C	-2.74085900	-2.88729000	-0.67579000
C	-1.89786400	-2.65770200	-1.80083400
H	-4.72524600	-2.96402500	0.09499000
H	-0.83085700	-2.83143900	-1.72757500
N	-2.29248000	-3.28950100	0.58390400
N	-1.07891600	-3.12812500	0.85432200
C	-0.79133800	-3.69547700	2.17789200
O	-1.54997000	-4.47753800	2.69845400
C	0.45617400	-3.23249000	2.82741100
C	0.48336500	-3.29321800	4.22698500
C	1.57041600	-2.76681900	2.12561200
C	1.60492500	-2.86634300	4.92225900
H	-0.39098200	-3.66739500	4.74924500
C	2.69457100	-2.34301800	2.82892800

H	1.57976000	-2.74664800	1.03745700
C	2.71113500	-2.38814400	4.21977800
H	1.61821900	-2.90248300	6.00637600
H	3.55415100	-1.96401100	2.28902500
H	3.59131400	-2.05005000	4.75788700

TSI'-1

Value of imaginary frequency = -231.8 cm^{-1}

C	5.80815700	4.11049500	1.71320200
C	5.08971000	3.22674600	0.94752200
C	3.66974700	3.27523300	0.92248700
C	3.00799500	4.24546000	1.72582200
C	3.77980700	5.15375500	2.49774100
C	5.14938000	5.09174800	2.49183400
H	6.89176300	4.05384100	1.72719600
C	2.88154300	2.36047300	0.15286600
C	1.58920100	4.29875000	1.73412400
H	3.26026000	5.89500500	3.09845800
H	5.73164900	5.78586000	3.08875100
C	0.82846900	3.39062700	1.04020200
C	1.50951000	2.38955500	0.29383300
H	1.09571500	5.08320800	2.30249100
C	3.46482600	1.37982500	-0.80176900
C	4.25909600	1.80033400	-1.91934800
C	3.14166000	0.04297900	-0.67720800
C	4.76224000	0.81780600	-2.81797100
C	4.53656200	3.16796700	-2.19740900
C	3.61727800	-0.94507000	-1.58628500
C	5.56227800	1.21828500	-3.92120500
C	4.42908700	-0.54561700	-2.61800800
C	5.30339100	3.52565500	-3.27761400
H	4.12658300	3.93489000	-1.55010100
C	5.83512700	2.54223100	-4.14549000
H	5.94438800	0.45146200	-4.58917600
H	4.81315200	-1.28915500	-3.31193600
H	5.49923700	4.57498600	-3.47325500
H	6.44365700	2.84075400	-4.99259800
O	2.37318700	-0.36510200	0.39388000
H	5.60111500	2.47013500	0.36144800
O	0.76135100	1.42467000	-0.34696800
P	0.75179500	-0.05418500	0.39855700
O	0.03100300	-0.99429500	-0.51681000
O	0.29721500	0.08611300	1.81580600
H	-0.70764100	-2.48499700	0.38605500
C	-0.65824800	3.53875700	0.96887200
C	-1.48753500	3.12520000	2.02769800
C	-1.21336800	4.17621000	-0.16072400
C	-0.97639600	2.45212100	3.18602000
C	-2.90409200	3.36298200	1.95409100
C	-2.62699000	4.42275200	-0.21483700

C	-0.41899100	4.58615300	-1.28176300
C	-1.81034900	2.05176300	4.18947800
H	0.08430500	2.23566200	3.23353000
C	-3.74412800	2.91929100	3.02568600
C	-3.43848500	4.00952800	0.84110000
C	-3.18228100	5.06777500	-1.36442600
H	0.65192400	4.41150600	-1.26203200
C	-0.98850500	5.18767300	-2.36680500
C	-3.21594500	2.28943300	4.11330700
H	-1.40421200	1.53864400	5.05572000
H	-4.81273500	3.10383100	2.95033000
H	-4.51121000	4.18271500	0.78869400
C	-2.39206300	5.43873100	-2.41083600
H	-4.25459400	5.24260100	-1.38575900
H	-0.36834700	5.48438100	-3.20665100
H	-3.85922500	1.95855000	4.92289900
H	-2.82316700	5.92176300	-3.28171000
C	3.26009300	-2.38131100	-1.39692200
C	4.08984100	-3.19382000	-0.60280800
C	2.11174200	-2.91598000	-2.01035900
C	5.30098900	-2.70305200	-0.01106000
C	3.71458700	-4.55641800	-0.34988200
C	1.74293400	-4.27960000	-1.74794400
C	1.29172000	-2.15306800	-2.90405700
C	6.06330800	-3.50124700	0.79115200
H	5.60066600	-1.67855100	-0.20632800
C	4.54006700	-5.35745600	0.50146100
C	2.54345600	-5.06233400	-0.91439300
C	0.55693400	-4.80846500	-2.35264100
H	1.55914600	-1.12064900	-3.10325100
C	0.19148000	-2.70469900	-3.49028600
C	5.67474300	-4.84796400	1.05968400
H	6.97580400	-3.11219300	1.23144600
H	4.23628100	-6.38243200	0.69575900
H	2.25253200	-6.08956600	-0.70632100
C	-0.19323500	-4.04880800	-3.19974800
H	0.27926600	-5.83465100	-2.12828400
H	-0.41347600	-2.11294100	-4.17059000
H	6.29157200	-5.46354400	1.70630100
H	-1.08798200	-4.45927900	-3.65718100
C	-3.01523500	0.75991900	-0.07435100
C	-4.41936600	0.64345200	-0.09889400
C	-5.13708000	1.11347700	-1.19636300
C	-4.42834800	1.67616500	-2.25631900

C	-3.03206400	1.75738500	-2.22574400
C	-2.29843700	1.29787700	-1.13460900
C	-3.61752200	-0.24823400	1.84122500
C	-4.80823300	-0.09487400	1.08773200
H	-6.21934500	1.01872500	-1.23613100
H	-4.96673900	2.04696600	-3.12327100
H	-2.50402800	2.20614100	-3.06137000
H	-1.21957500	1.36316000	-1.12137300
H	-1.59936900	0.18063000	1.45802900
N	-2.57683700	0.20699500	1.13143700
C	-3.42604500	-0.93013900	3.14578300
H	-4.23321400	-0.68050600	3.83806300
H	-3.41670600	-2.01867800	2.99103000
H	-2.47034500	-0.64017400	3.58928000
C	-6.18985300	-0.15053800	1.65870200
H	-6.93211300	-0.26657700	0.86413200
H	-6.30730400	-0.97740800	2.36508900
H	-6.42232300	0.78031200	2.18790100
C	-7.17767100	-1.61130400	-3.29076300
C	-5.80248500	-1.53229700	-3.43239100
C	-4.95729100	-1.73616300	-2.33116000
C	-5.53584200	-2.02618100	-1.06835400
C	-6.93738900	-2.12362100	-0.94782000
C	-7.75056600	-1.91447500	-2.04574100
H	-3.10869300	-1.42718400	-3.44437400
H	-7.81824000	-1.44800700	-4.15143000
H	-5.36241000	-1.31035800	-4.40020400
C	-3.51296500	-1.69762100	-2.47291800
C	-4.66950400	-2.21844900	0.05476400
H	-7.36744600	-2.38535700	0.01470300
H	-8.82773800	-1.99510400	-1.94900900
C	-3.25196500	-2.38953000	-0.17408000
C	-2.68217500	-2.00725200	-1.45566500
H	-5.06530100	-2.65389700	0.96789000
H	-1.60447100	-1.97712700	-1.57567800
N	-2.65206000	-2.91444600	0.86718100
N	-1.34780600	-3.03792400	0.98349500
C	-0.95303500	-3.69056500	2.17567600
O	-1.79118500	-4.24367400	2.85798000
C	0.47902200	-3.64055600	2.57463400
C	0.77437500	-4.20399400	3.82347400
C	1.49060800	-3.02920800	1.83249900
C	2.06169000	-4.14239600	4.33518800
H	-0.02679400	-4.67646100	4.37990400

C	2.77281200	-2.93756900	2.36866300
H	1.30690700	-2.61901400	0.84284300
C	3.06167500	-3.49469300	3.60974000
H	2.28221400	-4.58393300	5.30147300
H	3.54512200	-2.42581200	1.80800400
H	4.06817700	-3.42348700	4.01059400

IMI'-1

C	-5.87363500	3.95549200	-1.81756800
C	-5.12154300	3.12303700	-1.02711400
C	-3.71086400	3.27698200	-0.94604300
C	-3.09448700	4.29724500	-1.72322000
C	-3.90149200	5.15160900	-2.52046000
C	-5.26173100	4.98859300	-2.56658800
H	-6.94851500	3.81739800	-1.87412900
C	-2.88465500	2.42060000	-0.14717400
C	-1.68343400	4.44871800	-1.68943900
H	-3.41532400	5.93196200	-3.09912700
H	-5.87126200	5.64100300	-3.18292200
C	-0.88278400	3.59497100	-0.97255500
C	-1.51560900	2.55523200	-0.23438700
H	-1.22819400	5.26262500	-2.24827500
C	-3.44345600	1.38213900	0.76164700
C	-4.33688400	1.72373800	1.82890500
C	-3.04600100	0.06692400	0.61823800
C	-4.86725200	0.68451800	2.64245900
C	-4.69283200	3.06666400	2.13488500
C	-3.57224800	-0.98573000	1.42157200
C	-5.76427200	1.00639900	3.69570200
C	-4.47876900	-0.65683800	2.39953400
C	-5.55352500	3.34806200	3.16580500
H	-4.26599200	3.87470800	1.55099700
C	-6.10700100	2.30836800	3.95069300
H	-6.16569100	0.19745400	4.29962900
H	-4.90523000	-1.44667700	3.01295300
H	-5.80761600	4.37971000	3.38695600
H	-6.78966400	2.54737300	4.75934200
O	-2.16684700	-0.25595500	-0.39569100
H	-5.59963500	2.32763000	-0.46534100
O	-0.72345800	1.64816900	0.44481100
P	-0.58305200	0.17796600	-0.29788000
O	0.19075900	-0.71836800	0.60622300
O	-0.09673300	0.38413200	-1.70845500
H	0.80164900	-2.63289200	-0.18039100
C	0.59062000	3.83535600	-0.87413800
C	1.47515100	3.41427300	-1.88501000
C	1.07815900	4.54335700	0.24547300
C	1.03445200	2.69860400	-3.04851500
C	2.88110800	3.69451000	-1.75888300
C	2.47808000	4.84914400	0.33997400
C	0.22583400	4.96422100	1.31868600

C	1.92537500	2.26598100	-3.98693600
H	-0.02077600	2.47559800	-3.14925300
C	3.78384300	3.21531900	-2.76340900
C	3.34674600	4.41436400	-0.66107300
C	2.96432900	5.56031800	1.48181700
H	-0.83513000	4.74284000	1.26679500
C	0.72978400	5.63146500	2.39760800
C	3.32382000	2.52075100	-3.84249100
H	1.57254400	1.71739700	-4.85468300
H	4.84276400	3.43091600	-2.64599900
H	4.41045900	4.62372000	-0.57196400
C	2.11997500	5.93884400	2.48295800
H	4.02696000	5.78081700	1.53441600
H	0.06754800	5.93622000	3.20144500
H	4.01470000	2.16835200	-4.60287500
H	2.49779900	6.47289100	3.34873100
C	-3.20946000	-2.41692400	1.18648400
C	-4.07898900	-3.22861200	0.43400800
C	-2.04324600	-2.96395300	1.75761100
C	-5.28707800	-2.72636500	-0.15444700
C	-3.75047000	-4.61080900	0.21672000
C	-1.69981800	-4.33352400	1.49167300
C	-1.19220500	-2.21509000	2.63151500
C	-6.11173500	-3.54135300	-0.87376700
H	-5.53966200	-1.67973800	-0.01942900
C	-4.64913000	-5.43374700	-0.53435700
C	-2.55761900	-5.12195500	0.72323800
C	-0.49339500	-4.87033300	2.04336500
H	-1.44559100	-1.18299800	2.84726800
C	-0.07694800	-2.77779200	3.17963100
C	-5.79647200	-4.92089000	-1.06005200
H	-7.02178700	-3.14020800	-1.30866600
H	-4.38479000	-6.47720000	-0.68371800
H	-2.29645300	-6.15955600	0.52671300
C	0.29390400	-4.11875000	2.86468700
H	-0.23092800	-5.89713100	1.80355000
H	0.55084200	-2.19302100	3.84551100
H	-6.46963700	-5.55164400	-1.63167700
H	1.20467600	-4.53451400	3.28418700
C	3.06461000	0.92578200	0.09176300
C	4.40261300	0.54462700	0.14933600
C	5.20062800	0.98999500	1.19001900
C	4.60753100	1.77642500	2.18268700
C	3.24887200	2.09025200	2.13546000

C	2.44263900	1.66992400	1.07644800
C	3.38328400	-0.29261200	-1.77213100
C	4.67362000	-0.41396700	-0.98411200
H	6.24977100	0.71550500	1.25020700
H	5.21146800	2.13683800	3.00892600
H	2.80863300	2.69579500	2.92143900
H	1.39170900	1.92503000	1.02796500
H	1.50497000	0.51984400	-1.43583400
N	2.51624700	0.40834300	-1.11682500
C	3.09534600	-0.90231700	-3.08970700
H	3.68609300	-0.38648700	-3.85502400
H	3.38260700	-1.95658100	-3.07696700
H	2.03442000	-0.80999100	-3.32980500
C	5.89973600	-0.07133000	-1.83076200
H	6.79304200	-0.05366000	-1.20283400
H	6.04587700	-0.80863500	-2.62557300
H	5.77799500	0.91745400	-2.28168600
C	7.60809500	-2.10155000	2.78199800
C	6.24920300	-1.98926800	3.05825200
C	5.30943600	-1.96309200	2.02384200
C	5.75182800	-2.04060300	0.68816500
C	7.11199200	-2.17886600	0.42240800
C	8.04079000	-2.20599400	1.46220300
H	3.59114300	-1.67550000	3.35074900
H	8.32672900	-2.11905500	3.59474100
H	5.90412800	-1.92367200	4.08645700
C	3.87598100	-1.86438600	2.31856000
C	4.73955200	-1.92257500	-0.42512200
H	7.44868800	-2.27247800	-0.60655800
H	9.09741000	-2.31269900	1.24036100
C	3.36013200	-2.37585800	0.01799600
C	2.93129400	-2.03878300	1.37765500
H	5.03300300	-2.54167000	-1.27908600
H	1.87319800	-1.98724600	1.61224300
N	2.70656000	-3.02062600	-0.87954200
N	1.37871200	-3.29562200	-0.70518700
C	0.85922600	-4.21484700	-1.59874300
O	1.58106500	-5.04448300	-2.12897900
C	-0.58702100	-4.10687900	-1.96034100
C	-1.12791100	-5.12339600	-2.75445200
C	-1.34380100	-2.96984700	-1.68750000
C	-2.40391500	-4.98726000	-3.28619000
H	-0.52120800	-5.99728000	-2.96583300
C	-2.60891500	-2.81896600	-2.24719500

H	-0.96453000	-2.20416500	-1.02588700
C	-3.13711300	-3.82281000	-3.05232400
H	-2.82198400	-5.77911900	-3.89976400
H	-3.17491100	-1.91812800	-2.03584100
H	-4.12871400	-3.70884200	-3.47947300

TSI'-2

Value of imaginary frequency = -93.9 cm^{-1}

C	-5.37526900	-4.90868100	1.57996900
C	-4.82166800	-3.85340900	0.89940100
C	-3.41799200	-3.78582200	0.67935700
C	-2.60330400	-4.82044000	1.21335800
C	-3.20610100	-5.90830500	1.89985800
C	-4.56393200	-5.95662800	2.07687500
H	-6.44748600	-4.93771900	1.74464900
C	-2.78775500	-2.70239100	-0.01763200
C	-1.19790400	-4.73990800	1.06412700
H	-2.56514400	-6.69412900	2.28952000
H	-5.01969500	-6.78699700	2.60588500
C	-0.58733900	-3.66796900	0.45685000
C	-1.41282100	-2.63471600	-0.06559600
H	-0.58212900	-5.54502200	1.45732600
C	-3.59570400	-1.62225000	-0.63391600
C	-4.58694900	-1.92370600	-1.62225400
C	-3.41163300	-0.31356000	-0.22716600
C	-5.46749400	-0.89410600	-2.04542200
C	-4.71888400	-3.21059400	-2.21382100
C	-4.32912900	0.71553700	-0.59465600
C	-6.46885300	-1.17631500	-3.01298200
C	-5.33618900	0.39416200	-1.47782500
C	-5.68600700	-3.45218600	-3.15678800
H	-4.03577700	-4.00118700	-1.92211500
C	-6.57887100	-2.42865600	-3.55752600
H	-7.13788100	-0.37586500	-3.31615800
H	-6.05842300	1.15869000	-1.75243700
H	-5.76630400	-4.43737200	-3.60479200
H	-7.34136600	-2.63784700	-4.30050700
O	-2.40217100	-0.01511800	0.66148800
H	-5.45675200	-3.05342200	0.53582200
O	-0.83184200	-1.53398700	-0.66601400
P	-0.80395100	-0.16239800	0.27103200
O	-0.33753300	0.95349000	-0.60671200
O	-0.06465700	-0.49787500	1.53067600
H	1.05242100	2.06378900	0.26597400
C	0.89572700	-3.67677000	0.32737500
C	1.69444800	-3.67206100	1.49130600
C	1.48475200	-3.85072600	-0.94112300
C	1.15184400	-3.43328000	2.79710600
C	3.10559600	-3.91444500	1.38066700
C	2.90607600	-4.03313000	-1.04262900

C	0.71482500	-3.88911600	-2.15046500
C	1.94158500	-3.49527900	3.90866100
H	0.10082900	-3.18238900	2.88323600
C	3.89827800	-3.97877400	2.57247600
C	3.67696900	-4.08762300	0.11838000
C	3.50114100	-4.18983000	-2.33465200
H	-0.36369100	-3.78552500	-2.09366200
C	1.31920900	-4.04663700	-3.36321400
C	3.33365800	-3.79017500	3.79966600
H	1.51207600	-3.30873100	4.88751600
H	4.96093500	-4.18567700	2.47343800
H	4.74559100	-4.27698800	0.03719400
C	2.73533900	-4.19025400	-3.46100600
H	4.57965300	-4.30795300	-2.39276200
H	0.71869300	-4.06542400	-4.26697500
H	3.94131600	-3.84524100	4.69712500
H	3.19509200	-4.30516400	-4.43727700
C	-4.33560800	2.08557200	-0.00576900
C	-4.52549000	2.25990600	1.38271700
C	-4.34828200	3.20501300	-0.86746600
C	-4.60216300	1.16210500	2.30236000
C	-4.70999800	3.58377900	1.91135700
C	-4.62065000	4.50997600	-0.33319800
C	-4.10343800	3.10300800	-2.27853200
C	-4.78450600	1.36978900	3.63804000
H	-4.51886600	0.14840500	1.92847000
C	-4.88449800	3.76008300	3.32159300
C	-4.77263700	4.67263300	1.04239600
C	-4.72830500	5.62505100	-1.22561200
H	-3.83146700	2.13986300	-2.69484700
C	-4.18931000	4.19437600	-3.09397700
C	-4.91372100	2.68953700	4.16304800
H	-4.83623400	0.52103400	4.31216800
H	-5.00347900	4.77116800	3.70086500
H	-4.95506400	5.66646200	1.44548500
C	-4.52794700	5.47610000	-2.56534300
H	-4.97010600	6.59709500	-0.80322500
H	-3.99213900	4.09075000	-4.15605700
H	-5.04916600	2.83218400	5.23020200
H	-4.60904400	6.32794300	-3.23253800
C	2.97798700	-0.64541700	-1.01642200
C	4.31275800	-0.23600500	-0.97238800
C	5.03273600	-0.12053700	-2.15203800
C	4.37712400	-0.39429900	-3.35728100

C	3.03381900	-0.77114100	-3.37524900
C	2.30083400	-0.90164700	-2.19479400
C	3.32974600	-0.14523200	1.15194500
C	4.70125200	-0.00633200	0.47852500
H	6.07572000	0.18308300	-2.14486900
H	4.91974900	-0.30435300	-4.29227100
H	2.54589300	-0.97225700	-4.32357300
H	1.25491100	-1.18988800	-2.18867600
H	1.53131700	-0.93860900	0.60434700
N	2.48735100	-0.70516200	0.30531400
C	3.09227500	-0.23239300	2.61632300
H	3.43204700	-1.21626300	2.96150000
H	3.64157500	0.54589300	3.14684600
H	2.02140600	-0.14303900	2.81277500
C	5.58812800	-1.14828700	0.99914100
H	6.49024100	-1.22391300	0.39064900
H	5.86739500	-0.99089500	2.04596400
H	5.04503700	-2.09076600	0.91780000
C	9.06440100	2.30313800	-1.12817200
C	7.92686900	3.02497500	-1.46686800
C	6.70189900	2.76033200	-0.84452200
C	6.60642200	1.73395100	0.11302100
C	7.77028100	1.06615500	0.49337500
C	8.98766000	1.33657200	-0.12879300
H	5.68469600	4.39485500	-1.86768800
H	10.00936400	2.51196800	-1.61787800
H	7.98070500	3.81623900	-2.20924700
C	5.54767100	3.60785800	-1.13071700
C	5.27435800	1.41643800	0.75909800
H	7.73818600	0.33729200	1.29575600
H	9.87677600	0.79503500	0.17644400
C	4.14411700	2.35118400	0.37355600
C	4.36146200	3.47979400	-0.51159700
H	5.41277600	1.49305500	1.84685600
H	3.53096900	4.13337100	-0.74315800
N	3.01030200	1.91730200	0.78949500
N	1.86543800	2.63730200	0.52392900
C	1.72930000	3.88743700	1.08632400
O	2.62199900	4.40126900	1.74518000
C	0.47551600	4.62263000	0.74729600
C	0.20957700	5.78911000	1.46815100
C	-0.34723200	4.25092000	-0.31941100
C	-0.87575900	6.58599400	1.12571500
H	0.87289100	6.06129500	2.28197000

C	-1.42254200	5.06104400	-0.66795500
H	-0.15291400	3.34463600	-0.88479700
C	-1.68496900	6.22595400	0.05021900
H	-1.08367200	7.49124900	1.68677600
H	-2.52416700	6.85306400	-0.23401500
H	-2.05474100	4.78539200	-1.50573100

IMI'-2

C	5.40921900	-4.84813300	-1.07803100
C	4.76611900	-3.81060400	-0.45081200
C	3.34902700	-3.69686900	-0.49932800
C	2.62105000	-4.66817200	-1.23982000
C	3.31340100	-5.73676500	-1.86908900
C	4.67810200	-5.83045800	-1.78776500
H	6.49161700	-4.91350400	-1.03479900
C	2.63080300	-2.62728000	0.12934500
C	1.21237600	-4.55231700	-1.33640800
H	2.73722200	-6.47326500	-2.42214900
H	5.20146800	-6.64679500	-2.27436500
C	0.52891800	-3.50105800	-0.77506800
C	1.27268100	-2.51486200	-0.07161300
H	0.65765100	-5.32153200	-1.86795900
C	3.33827600	-1.59859900	0.93161900
C	4.10947200	-1.95015900	2.08463700
C	3.27994300	-0.27800300	0.53292800
C	4.90551300	-0.95246900	2.70866700
C	4.09017300	-3.25464700	2.64857900
C	4.16272800	0.70303800	1.06999200
C	5.67177300	-1.28573600	3.85731300
C	4.94549400	0.34594200	2.14440800
C	4.83027300	-3.54471300	3.76712600
H	3.46881900	-4.01842000	2.19244000
C	5.63656300	-2.55356300	4.37732300
H	6.28099000	-0.51268100	4.31730100
H	5.63344200	1.07685200	2.56194600
H	4.79451200	-4.54263800	4.19212500
H	6.21954800	-2.80090500	5.25823600
O	2.44131200	0.07655100	-0.49943600
H	5.34181900	-3.05913800	0.07778000
O	0.61469200	-1.43602700	0.47749400
P	0.80205000	0.03056200	-0.28587100
O	0.35251900	1.05427300	0.71518400
O	0.17624700	-0.04656400	-1.63576100
H	-1.02075700	1.84928700	0.00525300
C	-0.96069200	-3.49995000	-0.83324100
C	-1.62584400	-3.23961900	-2.04683400
C	-1.68058600	-3.92300400	0.30143200
C	-0.93887100	-2.76638000	-3.21166400
C	-3.04237500	-3.46027400	-2.13643900
C	-3.10428100	-4.08902300	0.21405100
C	-1.04173600	-4.23872100	1.54589400

C	-1.60542100	-2.56881900	-4.38621500
H	0.11989200	-2.54616500	-3.13534200
C	-3.70100300	-3.25573900	-3.39153100
C	-3.74637000	-3.87663300	-1.00538500
C	-3.83073200	-4.51163300	1.37218900
H	0.03662300	-4.14165700	1.62387800
C	-1.76854500	-4.65067100	2.62437000
C	-3.00471000	-2.83122300	-4.48501700
H	-1.07041300	-2.20366800	-5.25681100
H	-4.77001500	-3.44498000	-3.44927900
H	-4.81855200	-4.04885800	-1.07759200
C	-3.18673400	-4.78140100	2.54194100
H	-4.90977400	-4.61339300	1.29294000
H	-1.26602600	-4.87974500	3.55878900
H	-3.51145900	-2.67883000	-5.43253400
H	-3.74672600	-5.09744700	3.41623600
C	4.40231800	2.02949700	0.43037800
C	4.96923100	2.08117500	-0.86275400
C	4.24975600	3.21180300	1.18234300
C	5.17557500	0.91476000	-1.67166500
C	5.41090500	3.34258000	-1.39124000
C	4.74667200	4.45617500	0.66358500
C	3.59036900	3.23238900	2.45565000
C	5.72895400	1.00514700	-2.91535200
H	4.88847800	-0.05786700	-1.28847400
C	5.98276000	3.39538700	-2.70230600
C	5.31577800	4.49240200	-0.60743700
C	4.62360900	5.64390400	1.45398000
H	3.16258500	2.31061300	2.83512000
C	3.46867900	4.39048000	3.16834500
C	6.13234300	2.26498700	-3.44767500
H	5.86890900	0.10685200	-3.50796800
H	6.30011300	4.36174900	-3.08425600
H	5.68785300	5.43682200	-0.99916700
C	4.00837400	5.61491700	2.67036100
H	5.01979000	6.57226700	1.05126400
H	2.95131100	4.38580100	4.12223100
H	6.56621200	2.31461100	-4.44103600
H	3.91247500	6.52174900	3.25858800
C	-3.11305000	-0.77385300	1.01774500
C	-4.45095800	-0.34668900	1.00041400
C	-5.24671500	-0.51732300	2.12255200
C	-4.68438900	-1.07980500	3.27405200
C	-3.34484600	-1.46469700	3.28446400

C	-2.53451300	-1.31181000	2.15943400
C	-3.31497200	0.37775300	-0.95092300
C	-4.77359300	0.20157400	-0.38833800
H	-6.28898500	-0.21238800	2.11888600
H	-5.29321100	-1.20861700	4.16252000
H	-2.91688300	-1.89487300	4.18526900
H	-1.49104300	-1.60685900	2.15994800
H	-1.59964700	-0.80206900	-0.51495800
N	-2.53817100	-0.55384600	-0.22669800
C	-3.06582300	0.34746500	-2.44127600
H	-3.33761700	-0.63514500	-2.83337200
H	-3.63325300	1.12862800	-2.95251300
H	-1.99586500	0.50328200	-2.61233500
C	-5.58253500	-0.79150000	-1.21800200
H	-6.47120900	-1.11865000	-0.67465400
H	-5.88526800	-0.36447800	-2.17935300
H	-4.96808900	-1.67490600	-1.40445200
C	-8.77661100	2.92676300	1.85928900
C	-7.61325400	3.68243400	1.86728300
C	-6.48616400	3.25995300	1.14938100
C	-6.52766200	2.05384800	0.42153400
C	-7.71514200	1.32697700	0.38664200
C	-8.82669200	1.75164200	1.11069400
H	-5.33460600	5.02665600	1.68670500
H	-9.64403900	3.25439600	2.42138000
H	-7.56553000	4.61136900	2.42782300
C	-5.28796400	4.08785000	1.14076400
C	-5.32194800	1.65283000	-0.38998600
H	-7.78040900	0.42262300	-0.20727600
H	-9.73746900	1.16292600	1.08466300
C	-4.09728800	2.45409000	-0.08893100
C	-4.13306000	3.74369400	0.52504400
H	-5.55755100	1.90240000	-1.44079600
H	-3.23806400	4.35035000	0.57762000
N	-3.03602400	1.79609500	-0.44019200
N	-1.79290300	2.36769100	-0.47022000
C	-1.57550700	3.28591200	-1.48575500
O	-2.44696300	3.56508700	-2.29217900
C	-0.25222000	3.96280500	-1.44732400
C	0.19616400	4.58393700	-2.61513000
C	0.47395100	4.08247700	-0.26027500
C	1.37915000	5.31219800	-2.60002100
H	-0.39543000	4.49127300	-3.51979500
C	1.64129800	4.83646400	-0.24442700

H	0.12835800	3.60670500	0.65076900
C	2.09617000	5.44638400	-1.41112100
H	1.73536700	5.78574300	-3.50885600
H	3.01065100	6.03148800	-1.39061200
H	2.18174300	4.95969800	0.68710500

IMI'-3

C	6.42866000	-2.72822900	-2.53368400
C	5.54702600	-1.87593800	-1.91790100
C	4.25302500	-2.32091400	-1.53466500
C	3.88410200	-3.66550900	-1.82089700
C	4.82250600	-4.52625900	-2.44976600
C	6.06821900	-4.07170900	-2.79741400
H	7.40959300	-2.36912300	-2.82765100
C	3.30408200	-1.46067700	-0.89689700
C	2.59234700	-4.12596900	-1.45841500
H	4.52932600	-5.55203400	-2.65521000
H	6.77757500	-4.73526400	-3.28079200
C	1.65771500	-3.28759800	-0.90018100
C	2.02125600	-1.92839800	-0.68336600
H	2.34104700	-5.17050400	-1.62589100
C	3.64387700	-0.09438100	-0.41428200
C	4.66408900	0.12410300	0.56900900
C	2.85752500	0.96960900	-0.80702200
C	4.87194500	1.44462400	1.06000600
C	5.42337900	-0.93363800	1.14340400
C	3.02830600	2.28646700	-0.29733000
C	5.85530700	1.67454900	2.05967100
C	4.04649900	2.50111300	0.60009900
C	6.35177900	-0.68256800	2.12270900
H	5.24852800	-1.95210400	0.81582500
C	6.58220200	0.63647500	2.58124800
H	6.00357300	2.69019900	2.41566700
H	4.19834800	3.49842500	1.00550700
H	6.91125100	-1.50559700	2.55562700
H	7.32383700	0.81803700	3.35196500
O	1.85591200	0.73895100	-1.72062300
H	5.82576500	-0.84443900	-1.72730200
O	1.07600600	-1.08976600	-0.15160700
P	0.45730700	0.12404900	-1.10198500
O	-0.05497800	1.11076600	-0.08266300
O	-0.34493600	-0.40340400	-2.22591600
H	-0.70953400	0.71917700	1.20317400
C	0.33402600	-3.80496400	-0.44803100
C	-0.58399900	-4.32850100	-1.38047600
C	0.03179500	-3.81486700	0.93130700
C	-0.36532900	-4.27000900	-2.79680700
C	-1.80489500	-4.92793600	-0.91435100
C	-1.20933400	-4.38293300	1.38088000
C	0.91666900	-3.27947500	1.92437100

C	-1.27353200	-4.78902900	-3.67199300
H	0.52921900	-3.78175700	-3.16713700
C	-2.72761200	-5.47015700	-1.86618600
C	-2.08340600	-4.95048900	0.45234700
C	-1.53745200	-4.34186000	2.77471800
H	1.87348300	-2.86952400	1.61920400
C	0.56979300	-3.25837700	3.24305100
C	-2.47069700	-5.40758500	-3.20294500
H	-1.09247900	-4.72269100	-4.73976000
H	-3.64050200	-5.92774200	-1.49314100
H	-3.00942000	-5.40378300	0.80171400
C	-0.68374900	-3.78192000	3.67767100
H	-2.49061000	-4.75750400	3.09018900
H	1.24815900	-2.82176900	3.97072400
H	-3.17734900	-5.81687500	-3.91746100
H	-0.94620800	-3.73827500	4.72997300
C	2.11511300	3.40187500	-0.68035100
C	2.14962700	3.93330400	-1.98308200
C	1.25963600	3.96037800	0.29240000
C	2.99950700	3.39776700	-3.00550500
C	1.32697200	5.06508700	-2.31152100
C	0.46033100	5.10768500	-0.03875000
C	1.12429600	3.40750800	1.60941700
C	3.01224700	3.93207100	-4.25988700
H	3.63702000	2.55276700	-2.76821000
C	1.36913600	5.59458500	-3.64157300
C	0.51440500	5.63451500	-1.33051900
C	-0.38289200	5.68579100	0.96554400
H	1.68468000	2.51499000	1.86179200
C	0.29145600	3.97295200	2.53200600
C	2.18204900	5.04601700	-4.58746800
H	3.66004900	3.50948800	-5.02099100
H	0.73749400	6.44693400	-3.87580800
H	-0.09447200	6.50046400	-1.57978000
C	-0.46305600	5.14328700	2.21323800
H	-0.96827800	6.56169600	0.70066200
H	0.19889800	3.52396200	3.51719700
H	2.20724400	5.45386300	-5.59270100
H	-1.11324700	5.58281600	2.96298600
C	-2.60692700	2.62305500	-0.85045400
C	-3.88425800	2.06595100	-0.95078700
C	-4.41836700	1.76968200	-2.19823200
C	-3.64302200	2.00500200	-3.33581000
C	-2.35647000	2.53245900	-3.21576900

C	-1.81816200	2.85199000	-1.97125500
C	-3.20896500	2.21138900	1.32796100
C	-4.48614200	1.95806900	0.44552100
H	-5.41478700	1.34963700	-2.29494100
H	-4.03988600	1.76446200	-4.31615500
H	-1.75625700	2.69115500	-4.10649200
H	-0.80870900	3.23806500	-1.86406500
H	-1.32803000	2.94372500	0.74944400
N	-2.31038000	2.93979600	0.48075900
C	-3.37597700	2.83384900	2.69824000
H	-3.74285800	3.85626100	2.59514700
H	-4.06226500	2.25026600	3.31693200
H	-2.40245000	2.86474900	3.19695000
C	-5.56687100	3.01270100	0.67232300
H	-6.34230900	2.93670500	-0.09198700
H	-6.02878400	2.91771500	1.65955600
H	-5.12321700	4.00855900	0.58463200
C	-7.36621600	-1.94269500	-1.71266500
C	-6.15272600	-2.42182100	-1.24175800
C	-5.35028200	-1.62862700	-0.41057400
C	-5.76414700	-0.32668500	-0.06782600
C	-7.00898000	0.12233700	-0.50201400
C	-7.79855800	-0.67365400	-1.32904300
H	-3.86897100	-3.20212100	-0.15208700
H	-7.98122800	-2.55743600	-2.36033300
H	-5.81095900	-3.41753700	-1.50976000
C	-4.11724100	-2.18212300	0.12957000
C	-4.88853300	0.50298900	0.83587200
H	-7.37109700	1.09844000	-0.19879000
H	-8.75707800	-0.29994100	-1.67314800
C	-3.55728300	-0.12136500	1.12435900
C	-3.26209500	-1.50224400	0.92968300
H	-5.39309400	0.55239200	1.81703100
H	-2.32449400	-1.92045800	1.27935800
N	-2.71669100	0.79298400	1.50151200
N	-1.44758900	0.55454500	1.96173300
C	-1.32139500	0.13489900	3.26285100
O	-2.29686600	-0.07520000	3.96935100
C	0.08294600	-0.02390700	3.75453700
C	0.23880700	-0.29321800	5.11610000
C	1.20581300	0.05399100	2.92374900
C	1.50862700	-0.47498200	5.65298400
H	-0.64913900	-0.35882700	5.73565300
C	2.47575400	-0.13200700	3.46554900

H	1.11154400	0.23430700	1.85614700
C	2.62868300	-0.39448600	4.82627500
H	1.62539000	-0.67981800	6.71210300
H	3.34764900	-0.08170000	2.82050900
H	3.62214400	-0.53773800	5.24000600

IMI'-4

C	6.75977200	-3.47344600	-1.59010700
C	5.97160000	-2.45823600	-1.10932200
C	4.62246200	-2.69985200	-0.73246800
C	4.10010700	-4.01509500	-0.88864300
C	4.94512600	-5.04739900	-1.37582300
C	6.24661800	-4.78666800	-1.71763700
H	7.78532200	-3.26792700	-1.87958500
C	3.76537400	-1.66325400	-0.24059000
C	2.74495200	-4.27554000	-0.55584300
H	4.53302400	-6.04714900	-1.48099500
H	6.88357700	-5.58011700	-2.09427100
C	1.90386300	-3.27150500	-0.14576300
C	2.42847000	-1.95424400	-0.04039400
H	2.36749000	-5.29176000	-0.63816900
C	4.23757200	-0.28832800	0.08007000
C	5.26901200	-0.03988800	1.04565500
C	3.56429900	0.78802000	-0.46265100
C	5.60851100	1.30799800	1.35818400
C	5.94449600	-1.07940800	1.74401300
C	3.83601700	2.13421200	-0.09482000
C	6.64259300	1.57155600	2.29589100
C	4.86805200	2.37011300	0.77874200
C	6.93173100	-0.79294600	2.65309300
H	5.66775700	-2.11080200	1.55783900
C	7.29872500	0.54639100	2.92523000
H	6.89272900	2.60661000	2.51173600
H	5.09845600	3.39176200	1.07062900
H	7.43245300	-1.60243800	3.17444600
H	8.08532100	0.75568800	3.64262600
O	2.59136300	0.55364900	-1.40562100
H	6.36966900	-1.45267800	-1.02066100
O	1.56122400	-0.95453500	0.32657900
P	1.10102400	0.10122300	-0.86830600
O	0.41540600	1.22408100	-0.17274100
O	0.45686400	-0.63234500	-2.00505900
H	-1.27790100	-0.67425800	-2.04795400
C	0.49296600	-3.55381700	0.25420800
C	-0.48790300	-3.81172000	-0.72004200
C	0.16250400	-3.59717000	1.62719000
C	-0.21183300	-3.73262700	-2.12633400
C	-1.82526400	-4.14995700	-0.30976900
C	-1.17749000	-3.93018100	2.02491700
C	1.11654400	-3.31224000	2.65753700

C	-1.17867400	-4.01174400	-3.04432000
H	0.77574700	-3.41939900	-2.44366400
C	-2.81161600	-4.43434000	-1.31021900
C	-2.13917200	-4.19912700	1.04717700
C	-1.50408300	-3.97186400	3.41766600
H	2.13364400	-3.05900400	2.37657900
C	0.76511500	-3.35493000	3.97698100
C	-2.49640500	-4.38043600	-2.63279300
H	-0.95895900	-3.93190600	-4.10373200
H	-3.81723800	-4.68675300	-0.98439700
H	-3.15303800	-4.45237300	1.35024500
C	-0.56461700	-3.69236700	4.36733000
H	-2.52184500	-4.22820400	3.69866500
H	1.50408000	-3.13342400	4.74010300
H	-3.25244300	-4.58007200	-3.38508600
H	-0.82228700	-3.72477100	5.42098600
C	2.96050800	3.24297800	-0.57592700
C	3.11009700	3.75829600	-1.87566000
C	1.97714200	3.75997300	0.28960400
C	4.08265100	3.24399700	-2.79333400
C	2.26875700	4.83708400	-2.31213000
C	1.14087000	4.83866100	-0.15664600
C	1.73590200	3.21735700	1.59603200
C	4.20997700	3.76549600	-4.04731800
H	4.72083900	2.42644900	-2.47293700
C	2.43809900	5.35907800	-3.63427400
C	1.30827400	5.35509000	-1.44203300
C	0.13999200	5.35684900	0.72879500
H	2.32671700	2.36884700	1.92317600
C	0.75543600	3.71890000	2.39973900
C	3.37702700	4.84222500	-4.47616100
H	4.95015500	3.36137500	-4.73028900
H	1.79810400	6.17850400	-3.94964900
H	0.67426800	6.17412100	-1.77467100
C	-0.04944600	4.81627800	1.96581900
H	-0.46841800	6.19006900	0.38609400
H	0.56886100	3.27648300	3.37436600
H	3.49701900	5.24516700	-5.47653700
H	-0.81132800	5.21506700	2.62875900
C	-5.27229800	1.56072700	-0.93881600
C	-4.73246000	1.97343500	0.28751600
C	-5.53048300	2.00328800	1.42036100
C	-6.86579800	1.59714900	1.31971100
C	-7.38740800	1.19480300	0.09208700

C	-6.60011100	1.17820000	-1.06033100
C	-3.00913900	1.72991900	-1.31955100
C	-3.29408900	2.42196700	0.05847400
H	-5.12836800	2.32845300	2.37497500
H	-7.49654400	1.59920300	2.20198100
H	-8.42450900	0.88034500	0.02601500
H	-7.00359800	0.85391400	-2.01314100
H	-4.40668400	1.18744400	-2.83169600
N	-4.29325000	1.63698200	-1.93308400
C	-1.93800800	2.30871800	-2.22066200
H	-2.24485700	3.29719900	-2.56607100
H	-0.98259500	2.36625500	-1.69126400
H	-1.80775600	1.66067300	-3.09298700
C	-3.21243600	3.94410800	-0.06292900
H	-3.61731500	4.42938500	0.82714100
H	-2.18000800	4.27520500	-0.20634900
H	-3.81634000	4.27128700	-0.91474300
C	-2.06282900	1.84956500	5.28498700
C	-1.68869200	0.71517200	4.57880600
C	-1.79086400	0.67942900	3.18174800
C	-2.27860300	1.80399800	2.48254900
C	-2.63690900	2.94093400	3.20248300
C	-2.54075800	2.96164500	4.59253700
H	-0.98178200	-1.34216700	3.05994700
H	-1.98196200	1.87133800	6.36610900
H	-1.31079800	-0.16045600	5.09963200
C	-1.38915700	-0.52524800	2.46778300
C	-2.23006400	1.77767000	0.97762300
H	-2.99120400	3.82278200	2.68095200
H	-2.83465200	3.85416400	5.13510700
C	-2.07862000	0.41008400	0.40846900
C	-1.52317800	-0.68412800	1.13120200
H	-1.25546300	2.23731600	0.71813800
H	-1.24737900	-1.59045000	0.60480300
N	-2.51538600	0.37031900	-0.81961800
N	-2.25181800	-0.67566900	-1.67731700
C	-3.26263500	-1.24360800	-2.44642900
O	-3.03278800	-1.56525600	-3.59830900
C	-4.57190700	-1.53368500	-1.78758100
C	-5.67864200	-1.72652500	-2.61692900
C	-4.69598000	-1.71455700	-0.40657900
C	-6.90851100	-2.07666200	-2.07003200
H	-5.55550900	-1.60786200	-3.68904700
C	-5.92718100	-2.06540900	0.13690000

H	-3.82621400	-1.63157800	0.23830600
C	-7.03383400	-2.24146600	-0.69181600
H	-7.76714400	-2.22281700	-2.71737600
H	-6.02109900	-2.20840900	1.20849000
H	-7.99338900	-2.51334000	-0.26321000

TSI'-3

Value of imaginary frequency = -943.3 cm^{-1}

C	6.76512800	-3.04737100	-1.96023300
C	5.95205200	-2.12243300	-1.35561400
C	4.64689200	-2.47668500	-0.91627900
C	4.19030300	-3.80369900	-1.15437800
C	5.05994800	-4.74147700	-1.77291800
C	6.32213100	-4.37630300	-2.16285100
H	7.75635800	-2.75617600	-2.29218300
C	3.76581900	-1.54183100	-0.28338400
C	2.87050300	-4.16842500	-0.78301500
H	4.69827900	-5.75276200	-1.93657400
H	6.97968200	-5.09773800	-2.63640200
C	2.00261600	-3.26167900	-0.22498700
C	2.47253500	-1.94017100	-0.00329300
H	2.53829200	-5.18919400	-0.95520200
C	4.16513800	-0.14378000	0.03924400
C	5.26421300	0.17277600	0.90252400
C	3.39020200	0.88930900	-0.44493500
C	5.55807500	1.54123800	1.16712700
C	6.05133300	-0.82251700	1.54394800
C	3.64341300	2.25820100	-0.16118500
C	6.65223100	1.86934700	2.01170700
C	4.73401400	2.55737200	0.61809200
C	7.09413900	-0.47386200	2.36488100
H	5.81414100	-1.86862200	1.38440400
C	7.40927100	0.88671600	2.59428000
H	6.86858900	2.91821900	2.19420600
H	4.95777000	3.59621400	0.84784500
H	7.68001100	-1.24902900	2.84814900
H	8.24141500	1.14672500	3.24000000
O	2.31326200	0.58486800	-1.25115900
H	6.29882000	-1.10420700	-1.21688200
O	1.59441000	-1.03002500	0.54743400
P	0.95781600	0.07463300	-0.48868900
O	0.46194000	1.20121500	0.39551500
O	0.07953100	-0.55378600	-1.50865300
H	-1.71059400	-1.02830700	-2.04632100
C	0.62648100	-3.67700000	0.18154500
C	-0.35856900	-3.92572700	-0.79271000
C	0.34223700	-3.88070000	1.54806100
C	-0.15569500	-3.63718300	-2.18335600
C	-1.63641700	-4.45219400	-0.39209600
C	-0.93754100	-4.40578700	1.93669000

C	1.28357700	-3.57175100	2.58330400
C	-1.14203300	-3.86443600	-3.09641500
H	0.78814800	-3.20249900	-2.49221200
C	-2.63956300	-4.69017700	-1.38717600
C	-1.88941200	-4.69656300	0.95711900
C	-1.22090300	-4.60099200	3.32619500
H	2.25710700	-3.17853700	2.30943200
C	0.96919400	-3.75325700	3.89983400
C	-2.40011800	-4.41104800	-2.69753700
H	-0.98105900	-3.61711800	-4.14045800
H	-3.59819200	-5.08755600	-1.06491400
H	-2.85589300	-5.09671600	1.25536700
C	-0.30135600	-4.27864400	4.28102700
H	-2.19273000	-5.00159500	3.60109100
H	1.69320500	-3.50153200	4.66797000
H	-3.17029700	-4.57110400	-3.44397600
H	-0.52825100	-4.42222500	5.33238900
C	2.73134900	3.32324600	-0.67196900
C	2.71516100	3.63765300	-2.04483700
C	1.89858800	4.01761700	0.22754700
C	3.53762900	2.95430800	-2.99882900
C	1.85547900	4.68434700	-2.52260100
C	1.06390400	5.08238200	-0.25753200
C	1.81284600	3.68097400	1.61922300
C	3.49746000	3.27814600	-4.32320500
H	4.20031600	2.16810100	-2.65174800
C	1.84338700	4.99367200	-3.92028200
C	1.05860900	5.38761400	-1.61852700
C	0.23325700	5.79752700	0.66595300
H	2.39622600	2.84572900	1.98901800
C	0.98923200	4.36721200	2.46140200
C	2.63582700	4.31297600	-4.79526100
H	4.12659200	2.74590700	-5.02932300
H	1.18596500	5.78708400	-4.26502000
H	0.41833600	6.18804900	-1.98283600
C	0.19465600	5.45306200	1.98338400
H	-0.38037400	6.60842500	0.28235500
H	0.92552600	4.08009000	3.50615700
H	2.61937200	4.55450800	-5.85303800
H	-0.44674900	5.99287800	2.67360300
C	-5.16452400	1.85540000	-0.61963000
C	-4.45470500	2.14601700	0.55289500
C	-5.12923200	2.33618400	1.74704400
C	-6.52402800	2.21903900	1.76366300

C	-7.21730500	1.93055900	0.58984500
C	-6.54863700	1.74978700	-0.62266400
C	-2.95831200	1.51173200	-1.17160900
C	-2.96757200	2.23064100	0.22502700
H	-4.58488000	2.55778300	2.66073700
H	-7.06509900	2.35180300	2.69430700
H	-8.29864600	1.83569400	0.61462600
H	-7.08887800	1.51035400	-1.53244200
H	-4.56311200	1.24939100	-2.53063200
N	-4.27710000	1.74612800	-1.69592900
C	-1.86390100	1.90657600	-2.14503500
H	-2.06680400	2.91119400	-2.51903400
H	-0.88741500	1.89152900	-1.65743700
H	-1.84018500	1.21715300	-2.99337000
C	-2.49221200	3.67899500	0.11404900
H	-2.72350500	4.24118000	1.02054200
H	-1.41319200	3.72996300	-0.06005600
H	-3.01210800	4.17239200	-0.71309000
C	-1.11647900	1.37908200	5.25189300
C	-1.06137600	0.20278100	4.53137000
C	-1.43007400	0.17910600	3.17285500
C	-1.85483900	1.36899600	2.53032500
C	-1.87892700	2.55837600	3.27310900
C	-1.53052300	2.55724000	4.61461400
H	-1.02085000	-1.93708900	2.96639100
H	-0.83721000	1.39514400	6.29954900
H	-0.73350500	-0.72204800	4.99879100
C	-1.38789100	-1.05943200	2.43901200
C	-2.10057100	1.29748900	1.08242300
H	-2.16880200	3.48840100	2.79902000
H	-1.57052000	3.48649000	5.17458200
C	-2.25766200	-0.00696800	0.50211200
C	-1.79632000	-1.18408800	1.14486100
H	-0.88870500	1.35102800	0.69916700
H	-1.78108400	-2.12490400	0.60954600
N	-2.76709300	0.07488300	-0.72527700
N	-2.64503700	-0.95560500	-1.63160400
C	-3.73553800	-1.37346700	-2.37449000
O	-3.58248100	-1.76545700	-3.51860000
C	-5.07189900	-1.39509900	-1.70143600
C	-6.20373000	-1.29183500	-2.51346200
C	-5.21644500	-1.60535200	-0.32709600
C	-7.47407700	-1.37494000	-1.95316700
H	-6.07039900	-1.15591400	-3.58248100

C	-6.48841800	-1.70039500	0.22796700
H	-4.33988800	-1.72624800	0.30219600
C	-7.61590200	-1.57891900	-0.58164700
H	-8.35176300	-1.28863600	-2.58543100
H	-6.59960500	-1.87031100	1.29376200
H	-8.60653300	-1.64826000	-0.14348200

IMI'-5

C	6.59761700	-3.36078700	-2.08547600
C	5.86145600	-2.37887900	-1.47181200
C	4.56428800	-2.65595700	-0.96196100
C	4.03358600	-3.96647900	-1.13073000
C	4.82593300	-4.96409000	-1.75846300
C	6.08151700	-4.67170600	-2.22285200
H	7.58379500	-3.12986500	-2.47477100
C	3.75694200	-1.65869000	-0.32267300
C	2.72111100	-4.26039000	-0.68020400
H	4.40954600	-5.96091800	-1.87082300
H	6.67836500	-5.43805800	-2.70591100
C	1.91804300	-3.29531200	-0.12381500
C	2.46072600	-1.99180100	0.01120200
H	2.33991900	-5.27224200	-0.79065900
C	4.24969100	-0.28498000	-0.02303300
C	5.40399600	-0.04369100	0.79445300
C	3.53216400	0.80407400	-0.46589500
C	5.80541600	1.30061500	1.03950300
C	6.14445900	-1.09096800	1.40752400
C	3.88900300	2.15207900	-0.20008800
C	6.95596800	1.55254800	1.83347500
C	5.03249300	2.37378400	0.52546800
C	7.24481500	-0.81506300	2.17952200
H	5.82697000	-2.11818600	1.26869700
C	7.66648000	0.51961900	2.38640800
H	7.25318400	2.58378400	2.00123800
H	5.33816600	3.39432700	0.74109600
H	7.79331000	-1.62865600	2.64276600
H	8.54212900	0.72172400	2.99413200
O	2.39641600	0.59137700	-1.24120700
H	6.26322700	-1.37565400	-1.37924100
O	1.63032300	-1.00826100	0.54417000
P	1.06047700	0.05732300	-0.52780000
O	0.62737100	1.25940900	0.39139900
O	0.09419200	-0.45308800	-1.51340400
H	-1.77641700	-0.85304900	-2.03902100
C	0.54882800	-3.61546700	0.37563000
C	-0.48973200	-3.90377800	-0.52938900
C	0.32005500	-3.66531500	1.76696800
C	-0.33085000	-3.78669200	-1.95073000
C	-1.77962300	-4.29336500	-0.02516500
C	-0.97719300	-4.03915400	2.25716200
C	1.33456700	-3.34800300	2.72829400

C	-1.36502700	-4.05946600	-2.79546400
H	0.62291600	-3.45172600	-2.34330400
C	-2.83589100	-4.58026500	-0.94956000
C	-1.99038000	-4.35876200	1.35107900
C	-1.21307900	-4.05798900	3.66824600
H	2.32777900	-3.08199800	2.38154900
C	1.06838300	-3.36971900	4.06755300
C	-2.63478000	-4.47604200	-2.29132800
H	-1.23479200	-3.94321700	-3.86615500
H	-3.80340600	-4.87158900	-0.54977100
H	-2.97020400	-4.64491400	1.72695100
C	-0.22613500	-3.72575400	4.54885800
H	-2.20255500	-4.33689900	4.01941500
H	1.84972000	-3.11763400	4.77728300
H	-3.44406500	-4.67110100	-2.98642700
H	-0.41695500	-3.73534200	5.61686300
C	3.01051600	3.26281200	-0.67080000
C	3.02042900	3.63482700	-2.02860900
C	2.14833300	3.89965600	0.24099600
C	3.88451400	3.01291100	-2.98715400
C	2.13977700	4.67316400	-2.48385100
C	1.25831800	4.92539400	-0.22975800
C	2.07585200	3.52983100	1.62552200
C	3.87210000	3.39566900	-4.29651100
H	4.56060700	2.23156500	-2.65443000
C	2.15860000	5.04577400	-3.86563700
C	1.27829900	5.29068100	-1.57553100
C	0.34548500	5.53513800	0.69220000
H	2.72737300	2.74410600	1.99198100
C	1.17916000	4.11845200	2.46552500
C	2.99587600	4.42790900	-4.74604400
H	4.53584800	2.91449400	-5.00755800
H	1.48717400	5.83383200	-4.19519900
H	0.60169200	6.06636600	-1.92720700
C	0.29782700	5.13882200	1.99456700
H	-0.32064600	6.30859900	0.31908400
H	1.11712100	3.80058500	3.50160900
H	3.00236100	4.71689600	-5.79192700
H	-0.41140700	5.58933500	2.68203200
C	-5.44616400	1.78807400	-0.82507200
C	-4.82380900	2.16052300	0.37218700
C	-5.56626900	2.34161600	1.52541700
C	-6.95066000	2.14200200	1.47637600
C	-7.56139600	1.77260300	0.27903900

C	-6.81983500	1.59281600	-0.89105300
C	-3.19797500	1.53617600	-1.23142100
C	-3.32587400	2.31653200	0.12980800
H	-5.07708500	2.61527100	2.45742600
H	-7.54790500	2.26790200	2.37322800
H	-8.63473200	1.61039400	0.25279800
H	-7.29701700	1.28504400	-1.81576000
H	-4.70800800	1.10611400	-2.64226200
N	-4.49701200	1.70521800	-1.85178100
C	-2.06709200	1.95312800	-2.15411600
H	-2.22570500	2.97153400	-2.51038200
H	-1.10575400	1.89696200	-1.63668000
H	-2.02298900	1.28859100	-3.02188000
C	-2.94071700	3.79114600	-0.01508400
H	-3.31098700	4.37975400	0.82592200
H	-1.85558000	3.91966900	-0.08222600
H	-3.40609400	4.19679000	-0.91863400
C	-0.92018400	2.06626900	4.98067500
C	-0.76263700	0.86403000	4.34019800
C	-1.30475800	0.64709500	3.04653200
C	-2.00130500	1.71078200	2.38681200
C	-2.14764600	2.94525000	3.08123100
C	-1.62990600	3.11164000	4.34138800
H	-0.61778600	-1.39752400	2.92470700
H	-0.50944300	2.21876700	5.97310900
H	-0.22895200	0.04560800	4.81680800
C	-1.16666900	-0.61522400	2.40793800
C	-2.50094400	1.46143000	1.07953000
H	-2.68140600	3.76198100	2.61160000
H	-1.76128300	4.06088100	4.85218300
C	-2.36904700	0.20011000	0.51650900
C	-1.69379600	-0.85859300	1.16357100
H	-0.32566400	1.31135200	0.60160000
H	-1.57602300	-1.81179400	0.66104200
N	-2.99399300	0.14512200	-0.72036800
N	-2.70244800	-0.86713700	-1.60932400
C	-3.71872800	-1.44580200	-2.33578800
O	-3.51517400	-1.86526400	-3.46588700
C	-5.05516900	-1.58207400	-1.67326800
C	-6.18218600	-1.61157900	-2.49596400
C	-5.19392700	-1.75942500	-0.29307100
C	-7.44766100	-1.78546800	-1.94255700
H	-6.05013000	-1.50049300	-3.56804900
C	-6.45781600	-1.94841900	0.25503000

H	-4.31441200	-1.76816500	0.34378000
C	-7.58493600	-1.95210100	-0.56645900
H	-8.32326200	-1.79599400	-2.58349800
H	-6.56530700	-2.08964500	1.32555600
H	-8.57019600	-2.08961600	-0.13202100

COMII'

C	5.48186900	2.89215200	-3.83678500
C	4.65162000	2.81093200	-2.74755900
C	4.36079700	1.55482900	-2.14980900
C	4.92367700	0.38132900	-2.72484900
C	5.78973400	0.49996100	-3.84435700
C	6.06752600	1.72698400	-4.38747400
H	5.68685000	3.85857600	-4.28554500
C	3.48858600	1.41964100	-1.02153200
C	4.60984800	-0.88889200	-2.17774500
H	6.21872700	-0.40472700	-4.26532300
H	6.72629100	1.80855200	-5.24556600
C	3.73075300	-1.03104700	-1.13136700
C	3.16290300	0.15069500	-0.59429100
H	5.07111200	-1.77500900	-2.60616600
C	2.90422100	2.58867800	-0.31193200
C	3.72532500	3.59476600	0.29532100
C	1.53733300	2.68039200	-0.16297300
C	3.09811600	4.69525200	0.94452300
C	5.14520700	3.52145900	0.31058800
C	0.89178800	3.76143200	0.48917900
C	3.89938500	5.70668500	1.53868300
C	1.68375900	4.75461700	1.01270900
C	5.89211500	4.50806800	0.90280500
H	5.63876200	2.66968500	-0.14353500
C	5.26655900	5.62081100	1.51444300
H	3.40341700	6.54394500	2.02104300
H	1.21493200	5.59932600	1.51068400
H	6.97444600	4.43189200	0.90817600
H	5.87221300	6.39521000	1.97315700
O	0.72345300	1.69940200	-0.71876500
H	4.20063100	3.70931200	-2.34032200
O	2.21599700	0.01821400	0.42427800
P	0.70053200	0.21158300	-0.10461800
O	-0.13028000	0.29005300	1.22174600
O	0.25871700	-0.78909200	-1.09498700
C	3.46697600	-2.37954100	-0.54724700
C	2.65567500	-3.30598300	-1.22799700
C	4.14721700	-2.75020700	0.63055900
C	1.92136400	-2.96487500	-2.41114700
C	2.55389900	-4.65160600	-0.73310900
C	4.06215400	-4.10490500	1.09692600
C	4.96024700	-1.83367100	1.37408600
C	1.14857500	-3.89146100	-3.04685000

H	1.96416600	-1.94468000	-2.77489900
C	1.73617300	-5.59357100	-1.43481500
C	3.27133800	-5.02178200	0.40352700
C	4.81110400	-4.49351800	2.25183000
H	5.03511500	-0.80351400	1.04030200
C	5.64523600	-2.23951600	2.48294300
C	1.05712900	-5.22930800	-2.55758800
H	0.58829300	-3.61091200	-3.93317000
H	1.67041500	-6.60604700	-1.04552000
H	3.21028000	-6.04766300	0.76126500
C	5.58170400	-3.59304500	2.92543000
H	4.74195200	-5.52632600	2.58366600
H	6.25469900	-1.52816700	3.03127300
H	0.43715200	-5.94911100	-3.08247400
H	6.14460900	-3.89711100	3.80207700
C	-0.59277200	3.83656000	0.60323400
C	-1.36933200	4.14148700	-0.53144200
C	-1.20099200	3.67291500	1.86349600
C	-0.79712000	4.29214900	-1.83658400
C	-2.78797700	4.31601200	-0.39255100
C	-2.61800100	3.87149100	1.99322100
C	-0.46407600	3.30032000	3.03663100
C	-1.57872900	4.57460300	-2.91865800
H	0.27508000	4.17728500	-1.95920200
C	-3.57148500	4.62374100	-1.55071800
C	-3.37675200	4.18685000	0.86540400
C	-3.22663900	3.73438500	3.28308300
H	0.60136500	3.11750300	2.95004200
C	-1.08538000	3.15865600	4.24264000
C	-2.98847000	4.74291900	-2.77758500
H	-1.12690400	4.67754100	-3.89980400
H	-4.64307700	4.75495900	-1.42649600
H	-4.45043400	4.33324700	0.96828700
C	-2.48761300	3.38809600	4.37397400
H	-4.29648000	3.90932600	3.36782000
H	-0.51019000	2.86746300	5.11542500
H	-3.58979600	4.97185700	-3.65120600
H	-2.95902700	3.28111400	5.34530900
C	-3.40681200	-2.34324200	-2.03730200
C	-4.65100300	-1.70617300	-2.27494000
C	-5.78809600	-2.49632000	-2.50307000
C	-5.66312300	-3.87744100	-2.47573400
C	-4.41656700	-4.48900000	-2.22874700
C	-3.27344700	-3.73469300	-2.00739400

C	-3.10169100	-0.12511200	-1.85819000
C	-4.43504200	-0.29027000	-2.14855400
H	-6.75453500	-2.02951400	-2.67751400
H	-6.53570000	-4.50119500	-2.64550000
H	-4.35210100	-5.57256200	-2.20626000
H	-2.31553400	-4.19324600	-1.78359800
H	-1.49638700	-1.48202000	-1.59476000
N	-2.48382800	-1.35886300	-1.79754800
C	-2.32062500	1.12147300	-1.61102200
H	-2.89363500	2.00030000	-1.91267300
H	-2.06901400	1.24042000	-0.54788300
H	-1.38212300	1.11743200	-2.17239500
C	-5.48416400	0.76980900	-2.27282400
H	-6.36351200	0.51616900	-1.66844300
H	-5.11330800	1.73818700	-1.92337900
H	-5.82545800	0.89279700	-3.30730100
C	-8.12289600	0.76819800	0.78557300
C	-6.89285400	1.21933800	1.20221500
C	-5.77544400	0.34974900	1.21098400
C	-5.94762800	-0.99660000	0.78866800
C	-7.22589700	-1.43711900	0.36011400
C	-8.29184400	-0.57082900	0.35846900
H	-4.36872000	1.81108300	1.96892100
H	-8.97406700	1.44129300	0.77935200
H	-6.76007200	2.24780100	1.52727500
C	-4.48471800	0.78786800	1.62960500
C	-4.82501300	-1.85791300	0.79053700
H	-7.33674700	-2.46406800	0.02419200
H	-9.26866600	-0.90869700	0.02886000
C	-3.58497000	-1.39729800	1.18176200
C	-3.40821000	-0.05167000	1.62035800
H	-4.91841000	-2.88419900	0.44297500
H	-2.44251700	0.30609300	1.96118600
N	-2.57769600	-2.37163800	1.07796600
N	-1.39206400	-2.03220900	1.26446000
C	-0.51082600	-3.19330700	1.08295300
O	-0.68121200	-3.94807800	0.16095100
H	-0.70044100	-0.55835100	1.31988200
C	0.50329000	-3.38047700	2.14739100
C	0.83556200	-4.70230100	2.46784400
C	1.09196700	-2.32110700	2.84530400
C	1.72288100	-4.96320100	3.50232500
H	0.37485900	-5.50966500	1.90741000
C	2.01708800	-2.58947600	3.84954900

H	0.85340700	-1.29182600	2.60378500
C	2.31767600	-3.90591600	4.19016700
H	1.96397600	-5.98868500	3.76352800
H	2.49641800	-1.76840500	4.37161300
H	3.02841300	-4.10890200	4.98487600

TSII'-1

Value of imaginary frequency = -147.5 cm^{-1}

C	4.57355600	4.27081800	-3.49979400
C	3.78713400	3.91068400	-2.43436700
C	3.82619800	2.58783500	-1.91412400
C	4.67370400	1.63785600	-2.54988000
C	5.48651600	2.04468900	-3.64128300
C	5.44378300	3.33345800	-4.10556500
H	4.52303600	5.28342000	-3.88676500
C	3.02005300	2.16411600	-0.80635700
C	4.68195500	0.29403400	-2.09661800
H	6.13592800	1.30790900	-4.10569400
H	6.06351500	3.63491400	-4.94346800
C	3.86189800	-0.13015100	-1.08030800
C	3.02119300	0.83064900	-0.45807800
H	5.34474000	-0.42002800	-2.57924800
C	2.14206400	3.11080100	-0.06748200
C	2.66634800	4.28070300	0.57092600
C	0.78582000	2.85804600	0.01222700
C	1.76264200	5.20994000	1.15655600
C	4.06078100	4.53928400	0.67164700
C	-0.13716800	3.80652200	0.53669300
C	2.26908200	6.37734900	1.78774900
C	0.37014100	4.95885900	1.09078100
C	4.52160800	5.66913000	1.29904200
H	4.76282300	3.82389800	0.25712800
C	3.61848300	6.60631300	1.85669300
H	1.56275300	7.08079100	2.21945400
H	-0.31614200	5.70118400	1.49057000
H	5.58983000	5.84504100	1.37388400
H	3.99910600	7.49811800	2.34340400
O	0.28191700	1.69700600	-0.52382600
H	3.11607600	4.63654400	-1.98861300
O	2.19238800	0.41404200	0.56307100
P	0.60507200	0.24061900	0.17827100
O	-0.11308100	0.08800400	1.48331800
O	0.44005100	-0.76261000	-0.92119100
C	3.90115300	-1.54898100	-0.62025700
C	3.31308700	-2.56231200	-1.39939400
C	4.62792800	-1.87239300	0.54235400
C	2.59345500	-2.28271700	-2.60862300
C	3.44190700	-3.93403000	-0.98947700
C	4.77624200	-3.24821500	0.92496500
C	5.27215000	-0.87568400	1.34633400

C	2.07258300	-3.29108100	-3.36413800
H	2.45623800	-1.24881300	-2.90389500
C	2.85910500	-4.96115900	-1.80090700
C	4.16420100	-4.24428500	0.16303800
C	5.58088700	-3.57112800	2.06312200
H	5.16396500	0.16954500	1.07459000
C	6.02620800	-1.22441700	2.42942200
C	2.20824600	-4.65335800	-2.95799000
H	1.52948000	-3.06014400	-4.27491100
H	2.96213300	-5.99301900	-1.47590100
H	4.27539500	-5.28514200	0.45894000
C	6.19399500	-2.59413900	2.78969600
H	5.68735500	-4.61788700	2.33560700
H	6.51148200	-0.45437900	3.02066700
H	1.77447400	-5.43879000	-3.56892600
H	6.80461700	-2.85139300	3.64939300
C	-1.61643400	3.64141300	0.42745600
C	-2.23169300	3.61740400	-0.84329100
C	-2.40858300	3.65129400	1.59537300
C	-1.48530200	3.60234300	-2.06822700
C	-3.66587300	3.63849000	-0.93746900
C	-3.83905700	3.74107500	1.48472700
C	-1.84423500	3.55210600	2.91073500
C	-2.11378200	3.56073700	-3.27848500
H	-0.40224300	3.62203300	-2.02948000
C	-4.28703000	3.59572800	-2.22707700
C	-4.43353700	3.73210500	0.22331700
C	-4.63174400	3.79277200	2.67701000
H	-0.77092600	3.43434600	3.01095900
C	-2.63611100	3.57362000	4.02154300
C	-3.53749200	3.54872000	-3.36395300
H	-1.52547000	3.54253900	-4.19001800
H	-5.37262000	3.60282300	-2.27349800
H	-5.51672600	3.79452400	0.14100300
C	-4.05151900	3.71207500	3.90753500
H	-5.70995100	3.88734000	2.57440300
H	-2.18844600	3.47835600	5.00530300
H	-4.01606000	3.51244800	-4.33730400
H	-4.66109600	3.74095000	4.80462100
C	-1.87159100	-3.02328100	-1.72468100
C	-3.15402500	-3.51862100	-2.02813700
C	-3.34326300	-4.90646600	-2.11928900
C	-2.24955600	-5.73442500	-1.92027500
C	-0.97518600	-5.20851500	-1.62767700

C	-0.76215400	-3.84332600	-1.52116100
C	-3.20039300	-1.23752700	-1.94722100
C	-4.02931500	-2.37853000	-2.11743700
H	-4.32082800	-5.32213000	-2.34657200
H	-2.37348700	-6.81014300	-1.99135200
H	-0.14147500	-5.88572700	-1.47076800
H	0.20943000	-3.41751200	-1.28687800
H	-1.11500900	-1.06161500	-1.45851800
N	-1.94704300	-1.63754200	-1.69238600
C	-3.57410800	0.19780100	-2.07323200
H	-4.50846200	0.40595600	-1.54128000
H	-2.79121000	0.84976800	-1.67647700
H	-3.73583000	0.45243900	-3.12632200
C	-5.40300500	-2.35794300	-2.70038600
H	-5.97427800	-3.24098200	-2.39880400
H	-5.95961700	-1.46873000	-2.39205700
H	-5.35246700	-2.35926300	-3.79478200
C	-7.85588000	0.24302800	0.58467100
C	-6.59831800	0.69657000	0.94663500
C	-5.48462300	-0.15253100	0.86270500
C	-5.66125500	-1.47707100	0.38337100
C	-6.95414600	-1.92692700	0.04108500
C	-8.03814300	-1.07653600	0.14050100
H	-4.06510100	1.29563400	1.65347300
H	-8.71067900	0.90732800	0.65822600
H	-6.46044400	1.70768200	1.31883800
C	-4.17404200	0.27659800	1.29886700
C	-4.52057500	-2.33489400	0.29302900
H	-7.08640300	-2.95320200	-0.28806500
H	-9.03049600	-1.42773500	-0.11970600
C	-3.28435400	-1.93827600	0.89833000
C	-3.11392700	-0.55935900	1.31789500
H	-4.66008300	-3.39461100	0.10679900
H	-2.15344600	-0.20508500	1.67497700
N	-2.42249800	-2.92880400	1.05052700
N	-1.23818600	-2.71734100	1.57697100
C	-0.50119100	-3.87101700	1.93840800
O	-0.95945500	-4.97543500	1.74966000
H	-0.86569100	-1.76775100	1.72011200
C	0.79498500	-3.64802000	2.64169300
C	1.32031900	-4.76259900	3.30588600
C	1.46896300	-2.42430100	2.69864800
C	2.48588200	-4.64812500	4.05061700
H	0.78790200	-5.70493500	3.23988000

C	2.64430600	-2.31859800	3.43631000
H	1.09365000	-1.54304100	2.19090800
C	3.14400800	-3.42115000	4.12430200
H	2.87880900	-5.51171100	4.57725000
H	3.17521300	-1.37215800	3.46115400
H	4.05642400	-3.32836100	4.70410100

IMII'-1

C	5.10632400	4.36089500	-2.92779600
C	4.18693800	3.93227600	-2.00355100
C	4.10620700	2.56025600	-1.63901600
C	4.97726200	1.63813800	-2.28424700
C	5.92770000	2.11476500	-3.22600800
C	5.99744800	3.44721800	-3.53888100
H	5.14716500	5.41127600	-3.19739900
C	3.15865800	2.06659100	-0.68071700
C	4.88182900	0.25495600	-1.98281900
H	6.59345400	1.39746700	-3.69760500
H	6.72366200	3.80400900	-4.26160400
C	3.93504800	-0.22836900	-1.11505200
C	3.06170700	0.70484800	-0.49492200
H	5.57428700	-0.43693700	-2.45571100
C	2.25956700	2.98144600	0.07423800
C	2.77778000	4.03704100	0.89226000
C	0.89104400	2.81209700	-0.00142000
C	1.86941200	4.95674600	1.48606300
C	4.16543900	4.18778900	1.16150500
C	-0.03260000	3.74606800	0.54684200
C	2.37021200	6.01364100	2.29233800
C	0.47870900	4.80206800	1.26530800
C	4.61881700	5.20974300	1.95690400
H	4.86617000	3.47377500	0.74234200
C	3.71504400	6.14142200	2.52251400
H	1.66227400	6.71220500	2.72928300
H	-0.20312400	5.53699000	1.68560900
H	5.68074600	5.30300000	2.15978000
H	4.08999600	6.94695700	3.14504400
O	0.38365800	1.75746300	-0.72312500
H	3.50243800	4.64234300	-1.55277900
O	2.09195600	0.21652600	0.36258100
P	0.56569500	0.20596000	-0.22099300
O	-0.34882700	-0.13985100	0.90204500
O	0.51405700	-0.57965100	-1.51274100
C	3.89030300	-1.67646400	-0.75582700
C	3.29137700	-2.61818700	-1.61204200
C	4.54038900	-2.09320000	0.42276600
C	2.67304300	-2.24788300	-2.85220800
C	3.31978500	-4.01202100	-1.25953100
C	4.56332200	-3.48784200	0.76372300
C	5.22498300	-1.17639100	1.28753500
C	2.15353300	-3.19285600	-3.68732200

H	2.61838200	-1.19615400	-3.10829200
C	2.74401300	-4.97043900	-2.15632000
C	3.93883800	-4.41127900	-0.07542200
C	5.26044400	-3.90665500	1.94060900
H	5.22244200	-0.11914500	1.04214000
C	5.88730600	-1.61756900	2.39692700
C	2.19114200	-4.57769700	-3.33863300
H	1.69559100	-2.89330700	-4.62463400
H	2.77425100	-6.01975700	-1.87538500
H	3.96138100	-5.46716400	0.18426500
C	5.90994700	-3.00431000	2.72938200
H	5.26226300	-4.96490400	2.18699900
H	6.40678200	-0.90874700	3.03390100
H	1.76684900	-5.31159700	-4.01652700
H	6.44329600	-3.33323600	3.61566400
C	-1.50471900	3.65168500	0.32129800
C	-2.03519500	3.72561800	-0.98564000
C	-2.37399500	3.60663500	1.43281600
C	-1.21225900	3.78662200	-2.15885500
C	-3.46029600	3.75931700	-1.17088200
C	-3.79050200	3.75229100	1.23576100
C	-1.90677400	3.40116200	2.77405100
C	-1.76180000	3.80352200	-3.40760700
H	-0.13438700	3.81669800	-2.04922600
C	-3.99769000	3.77436400	-2.49799800
C	-4.30267800	3.80486800	-0.05943900
C	-4.65478900	3.80563300	2.37770400
H	-0.85024600	3.22187300	2.93795800
C	-2.76908900	3.40306100	3.83167700
C	-3.17675600	3.78244400	-3.58547100
H	-1.11657300	3.83935000	-4.27922900
H	-5.07804000	3.78267000	-2.61335900
H	-5.37769700	3.88213500	-0.20813100
C	-4.16321600	3.63687300	3.63763000
H	-5.71564300	3.97486500	2.21171500
H	-2.39275700	3.22847800	4.83422200
H	-3.59159700	3.79126100	-4.58811800
H	-4.82665500	3.66677500	4.49552100
C	-1.82945500	-3.03895900	-1.73034500
C	-3.16718100	-3.41243000	-1.70250300
C	-3.49633600	-4.75790200	-1.68622900
C	-2.45431300	-5.68907400	-1.68888300
C	-1.11573700	-5.28468100	-1.68837200
C	-0.77345300	-3.93272700	-1.70601400

C	-2.93038300	-1.08879200	-1.70175600
C	-4.00561300	-2.15963700	-1.58593400
H	-4.53088700	-5.08723300	-1.65352600
H	-2.68818700	-6.74829800	-1.67813700
H	-0.32689100	-6.02982900	-1.67200700
H	0.25673000	-3.59135500	-1.69345600
H	-0.76902300	-1.10486100	-1.72761400
N	-1.75532100	-1.62711900	-1.74896500
C	-3.15192600	0.37470500	-1.82694200
H	-4.04047300	0.68967400	-1.27756200
H	-2.28278400	0.94089100	-1.47885000
H	-3.31626500	0.61055000	-2.88578300
C	-5.04114200	-2.02118000	-2.70521500
H	-5.76303100	-2.83989100	-2.65029500
H	-5.58243600	-1.07546200	-2.63384600
H	-4.54187700	-2.07449200	-3.67607100
C	-7.90431300	0.64315800	0.35478300
C	-6.64911900	0.95313500	0.86288700
C	-5.58545400	0.05186800	0.73905300
C	-5.78072700	-1.17051100	0.07196900
C	-7.05573600	-1.48693200	-0.39738500
C	-8.11111200	-0.58765000	-0.26590700
H	-4.17318900	1.30574000	1.84099400
H	-8.72277400	1.34758200	0.45925100
H	-6.48122300	1.89044400	1.38595100
C	-4.29537000	0.33967900	1.36117400
C	-4.63213100	-2.13830900	-0.10384200
H	-7.22870200	-2.45261200	-0.86407800
H	-9.09414600	-0.85207500	-0.64113400
C	-3.49159100	-1.90988300	0.87919600
C	-3.30180900	-0.56286900	1.41943500
H	-5.01061800	-3.15593300	0.03349800
H	-2.38185000	-0.30830200	1.92854000
N	-2.75204700	-2.93743600	1.11342000
N	-1.58436600	-2.74939300	1.79405700
C	-0.94141000	-3.86057400	2.28351800
O	-1.44510200	-4.97242800	2.27255600
H	-1.11346900	-1.84461700	1.74072400
C	0.39216900	-3.60114400	2.91667200
C	0.81287700	-4.50661000	3.89381300
C	1.20802700	-2.51865900	2.57565900
C	2.02293800	-4.31463400	4.55104500
H	0.17273700	-5.34981000	4.13086100
C	2.42326700	-2.33572200	3.22786900

H	0.91308300	-1.81263200	1.80589600
C	2.82681500	-3.22457200	4.22139800
H	2.33908100	-5.01278800	5.31956500
H	3.05889000	-1.50071400	2.95054100
H	3.77543300	-3.07357000	4.72668300

TSII'-2

Value of imaginary frequency = -81.2 cm^{-1}

C	-7.38522900	-1.98831400	-0.67820500
C	-6.04429800	-1.99349200	-0.38832400
C	-5.29661900	-0.78439600	-0.38085600
C	-5.96436800	0.42810500	-0.71353900
C	-7.35599500	0.40183100	-0.99864300
C	-8.05429900	-0.77724500	-0.97777300
H	-7.93868300	-2.92170800	-0.68394000
C	-3.89823000	-0.74503300	-0.07836100
C	-5.22999500	1.64029100	-0.76755400
H	-7.85284200	1.33714400	-1.24067200
H	-9.11612400	-0.78864400	-1.20013900
C	-3.87422400	1.67478200	-0.54410100
C	-3.22365100	0.45218900	-0.21943200
H	-5.75531600	2.56162100	-1.00680300
C	-3.13086500	-1.94445500	0.35652500
C	-3.46045400	-2.67894000	1.54277200
C	-1.99911100	-2.29941200	-0.34791200
C	-2.63512100	-3.77278400	1.92689800
C	-4.53957400	-2.31522200	2.39542800
C	-1.16442200	-3.39292500	0.01742700
C	-2.93555800	-4.49057600	3.11516900
C	-1.50759500	-4.11368900	1.13508700
C	-4.79465600	-3.01800700	3.54671100
H	-5.15417700	-1.45978500	2.13787100
C	-3.99202600	-4.12576000	3.90892300
H	-2.30126700	-5.32907200	3.38832600
H	-0.89074200	-4.95681600	1.43596700
H	-5.61809500	-2.71927500	4.18722700
H	-4.20944100	-4.67539200	4.81860300
O	-1.63763100	-1.53388300	-1.44110900
H	-5.53821900	-2.92780300	-0.16916800
O	-1.87534800	0.49810500	0.03438000
P	-0.80897300	-0.17921700	-1.01915400
O	0.36844600	-0.57100000	-0.18218700
O	-0.60833100	0.66160900	-2.23683700
C	-3.10660400	2.95159400	-0.61665900
C	-3.02197900	3.65225600	-1.83825600
C	-2.49080200	3.46761100	0.54385800
C	-3.55654600	3.14043800	-3.06803600
C	-2.35188900	4.92406300	-1.87907500
C	-1.79939900	4.72490700	0.48174700
C	-2.52705700	2.78872100	1.80580000

C	-3.46003200	3.85010700	-4.22899400
H	-4.02797900	2.16413700	-3.06763100
C	-2.28222300	5.64113500	-3.11678600
C	-1.76762100	5.43378000	-0.71991900
C	-1.14984900	5.22846600	1.65397900
H	-3.05453200	1.84446700	1.88907100
C	-1.89025000	3.29635000	2.89981100
C	-2.82261200	5.12626700	-4.25603100
H	-3.86390700	3.43789300	-5.14801700
H	-1.77911500	6.60425900	-3.12324700
H	-1.26845100	6.40015900	-0.75721700
C	-1.18448400	4.53332300	2.82549200
H	-0.62287700	6.17623700	1.58121700
H	-1.91056600	2.74592900	3.83562600
H	-2.76174700	5.67514400	-5.19010000
H	-0.67885600	4.91490500	3.70674300
C	0.02592500	-3.76579100	-0.80238600
C	-0.17253400	-4.33033800	-2.07932400
C	1.32994700	-3.60279000	-0.29100000
C	-1.47713500	-4.52085800	-2.64264900
C	0.96064300	-4.75165800	-2.85452600
C	2.45565500	-4.04218600	-1.07213500
C	1.60000100	-2.96788500	0.96690500
C	-1.63741000	-5.06891900	-3.88141400
H	-2.34823700	-4.22535100	-2.06760500
C	0.74967300	-5.32304700	-4.15020400
C	2.24515900	-4.60627600	-2.33018600
C	3.78085300	-3.87144800	-0.55382100
H	0.76703000	-2.58588700	1.54737300
C	2.87844000	-2.79761900	1.41219100
C	-0.50774800	-5.47522000	-4.65228500
H	-2.63450100	-5.20106800	-4.28884600
H	1.62010600	-5.63180600	-4.72251400
H	3.10060600	-4.93278800	-2.91740800
C	3.98998500	-3.26552300	0.64890300
H	4.61557600	-4.22018000	-1.15604300
H	3.05586200	-2.28483300	2.35256100
H	-0.65781100	-5.90872800	-5.63564800
H	4.99882300	-3.12041600	1.02513900
C	2.27717700	2.88651000	-1.21696200
C	3.61772800	2.99842900	-0.83724100
C	4.10943300	4.22317100	-0.41876400
C	3.22729100	5.30725900	-0.35447900
C	1.88883400	5.16682600	-0.72361600

C	1.38573000	3.94408100	-1.17143100
C	3.05959100	0.79070800	-1.29336200
C	4.29704700	1.66185800	-1.10235100
H	5.15193100	4.34515900	-0.13775300
H	3.58924500	6.27008200	-0.01046500
H	1.22249000	6.02123100	-0.66140600
H	0.34538400	3.82094500	-1.45692100
H	1.09643100	1.20252500	-1.88387300
N	2.02587400	1.55443100	-1.59695300
C	3.11953400	-0.65225000	-1.64428500
H	3.99595600	-1.11544500	-1.18683400
H	2.21250500	-1.15507800	-1.29867900
H	3.19324100	-0.74782400	-2.73304600
C	4.94294000	1.76502700	-2.50382600
H	5.77439900	2.47274000	-2.48527800
H	5.28936700	0.79603300	-2.86605100
H	4.19629300	2.14759400	-3.20420700
C	8.66720600	-1.45770900	-0.25357500
C	7.86257100	-1.45313400	0.87734600
C	6.74741100	-0.61323100	0.96583800
C	6.39952000	0.23479200	-0.11286100
C	7.27114500	0.27363400	-1.20293800
C	8.37656800	-0.57287900	-1.28486200
H	6.42450700	-1.13173600	3.06209000
H	9.52506200	-2.11843800	-0.31497400
H	8.09911800	-2.09631500	1.72037900
C	6.00218700	-0.58195300	2.22461800
C	5.20374400	1.18124300	0.07819000
H	7.12138300	0.97616000	-2.00723700
H	9.01466200	-0.52525100	-2.16105000
C	4.27093300	0.65712500	1.15954800
C	4.83896800	0.06973500	2.36718700
H	5.64448400	2.09892600	0.50216600
H	4.27560400	0.07491700	3.29024100
N	3.03761100	0.68287500	0.83061300
N	2.02307600	0.33159000	1.68074400
C	1.82770900	0.97576300	2.87577500
O	2.67007700	1.70913700	3.37798200
H	1.22498500	-0.01734900	1.12388100
C	0.52712200	0.67203200	3.56243400
C	-0.51829600	-0.04895500	2.97485200
C	0.38665400	1.15440600	4.86687800
C	-1.68720300	-0.28196400	3.69478200
H	-0.45590000	-0.42217100	1.95651100

C	-0.77808600	0.91047000	5.58587500
H	1.20622500	1.71660200	5.30127700
C	-1.81856500	0.19013200	4.99917300
H	-2.49689000	-0.83641000	3.23004000
H	-0.87563700	1.28267100	6.60055500
H	-2.73067800	-0.00287900	5.55548200

IMII'-2

C	-7.66512900	-1.36705300	-0.50479700
C	-6.31925200	-1.50429200	-0.27527800
C	-5.46569200	-0.36771700	-0.24876700
C	-6.03357800	0.91263300	-0.50158800
C	-7.43218900	1.02332800	-0.72383000
C	-8.23367500	-0.08856100	-0.72063700
H	-8.29988500	-2.24692200	-0.52568700
C	-4.05919100	-0.46601500	-0.00169600
C	-5.19378200	2.05498500	-0.54608800
H	-7.85184700	2.00909800	-0.90411800
H	-9.30051200	0.00497100	-0.89444100
C	-3.83284200	1.95767400	-0.38405500
C	-3.28399300	0.67099800	-0.12301200
H	-5.64153700	3.02824600	-0.73179900
C	-3.38810100	-1.74486800	0.35964800
C	-3.74431400	-2.49377100	1.52961500
C	-2.31239300	-2.16705400	-0.39441800
C	-3.01205000	-3.67367300	1.84116400
C	-4.75368600	-2.06680300	2.43660800
C	-1.56351900	-3.33993000	-0.09347800
C	-3.33959300	-4.41104400	3.01016200
C	-1.94173200	-4.07711100	1.00199200
C	-5.03602500	-2.79181200	3.56766700
H	-5.29237700	-1.14743800	2.23607200
C	-4.33100600	-3.98453200	3.85530600
H	-2.77723200	-5.31475100	3.22731800
H	-1.38990100	-4.97941500	1.25369600
H	-5.80430800	-2.44429100	4.25074600
H	-4.56971700	-4.55025200	4.74966000
O	-1.91542800	-1.39367200	-1.46929600
H	-5.89065100	-2.48889300	-0.11957100
O	-1.93016600	0.58611900	0.08793900
P	-0.95849100	-0.13087300	-1.03062400
O	0.18746100	-0.68336600	-0.23007800
O	-0.70656500	0.73956900	-2.20816000
C	-2.94755100	3.15419700	-0.46724400
C	-2.83244500	3.86095500	-1.68216300
C	-2.23633300	3.57924900	0.67421700
C	-3.48331200	3.44320000	-2.89097100
C	-2.01303200	5.04130900	-1.73790400
C	-1.39257800	4.73819400	0.59496000
C	-2.31911600	2.89801600	1.93222000
C	-3.35495600	4.15856300	-4.04526100

H	-4.07387200	2.53441500	-2.88193500
C	-1.91234600	5.76780400	-2.96782700
C	-1.31702200	5.45250100	-0.60154400
C	-0.63603100	5.13579400	1.74355400
H	-2.96703100	2.03275500	2.02647700
C	-1.58536800	3.30795700	3.00573600
C	-2.56571100	5.34635000	-4.08619600
H	-3.85117300	3.81824700	-4.94845200
H	-1.29477200	6.66158200	-2.98566400
H	-0.69074100	6.34112200	-0.65265600
C	-0.72001500	4.43770300	2.91089800
H	0.01319900	6.00296000	1.65616600
H	-1.64806700	2.75942000	3.94025100
H	-2.48137700	5.90165900	-5.01465700
H	-0.13383200	4.73632700	3.77418200
C	-0.40879100	-3.76280900	-0.93811100
C	-0.63956500	-4.22610600	-2.24891200
C	0.89908800	-3.74255000	-0.41096600
C	-1.95000000	-4.27684300	-2.82765700
C	0.46400700	-4.68678300	-3.04459600
C	1.99380200	-4.21573900	-1.21437200
C	1.20508200	-3.22359900	0.89067300
C	-2.14227000	-4.73263500	-4.09889300
H	-2.79962000	-3.94976600	-2.23755900
C	0.22009700	-5.15722200	-4.37432100
C	1.75128200	-4.67730300	-2.50776300
C	3.32274200	-4.18708600	-0.67946200
H	0.39836200	-2.82524700	1.49636800
C	2.48796300	-3.19008800	1.35495700
C	-1.04110800	-5.17796200	-4.88958000
H	-3.14331300	-4.76108400	-4.51696400
H	1.06863400	-5.49683900	-4.96179300
H	2.58358900	-5.03140800	-3.11194600
C	3.56742100	-3.68637300	0.56426000
H	4.13302100	-4.55856900	-1.30107700
H	2.69185900	-2.77221900	2.33637400
H	-1.21633700	-5.53584000	-5.89887600
H	4.57998100	-3.65270800	0.95536900
C	2.62564200	2.77737400	-1.07293400
C	4.01803800	2.72500400	-0.91755200
C	4.75070800	3.88811600	-0.76117200
C	4.07777300	5.11521900	-0.74921000
C	2.69321200	5.15385000	-0.91224000
C	1.94281500	3.98757100	-1.07516600

C	3.11184800	0.54795400	-0.89007300
C	4.48067000	1.27994100	-1.07443500
H	5.83271000	3.85242000	-0.65288100
H	4.63387000	6.03681000	-0.61725000
H	2.18040400	6.11144600	-0.90491700
H	0.86399700	4.01830200	-1.19091000
H	1.18827300	1.25096300	-1.54078000
N	2.11799500	1.49183900	-1.20528000
C	2.96813200	-0.81047700	-1.55071700
H	3.83770500	-1.43111500	-1.31701900
H	2.06595000	-1.31531200	-1.19952000
H	2.89858700	-0.67580800	-2.63212100
C	5.00714900	1.08429800	-2.49715300
H	5.80896200	1.79374000	-2.71108900
H	5.36497700	0.06743000	-2.67501500
H	4.19313500	1.29711600	-3.19646800
C	9.03739600	-1.51168600	-0.00913500
C	8.14032900	-1.64029600	1.04205400
C	6.94759600	-0.90876100	1.05590600
C	6.63603900	-0.03841500	-0.01358700
C	7.57557900	0.12613700	-1.02861900
C	8.75623400	-0.61609600	-1.03668200
H	6.40692200	-1.64188000	3.03640300
H	9.95619900	-2.08743500	-0.01705800
H	8.35892900	-2.30621900	1.87169000
C	6.06003000	-1.02814600	2.20894200
C	5.37986000	0.80895600	0.11733300
H	7.40503800	0.84040200	-1.82240700
H	9.46153900	-0.48299900	-1.85016600
C	4.39836700	0.20589000	1.08200300
C	4.83669500	-0.46420600	2.27787900
H	5.72231600	1.71816100	0.64118100
H	4.16975000	-0.61080600	3.11577700
N	3.18516400	0.29408400	0.64277500
N	2.06780100	0.06122700	1.39169600
C	1.94276400	0.76438600	2.58104400
O	2.85385100	1.44918800	3.01802100
H	1.23774700	-0.22894900	0.80055200
C	0.67769900	0.53719800	3.34851200
C	-0.43393300	-0.14528200	2.84539100
C	0.65908700	1.02903200	4.65793900
C	-1.55283800	-0.32921700	3.65420700
H	-0.45558200	-0.52267200	1.82834300
C	-0.45292700	0.82695700	5.46636100

H	1.53132400	1.55842200	5.02573900
C	-1.56239300	0.14674200	4.96349200
H	-2.41776400	-0.85196000	3.25581900
H	-0.45661200	1.20009100	6.48526500
H	-2.43406300	-0.01167400	5.59114500

IMII'-3

C	7.23556500	-3.23270900	-0.72778500
C	6.32330700	-2.28784200	-0.33059100
C	4.93358500	-2.58453100	-0.30035300
C	4.50600600	-3.87645300	-0.72010300
C	5.47587400	-4.83593900	-1.11491700
C	6.81114900	-4.52577900	-1.11669700
H	8.29203300	-2.98557600	-0.75043400
C	3.95092200	-1.62142400	0.09611900
C	3.12038400	-4.18586400	-0.74026400
H	5.13483200	-5.81963300	-1.42530200
H	7.54410400	-5.26377400	-1.42575300
C	2.17279700	-3.24737400	-0.41482100
C	2.61612800	-1.95102300	-0.03590300
H	2.80856100	-5.18729600	-1.02660700
C	4.28893500	-0.27303100	0.62873600
C	5.07516500	-0.08656600	1.81287600
C	3.72225300	0.83364900	0.02888400
C	5.30198500	1.23681400	2.28788700
C	5.60545000	-1.17030200	2.56594800
C	3.89857200	2.15635400	0.52102900
C	6.09162400	1.43728900	3.45134000
C	4.70068700	2.33505200	1.62047200
C	6.35449000	-0.94558400	3.69369500
H	5.40508700	-2.18652500	2.24545100
C	6.61443900	0.37254700	4.13790800
H	6.26256200	2.45499200	3.79134500
H	4.85871900	3.33751400	2.01065800
H	6.74712700	-1.78775700	4.25451700
H	7.21339900	0.53515300	5.02795400
O	2.96186500	0.65801600	-1.10372500
H	6.65549100	-1.29563400	-0.04348400
O	1.65806000	-1.01077900	0.25405300
P	1.40801200	0.15371000	-0.89898100
O	0.65225400	1.22709900	-0.15600700
O	0.93433600	-0.41755900	-2.18025000
C	0.71739100	-3.57325600	-0.38024800
C	0.00419000	-3.80928400	-1.57035600
C	0.06856900	-3.67140200	0.86813700
C	0.60268500	-3.66850700	-2.86565000
C	-1.38108200	-4.18972600	-1.50302000
C	-1.31860000	-4.04022700	0.92083800
C	0.73995600	-3.41545100	2.10871900
C	-0.11062400	-3.91910000	-4.00045400

H	1.63112900	-3.33151800	-2.92665200
C	-2.08815600	-4.45863900	-2.71868400
C	-2.01033200	-4.29738000	-0.26326800
C	-1.97174100	-4.13339900	2.19120800
H	1.79057500	-3.14462200	2.09318700
C	0.08076200	-3.50390700	3.30054300
C	-1.47495500	-4.33278200	-3.92882200
H	0.35767500	-3.79714200	-4.97165000
H	-3.12479300	-4.77541900	-2.64689200
H	-3.05762200	-4.59064400	-0.21538400
C	-1.29781900	-3.86787600	3.34698600
H	-3.02219600	-4.41619700	2.20560000
H	0.60859400	-3.29938800	4.22641800
H	-2.01945100	-4.54094500	-4.84431900
H	-1.80278100	-3.93565000	4.30557300
C	3.20748300	3.30159300	-0.13853400
C	3.67992500	3.77882000	-1.37545300
C	2.08865300	3.89642700	0.47561500
C	4.81616400	3.20353700	-2.03228400
C	3.01831500	4.88224000	-2.01147200
C	1.43209600	4.99793500	-0.17126800
C	1.55282500	3.43300400	1.72253500
C	5.25819000	3.68921600	-3.22764800
H	5.32861500	2.37113600	-1.56107200
C	3.51420900	5.36308400	-3.26550500
C	1.90996300	5.46469800	-1.39611600
C	0.29218200	5.59840000	0.45452300
H	2.01793000	2.58129500	2.20628700
C	0.47028000	4.03813400	2.29285500
C	4.59876100	4.78711200	-3.85694700
H	6.12006800	3.23874000	-3.70922500
H	3.00220800	6.19855100	-3.73480000
H	1.40669100	6.29731600	-1.88203000
C	-0.17270100	5.14072600	1.65057900
H	-0.19136400	6.43068500	-0.04915000
H	0.09198800	3.68141700	3.24728000
H	4.96656600	5.15828900	-4.80798000
H	-1.02970400	5.61227100	2.12103400
C	-3.61134000	2.23837400	2.49144800
C	-4.57630500	1.24672600	2.27700100
C	-5.92277200	1.53483700	2.41687500
C	-6.30316600	2.83738700	2.75893600
C	-5.33340400	3.81724700	2.96971800
C	-3.97136100	3.53237100	2.84597800

C	-2.46442900	0.48784300	1.56720500
C	-3.88471700	-0.05992000	1.90935500
H	-6.67471500	0.76668900	2.25039900
H	-7.35410300	3.08501400	2.85976900
H	-5.63912600	4.82520900	3.23071900
H	-3.22019700	4.29980300	2.99859000
H	-1.55520600	2.31405600	2.05206400
N	-2.33239800	1.70614200	2.29455200
C	-1.29488600	-0.45933100	1.74036700
H	-1.45312500	-1.37021200	1.15408600
H	-0.36706700	0.01172600	1.41043700
H	-1.20412500	-0.72840300	2.79435300
C	-3.84729300	-0.98306800	3.12671400
H	-4.85514600	-1.15339800	3.51053200
H	-3.36725100	-1.93948600	2.90588400
H	-3.28059600	-0.48477000	3.91904500
C	-5.91108700	-4.55916400	-0.49360100
C	-5.37813300	-3.70600000	-1.45012100
C	-4.83153300	-2.47054600	-1.08116100
C	-4.84984200	-2.06254000	0.27366700
C	-5.41949400	-2.91413600	1.21636300
C	-5.92072400	-4.16123700	0.84081900
H	-4.21779800	-2.02727800	-3.12095800
H	-6.32197600	-5.51936700	-0.78496600
H	-5.37711500	-3.99009500	-2.49874200
C	-4.21630100	-1.63900000	-2.10576500
C	-4.43550800	-0.63118900	0.55416500
H	-5.48961800	-2.61996900	2.25403800
H	-6.33875800	-4.81459500	1.59943000
C	-3.49146400	-0.08836000	-0.47801400
C	-3.57273600	-0.47594900	-1.85246800
H	-5.35613000	-0.05885400	0.32964600
H	-3.01617400	0.04916700	-2.61759800
N	-2.64426000	0.73642200	0.06243900
N	-1.82937700	1.61816200	-0.58811700
C	-2.26815800	2.49539600	-1.56245500
O	-1.44177700	3.10914800	-2.21319000
H	-0.75597000	1.48564600	-0.44553300
C	-3.73930200	2.65621000	-1.82342900
C	-4.69090400	2.81416200	-0.81386900
C	-4.13497400	2.68347500	-3.16299900
C	-6.03535100	2.96327000	-1.14536200
H	-4.38909900	2.84406200	0.22746800
C	-5.47962700	2.81980900	-3.49024000

H	-3.38017100	2.58590100	-3.93710000
C	-6.43207400	2.95313400	-2.48101600
H	-6.76679000	3.09052100	-0.35347400
H	-5.78418800	2.82495500	-4.53153500
H	-7.48157000	3.05943600	-2.73583800

IMII'-4

C	7.00623800	-1.91678900	-2.14755800
C	6.05022500	-1.18362300	-1.49096600
C	4.82620300	-1.78109600	-1.08102400
C	4.60520700	-3.15061500	-1.39964300
C	5.61953500	-3.88681800	-2.06788800
C	6.79733800	-3.28769300	-2.43152800
H	7.93032900	-1.44006300	-2.45857500
C	3.80014600	-1.04653600	-0.40185300
C	3.37106400	-3.75702700	-1.05216100
H	5.43569900	-4.93367700	-2.29313500
H	7.56545400	-3.85487800	-2.94676000
C	2.36260500	-3.03855600	-0.46072900
C	2.58304600	-1.66335700	-0.17151900
H	3.22120600	-4.81182300	-1.26899200
C	3.97799600	0.36829400	0.02363900
C	5.01865700	0.79007700	0.91398300
C	3.05271200	1.29850600	-0.40217000
C	5.10567100	2.16768600	1.26517000
C	5.95058500	-0.11295000	1.49576200
C	3.10598000	2.67103500	-0.03419800
C	6.14094700	2.60334100	2.13413500
C	4.13942300	3.08210000	0.77035900
C	6.93357400	0.33679900	2.34139700
H	5.87272800	-1.17092000	1.26991800
C	7.04095000	1.71197300	2.65779900
H	6.19708700	3.65958600	2.38248000
H	4.20971500	4.12784400	1.05989400
H	7.63311200	-0.36987400	2.77626100
H	7.82684200	2.05339400	3.32337600
O	2.04542800	0.88709000	-1.23662500
H	6.21682900	-0.13116500	-1.28819800
O	1.55686200	-0.96118800	0.41085600
P	0.74900300	0.15525500	-0.51628300
O	0.08554200	1.09254800	0.42663000
O	0.04884900	-0.52332000	-1.65248800
C	1.08805300	-3.70037800	-0.05411000
C	0.06484400	-3.92480500	-0.99153500
C	0.94750500	-4.14367600	1.27741200
C	0.16386400	-3.48091400	-2.35248800
C	-1.12807900	-4.61941800	-0.58652800
C	-0.26334600	-4.80264500	1.68173500
C	1.98017400	-3.96756600	2.25639300
C	-0.83684400	-3.72645200	-3.24231200

H	1.04128600	-2.91800600	-2.64838900
C	-2.15144400	-4.86950500	-1.56045000
C	-1.27259600	-5.02516600	0.74022800
C	-0.40145600	-5.23424400	3.03919100
H	2.90297100	-3.47809800	1.96252500
C	1.81419500	-4.40518500	3.53938400
C	-2.01012300	-4.43920200	-2.84441300
H	-0.76414000	-3.36119900	-4.26025400
H	-3.04082700	-5.40973500	-1.24532200
H	-2.18312900	-5.53614000	1.04595200
C	0.60402900	-5.04490400	3.94051000
H	-1.32667500	-5.72291500	3.33167900
H	2.60749200	-4.26371300	4.26608600
H	-2.78914200	-4.62301500	-3.57697100
H	0.49034300	-5.37945500	4.96641700
C	2.05706200	3.62004300	-0.50510900
C	2.00341100	3.98518500	-1.86455800
C	1.13729300	4.16099500	0.41464800
C	2.92229000	3.46558400	-2.83404300
C	1.00884800	4.91900100	-2.31210900
C	0.16186300	5.11301100	-0.03996600
C	1.11066800	3.78060100	1.79732500
C	2.84696300	3.83359200	-4.14514800
H	3.68884900	2.76954700	-2.50954200
C	0.96379500	5.28044700	-3.69683800
C	0.11618500	5.46582500	-1.38891100
C	-0.75197700	5.67978300	0.90554400
H	1.80766500	3.02625400	2.14313900
C	0.21038800	4.32908400	2.66190500
C	1.85064100	4.75402700	-4.58763800
H	3.55140100	3.42592100	-4.86291300
H	-0.62751900	6.18455700	-1.72769600
C	-0.73029800	5.30456400	2.21456600
H	-1.47244300	6.41058000	0.54823800
H	0.20009400	4.01705300	3.70140200
H	-1.43849200	5.73099200	2.91800400
C	-1.59742700	-1.25225300	2.46665400
C	-2.68465100	-0.46029500	2.86274200
C	-2.89657900	-0.17451000	4.20086800
C	-1.99056900	-0.66087100	5.14957000
C	-0.89152700	-1.41393200	4.73948800
C	-0.67600600	-1.72108000	3.39474900
C	-2.94799600	-1.13505400	0.60016000
C	-3.43954000	-0.04492000	1.62111900

H	-3.76245300	0.40241900	4.51577900
H	-2.14594300	-0.45298800	6.20247500
H	-0.18860000	-1.78610900	5.47896300
H	0.17577900	-2.31588200	3.08575400
H	-1.19518700	-2.31774900	0.73108100
N	-1.61771400	-1.46481200	1.08512600
C	-3.83434700	-2.35194600	0.43216400
H	-4.85162200	-2.07879600	0.14412400
H	-3.41594300	-3.01405900	-0.33153000
H	-3.85893700	-2.89015700	1.38430200
C	-4.95281200	0.03867400	1.76454500
H	-5.22768000	0.83813200	2.45602300
H	-5.42993000	0.25078800	0.80141800
H	-5.35286300	-0.89952400	2.15502300
C	-4.27993700	5.23007900	1.74496500
C	-3.88696100	4.85785800	0.46906600
C	-3.41432500	3.56114200	0.22103300
C	-3.35412100	2.62111900	1.27098900
C	-3.69762500	3.02449600	2.55890600
C	-4.16919000	4.31363000	2.79218300
H	-2.94883200	3.98372000	-1.86114200
H	-4.65264000	6.23133800	1.93146000
H	-3.93508400	5.56846500	-0.35162500
C	-2.97008700	3.19570500	-1.11196900
C	-2.82628500	1.24787500	0.97503600
H	-3.59745400	2.32650700	3.38343900
H	-4.45182500	4.60444700	3.79872600
C	-2.75485500	0.93481000	-0.46920400
C	-2.62108300	1.93424700	-1.47400600
H	-1.73975200	1.25665200	1.21513400
H	-2.34033300	1.66723300	-2.48533400
N	-2.84947600	-0.35629100	-0.67114400
N	-2.53148900	-0.94043000	-1.87632800
C	-3.45681900	-1.36211600	-2.80089000
O	-3.08104000	-1.82578000	-3.86359900
H	-1.50103700	-0.93927400	-2.05094300
H	1.80789400	5.03371700	-5.63534500
H	0.20391800	5.98730800	-4.01928000
C	-4.91357200	-1.30614500	-2.44741500
C	-5.56039000	-0.15667700	-1.98995700
C	-5.63797500	-2.48560300	-2.63450500
C	-6.92149000	-0.20038900	-1.69455900
H	-5.01937700	0.77930700	-1.88614000
C	-6.99090400	-2.53146800	-2.31762200

H	-5.12390700	-3.36515500	-3.01011700
C	-7.63284000	-1.38882500	-1.84241500
H	-7.42456600	0.69648600	-1.34777900
H	-7.54491800	-3.45548900	-2.44496800
H	-8.68948500	-1.42118600	-1.59791800

TSII'-3

Value of imaginary frequency = -480.9 cm^{-1}

C	5.69108300	-4.29884000	-2.03263000
C	5.06154000	-3.23115000	-1.44494500
C	3.73094100	-3.34900000	-0.95634600
C	3.05566500	-4.58852200	-1.12950300
C	3.73820400	-5.68044100	-1.73066100
C	5.02942600	-5.54331900	-2.16837200
H	6.70445100	-4.18774000	-2.40458100
C	3.03669300	-2.26282300	-0.33439900
C	1.70213600	-4.70263200	-0.72890600
H	3.20994400	-6.62276700	-1.84537900
H	5.54275300	-6.37942000	-2.63156300
C	1.00610200	-3.64179600	-0.19733500
C	1.70318500	-2.41559200	-0.00317700
H	1.19215000	-5.65186500	-0.87342600
C	3.67812800	-0.94478200	-0.09052700
C	4.84910500	-0.79496100	0.71877000
C	3.06807700	0.18209700	-0.60623700
C	5.39371900	0.50698400	0.89997900
C	5.47206600	-1.88561700	1.38667400
C	3.57230100	1.49324200	-0.39509000
C	6.56443200	0.67305900	1.68807600
C	4.73546100	1.62290300	0.32772000
C	6.59438800	-1.69268600	2.15164600
H	5.04501300	-2.87797400	1.29245700
C	7.15773000	-0.40162000	2.29665300
H	6.97208400	1.67315000	1.80601200
H	5.14550500	2.61535300	0.49737400
H	7.05361500	-2.53685500	2.65589000
H	8.04955700	-0.26678500	2.89989400
O	1.91639500	0.02443100	-1.34858100
H	5.57465100	-2.27980400	-1.35606800
O	1.03034000	-1.35145200	0.56225800
P	0.53598900	-0.15563800	-0.46578800
O	0.37181200	1.10584200	0.34484600
O	-0.52778000	-0.67076500	-1.37499500
C	-0.43090500	-3.81208200	0.16200900
C	-1.36934400	-4.13957700	-0.84097500
C	-0.82835600	-3.76286400	1.51298000
C	-1.03357100	-4.17729600	-2.23502800
C	-2.72082600	-4.46285500	-0.46956100
C	-2.20217500	-4.00428600	1.86114000
C	0.09456800	-3.49505900	2.57796000

C	-1.94038100	-4.59534400	-3.16398400
H	-0.04310300	-3.86316200	-2.54358400
C	-3.63728400	-4.90507200	-1.47584900
C	-3.11131600	-4.36240800	0.86545800
C	-2.60483000	-3.89539500	3.23212200
H	1.14336400	-3.34937500	2.34086000
C	-0.32672300	-3.41296200	3.87398000
C	-3.25427300	-4.99247000	-2.77915900
H	-1.66374000	-4.61923200	-4.21317800
H	-4.64565200	-5.17046800	-1.17051200
H	-4.14075500	-4.58498900	1.13837900
C	-1.70158200	-3.59658300	4.20865300
H	-3.65176100	-4.06026200	3.47321200
H	0.38913000	-3.20333400	4.66240200
H	-3.95339500	-5.33505900	-3.53507600
H	-2.01775900	-3.51320100	5.24308600
C	2.87908800	2.71862000	-0.88596300
C	2.81083100	3.00976800	-2.26151900
C	2.39095300	3.64308600	0.06115200
C	3.28475200	2.10250400	-3.26468000
C	2.27020300	4.27011500	-2.69271100
C	1.93398800	4.93176400	-0.37736400
C	2.31214200	3.34458700	1.46199400
C	3.19368700	2.40822200	-4.59081600
H	3.71643900	1.15670700	-2.95440900
C	2.19243600	4.55139500	-4.09438300
C	1.87175300	5.21111000	-1.74263800
C	1.56351400	5.90871500	0.60126600
H	2.54126400	2.33780100	1.79329800
C	1.91293400	4.29059100	2.36044300
C	2.63314400	3.64990100	-5.01621500
H	3.55251500	1.70342800	-5.33393100
H	1.50868500	6.18223000	-2.07243800
C	1.56936200	5.60647700	1.92960300
H	1.25907400	6.89244300	0.25347000
H	1.84279300	4.03614300	3.41318000
H	1.27973000	6.35308200	2.66314300
C	-0.87642600	0.29727800	2.88462400
C	-1.53585100	1.52504600	3.02311300
C	-1.11054300	2.44822600	3.96409000
C	0.01204200	2.15404900	4.74536600
C	0.69681800	0.95455000	4.55597700
C	0.26356400	0.00823600	3.62557900
C	-2.82769900	0.05642800	1.65797700

C	-2.63867600	1.58285100	1.98853500
H	-1.64675900	3.38232800	4.11167000
H	0.35281100	2.86282700	5.49272900
H	1.57955700	0.74151100	5.15114700
H	0.79410300	-0.92431000	3.47654100
H	-1.45784900	-1.50530000	2.06523800
N	-1.50603100	-0.50171600	1.92348500
C	-3.91170100	-0.67467900	2.42393100
H	-4.87854100	-0.17767900	2.33343600
H	-3.99141800	-1.70036900	2.04995900
H	-3.62955600	-0.71090800	3.47985500
C	-3.91971100	2.28985600	2.41537300
H	-3.73917500	3.35901400	2.54792300
H	-4.69744600	2.17515200	1.65222400
H	-4.28860300	1.88831600	3.36243800
C	-1.67633800	6.15628800	-0.69011200
C	-1.89491100	5.14236500	-1.60285400
C	-2.07166200	3.81737700	-1.16539700
C	-2.00502400	3.51385500	0.21650500
C	-1.73904700	4.54566700	1.12131200
C	-1.59972100	5.85059500	0.67453800
H	-2.30494900	3.03060500	-3.17138400
H	-1.55140800	7.17962100	-1.02771800
H	-1.93854200	5.35499700	-2.66734500
C	-2.32842900	2.76624200	-2.11735500
C	-2.12807200	2.09962100	0.61232100
H	-1.62927600	4.32085900	2.17570200
H	-1.40954000	6.64119300	1.39342800
C	-2.65207200	1.19406600	-0.37496800
C	-2.61109900	1.48229600	-1.76586300
H	-0.97414900	1.67157600	0.49852600
H	-2.79383000	0.71320200	-2.50526300
N	-3.09098000	0.06977500	0.19623400
N	-3.15985500	-1.13175400	-0.50235700
C	-4.07429800	-1.24161000	-1.55259800
O	-3.79008500	-1.91528900	-2.52283700
H	-2.21491900	-1.42840600	-0.79302400
H	2.56903800	3.87267600	-6.07638100
H	1.77601400	5.50619000	-4.40429000
C	-5.37745300	-0.51599000	-1.45050600
C	-5.88006900	0.06245700	-2.61779700
C	-6.11461400	-0.45596900	-0.26797500
C	-7.09824400	0.73251200	-2.59202700
H	-5.30679100	-0.01639300	-3.53634700

C	-7.34097800	0.20116600	-0.24757700
H	-5.74194800	-0.95251400	0.61954800
C	-7.82703200	0.80534000	-1.40589300
H	-7.48155100	1.19278900	-3.49653600
H	-7.91938000	0.23645800	0.66969300
H	-8.77925300	1.32548500	-1.38626400

IMII'-5

C	7.09868700	-2.40014000	-1.76326600
C	6.15864100	-1.54265400	-1.24979400
C	4.92455200	-2.03472700	-0.74541700
C	4.67011100	-3.43363600	-0.82052600
C	5.66989400	-4.29674200	-1.34399300
C	6.86016700	-3.79469000	-1.80085600
H	8.03248500	-2.00533000	-2.14983500
C	3.91391800	-1.17506600	-0.20210800
C	3.41581000	-3.94787000	-0.40187800
H	5.46436400	-5.36253600	-1.38433000
H	7.61577000	-4.46068500	-2.20373200
C	2.41193400	-3.12297200	0.04483900
C	2.69829200	-1.73551100	0.12836800
H	3.23830600	-5.01821800	-0.46891600
C	4.11047900	0.28842700	-0.00086400
C	5.18237300	0.81152200	0.79946900
C	3.19545800	1.18336000	-0.51468700
C	5.31839900	2.22240000	0.93997600
C	6.09740700	-0.02377300	1.49708600
C	3.27594400	2.58825000	-0.32890300
C	6.38855200	2.74952700	1.71073600
C	4.35090400	3.08490800	0.36200600
C	7.11297100	0.51503500	2.24643200
H	5.98163600	-1.10019500	1.44321100
C	7.27319900	1.91727700	2.34516300
H	6.48098900	3.82845900	1.79666900
H	4.43946600	4.15698700	0.51722900
H	7.79644700	-0.14141700	2.77508400
H	8.08513100	2.32807800	2.93597000
O	2.13732100	0.72610800	-1.29173200
H	6.34828500	-0.47498100	-1.23446500
O	1.67974400	-0.89876800	0.56966800
P	0.92994300	-0.09531700	-0.62522400
O	0.05273600	0.92067700	0.16282800
O	0.26692000	-0.95896900	-1.62357800
C	1.06634400	-3.64487400	0.41934400
C	0.25987400	-4.26801800	-0.55656200
C	0.60843000	-3.52155600	1.74872800
C	0.63306400	-4.34855900	-1.93911900
C	-1.01005700	-4.82500700	-0.17512300
C	-0.67436700	-4.05812000	2.10825800
C	1.37422700	-2.87927700	2.77823300
C	-0.17260700	-4.96430300	-2.85023100

H	1.55991700	-3.88713300	-2.25918600
C	-1.82281700	-5.46901400	-1.16222400
C	-1.44062000	-4.71624500	1.14526500
C	-1.15556900	-3.88969500	3.44745600
H	2.36494600	-2.50452700	2.54469000
C	0.87914000	-2.73330800	4.04185700
C	-1.41518800	-5.54435300	-2.45888100
H	0.12434600	-4.99979300	-3.89328700
H	-2.77625600	-5.88582900	-0.84868500
H	-2.40324700	-5.13868300	1.42829800
C	-0.41388700	-3.23194100	4.38289900
H	-2.13390000	-4.29356900	3.69499800
H	1.47539000	-2.23710600	4.80114400
H	-2.04029600	-6.02434100	-3.20456900
H	-0.79269800	-3.09841400	5.39071100
C	2.13894200	3.43561800	-0.78782300
C	2.00821600	3.78789700	-2.14223200
C	1.15120100	3.79276800	0.14843200
C	2.99178800	3.43678200	-3.12241200
C	0.84870000	4.51688300	-2.57392100
C	-0.01679600	4.49687200	-0.30026900
C	1.23283600	3.44070400	1.53624600
C	2.83731400	3.79223400	-4.43055000
H	3.87129400	2.88450400	-2.80557600
C	0.72574500	4.87112500	-3.95510400
C	-0.13923600	4.84585000	-1.64523900
C	-1.05120500	4.80281200	0.63889300
H	2.10389700	2.89965500	1.89036400
C	0.22678900	3.75556300	2.40136500
C	1.68711300	4.52237200	-4.85631900
H	3.59371200	3.51890900	-5.15933400
H	-1.02941500	5.37771700	-1.97503400
C	-0.94040900	4.43755300	1.94683700
H	-1.93596000	5.31670500	0.27561600
H	0.30026700	3.47032800	3.44538000
H	-1.74314300	4.65145200	2.64666700
C	-1.64489200	0.43822500	2.85717300
C	-2.84255200	1.15466600	2.85324100
C	-3.10305000	2.04769300	3.88319400
C	-2.14535300	2.23027300	4.88603800
C	-0.94975900	1.51434500	4.86202100
C	-0.68133000	0.60199100	3.83940200
C	-3.00732000	-0.66492400	1.30916500
C	-3.69603500	0.70406400	1.68045800

H	-4.04825900	2.58069100	3.93509700
H	-2.34313500	2.92304100	5.69701300
H	-0.21788200	1.66077700	5.65002400
H	0.24008800	0.02818800	3.81355500
H	-1.09402000	-1.31385700	1.94414800
N	-1.57812000	-0.43732000	1.73225500
C	-3.56631200	-1.88599300	2.00497500
H	-4.63345700	-1.99040800	1.80451000
H	-3.04764400	-2.77537400	1.63952600
H	-3.40774500	-1.80420300	3.08458000
C	-5.18553900	0.57088400	2.00501400
H	-5.63308100	1.55948400	2.13372400
H	-5.70565900	0.07296900	1.18079200
H	-5.34166100	0.00136300	2.92512700
C	-4.35113100	5.47769800	-0.74885300
C	-3.82868000	4.59303000	-1.65846200
C	-3.52736000	3.25431900	-1.29071500
C	-3.75459100	2.83500100	0.05717200
C	-4.26626400	3.78563200	0.98372700
C	-4.56975200	5.06446600	0.58864400
H	-2.83198700	2.68141800	-3.25538700
H	-4.59375100	6.49242300	-1.04645700
H	-3.65353000	4.89810800	-2.68734000
C	-3.03687300	2.32599400	-2.24932000
C	-3.49082000	1.48114300	0.37871100
H	-4.42444600	3.48735000	2.01368400
H	-4.97535300	5.76922200	1.30765400
C	-3.12395400	0.60062200	-0.61450000
C	-2.84825700	1.00269400	-1.93781200
H	-0.65860200	0.43108500	0.72979800
H	-2.48580200	0.28918600	-2.67141800
N	-3.12725800	-0.72257000	-0.13472900
N	-2.44220200	-1.70712200	-0.84215900
C	-3.07697200	-2.22037900	-1.96878400
O	-2.43725200	-2.51922800	-2.96046100
H	-1.45201000	-1.51174500	-1.04302300
H	1.58403600	4.79481800	-5.90162100
H	-0.15616600	5.42449000	-4.26658300
C	-4.55997700	-2.40332300	-1.90465600
C	-5.32359600	-2.01089400	-3.00372100
C	-5.16885700	-3.02742500	-0.81536300
C	-6.70158900	-2.20767500	-2.99629000
H	-4.83114100	-1.54704300	-3.85285900
C	-6.54348000	-3.24141700	-0.81794100

H	-4.55705100	-3.36497100	0.01429300
C	-7.31132400	-2.82102900	-1.90355400
H	-7.29843300	-1.88924000	-3.84459300
H	-7.01625500	-3.73768200	0.02340000
H	-8.38486200	-2.98003700	-1.90106800

COMIII'

C	5.00908500	5.15122100	1.10868200
C	4.47458000	3.92627500	0.79923000
C	3.09832500	3.79679700	0.46733000
C	2.28176900	4.96097100	0.50577700
C	2.86777500	6.21841500	0.81260600
C	4.20325700	6.31531600	1.10166000
H	6.05985800	5.22841700	1.36793400
C	2.49822200	2.53885900	0.12804100
C	0.89121200	4.84861200	0.26384500
H	2.23089600	7.09799700	0.82406900
H	4.64407700	7.27758300	1.33963700
C	0.28472300	3.63457000	0.03880200
C	1.12333000	2.48829900	-0.00686700
H	0.28141700	5.74800000	0.28697800
C	3.31574900	1.30689500	-0.05674400
C	4.41068900	1.24624200	-0.98561200
C	2.99773500	0.16127700	0.63868200
C	5.16946500	0.04620900	-1.07990400
C	4.73686000	2.31619000	-1.86373200
C	3.72245900	-1.05385000	0.54142500
C	6.26417000	-0.02381800	-1.98268000
C	4.80673000	-1.08068300	-0.29960900
C	5.78690300	2.21239100	-2.74238400
H	4.13853100	3.22041500	-1.84598800
C	6.57513300	1.03741600	-2.79219200
H	6.84032000	-0.94355900	-2.02607000
H	5.39137100	-1.99293300	-0.38580700
H	6.01381700	3.03944200	-3.40707300
H	7.40962200	0.97555300	-3.48254300
O	1.93059800	0.18726500	1.53113600
H	5.10102300	3.04165600	0.82019100
O	0.51553600	1.26289100	-0.26174900
P	0.44497300	0.16083900	0.92534000
O	0.37173900	-1.18562100	0.12740300
O	-0.56537400	0.40542900	1.96913200
C	-1.19499300	3.57076500	-0.14896100
C	-2.03897000	4.03193900	0.88739600
C	-1.74991500	3.13347200	-1.37024900
C	-1.55359900	4.37635400	2.19323000
C	-3.45416800	4.13731200	0.65450300
C	-3.17157000	3.19620200	-1.56693700
C	-0.95544000	2.60469300	-2.43965300
C	-2.40057600	4.81369100	3.16958700

H	-0.49723700	4.26374000	2.40853500
C	-4.30602300	4.61637300	1.70101000
C	-3.98394200	3.73407300	-0.57043100
C	-3.74067500	2.66021100	-2.76562500
H	0.12608000	2.60777200	-2.34824800
C	-1.53526100	2.08587100	-3.56120100
C	-3.79841500	4.94837300	2.92122000
H	-2.00929800	5.05402000	4.15280300
H	-5.37062600	4.69688300	1.49729600
H	-5.05852600	3.78962400	-0.73054500
C	-2.95269200	2.09858400	-3.72468100
H	-4.82098300	2.69230200	-2.87805900
H	-0.91040100	1.66549900	-4.34356200
H	-4.45213100	5.30387200	3.71076200
H	-3.39256400	1.67181500	-4.61986400
C	3.32854800	-2.24852200	1.34117300
C	3.54037100	-2.25462500	2.73419000
C	2.78840100	-3.37580000	0.69339900
C	4.09848300	-1.13496300	3.43323300
C	3.20368200	-3.42418000	3.49558900
C	2.48294500	-4.55063600	1.46370600
C	2.50717000	-3.40083100	-0.71395400
C	4.28788500	-1.17194800	4.78375800
H	4.37664500	-0.24838200	2.87275700
C	3.41670100	-3.42219500	4.91098000
C	2.69112900	-4.54541300	2.84244500
C	1.97456800	-5.71170600	0.79703600
H	2.68567500	-2.50552800	-1.30203500
C	2.01023500	-4.52456000	-1.30818500
C	3.93899200	-2.33113600	5.53869200
H	4.71136100	-0.31252600	5.29341700
H	3.15223200	-4.31450400	5.47132500
H	2.45078600	-5.43502600	3.41989500
C	1.75910400	-5.70666300	-0.54773600
H	1.76377800	-6.59562100	1.39232900
H	1.79082300	-4.52300800	-2.37136000
H	4.09691800	-2.33821700	6.61207900
H	1.37810000	-6.59247400	-1.04587700
C	-2.19107700	-3.22743100	0.89928000
C	-3.56680900	-3.51279000	0.70459300
C	-3.93445100	-4.48316000	-0.23921900
C	-2.94278100	-5.13775900	-0.95309900
C	-1.58218400	-4.85739200	-0.72586600
C	-1.18441000	-3.90628600	0.20131200

C	-3.39053900	-1.86400800	2.22717000
C	-4.31351200	-2.63550800	1.56534100
H	-4.98327600	-4.71105700	-0.41269300
H	-3.21417200	-5.88368200	-1.69395000
H	-0.82578500	-5.38407900	-1.29786600
H	-0.13274200	-3.69017200	0.37060200
H	-1.29443500	-1.69789600	2.08598700
N	-2.11656100	-2.23700500	1.84892500
C	-3.58469300	-0.76390700	3.21686400
H	-4.57372600	-0.31526500	3.09085500
H	-3.50610200	-1.12712000	4.24719000
H	-2.82613500	0.01068800	3.06996000
C	-5.80283100	-2.59636000	1.71193900
H	-6.15932000	-3.25448500	2.51270500
H	-6.15895000	-1.58240300	1.92699700
H	-6.28779700	-2.91595800	0.78449400
C	-7.27731000	0.97049900	0.81076900
C	-5.92318400	1.17065400	0.94092800
C	-5.00903300	0.44640200	0.13592800
C	-5.51215300	-0.48784200	-0.81539800
C	-6.91541000	-0.67297200	-0.92693100
C	-7.77807000	0.03992600	-0.13215800
H	-3.22249100	1.40390000	0.91925700
H	-7.97093400	1.52906400	1.43104400
H	-5.52974600	1.88891000	1.65672000
C	-3.60566300	0.66192000	0.22338900
C	-4.59729500	-1.20080700	-1.62771900
H	-7.29276100	-1.38976400	-1.65095400
H	-8.84928500	-0.10624500	-0.22314500
C	-3.24430300	-0.97928700	-1.50273400
C	-2.74563100	-0.01133600	-0.59160400
H	-4.95210400	-1.93769200	-2.34248600
H	-1.69748500	0.25457100	-0.60919200
N	-2.40820500	-1.72908400	-2.35961200
N	-1.20319400	-1.73390500	-2.04583600
C	-0.36344600	-2.44699100	-3.00101400
O	-0.66448100	-3.53024400	-3.43492100
H	-0.31747200	-1.31634000	-0.59836300
C	0.88660000	-1.71457300	-3.31614200
C	1.88540100	-2.35568000	-4.05645500
C	1.06345800	-0.39215700	-2.89827000
C	3.07535100	-1.69130300	-4.32984600
H	1.71722000	-3.37020100	-4.40443200
C	2.24380800	0.27586900	-3.19608200

H	0.28326200	0.12522900	-2.35239800
C	3.25849500	-0.37745300	-3.89333700
H	3.86018300	-2.19364500	-4.88516000
H	2.37742300	1.30369600	-2.87310600
H	4.19123200	0.14112800	-4.09665800

TSIII'-1

Value of imaginary frequency = -159.0 cm^{-1}

C	-4.68604100	5.37872400	-1.85274100
C	-4.25390400	4.23056400	-1.23766600
C	-2.92664300	4.12620600	-0.73648000
C	-2.04733200	5.22856900	-0.93118300
C	-2.52786600	6.40810000	-1.55997400
C	-3.82072100	6.48790600	-2.00638400
H	-5.70126000	5.43493100	-2.23198900
C	-2.42602300	2.94752100	-0.09012500
C	-0.69423100	5.12565000	-0.52255900
H	-1.84256500	7.24125300	-1.68778400
H	-4.17996100	7.39082600	-2.48889400
C	-0.19521400	3.97809800	0.04386700
C	-1.08910600	2.89365800	0.24683600
H	-0.03149100	5.97285500	-0.68098300
C	-3.28311900	1.74790900	0.11624000
C	-4.51094000	1.79275900	0.85149900
C	-2.89367700	0.54849900	-0.44690700
C	-5.34755100	0.64175100	0.86729100
C	-4.91587900	2.93632700	1.59203200
C	-3.74347400	-0.59227700	-0.49652500
C	-6.57017700	0.67870100	1.58967600
C	-4.95308100	-0.51810300	0.15266100
C	-6.09709600	2.93796500	2.29026800
H	-4.27145100	3.80905300	1.60757000
C	-6.94034500	1.80072700	2.28458100
H	-7.20205100	-0.20494800	1.58489800
H	-5.62706200	-1.37058300	0.12238900
H	-6.38628500	3.81675800	2.85742200
H	-7.87313800	1.81891700	2.83828000
O	-1.67522000	0.46706500	-1.07646200
H	-4.92732800	3.38668200	-1.14108300
O	-0.59809900	1.74479400	0.83016700
P	-0.30026000	0.48031800	-0.17308100
O	-0.21818600	-0.72843400	0.70696300
O	0.78858500	0.81468000	-1.14589100
C	1.24117400	3.91743800	0.44547400
C	2.24303200	3.86456000	-0.54341400
C	1.58753300	4.03375300	1.80603900
C	1.94253800	3.66658600	-1.93160500
C	3.62193000	4.00599500	-0.16314600
C	2.96953200	4.15791300	2.17744300
C	0.60404700	4.06365700	2.84815400

C	2.93468900	3.62607200	-2.86656300
H	0.90948200	3.51763300	-2.22331100
C	4.63228000	3.97008400	-1.17848300
C	3.95012400	4.17135600	1.18357400
C	3.31116800	4.28355800	3.56185100
H	-0.44529400	3.98819400	2.58239800
C	0.97009500	4.18162800	4.15690400
C	4.30185300	3.78653300	-2.48784500
H	2.68828000	3.46035800	-3.91037000
H	5.66991200	4.09285500	-0.87883800
H	4.99172300	4.30778500	1.46842500
C	2.34491400	4.29027200	4.52289400
H	4.36131000	4.37219800	3.82598600
H	0.21063000	4.19599000	4.93201300
H	5.07520800	3.75569000	-3.24885900
H	2.61361400	4.38261100	5.57011600
C	-3.37398300	-1.79744300	-1.29374600
C	-3.20893000	-1.68646900	-2.69216800
C	-3.27477900	-3.05788200	-0.66792500
C	-3.34890400	-0.44390600	-3.39412300
C	-2.91958100	-2.86066200	-3.46753100
C	-3.04797600	-4.23262900	-1.46552300
C	-3.37392100	-3.22706900	0.75165400
C	-3.17319800	-0.37147600	-4.74490200
H	-3.60405200	0.45251100	-2.83961500
C	-2.73183600	-2.74072000	-4.88170500
C	-2.85685800	-4.10500700	-2.83983600
C	-3.01292400	-5.51613600	-0.83040100
H	-3.48405300	-2.34929300	1.37856900
C	-3.31130600	-4.46441500	1.32278800
C	-2.84845000	-1.53460600	-5.50404100
H	-3.28444200	0.58162200	-5.25170600
H	-2.49969300	-3.63985500	-5.44557100
H	-2.66265400	-4.99391900	-3.43586800
C	-3.14681000	-5.63262500	0.52087800
H	-2.86130900	-6.39267600	-1.45487800
H	-3.37411500	-4.56048600	2.40200100
H	-2.70604500	-1.45276300	-6.57664800
H	-3.11134300	-6.60813200	0.99529200
C	1.73030800	-2.73262900	-1.51006700
C	2.88979300	-3.53026500	-1.61709600
C	2.80492800	-4.89878300	-1.32616600
C	1.57494700	-5.42106200	-0.95384100
C	0.43211900	-4.60559000	-0.87051200

C	0.48519800	-3.24664100	-1.15631800
C	3.40760400	-1.35192100	-2.03771700
C	3.98753800	-2.64722800	-1.90538400
H	3.68461500	-5.53392900	-1.38071200
H	1.49088300	-6.47530700	-0.71211800
H	-0.51292400	-5.04254000	-0.56310200
H	-0.39011500	-2.60951800	-1.06427400
H	1.50359500	-0.57068100	-1.64979000
N	2.09540200	-1.42108400	-1.79004500
C	4.05093500	-0.06915000	-2.43014500
H	5.07759800	-0.01361200	-2.05990300
H	4.08681000	0.00503700	-3.52278700
H	3.47737800	0.78004900	-2.04523100
C	5.33288500	-3.04407200	-2.42304600
H	5.25882600	-3.37416600	-3.46432200
H	6.03650500	-2.20838000	-2.38927200
H	5.75373200	-3.87376400	-1.84583600
C	7.47252800	0.92319000	0.16606300
C	6.16629200	1.22642300	0.51471300
C	5.19283800	0.21977400	0.58381600
C	5.56568600	-1.11698800	0.29199400
C	6.90373300	-1.41147100	-0.03610600
C	7.84653500	-0.40149600	-0.10351900
H	3.56233900	1.54980700	1.15945800
H	8.21433400	1.71347000	0.11301800
H	5.87868200	2.24682700	0.74532600
C	3.82838500	0.51285800	0.97434000
C	4.56173500	-2.14131600	0.35381800
H	7.18660800	-2.44294200	-0.22369900
H	8.87533400	-0.63420800	-0.35571200
C	3.29589400	-1.85012400	0.95666200
C	2.91409100	-0.46353600	1.15738000
H	4.86557400	-3.18365900	0.34143000
H	1.91388500	-0.21858500	1.49420100
N	2.61981000	-2.92580300	1.32552800
N	1.40850300	-2.80190100	1.80914800
C	0.84621900	-3.93918300	2.42615200
O	1.42884800	-5.00083700	2.42422400
H	0.84793800	-1.95750400	1.62049800
C	-0.42449100	-3.71731900	3.18132700
C	-0.86490100	-4.79665000	3.95614700
C	-1.12672100	-2.50821900	3.21295500
C	-1.98412500	-4.66955300	4.76779900
H	-0.30278900	-5.72309900	3.91869300

C	-2.25257900	-2.38840200	4.02483900
H	-0.83295100	-1.65924200	2.60344000
C	-2.67870300	-3.45983000	4.80642100
H	-2.31235400	-5.50822600	5.37275900
H	-2.79676500	-1.44960000	4.04544900
H	-3.55107500	-3.35429100	5.44363500

IMIII'-1

C	-4.01926300	5.94225600	-0.56409000
C	-3.61988300	4.66101100	-0.27812900
C	-2.23973500	4.31485800	-0.24908400
C	-1.29086100	5.32608800	-0.56504400
C	-1.73314100	6.64675500	-0.84343100
C	-3.06814200	6.95401700	-0.83746600
H	-5.07760700	6.18102800	-0.58795400
C	-1.77598700	2.98868400	0.04713100
C	0.08517600	4.99480800	-0.61720900
H	-0.98843600	7.40459700	-1.06990200
H	-3.40028800	7.96355700	-1.05547300
C	0.52784300	3.71142800	-0.41374900
C	-0.42969000	2.70653600	-0.10299000
H	0.80705000	5.77701500	-0.83832000
C	-2.73766000	1.91782300	0.42730600
C	-3.64536900	2.03878100	1.53022400
C	-2.78349900	0.76662500	-0.32613200
C	-4.63737700	1.03651900	1.72084800
C	-3.55655400	3.09428000	2.47721800
C	-3.77836700	-0.23575500	-0.16880500
C	-5.53336100	1.14309400	2.81679000
C	-4.69577000	-0.07409500	0.83882300
C	-4.41737500	3.15379100	3.54543800
H	-2.78313100	3.84590300	2.35882100
C	-5.42607500	2.17487800	3.71416200
H	-6.29225300	0.37572500	2.94234000
H	-5.47751200	-0.81682700	0.97670200
H	-4.32317300	3.95680700	4.26907400
H	-6.10547300	2.23992900	4.55753300
O	-1.84810900	0.59072200	-1.32327100
H	-4.36453800	3.89723400	-0.08570000
O	0.04553300	1.43700900	0.13904100
P	-0.36260600	0.14786000	-0.80179600
O	-0.40817500	-1.02935000	0.11421000
O	0.48252000	0.08435100	-2.04735100
C	1.99610500	3.43819300	-0.47863000
C	2.58822900	3.00971600	-1.68132100
C	2.79686000	3.74712900	0.63865400
C	1.81366500	2.70006100	-2.84632600
C	4.01963300	2.90735500	-1.77169700
C	4.22789200	3.65782000	0.53299200
C	2.23673800	4.15114600	1.89555300
C	2.41705200	2.32136300	-4.00979200

H	0.73252000	2.75886500	-2.78553300
C	4.61302200	2.50209300	-3.01039200
C	4.80502800	3.23851500	-0.66669400
C	5.03142900	3.99414600	1.66997400
H	1.15761700	4.21203700	1.99091300
C	3.03707800	4.44464000	2.96049600
C	3.83809300	2.22296500	-4.09689200
H	1.81310700	2.08519900	-4.87965000
H	5.69601200	2.43138700	-3.06312400
H	5.88854000	3.17750500	-0.74575500
C	4.45756600	4.37172000	2.84728700
H	6.11280600	3.94209900	1.56965400
H	2.59356600	4.73954600	3.90590800
H	4.29637000	1.92198000	-5.03368600
H	5.07550500	4.62075700	3.70357000
C	-3.86435300	-1.36215700	-1.14202300
C	-4.26738100	-1.08116500	-2.46524500
C	-3.59165600	-2.68460700	-0.74445500
C	-4.57179000	0.24588800	-2.91440100
C	-4.39832000	-2.15340400	-3.41041300
C	-3.75569400	-3.75235300	-1.69567400
C	-3.13850700	-3.02125600	0.57557100
C	-4.95328100	0.48512200	-4.20225900
H	-4.49998100	1.07074600	-2.21321900
C	-4.79928500	-1.86096400	-4.75293400
C	-4.14679500	-3.46319600	-3.00170100
C	-3.51955300	-5.10250400	-1.28022000
H	-2.96313300	-2.22425400	1.29185700
C	-2.90933600	-4.31998400	0.92452700
C	-5.06548500	-0.58233700	-5.14136500
H	-5.17730900	1.49861700	-4.51896100
H	-4.88736100	-2.68661900	-5.45368300
H	-4.26286400	-4.27549800	-3.71561200
C	-3.12288900	-5.38005400	-0.00699000
H	-3.66820300	-5.89699000	-2.00647000
H	-2.55672500	-4.55539000	1.92284100
H	-5.36771400	-0.36936700	-6.16155600
H	-2.95045600	-6.40618900	0.30334800
C	1.47281000	-3.42444600	-1.36455800
C	2.64357100	-4.06120200	-0.95947800
C	2.60435600	-5.38259300	-0.54930600
C	1.37300200	-6.03960500	-0.57636600
C	0.20918800	-5.37714400	-0.97214000
C	0.23186100	-4.03870000	-1.36798100

C	3.07879100	-1.86910800	-1.61109400
C	3.76412900	-3.05021100	-0.95826700
H	3.50046100	-5.89561600	-0.21255200
H	1.31593500	-7.07990300	-0.27439300
H	-0.73619900	-5.90643900	-0.96961400
H	-0.67247400	-3.51064600	-1.65416200
H	1.14669800	-1.30324800	-2.03323200
N	1.81237000	-2.10376800	-1.75728200
C	3.70636000	-0.62634800	-2.11910000
H	4.54712300	-0.31294700	-1.49931600
H	4.09918200	-0.84083700	-3.12142700
H	2.96221400	0.17096700	-2.20063700
C	5.01308200	-3.49212900	-1.72073800
H	4.74422900	-3.77714600	-2.74059800
H	5.75780000	-2.69432200	-1.75959000
H	5.46216700	-4.36021300	-1.23061800
C	7.49581400	-0.12574000	1.10720700
C	6.21246400	0.40827000	1.12314100
C	5.09551700	-0.41890800	0.96514700
C	5.27385600	-1.80179300	0.77539000
C	6.56476500	-2.32808600	0.78168800
C	7.67198500	-1.49810700	0.94190200
H	3.63311400	1.21387700	1.03907400
H	8.35556500	0.52342100	1.23633900
H	6.05751800	1.47174700	1.28119100
C	3.74074200	0.13240900	1.03051600
C	4.06943500	-2.69426700	0.58350400
H	6.70569300	-3.39952500	0.66864600
H	8.66956700	-1.92454900	0.94574700
C	2.82283500	-2.10999900	1.21815400
C	2.65368200	-0.65148400	1.13532000
H	4.26192000	-3.66953900	1.04162400
H	1.67123200	-0.20627700	1.23746500
N	2.01451400	-2.94170800	1.77423300
N	0.82167400	-2.41749500	2.20460800
C	0.07389200	-3.12220900	3.10672500
O	0.41972200	-4.18498700	3.59947300
H	0.35070700	-1.74652700	1.58510400
C	-1.20085400	-2.43625000	3.51126900
C	-2.16492600	-3.21189900	4.15853300
C	-1.42542600	-1.06693700	3.32477600
C	-3.36145000	-2.64134500	4.57821700
H	-1.95563100	-4.26399400	4.32451800
C	-2.61077900	-0.49185200	3.77447700

H	-0.67939500	-0.43981600	2.84635700
C	-3.58431700	-1.27902300	4.38688100
H	-4.11296400	-3.25445400	5.06499400
H	-2.77419600	0.57475300	3.65480800
H	-4.51010300	-0.82258700	4.72392200

TSIII'-2

Value of imaginary frequency = -106.7 cm^{-1}

C	-6.14503800	4.30626600	-0.93887000
C	-5.38616000	3.22038500	-0.58157900
C	-3.96957600	3.31450100	-0.50708900
C	-3.35524700	4.55391900	-0.84180900
C	-4.16872700	5.66383000	-1.19446100
C	-5.53355800	5.54712000	-1.23914000
H	-7.22456400	4.21235100	-0.99784300
C	-3.14319200	2.20411700	-0.13821900
C	-1.94118200	4.66041500	-0.82970600
H	-3.68336200	6.60513300	-1.43667000
H	-6.14694400	6.39849600	-1.51458200
C	-1.14014000	3.57933800	-0.55173700
C	-1.77123500	2.34332000	-0.23837000
H	-1.48387000	5.61936400	-1.06098100
C	-3.70037300	0.90711900	0.33609000
C	-4.54720400	0.80792700	1.49052100
C	-3.30311500	-0.25733400	-0.28595800
C	-4.97685100	-0.48050000	1.91952700
C	-4.90462400	1.93408000	2.28285500
C	-3.72960200	-1.55019200	0.12232300
C	-5.77764700	-0.59828100	3.08626600
C	-4.56423400	-1.63691000	1.20729800
C	-5.66419400	1.78583500	3.41683100
H	-4.55237500	2.91823400	1.99542200
C	-6.11646100	0.50799600	3.82209500
H	-6.10177700	-1.58909000	3.39261200
H	-4.90826000	-2.61184100	1.54341200
H	-5.91669900	2.65749400	4.01183900
H	-6.72022200	0.40812200	4.71804200
O	-2.44895400	-0.17417900	-1.36562100
H	-5.86375300	2.27103000	-0.36291600
O	-0.95566900	1.27824200	0.05302100
P	-0.86382800	-0.00778300	-0.97858700
O	-0.38147800	-1.14075000	-0.12794600
O	-0.13259800	0.34083100	-2.23567300
C	0.34664900	3.69667000	-0.54570800
C	1.03336200	4.01301800	-1.73645600
C	1.06053500	3.51695600	0.65945500
C	0.37570100	4.11781500	-3.00755100
C	2.45721200	4.21336500	-1.70153000
C	2.48742600	3.67864000	0.66983300
C	0.42079600	3.17660400	1.89617200

C	1.07234800	4.42613700	-4.13884100
H	-0.69025200	3.92864500	-3.06239800
C	3.14840700	4.54885600	-2.91026100
C	3.14747600	4.05120400	-0.50175000
C	3.21349000	3.43506600	1.87872900
H	-0.66054800	3.08633300	1.92556800
C	1.14678700	2.95270800	3.03008700
C	2.47988000	4.65658000	-4.09208600
H	0.55457200	4.48984400	-5.09040300
H	4.22215200	4.70743600	-2.85978200
H	4.22675800	4.18832700	-0.48461700
C	2.56792200	3.07031300	3.02236900
H	4.29538300	3.53799200	1.85648900
H	0.63827300	2.67698900	3.94871500
H	3.01260900	4.90639800	-5.00375800
H	3.12776600	2.87490400	3.93164300
C	-3.31980200	-2.75604300	-0.65448700
C	-3.90651500	-2.97422200	-1.91821700
C	-2.38987000	-3.67297900	-0.12883700
C	-4.86186700	-2.07029100	-2.48842900
C	-3.55542600	-4.14387200	-2.67211800
C	-2.05527700	-4.84692500	-0.89011400
C	-1.73533000	-3.47938900	1.13397400
C	-5.41577500	-2.30922900	-3.71199500
H	-5.14852100	-1.18512300	-1.93034500
C	-4.15866000	-4.35814000	-3.95251900
C	-2.64139700	-5.05360700	-2.13884000
C	-1.11670500	-5.78619100	-0.35288200
H	-1.93932600	-2.57503700	1.70053100
C	-0.83753300	-4.39282500	1.60193500
C	-5.05966300	-3.47046400	-4.45994300
H	-6.13675400	-1.61063500	-4.12410600
H	-3.88025600	-5.24876200	-4.50914600
H	-2.38123000	-5.94313200	-2.70831900
C	-0.52548800	-5.56798100	0.85440700
H	-0.88699700	-6.67422900	-0.93613900
H	-0.34435300	-4.22031200	2.55294200
H	-5.51207100	-3.64103400	-5.43143300
H	0.19224200	-6.27954100	1.25035700
C	2.40046400	-2.70613500	-1.68259600
C	3.73324900	-2.82157700	-1.27488900
C	4.29549200	-4.07525700	-1.10807700
C	3.48874600	-5.19877300	-1.31580300
C	2.15034200	-5.05991200	-1.68417400

C	1.57607200	-3.80115000	-1.87551400
C	3.03894000	-0.61044900	-1.23299000
C	4.33084000	-1.42722300	-1.16237100
H	5.33513700	-4.18832500	-0.81166600
H	3.90617100	-6.19017500	-1.17654800
H	1.53532600	-5.94428000	-1.81315300
H	0.52847200	-3.68449000	-2.13435300
H	1.17980500	-0.92783900	-2.05436700
N	2.08740000	-1.33838100	-1.78863600
C	3.00133600	0.87844600	-1.28595900
H	3.75227100	1.30332500	-0.61743700
H	3.21502100	1.20290000	-2.31034700
H	2.00996300	1.25572200	-1.01723500
C	5.07877800	-1.11498900	-2.47823200
H	4.36564700	-1.16315300	-3.30581400
H	5.53443100	-0.12258200	-2.46104300
H	5.84697100	-1.86360000	-2.67247900
C	8.81912800	1.05646900	0.43456700
C	7.82521500	1.21959900	1.38915300
C	6.62386500	0.50474300	1.30686800
C	6.39134100	-0.36906500	0.22411900
C	7.43631300	-0.58265000	-0.67638600
C	8.62889600	0.13139000	-0.58772300
H	5.94310000	1.23288600	3.24711700
H	9.74445600	1.61793900	0.50480400
H	7.97665600	1.89385500	2.22740700
C	5.66467000	0.60572800	2.40370200
C	5.10299400	-1.18459300	0.18471700
H	7.34075600	-1.32720500	-1.45515600
H	9.41233000	-0.04750000	-1.31655800
C	4.07175900	-0.72676800	1.20782000
C	4.48379100	-0.03496000	2.41646500
H	5.40232400	-2.18534500	0.53658400
H	3.78525700	0.06790000	3.23495400
N	2.87196600	-0.91318800	0.79969700
N	1.74901800	-0.68172500	1.54795200
C	1.59257200	-1.31104600	2.77400800
O	2.50057600	-1.88699700	3.35213900
H	0.90584400	-0.73344300	0.94150300
C	0.20865500	-1.21557800	3.33075300
C	-0.16812200	-2.14988300	4.29811300
C	-0.68992100	-0.22471700	2.92640500
C	-1.45315600	-2.12247100	4.82978400
H	0.55398800	-2.89654100	4.61381200

C	-1.96318800	-0.18121900	3.48531300
H	-0.40064800	0.51694500	2.18902200
C	-2.35208500	-1.13677900	4.42270700
H	-1.75130400	-2.86297300	5.56491000
H	-2.65426600	0.59990500	3.18674600
H	-3.35544900	-1.10508400	4.83725900

IMIII'-2

C	-6.65700900	-3.16141000	1.83270000
C	-5.85948500	-2.35091900	1.06469100
C	-4.49589500	-2.67950200	0.83398000
C	-3.96817200	-3.85283300	1.44327200
C	-4.82246900	-4.67767600	2.22254600
C	-6.13849100	-4.34440000	2.41168300
H	-7.69388700	-2.89102400	2.00438600
C	-3.62656500	-1.85499600	0.04910600
C	-2.59824100	-4.17949600	1.26820100
H	-4.40699200	-5.57510300	2.67222600
H	-6.78227400	-4.97751200	3.01322500
C	-1.74862400	-3.36199500	0.56474000
C	-2.28683300	-2.18102400	-0.01116700
H	-2.21473900	-5.09626300	1.70918000
C	-4.09154600	-0.64970400	-0.69016100
C	-5.10247800	-0.72232300	-1.70371500
C	-3.46255200	0.55890800	-0.46305700
C	-5.48190300	0.46850400	-2.38549500
C	-5.72066500	-1.94406200	-2.08963500
C	-3.80887600	1.74858500	-1.16005100
C	-6.49459400	0.41410400	-3.38030000
C	-4.82003500	1.68637400	-2.08663300
C	-6.68806900	-1.96687300	-3.06224800
H	-5.41332900	-2.86779900	-1.61214600
C	-7.09188800	-0.77450500	-3.70907300
H	-6.77758900	1.33532500	-3.88188700
H	-5.10693300	2.58676700	-2.62411000
H	-7.14465000	-2.91022200	-3.34413100
H	-7.86256600	-0.80915300	-4.47208600
O	-2.48610600	0.63322100	0.50606900
H	-6.26195200	-1.44011800	0.63410000
O	-1.42262100	-1.33600100	-0.67480700
P	-0.99867800	0.01188700	0.17387800
O	-0.28360300	0.88614800	-0.81779900
O	-0.36664000	-0.33664900	1.47906400
C	-0.32312800	-3.74842400	0.34295900
C	0.61509800	-3.65908700	1.38653500
C	0.04882800	-4.28486700	-0.90815900
C	0.29700800	-3.07521200	2.65771900
C	1.94606100	-4.16640300	1.18863700
C	1.38201900	-4.78417000	-1.09636200
C	-0.86321500	-4.37206000	-2.00986200
C	1.22851100	-3.01163300	3.65113100

H	-0.69143700	-2.65541800	2.80270400
C	2.89003800	-4.08809800	2.26359400
C	2.29363900	-4.72772400	-0.03933600
C	1.74927200	-5.33389000	-2.36536200
H	-1.87766200	-4.00833100	-1.88324600
C	-0.47388000	-4.89933400	-3.20693300
C	2.54506400	-3.52986400	3.45640200
H	0.97297800	-2.55677700	4.60317400
H	3.88907700	-4.48482600	2.10102600
H	3.29766600	-5.12312600	-0.18103700
C	0.85289800	-5.38844400	-3.39104100
H	2.76225100	-5.70671100	-2.49010500
H	-1.17925300	-4.95080000	-4.02997000
H	3.27028800	-3.46108200	4.26088000
H	1.14196500	-5.80525100	-4.35039500
C	-3.09392600	3.03171200	-0.89384500
C	-3.47327400	3.82151300	0.20723100
C	-2.07675600	3.46450000	-1.76499300
C	-4.49906900	3.41340700	1.12156100
C	-2.81299000	5.07453000	0.44426300
C	-1.41708900	4.71622300	-1.51477100
C	-1.66141300	2.69760100	-2.90248000
C	-4.83049000	4.18678900	2.19653900
H	-5.00826600	2.47034500	0.95091400
C	-3.19493000	5.85831000	1.57925000
C	-1.79936700	5.49059900	-0.41883800
C	-0.37923900	5.14684800	-2.40256800
H	-2.13627900	1.74038500	-3.08603000
C	-0.67555000	3.14679200	-3.72993200
C	-4.16850300	5.42919000	2.43219800
H	-5.60474000	3.85721200	2.88182000
H	-2.68181700	6.80069400	1.74976600
H	-1.29670800	6.43703500	-0.23297200
C	-0.02139300	4.39055000	-3.47793100
H	0.11084600	6.09494400	-2.19901400
H	-0.37405000	2.55088100	-4.58525900
H	-4.44582900	6.02760100	3.29385100
H	0.76331600	4.72748800	-4.14780000
C	3.49233400	-0.47885800	2.23393600
C	4.74489800	-0.47471400	1.60814500
C	5.90309200	-0.32956000	2.35057500
C	5.80277800	-0.16046600	3.73616900
C	4.54907800	-0.13954100	4.34624600
C	3.37438000	-0.29456400	3.60728500

C	3.01590100	-0.44524100	0.00004400
C	4.56002500	-0.68172300	0.10772600
H	6.87759100	-0.33733100	1.86611400
H	6.69985500	-0.03693200	4.33294400
H	4.48003400	0.00684900	5.41986400
H	2.39878500	-0.27018300	4.08153800
H	1.49113100	-0.61607600	1.48220300
N	2.49557100	-0.68733500	1.29124900
C	2.27849900	-1.14473000	-1.12429900
H	2.79473400	-0.97873200	-2.07450600
H	2.23979200	-2.21574100	-0.91329500
H	1.26098600	-0.75952500	-1.21579700
C	4.92766100	-2.11545300	-0.26647900
H	4.27548700	-2.78571600	0.30056500
H	4.79453600	-2.31832000	-1.33239300
H	5.95884400	-2.33511300	0.01994400
C	7.70130300	0.52849200	-4.23316600
C	6.92374800	1.62391600	-3.88133700
C	6.09678300	1.57873800	-2.75354700
C	6.04441000	0.40650900	-1.96184100
C	6.86506600	-0.66509000	-2.29960200
C	7.67299900	-0.61145800	-3.43556800
H	5.45752200	3.64654200	-3.01328200
H	8.33316000	0.56690700	-5.11351900
H	6.94968400	2.52965600	-4.47996200
C	5.30416500	2.75698800	-2.40756900
C	5.23012500	0.49552000	-0.68314900
H	6.88985600	-1.55346000	-1.68421000
H	8.28709400	-1.46869400	-3.69056900
C	4.13474200	1.50852000	-0.79897700
C	4.36096200	2.77240800	-1.44107400
H	5.92049000	0.98885700	0.02335500
H	3.70465800	3.61383000	-1.26020000
N	3.01772800	1.07305800	-0.31658600
N	2.00876400	1.90142500	0.10012500
C	2.33018500	2.61242400	1.25854400
O	3.49735900	2.79886800	1.55859100
H	1.05075900	1.55325700	-0.15100100
C	1.20011000	3.09549700	2.10441100
C	1.55892200	3.59982800	3.35952300
C	-0.14885000	3.00301700	1.74857800
C	0.58011000	3.99483700	4.26168200
H	2.61165700	3.65885100	3.61228900
C	-1.12524500	3.37884300	2.66755300

H	-0.45740800	2.64634500	0.76844500
C	-0.76517100	3.87439800	3.91779700
H	0.86536200	4.38269800	5.23406600
H	-2.17304500	3.27698900	2.40739800
H	-1.53746500	4.16698000	4.62271300

IMIII'-3

C	-7.18638200	0.86523900	-2.58904600
C	-5.85641900	1.04007600	-2.29924100
C	-5.10727200	0.01272800	-1.66385600
C	-5.77848700	-1.19067900	-1.30566000
C	-7.15181900	-1.34701100	-1.63168500
C	-7.84269900	-0.34544400	-2.26304500
H	-7.74204400	1.66500200	-3.06793700
C	-3.71862300	0.15860300	-1.33927600
C	-5.07107100	-2.21203500	-0.61863100
H	-7.64591100	-2.27576500	-1.36012300
H	-8.89316400	-0.47206000	-2.50310400
C	-3.76255500	-2.04596700	-0.23962600
C	-3.11292300	-0.82931300	-0.58819400
H	-5.58806600	-3.13662900	-0.37374500
C	-2.90202900	1.32613700	-1.77115500
C	-2.76656600	1.68473500	-3.15281200
C	-2.18011800	2.03240200	-0.82644600
C	-1.98281000	2.82286600	-3.49528200
C	-3.35418300	0.93394300	-4.20894900
C	-1.33678500	3.12962700	-1.16272900
C	-1.86519000	3.21146000	-4.85693500
C	-1.28880300	3.52423700	-2.47868400
C	-3.20991000	1.32421800	-5.51648000
H	-3.91530800	0.03696400	-3.97309400
C	-2.47024500	2.48482900	-5.84829900
H	-1.27424200	4.09139100	-5.09529900
H	-0.67058300	4.37386600	-2.75806800
H	-3.66413300	0.73438800	-6.30616100
H	-2.37331000	2.78536800	-6.88627300
O	-2.31615600	1.70678500	0.49906100
H	-5.36491500	1.97590500	-2.54297400
O	-1.80960300	-0.66372100	-0.18529400
P	-1.57451200	0.36118700	1.09456000
O	-0.08503100	0.55920500	1.09328200
O	-2.32085500	-0.05108200	2.30452500
C	-3.00173400	-3.10547700	0.48211700
C	-3.32257600	-3.43230900	1.81346600
C	-1.96157900	-3.78242800	-0.18712800
C	-4.35746500	-2.76103800	2.54492500
C	-2.58218600	-4.46425100	2.48703800
C	-1.21382100	-4.79444800	0.50278100
C	-1.62487400	-3.51337500	-1.55477500
C	-4.65423500	-3.11426500	3.82776000

H	-4.89363800	-1.95110900	2.06435200
C	-2.92724800	-4.80492800	3.83475900
C	-1.54084300	-5.11194000	1.82179600
C	-0.15058000	-5.46812700	-0.18041300
H	-2.19119200	-2.76463100	-2.09914600
C	-0.62093200	-4.19395700	-2.17943500
C	-3.93508700	-4.15794200	4.48379800
H	-5.43933000	-2.59108000	4.36389600
H	-2.36326400	-5.59319800	4.32581600
H	-0.97387600	-5.88285600	2.33970400
C	0.13828800	-5.18136800	-1.48035700
H	0.42262800	-6.21107200	0.36763100
H	-0.39208100	-3.98335500	-3.22018100
H	-4.18965500	-4.42357400	5.50475900
H	0.94501600	-5.69839600	-1.99086100
C	-0.49253200	3.81037300	-0.13863600
C	-1.08422900	4.53257000	0.91813000
C	0.91460900	3.76876000	-0.26865400
C	-2.50523100	4.63785600	1.07725700
C	-0.25049400	5.22240500	1.86240100
C	1.73455800	4.48532000	0.67001000
C	1.58316000	3.03123600	-1.30342200
C	-3.04816300	5.33685100	2.11457200
H	-3.15224700	4.14864500	0.35750800
C	-0.85976100	5.94078800	2.94177000
C	1.13529600	5.19053800	1.71290800
C	3.15804200	4.46427800	0.52143500
H	0.98855100	2.47112500	-2.01497800
C	2.94400800	3.02940300	-1.40871700
C	-2.21502600	5.99143400	3.07065300
H	-4.12648500	5.39884100	2.21852800
H	-0.21090000	6.44360700	3.65394800
H	1.76134200	5.71990800	2.42772200
C	3.74697400	3.77057700	-0.49224100
H	3.75525800	5.02652800	1.23397900
H	3.42609600	2.46258900	-2.20125700
H	-2.66948000	6.53482400	3.89264100
H	4.82598300	3.77712500	-0.60825300
C	2.07548100	-2.91415200	0.91866300
C	3.18868600	-3.17835700	0.11372700
C	3.99886300	-4.27073900	0.37346800
C	3.69736400	-5.09139800	1.46609200
C	2.59444400	-4.80587700	2.27155900
C	1.76657500	-3.71237700	2.01408800

C	2.16889600	-1.13548700	-0.53397300
C	3.24715400	-2.16487800	-1.02430800
H	4.85822900	-4.48579800	-0.25847500
H	4.32472300	-5.94714700	1.69002200
H	2.37220300	-5.44543800	3.12049500
H	0.90154800	-3.49868200	2.63331800
H	0.65234800	-1.31359600	0.90649000
N	1.37804300	-1.82508700	0.41371500
C	1.35152700	-0.40487600	-1.58461200
H	2.00524600	0.09933500	-2.30208000
H	0.72013700	-1.12886900	-2.10368800
H	0.69598000	0.32426600	-1.10227400
C	2.81506900	-2.82974900	-2.33058600
H	1.77773900	-3.15576000	-2.21940800
H	2.88656600	-2.15433100	-3.18707300
H	3.41067800	-3.72450800	-2.52275400
C	7.37751900	-0.63437100	-4.25825300
C	7.24406200	0.25968500	-3.20488200
C	6.31892200	0.02368400	-2.18133800
C	5.49983200	-1.12828700	-2.21834000
C	5.68737700	-2.04351000	-3.25051200
C	6.60343300	-1.79098200	-4.27099700
H	6.95790300	1.77728100	-1.05472200
H	8.09202300	-0.44236900	-5.05096000
H	7.86238200	1.15141800	-3.16083400
C	6.23977400	0.96083900	-1.06508000
C	4.61344800	-1.39016100	-1.01272900
H	5.12913500	-2.96898600	-3.27134800
H	6.71496300	-2.51198400	-5.07384600
C	4.31289900	-0.13166900	-0.25638300
C	5.30531300	0.89499300	-0.09293600
H	5.27511000	-1.93706200	-0.31876800
H	5.21026500	1.63900300	0.68591700
N	3.08247100	-0.09390700	0.14089100
N	2.59526900	0.78019700	1.07585100
C	3.19729600	0.72130200	2.33675300
O	4.25784000	0.14520400	2.49900400
H	1.56393600	0.87317500	1.02851200
C	2.48803200	1.44356800	3.43171200
C	3.02516000	1.29464000	4.71530500
C	1.35294100	2.23623500	3.23623000
C	2.42745200	1.92232500	5.79958600
H	3.90889000	0.67853900	4.84087400
C	0.75888200	2.86383600	4.32827900

H	0.91605100	2.36978700	2.25223400
C	1.29067500	2.70680800	5.60569700
H	2.84446000	1.79969100	6.79353900
H	-0.12367800	3.47685700	4.17384700
H	0.81859100	3.19608700	6.45176000

IMIII'-4

C	-5.75981900	3.79586300	2.30663900
C	-4.69516100	3.47919700	1.50064600
C	-4.50273600	2.14858000	1.03515100
C	-5.42229300	1.14984000	1.45904500
C	-6.52131100	1.51007100	2.28369400
C	-6.69307700	2.80553700	2.69575000
H	-5.88485200	4.81592000	2.65542300
C	-3.40362800	1.76799000	0.19682100
C	-5.22603800	-0.19296100	1.05219700
H	-7.21796800	0.73324700	2.58659500
H	-7.53371000	3.07371200	3.32703100
C	-4.14556300	-0.57228600	0.29379600
C	-3.21648100	0.43093900	-0.10080600
H	-5.95359800	-0.94361200	1.35145600
C	-2.42468800	2.76841800	-0.30694900
C	-2.81850400	3.89507600	-1.09926400
C	-1.08672300	2.59777900	-0.00877100
C	-1.83917400	4.86457500	-1.45374700
C	-4.14676600	4.07273600	-1.57523400
C	-0.10174200	3.57110300	-0.33545500
C	-2.21938800	5.99306100	-2.22850600
C	-0.49672600	4.68540200	-1.03530200
C	-4.48143300	5.16648200	-2.33341900
H	-4.89562900	3.32295500	-1.34257300
C	-3.51211800	6.14596800	-2.65689100
H	-1.45974300	6.72784100	-2.48082600
H	0.23880100	5.44523900	-1.28863600
H	-5.49838400	5.27976100	-2.69495800
H	-3.79381000	7.00812300	-3.25223200
O	-0.69298300	1.49500600	0.69917700
H	-3.98174200	4.24695400	1.22226400
O	-2.12013900	0.06411400	-0.84558000
P	-0.66761500	0.01202400	-0.05045400
O	0.39304300	-0.02191600	-1.10061900
O	-0.73116400	-0.96581000	1.07678800
C	-4.06097000	-1.99519000	-0.16007900
C	-3.56205700	-2.99750000	0.69271000
C	-4.62739100	-2.33740200	-1.40470800
C	-2.94101400	-2.69355500	1.94823100
C	-3.66320200	-4.37785500	0.30120000
C	-4.73909000	-3.72039600	-1.77893600
C	-5.11861300	-1.34979200	-2.32027000
C	-2.44090500	-3.68496000	2.74105700

H	-2.82927500	-1.65405600	2.23060500
C	-3.13043200	-5.38764200	1.16548100
C	-4.26842800	-4.70811500	-0.91185600
C	-5.32437300	-4.05584700	-3.04161500
H	-5.04363400	-0.30145800	-2.05010300
C	-5.66459700	-1.71017500	-3.51743500
C	-2.53575200	-5.05375200	2.34600300
H	-1.95244400	-3.43343400	3.67723900
H	-3.20845700	-6.42524700	0.85280300
H	-4.35395800	-5.75390700	-1.19849000
C	-5.77112600	-3.08426800	-3.88650400
H	-5.39899900	-5.10605000	-3.31018200
H	-6.02348300	-0.94704800	-4.20041100
H	-2.12986600	-5.82599000	2.99202200
H	-6.20997200	-3.34872500	-4.84313200
C	1.31810500	3.41949100	0.09519600
C	1.65569700	3.51947900	1.46308700
C	2.32681500	3.24832600	-0.87291600
C	0.66831200	3.67000200	2.49032900
C	3.03602200	3.47066700	1.85847400
C	3.70648500	3.22617600	-0.46772500
C	2.03333900	3.06218100	-2.26652300
C	1.02474800	3.74451800	3.80660200
H	-0.37854500	3.72122700	2.21056200
C	3.36909300	3.55791600	3.24764700
C	4.02915000	3.33623300	0.88407800
C	4.72699900	3.08930800	-1.46501200
H	0.99653900	3.01840600	-2.58016700
C	3.03334400	2.92130900	-3.18137000
C	2.39590900	3.68620700	4.19521300
H	0.25932400	3.85293100	4.56788800
H	4.41809500	3.51873700	3.52797900
H	5.07420100	3.31360300	1.18657700
C	4.40385000	2.95507600	-2.78027900
H	5.76431200	3.08474200	-1.14092300
H	2.79254200	2.76301600	-4.22727900
H	2.65822700	3.74965900	5.24629300
H	5.18110200	2.83349400	-3.52738800
C	1.64098700	-3.30732600	-2.16341800
C	1.07985300	-3.43245900	-0.88986300
C	-0.29155200	-3.55252600	-0.74014800
C	-1.09179000	-3.52607700	-1.88735100
C	-0.51828100	-3.40194900	-3.15099700
C	0.86381300	-3.29700300	-3.31263700

C	3.34230800	-2.80852600	-0.72311100
C	2.18800400	-3.38318200	0.16181100
H	-0.74847000	-3.62031900	0.24590800
H	-2.16804600	-3.58636100	-1.79107800
H	-1.15870700	-3.37497200	-4.02708000
H	1.31301800	-3.18493600	-4.29384300
H	3.56688700	-2.79846400	-2.81429800
N	3.03901300	-3.21227900	-2.05455300
C	4.75863900	-3.14095000	-0.29521800
H	4.95638700	-2.75658300	0.70944900
H	4.88333200	-4.22486100	-0.29962700
H	5.49014300	-2.70836600	-0.97970700
C	2.49382300	-4.78208200	0.68832800
H	2.82266400	-5.41155400	-0.14388300
H	3.27370100	-4.77533200	1.45474900
H	1.58829600	-5.23297900	1.10099100
C	1.63950900	-2.06886600	5.50406200
C	1.78492400	-0.92645900	4.73262200
C	1.91733000	-1.01705700	3.34045400
C	1.90599100	-2.28640900	2.70780800
C	1.72026000	-3.42204600	3.49350100
C	1.60648500	-3.31421000	4.87797500
H	2.00280900	1.14793900	3.10567900
H	1.54157700	-1.99365400	6.58140300
H	1.79394600	0.05638600	5.19606300
C	2.06866400	0.20447900	2.56630300
C	1.88171500	-2.25999800	1.20392200
H	1.65870400	-4.40108000	3.03815400
H	1.48361000	-4.21518200	5.47045600
C	2.48491400	-1.04689900	0.62081300
C	2.34231900	0.22516200	1.23865000
H	0.80519000	-1.96613200	1.04881800
H	2.52272700	1.12936100	0.67258700
N	3.08495700	-1.30034900	-0.51391800
N	3.15718100	-0.34920400	-1.50839400
C	4.28891800	-0.19379100	-2.29961900
O	4.17279400	0.02011300	-3.49196200
H	2.23676200	-0.18130500	-1.92752200
C	5.60924300	-0.22891400	-1.60862900
C	5.74880000	0.13294600	-0.26507900
C	6.72910700	-0.58907800	-2.36009300
C	7.00625900	0.10838100	0.32731200
H	4.88303500	0.46127200	0.30395200
C	7.98311000	-0.62618500	-1.75968000

H	6.59920800	-0.84448400	-3.40691200
C	8.12026500	-0.28212600	-0.41562000
H	7.11901100	0.39662500	1.36721800
H	8.85281600	-0.91879100	-2.33812500
H	9.09910600	-0.30983900	0.05219700

TSIII'-3

Value of imaginary frequency = -321.0 cm^{-1}

C	-5.55919100	4.10725700	2.10553500
C	-4.49610600	3.70912500	1.33497100
C	-4.37885700	2.36161500	0.89278500
C	-5.37270900	1.43268100	1.30591800
C	-6.46877600	1.87651000	2.09296500
C	-6.56697800	3.18682800	2.48084400
H	-5.62524400	5.13851900	2.43704300
C	-3.28743900	1.89856000	0.08644300
C	-5.24343900	0.07166400	0.93715500
H	-7.22177400	1.15092500	2.38790300
H	-7.40496500	3.51863200	3.08484600
C	-4.16410900	-0.39124000	0.22429400
C	-3.17129200	0.54645900	-0.17877600
H	-6.01749600	-0.62946200	1.23962200
C	-2.24488500	2.84016800	-0.40104900
C	-2.55889400	3.98604100	-1.20123700
C	-0.92871200	2.60976700	-0.05735900
C	-1.52526200	4.91306200	-1.51119500
C	-3.85893500	4.22081500	-1.72647200
C	0.10842000	3.54501100	-0.32468900
C	-1.82585800	6.05776100	-2.29707600
C	-0.21168900	4.67904000	-1.03174300
C	-4.11591100	5.32838100	-2.49439100
H	-4.64703300	3.50326900	-1.52403300
C	-3.09277100	6.26521900	-2.77665300
H	-1.02678900	6.76050600	-2.51602500
H	0.56283500	5.41283100	-1.24098900
H	-5.11185300	5.48581400	-2.89563600
H	-3.31441900	7.13904600	-3.38031000
O	-0.61176900	1.46431000	0.63162800
H	-3.72686900	4.42499500	1.06826400
O	-2.09656500	0.09968100	-0.91690600
P	-0.60693400	0.04488900	-0.21419600
O	0.41065200	0.06136000	-1.30036300
O	-0.59926200	-1.00869600	0.86250300
C	-4.12364000	-1.84269100	-0.13439000
C	-3.56561900	-2.77986700	0.75514300
C	-4.77618300	-2.27359500	-1.30615800
C	-2.90108300	-2.38692300	1.96195500
C	-3.66606900	-4.18434700	0.46240600
C	-4.89508700	-3.68029400	-1.57621500
C	-5.34231900	-1.35504100	-2.25009400

C	-2.34472300	-3.31460200	2.79188600
H	-2.81592100	-1.33105400	2.18889300
C	-3.06636700	-5.12706100	1.35937500
C	-4.34169800	-4.60179900	-0.68479900
C	-5.56870600	-4.10637800	-2.76530700
H	-5.25552400	-0.29021500	-2.05984400
C	-5.97339000	-1.80185000	-3.37404300
C	-2.41931900	-4.70657800	2.48378500
H	-1.82511500	-2.99369700	3.68936100
H	-3.13890400	-6.18399800	1.11821000
H	-4.42719000	-5.66529700	-0.89654100
C	-6.09198800	-3.19908500	-3.63726900
H	-5.64950300	-5.17306600	-2.95552200
H	-6.38916100	-1.09033200	-4.08006900
H	-1.96298700	-5.42726800	3.15600200
H	-6.59911100	-3.53241700	-4.53689200
C	1.49627400	3.34207900	0.18193900
C	1.75668700	3.40529200	1.56919900
C	2.55350900	3.16673900	-0.73115200
C	0.71799600	3.56092600	2.54375500
C	3.11090700	3.31309700	2.04035900
C	3.90725900	3.10400500	-0.24909500
C	2.33491400	3.01894800	-2.14290300
C	1.00213400	3.59645400	3.87925000
H	-0.31002100	3.64918400	2.20915600
C	3.36778000	3.35930600	3.44753500
C	4.15479900	3.17672600	1.12080400
C	4.97898900	2.96236100	-1.19051100
H	1.31646900	3.00207500	-2.51300200
C	3.38189300	2.87808700	-3.00311600
C	2.34670400	3.49175100	4.34251500
H	0.19847600	3.70916500	4.59946000
H	4.39803300	3.28515500	3.78438100
H	5.17983100	3.12065900	1.48160500
C	4.72761400	2.86786900	-2.52445900
H	5.99551200	2.92081000	-0.80838800
H	3.19768300	2.74870100	-4.06418900
H	2.55087700	3.52369700	5.40776100
H	5.54259600	2.74311800	-3.22971800
C	1.46570700	-3.26046200	-2.27347600
C	0.89290200	-3.41198400	-1.00903700
C	-0.47960900	-3.51575800	-0.86804400
C	-1.27610500	-3.44769800	-2.01553100
C	-0.69241900	-3.29762700	-3.27268100

C	0.69212100	-3.20756400	-3.42482600
C	3.18830100	-2.89125000	-0.80407800
C	1.98901200	-3.42964700	0.05089800
H	-0.93225500	-3.60509100	0.11756000
H	-2.35413200	-3.49802500	-1.92433700
H	-1.32655400	-3.24081100	-4.15198300
H	1.14666800	-3.08065200	-4.40181300
H	3.40295100	-2.77371100	-2.89508100
N	2.86406100	-3.21391500	-2.15810300
C	4.57558600	-3.35595000	-0.40012000
H	4.79972600	-3.04688500	0.62487900
H	4.63036700	-4.44308500	-0.47260100
H	5.33421400	-2.92954600	-1.05932200
C	2.22232700	-4.85410500	0.55036400
H	2.56785300	-5.47198100	-0.28370100
H	2.96263700	-4.89686400	1.35426900
H	1.28390500	-5.28787100	0.90250200
C	0.93140500	-2.27384000	5.33234500
C	1.29628800	-1.12454000	4.65603600
C	1.61016600	-1.16795100	3.28668400
C	1.55456800	-2.40152700	2.58297600
C	1.14465300	-3.54614700	3.27669100
C	0.85830600	-3.48403400	4.63407000
H	1.95305800	0.97612800	3.17898300
H	0.69542900	-2.23758800	6.39008400
H	1.34280200	-0.16904500	5.17145000
C	1.98353600	0.05101000	2.60601300
C	1.75497500	-2.31911000	1.11715900
H	1.04625700	-4.49197600	2.76184300
H	0.56232700	-4.38963100	5.15474400
C	2.46497800	-1.15395900	0.63346900
C	2.40450800	0.08970100	1.31378200
H	0.66925000	-1.81146100	0.89301300
H	2.73020300	0.99531700	0.81900400
N	3.06720800	-1.39080500	-0.52035200
N	3.21269000	-0.41005100	-1.47750100
C	4.38389100	-0.27490100	-2.20983700
O	4.33144700	-0.00547700	-3.39681500
H	2.32713100	-0.19862800	-1.94710200
C	5.67704000	-0.40540100	-1.47607300
C	5.79330000	-0.11702500	-0.11317100
C	6.80353800	-0.77661100	-2.21224800
C	7.03125400	-0.22245800	0.51120900
H	4.92624500	0.21585100	0.44964100

C	8.03763400	-0.89489000	-1.58142100
H	6.69411100	-0.97433800	-3.27375000
C	8.15039200	-0.62153800	-0.21920000
H	7.12447500	0.00934000	1.56706200
H	8.91081200	-1.19512300	-2.15079100
H	9.11355400	-0.71191600	0.27264100

IMIII'-5

C	-5.54941700	4.12058400	2.09199900
C	-4.47889600	3.72712200	1.32940000
C	-4.38022600	2.39252600	0.84707100
C	-5.39843700	1.46941500	1.21146700
C	-6.50223200	1.90993700	1.98947300
C	-6.58231800	3.20905700	2.41647800
H	-5.60209200	5.14138200	2.45609500
C	-3.28183900	1.93320000	0.04607300
C	-5.28716900	0.11583800	0.80988300
H	-7.27491300	1.19072700	2.24558700
H	-7.42582300	3.53843800	3.01388500
C	-4.20130000	-0.34784400	0.10806700
C	-3.19453700	0.58833100	-0.24737900
H	-6.07754400	-0.57965100	1.08049500
C	-2.21622800	2.87075000	-0.39719300
C	-2.50054400	4.04955300	-1.15985100
C	-0.90925000	2.62024500	-0.04431000
C	-1.44949500	4.97534300	-1.41031200
C	-3.78589100	4.31509900	-1.70376900
C	0.14617900	3.55031200	-0.23510800
C	-1.72103800	6.15070300	-2.16048600
C	-0.15062800	4.71420000	-0.90376400
C	-4.01369300	5.45208400	-2.43666800
H	-4.58508400	3.59896500	-1.54571600
C	-2.97472600	6.38718900	-2.66100200
H	-0.91147300	6.85333400	-2.33535000
H	0.63175500	5.45283200	-1.05767900
H	-4.99837500	5.63449100	-2.85444700
H	-3.17385900	7.28439500	-3.23743700
O	-0.61095700	1.42531000	0.59758300
H	-3.69131300	4.43647800	1.10233400
O	-2.10526900	0.12505600	-0.97894800
P	-0.64286500	0.08077200	-0.29930400
O	0.41699200	-0.07637100	-1.30698900
O	-0.75194100	-0.98482300	0.85415400
C	-4.15525100	-1.78925400	-0.28308200
C	-3.70260800	-2.75406300	0.63527700
C	-4.68258200	-2.17922100	-1.52928300
C	-3.14389100	-2.39936400	1.90640800
C	-3.79683900	-4.14939600	0.30104000
C	-4.79492600	-3.57681000	-1.84380000
C	-5.12833000	-1.22835100	-2.50444800
C	-2.67622600	-3.35464700	2.75869000

H	-3.07349400	-1.35047300	2.17229600
C	-3.29597600	-5.12191900	1.22609700
C	-4.36006200	-4.52791900	-0.91828300
C	-5.33896100	-3.96317000	-3.11016600
H	-5.05230900	-0.16969600	-2.27797200
C	-5.63658000	-1.63767800	-3.70239000
C	-2.74410400	-4.73838600	2.41225200
H	-2.23612500	-3.06299800	3.70656800
H	-3.36157400	-6.17161800	0.95367500
H	-4.44002200	-5.58458100	-1.16331800
C	-5.74520100	-3.02607600	-4.01266500
H	-5.41555300	-5.02335300	-3.33467800
H	-5.96430700	-0.90300500	-4.43073700
H	-2.35657800	-5.48054700	3.10343100
H	-6.15280000	-3.32968900	-4.97133000
C	1.50696000	3.31092900	0.32606300
C	1.68523300	3.27496700	1.72738600
C	2.61431300	3.20195900	-0.53700700
C	0.59661200	3.39975600	2.65101700
C	3.00739400	3.12535000	2.26866500
C	3.93630100	3.09108600	0.01937000
C	2.48379500	3.18674900	-1.96671700
C	0.80322900	3.34450600	3.99973300
H	-0.40835900	3.54574300	2.26943200
C	3.18216000	3.06799300	3.68763600
C	4.10141700	3.04660200	1.40279100
C	5.06310400	3.02923300	-0.86394600
H	1.49135300	3.21580400	-2.40217700
C	3.58174700	3.12160400	-2.77041800
C	2.11481900	3.16916600	4.53074700
H	-0.03819900	3.43812700	4.67851600
H	4.18906300	2.94421100	4.07632800
H	5.10302400	2.94872700	1.81641900
C	4.89496400	3.05597500	-2.21381400
H	6.05405000	2.94199300	-0.42663000
H	3.46193700	3.09370300	-3.84815000
H	2.25734200	3.12393300	5.60540900
H	5.75232600	2.98872200	-2.87537800
C	1.55730500	-3.19101600	-2.21165200
C	1.05813500	-3.47002800	-0.93351300
C	-0.30861600	-3.56250500	-0.72527100
C	-1.17047900	-3.32980300	-1.80433300
C	-0.66048500	-3.04125000	-3.06718500
C	0.71499600	-2.97818000	-3.29422600

C	3.37377300	-2.96310100	-0.82816700
C	2.22632900	-3.58653400	0.04610400
H	-0.71980000	-3.78004800	0.26269300
H	-2.24063300	-3.36807300	-1.65616000
H	-1.34687100	-2.85652500	-3.88809600
H	1.11500900	-2.74862500	-4.27678000
H	3.43862500	-2.65989500	-2.90650100
N	2.95858700	-3.19505100	-2.19082300
C	4.77993500	-3.47035200	-0.56181800
H	5.05426800	-3.27340500	0.47867700
H	4.85466400	-4.53997000	-0.76497300
H	5.49068200	-2.94036700	-1.20209200
C	2.49688800	-5.04603800	0.41263900
H	2.82913700	-5.58480900	-0.47975600
H	3.26436400	-5.13557500	1.18656800
H	1.58522100	-5.53648700	0.75806800
C	0.24747300	-2.60504400	5.01849700
C	0.70191500	-1.43198400	4.47176800
C	1.31085800	-1.40564300	3.19084000
C	1.43928800	-2.62665800	2.44644600
C	0.92102900	-3.81900000	3.02939300
C	0.35899200	-3.80802200	4.28121500
H	1.60021400	0.74199400	3.18697100
H	-0.20384200	-2.61435600	6.00516000
H	0.61275400	-0.49501800	5.01577900
C	1.76678200	-0.17894800	2.63307600
C	2.07147400	-2.56187700	1.17341400
H	0.98507800	-4.75256100	2.48568900
H	-0.01424700	-4.73451500	4.70758800
C	2.58576800	-1.35521300	0.72791000
C	2.40230200	-0.13874600	1.41883400
H	-0.03621700	-1.64615000	0.82827100
H	2.74101100	0.79083800	0.97263200
N	3.31699800	-1.50474700	-0.44083200
N	3.28070100	-0.52334700	-1.40477800
C	4.41643400	-0.17180500	-2.09639000
O	4.33777600	0.21982900	-3.25216400
H	2.39031400	-0.39443400	-1.88820900
C	5.73149300	-0.25412000	-1.38349800
C	5.85917300	-0.07044300	-0.00302900
C	6.86965000	-0.44272600	-2.16763900
C	7.11990500	-0.08791900	0.58270800
H	4.97854200	0.10917800	0.60569700
C	8.12942800	-0.47867600	-1.57635900

H	6.75088700	-0.55956200	-3.24014700
C	8.25466600	-0.30133800	-0.20060900
H	7.21902800	0.06581400	1.65249400
H	9.01129600	-0.63888900	-2.18803000
H	9.23621000	-0.32429300	0.26225900

COMIV'

C	5.43328900	3.74052300	-3.22015300
C	4.52269300	3.42168900	-2.24471200
C	4.26954300	2.06568500	-1.90276300
C	4.95628200	1.04348500	-2.61903100
C	5.90143700	1.40750400	-3.61483400
C	6.13984900	2.72500400	-3.90771300
H	5.61070100	4.78112200	-3.47131900
C	3.32173100	1.68907300	-0.89657700
C	4.67723900	-0.32178000	-2.34523100
H	6.42430000	0.61738700	-4.14598700
H	6.86013900	2.99359600	-4.67331800
C	3.72959000	-0.68817600	-1.42216400
C	3.05886300	0.34778200	-0.72344400
H	5.21765000	-1.09057500	-2.89141300
C	2.57330800	2.67492100	-0.06776500
C	3.22695500	3.62447800	0.78365200
C	1.19582700	2.62407300	-0.04888300
C	2.43174600	4.52402100	1.54988000
C	4.63993700	3.67753100	0.93043900
C	0.38256400	3.50176100	0.71373100
C	3.06872700	5.47494800	2.39090700
C	1.01641200	4.44543500	1.48411000
C	5.22528700	4.60069700	1.75966100
H	5.25655900	2.97181200	0.38479000
C	4.43475400	5.51885300	2.49112400
H	2.44765700	6.15994100	2.96093600
H	0.42239400	5.13962100	2.07306800
H	6.30532800	4.62370600	1.86140800
H	4.91273000	6.24621200	3.13878100
O	0.54750200	1.67595100	-0.83034100
H	3.97926900	4.20749200	-1.73110900
O	2.08846800	-0.02727000	0.19750300
P	0.56241100	0.14617900	-0.31624800
O	-0.21984200	0.16863700	1.03051500
O	0.14274700	-0.77279400	-1.38728200
C	3.41908600	-2.11388000	-1.10980600
C	2.65430200	-2.89061000	-2.00092200
C	3.90644000	-2.67080800	0.08871700
C	2.10525800	-2.35921200	-3.21495400
C	2.39176600	-4.26904100	-1.68826300
C	3.62820500	-4.04601100	0.39609500
C	4.69169400	-1.91760800	1.02188900
C	1.37469700	-3.14496600	-4.05877800

H	2.26832200	-1.31243800	-3.44641500
C	1.61949600	-5.05784600	-2.60093000
C	2.88538900	-4.81299800	-0.50143800
C	4.13182900	-4.60453100	1.61467200
H	4.92047900	-0.87995300	0.80141500
C	5.15857800	-2.48811500	2.16937700
C	1.12959100	-4.51756200	-3.75202500
H	0.96777500	-2.72370600	-4.97255100
H	1.42923600	-6.09742700	-2.34798700
H	2.68211400	-5.85651700	-0.27012100
C	4.87354800	-3.85236700	2.47516700
H	3.90810900	-5.64496800	1.83387800
H	5.75544100	-1.90108000	2.86041700
H	0.53857200	-5.12056400	-4.43336800
H	5.25248900	-4.28375800	3.39649500
C	-1.10590900	3.40982900	0.65088900
C	-1.77655500	3.88531100	-0.49383100
C	-1.83200500	2.88583400	1.73638000
C	-1.07901400	4.41665800	-1.62718400
C	-3.21075100	3.85464800	-0.53854700
C	-3.26833200	2.86254500	1.67992500
C	-1.19706500	2.34449700	2.90367000
C	-1.75653000	4.86975700	-2.72150800
H	0.00524900	4.45774100	-1.60653500
C	-3.88360300	4.34418300	-1.70273800
C	-3.92364400	3.35044100	0.55041300
C	-4.00290600	2.33365600	2.79057400
H	-0.11259100	2.33366300	2.94957600
C	-1.93306400	1.82998200	3.93087800
C	-3.18161400	4.83367200	-2.76404700
H	-1.20872500	5.26520400	-3.57088100
H	-4.96938800	4.31010100	-1.71709100
H	-5.01185600	3.31822600	0.50709900
C	-3.36020200	1.82899000	3.88043400
H	-5.08859000	2.33356700	2.73060900
H	-1.43177600	1.41581700	4.80066000
H	-3.70032400	5.20150500	-3.64339600
H	-3.92469600	1.42014500	4.71230300
C	-2.35382400	-2.87263200	-2.36156000
C	-3.47559800	-3.29133300	-1.60423800
C	-4.76274900	-3.00842400	-2.08332000
C	-4.89765900	-2.31526900	-3.27710100
C	-3.76759700	-1.90423400	-4.01181700
C	-2.48221700	-2.17769700	-3.56663700

C	-1.60091100	-3.81055400	-0.46571900
C	-2.97202800	-3.88339000	-0.39169700
H	-5.64034200	-3.31087600	-1.51763600
H	-5.88842000	-2.07938900	-3.65353200
H	-3.90623700	-1.36098300	-4.94166100
H	-1.60473000	-1.85124900	-4.11690300
H	-0.31622200	-2.82918900	-1.83413700
N	-1.22895600	-3.23787500	-1.66677800
C	-0.54447200	-4.26763500	0.48394500
H	0.04224100	-5.08403000	0.04921000
H	0.16046000	-3.45752100	0.71484100
H	-0.98936000	-4.62493000	1.41424000
C	-3.81083800	-4.41979300	0.72589000
H	-4.24841700	-5.39548200	0.48556400
H	-3.23602300	-4.51761500	1.65060500
H	-4.64078600	-3.73488800	0.93615900
C	-6.82696000	1.92599400	-1.63809300
C	-5.57616600	1.41365800	-1.88534600
C	-4.90382800	0.64945600	-0.90104200
C	-5.56148900	0.39260600	0.33703400
C	-6.85656500	0.93066000	0.56494000
C	-7.47242700	1.68892500	-0.39910600
H	-3.12131400	0.28650300	-2.08472600
H	-7.32886100	2.51930100	-2.39601300
H	-5.07704900	1.60041300	-2.83195200
C	-3.59506800	0.13328000	-1.11943100
C	-4.89590800	-0.38377600	1.31288500
H	-7.34565200	0.73466900	1.51520900
H	-8.45872500	2.10416300	-0.22099900
C	-3.60856000	-0.82822800	1.08773700
C	-2.95359500	-0.58510500	-0.15354400
H	-5.37356200	-0.60387100	2.26354800
H	-1.99245300	-1.04029700	-0.36282300
N	-3.04244500	-1.55901200	2.14313700
N	-1.79619200	-1.66226900	2.14086800
C	-1.31451300	-2.57852400	3.17161500
O	-1.98298300	-3.52160300	3.52210600
C	0.07250000	-2.33191600	3.62833000
C	0.81644700	-3.43291900	4.06751500
C	0.63141000	-1.05154400	3.64216700
C	2.12691900	-3.25652800	4.48819500
H	0.35724900	-4.41636300	4.05604000
C	1.94028200	-0.87852300	4.08197700
H	0.04688100	-0.19422900	3.32600700

C	2.68876100	-1.97923900	4.49248200
H	2.71511700	-4.11141800	4.80434600
H	2.37588800	0.11503200	4.09789700
H	3.71567400	-1.84309000	4.81713500
H	-0.78050300	-0.62813100	1.32035400

TSIV'-1

Value of imaginary frequency = -222.1 cm^{-1}

C	4.61329400	3.75753600	-3.79593100
C	3.90898700	3.48431900	-2.65031200
C	3.82520000	2.15755800	-2.14631100
C	4.46327100	1.11484900	-2.87546300
C	5.19603900	1.43168400	-4.05029700
C	5.27479600	2.72363300	-4.50113500
H	4.66055000	4.77556600	-4.16883600
C	3.08999200	1.82422300	-0.96293500
C	4.35106900	-0.22561100	-2.42393600
H	5.68635500	0.62488700	-4.58785500
H	5.83321200	2.95701500	-5.40156400
C	3.60351000	-0.55586200	-1.32047200
C	2.95763900	0.49526800	-0.61603000
H	4.86563200	-1.01050800	-2.97266900
C	2.41814300	2.84858300	-0.11825000
C	3.13987900	3.91562500	0.50844600
C	1.06161800	2.73455300	0.11733400
C	2.42349300	4.87582800	1.27655100
C	4.55474300	4.03784300	0.42665500
C	0.33132300	3.69317100	0.87041800
C	3.12691500	5.94224900	1.89779800
C	1.01891700	4.74641000	1.42113100
C	5.20778500	5.07343700	1.04590100
H	5.11889900	3.29360300	-0.12479900
C	4.48846500	6.04478600	1.78288800
H	2.56120200	6.66994700	2.47289900
H	0.47694100	5.49782200	1.98990300
H	6.28834600	5.14611400	0.97593600
H	5.01900300	6.85974100	2.26400200
O	0.36690800	1.68742000	-0.44377000
H	3.39751700	4.28282200	-2.12362100
O	2.17619500	0.17316800	0.47267300
P	0.55197700	0.17490900	0.18910600
O	-0.09164400	0.08630100	1.54166500
O	0.20904000	-0.78501600	-0.89826200
C	3.55184500	-1.96848100	-0.83677300
C	2.72868000	-2.91873300	-1.46837900
C	4.42881400	-2.35899000	0.19600400
C	1.83326500	-2.57650800	-2.53599200
C	2.78428100	-4.29261400	-1.04845900
C	4.50327800	-3.73991500	0.57971400
C	5.28795000	-1.42917100	0.86744900

C	1.06296200	-3.52781000	-3.13855500
H	1.76095600	-1.53819700	-2.83778100
C	1.95204300	-5.25784000	-1.70181900
C	3.66963100	-4.67091300	-0.04051000
C	5.45544500	-4.13946700	1.56934200
H	5.23551700	-0.37821300	0.60171000
C	6.17451300	-1.84779800	1.81765200
C	1.12546500	-4.89288000	-2.72031800
H	0.39335400	-3.24744800	-3.94706900
H	2.00340300	-6.28992900	-1.36651000
H	3.72146500	-5.71540500	0.25980600
C	6.27337300	-3.22663100	2.16592200
H	5.50486300	-5.19182200	1.83684700
H	6.81973600	-1.12634300	2.30901000
H	0.50863400	-5.63557800	-3.21686900
H	6.99390500	-3.54109900	2.91435300
C	-1.15312200	3.61043400	1.01808900
C	-1.97074800	4.15323700	0.00799500
C	-1.72411500	3.08190700	2.19001200
C	-1.43255600	4.69512700	-1.20551600
C	-3.39521800	4.18801100	0.18948600
C	-3.14992100	3.12802700	2.36513100
C	-0.93304000	2.49912800	3.23357700
C	-2.24844600	5.22993100	-2.16070300
H	-0.35820200	4.67548600	-1.35721200
C	-4.21584200	4.75835300	-0.83572200
C	-3.95047800	3.68079400	1.36451500
C	-3.72220800	2.59601500	3.56540300
H	0.13980300	2.43219700	3.09436200
C	-1.51621400	2.00491900	4.36261200
C	-3.66336800	5.26470000	-1.97514300
H	-1.82182800	5.63251200	-3.07358900
H	-5.29131500	4.77852800	-0.68136000
H	-5.02933200	3.71825000	1.50460500
C	-2.93247400	2.05387900	4.53439600
H	-4.80242400	2.63338100	3.68095800
H	-0.90201800	1.55836900	5.13777700
H	-4.29395700	5.69495400	-2.74629100
H	-3.37471800	1.65180000	5.44020500
C	-2.74502000	-0.72326800	-2.11395300
C	-4.10225100	-1.07578100	-2.22697100
C	-5.07743200	-0.08016800	-2.27317300
C	-4.66373000	1.24829200	-2.20681000
C	-3.30519400	1.57828900	-2.10915600

C	-2.31746400	0.59860100	-2.06161800
C	-2.82675500	-2.97007300	-2.13126400
C	-4.16879400	-2.52576500	-2.17020600
H	-6.13167200	-0.33503300	-2.34289700
H	-5.39956700	2.04671800	-2.23479800
H	-3.01160000	2.62159700	-2.07821900
H	-1.26816700	0.85076200	-1.97440300
H	-1.01705600	-1.90577800	-1.80773600
N	-2.01113000	-1.90725600	-2.05470800
C	-2.30608900	-4.36056300	-2.07150700
H	-1.80009100	-4.61834300	-3.00721600
H	-1.58895100	-4.46584800	-1.24819700
H	-3.12310400	-5.06850600	-1.92180800
C	-5.33963000	-3.34581500	-2.60828300
H	-5.36883300	-3.41782500	-3.70026500
H	-5.30385500	-4.36282700	-2.20664000
H	-6.27599200	-2.88287700	-2.28626800
C	-8.00011900	-0.62009300	0.67556100
C	-6.80047200	0.03891100	0.88723800
C	-5.57991600	-0.63685600	0.74018700
C	-5.59122400	-2.00086600	0.35381900
C	-6.82212200	-2.66199700	0.16730600
C	-8.01401300	-1.97915300	0.32541900
H	-4.34451100	1.07611500	1.27585600
H	-8.93779000	-0.08717000	0.79527400
H	-6.79016700	1.08588300	1.17794400
C	-4.32057800	0.01861200	1.03443000
C	-4.33571700	-2.67114500	0.16399900
H	-6.82171600	-3.71737800	-0.08949600
H	-8.95868600	-2.49309300	0.18597400
C	-3.13601900	-2.06075000	0.69130000
C	-3.14955900	-0.65123700	1.05150200
H	-4.32512200	-3.75339300	0.07391000
H	-2.22153600	-0.14888800	1.31506800
N	-2.14809100	-2.92344900	0.79822500
N	-0.99314200	-2.63565000	1.34200900
C	-0.07628100	-3.71374600	1.40603800
O	-0.32548500	-4.75787500	0.84094300
H	-0.73800700	-1.67554100	1.63200400
C	1.12690200	-3.54252700	2.26779800
C	1.73444000	-4.72894200	2.70143000
C	1.65252000	-2.30994200	2.66038600
C	2.83528500	-4.68229400	3.54273900
H	1.31928000	-5.67617300	2.37438300

C	2.78100100	-2.27038200	3.47732800
H	1.20534400	-1.37618100	2.34035900
C	3.36321100	-3.44958800	3.92916700
H	3.29184900	-5.60413200	3.88908100
H	3.20014300	-1.31060300	3.76091900
H	4.23797300	-3.41238600	4.57055900

IMIV'-1

C	-7.03073800	-0.81717600	-2.77221300
C	-5.88633900	-1.08081800	-2.06194800
C	-5.03915400	-0.02533700	-1.62915800
C	-5.38852300	1.31116100	-1.97577400
C	-6.58491700	1.55180400	-2.70188300
C	-7.39230000	0.51393600	-3.08955700
H	-7.66231600	-1.63705000	-3.09851900
C	-3.83464200	-0.25776100	-0.88976300
C	-4.53539500	2.38300300	-1.60274600
H	-6.84187000	2.57768000	-2.95053600
H	-8.30275600	0.70774800	-3.64681600
C	-3.34787300	2.16162600	-0.95001100
C	-3.01167300	0.81857400	-0.62785900
H	-4.82730400	3.39952800	-1.85482200
C	-3.41506400	-1.59841300	-0.39498400
C	-4.22723200	-2.37617000	0.49426600
C	-2.14525000	-2.05279700	-0.69218000
C	-3.72691400	-3.62071500	0.97428200
C	-5.48636200	-1.92508300	0.97936200
C	-1.60492500	-3.25898100	-0.17117800
C	-4.51919200	-4.39790300	1.86160300
C	-2.41738400	-4.03411800	0.62112300
C	-6.21959900	-2.69003800	1.85125300
H	-5.86063400	-0.95762200	0.66444000
C	-5.74118100	-3.94824200	2.28856200
H	-4.12555600	-5.34903300	2.20860800
H	-2.03167900	-4.96329400	1.03291300
H	-7.17413900	-2.32363700	2.21468700
H	-6.33634100	-4.54437000	2.97217400
O	-1.34749700	-1.30032800	-1.52848400
H	-5.61304700	-2.10523700	-1.83103400
O	-1.81624300	0.60795000	0.02274100
P	-0.58641200	-0.01651700	-0.85753100
O	0.48270500	-0.41291400	0.09917000
O	-0.26104100	0.89291700	-2.02113400
C	-2.43418600	3.27001000	-0.55108900
C	-1.79805200	4.05579100	-1.53302500
C	-2.20718900	3.51989300	0.81926900
C	-1.92716600	3.79662400	-2.93823500
C	-0.94996400	5.14402700	-1.12676600
C	-1.32209600	4.58080000	1.21043900
C	-2.82381900	2.74780100	1.85720500
C	-1.29259000	4.57599100	-3.86026500

H	-2.52376700	2.95048600	-3.25954100
C	-0.31018600	5.94397400	-2.12795000
C	-0.73159100	5.37988800	0.23040900
C	-1.05374500	4.79250400	2.60077500
H	-3.51382700	1.95403300	1.59083600
C	-2.54241800	2.97844700	3.17107700
C	-0.47765400	5.67462500	-3.45290200
H	-1.39840400	4.35571000	-4.91764000
H	0.31893800	6.76769800	-1.80128300
H	-0.07289500	6.19208900	0.53069300
C	-1.63252000	4.00781400	3.55287000
H	-0.36694500	5.58834300	2.87534200
H	-2.99963900	2.35835200	3.93687500
H	0.01403400	6.28425600	-4.20407500
H	-1.40584000	4.15892600	4.60321600
C	-0.17527800	-3.62150300	-0.39505200
C	0.29154200	-3.98657300	-1.67132600
C	0.70972100	-3.59051700	0.70246900
C	-0.55740800	-3.99404000	-2.82597500
C	1.66692500	-4.36517100	-1.84171900
C	2.06650600	-4.03080000	0.53300000
C	0.32760200	-3.08383900	1.98822900
C	-0.06816200	-4.31759100	-4.05741900
H	-1.60312600	-3.72884200	-2.70857500
C	2.13843600	-4.70799300	-3.14966700
C	2.51472500	-4.40423800	-0.73433900
C	2.93951900	-4.05111800	1.66925000
H	-0.67496300	-2.69484400	2.12216500
C	1.20991500	-3.05366800	3.02893000
C	1.30326500	-4.67600500	-4.22638500
H	-0.72515100	-4.30810300	-4.92093600
H	3.18064000	-4.99601100	-3.26043700
H	3.54767900	-4.72067300	-0.86396000
C	2.53066300	-3.57347700	2.87822500
H	3.94570300	-4.44030700	1.53613400
H	0.90165100	-2.63473900	3.98240400
H	1.67115100	-4.93346900	-5.21431100
H	3.20770400	-3.57222300	3.72604300
C	3.17603500	0.30062800	-2.26236400
C	4.43246800	0.69208700	-1.80638300
C	5.54935500	-0.03853000	-2.18233600
C	5.35386100	-1.18812900	-2.95443800
C	4.07547100	-1.59312300	-3.34522200
C	2.94829100	-0.84052000	-3.01138500

C	2.77115900	2.17426200	-1.10422700
C	4.25651700	1.91288800	-0.92885600
H	6.54706600	0.25386000	-1.86840900
H	6.21289300	-1.78120700	-3.25004900
H	3.95146600	-2.49997200	-3.92777400
H	1.94961700	-1.13425000	-3.31879200
H	1.12832800	1.15711300	-1.99167500
N	2.22453700	1.25321500	-1.82515300
C	1.99215800	3.29618500	-0.53036400
H	2.34735100	4.24523400	-0.94628200
H	0.93090800	3.17854600	-0.76083300
H	2.12978600	3.32234300	0.55545400
C	5.09527700	3.10851200	-1.39555600
H	4.84872500	3.36495400	-2.42882400
H	4.92082200	3.98205700	-0.76084700
H	6.15599400	2.85162900	-1.35299400
C	8.33063300	-0.36315300	0.94838500
C	7.15511000	-1.10544000	0.88585200
C	5.91336800	-0.46865500	0.81731100
C	5.85892100	0.93841900	0.79871300
C	7.03814000	1.67380900	0.88224000
C	8.27257300	1.02842400	0.95528200
H	4.75376900	-2.31733800	0.60795600
H	9.28911900	-0.86886400	1.00160100
H	7.19318500	-2.19126300	0.89236500
C	4.67003300	-1.24456100	0.76219300
C	4.51536400	1.60647600	0.61693200
H	6.99209700	2.75944100	0.89671900
H	9.18431200	1.61292900	1.01985800
C	3.41158900	0.75948000	1.21820300
C	3.46180900	-0.68359200	0.93762800
H	4.49772000	2.57607200	1.12490900
H	2.55399500	-1.27907400	0.92436800
N	2.58575200	1.38175500	1.98213500
N	1.53258900	0.67681700	2.49861000
C	0.86170100	1.21086800	3.56830300
O	1.29441700	2.14877900	4.22042600
H	1.11998200	-0.05866700	1.92347000
C	-0.42295300	0.52599200	3.93001600
C	-0.88760800	0.68130200	5.23813500
C	-1.19094300	-0.17819900	3.00109500
C	-2.10092200	0.11901300	5.62029400
H	-0.28778000	1.25319700	5.93863200
C	-2.41317000	-0.72782700	3.38061000

H	-0.86666400	-0.27322600	1.97083200
C	-2.86717000	-0.58535800	4.69018300
H	-2.45432700	0.23358900	6.64001200
H	-3.01281700	-1.25812200	2.64446900
H	-3.81876800	-1.01716700	4.98500000

TSIV'-2

Value of imaginary frequency = -156.5 cm^{-1}

C	5.58415600	3.56372500	-3.13603000
C	4.67038500	3.29104800	-2.14915900
C	4.36978500	1.94978100	-1.78653000
C	5.01923200	0.89557400	-2.48817800
C	5.96861100	1.21017200	-3.49621600
C	6.24940900	2.51389000	-3.81364200
H	5.79669600	4.59383900	-3.40342400
C	3.41222800	1.62028400	-0.77416900
C	4.71310100	-0.45265500	-2.16518900
H	6.46288800	0.39385900	-4.01548800
H	6.97311700	2.74467300	-4.58844000
C	3.76039700	-0.77353600	-1.23044800
C	3.09057500	0.29391700	-0.57046700
H	5.25203200	-1.24950500	-2.67182800
C	2.72598200	2.64577600	0.05797300
C	3.45107500	3.54089900	0.90920900
C	1.34503300	2.67316200	0.08377900
C	2.72883100	4.48492900	1.69247200
C	4.86710100	3.49962000	1.04011600
C	0.61133300	3.60533400	0.86441000
C	3.43692200	5.38205000	2.53627800
C	1.31221800	4.49851700	1.63762700
C	5.52226300	4.37174200	1.87201400
H	5.42910600	2.75914800	0.48164600
C	4.80365000	5.33322500	2.62249000
H	2.86888400	6.10183700	3.11900500
H	0.76911400	5.22532400	2.23659400
H	6.60257800	4.32013800	1.96183000
H	5.33733100	6.01913000	3.27206000
O	0.64034600	1.79790000	-0.70853300
H	4.15855000	4.10196400	-1.64169500
O	2.08654300	-0.00778100	0.32568700
P	0.56373300	0.20547200	-0.27701200
O	-0.37937200	0.02611500	0.87252800
O	0.42958300	-0.55759600	-1.55442300
C	3.53935300	-2.19519300	-0.82346600
C	2.70120600	-3.05509900	-1.55765300
C	4.26882500	-2.68387800	0.27971300
C	1.98949800	-2.62727300	-2.72668400
C	2.55514600	-4.42406400	-1.14208500
C	4.16642700	-4.06910700	0.64217100
C	5.15070200	-1.85407900	1.04865000

C	1.17732700	-3.48584800	-3.40859900
H	2.08650300	-1.59532600	-3.04044000
C	1.67902000	-5.28780200	-1.87535400
C	3.28985100	-4.89855700	-0.05607100
C	4.98842300	-4.57832700	1.69678300
H	5.22208000	-0.79809100	0.80878500
C	5.90688200	-2.37525500	2.05861800
C	1.01359200	-4.83724800	-2.97597800
H	0.64528800	-3.14211700	-4.29078600
H	1.56784800	-6.31394800	-1.53599000
H	3.19232900	-5.94063800	0.24048400
C	5.84284200	-3.76347500	2.37710600
H	4.90918500	-5.63404800	1.94299700
H	6.57280400	-1.72994900	2.62290100
H	0.35760800	-5.50111400	-3.53100600
H	6.46588900	-4.16052800	3.17225600
C	-0.88147900	3.64721700	0.84140300
C	-1.53815200	4.34060000	-0.19324800
C	-1.61808200	3.08566400	1.89962400
C	-0.83200900	4.90066700	-1.30766700
C	-2.96369400	4.50704600	-0.14304700
C	-3.04357900	3.26097300	1.94166600
C	-0.99687800	2.33938700	2.95448500
C	-1.49397900	5.57048100	-2.29598100
H	0.24549900	4.78001100	-1.35867900
C	-3.61852200	5.22810900	-1.19243500
C	-3.68245700	3.96751400	0.92352600
C	-3.77715400	2.72526000	3.04842900
H	0.07295200	2.16884000	2.90897800
C	-1.73316100	1.83106800	3.98367500
C	-2.91004500	5.74167200	-2.23844900
H	-0.94232500	5.98157600	-3.13529500
H	-4.69684200	5.35282600	-1.13561400
H	-4.76123300	4.10254500	0.96201200
C	-3.14537900	2.03521700	4.04002900
H	-4.85189000	2.88771800	3.07831900
H	-1.24557200	1.26496000	4.77070200
H	-3.41623000	6.28192700	-3.03174100
H	-3.71088800	1.63531700	4.87634300
C	-2.63684900	-0.33230000	-2.02858400
C	-3.99301000	-0.53819100	-1.79048000
C	-4.86692800	0.54132200	-1.78768800
C	-4.34498800	1.81657800	-2.01695300
C	-2.98435100	1.99817200	-2.26900900

C	-2.10020600	0.92149000	-2.28561800
C	-2.79181400	-2.57756200	-1.69695800
C	-4.23705000	-2.02721200	-1.62641200
H	-5.93026300	0.40058600	-1.61814800
H	-5.00363200	2.67937200	-2.00853700
H	-2.60244100	2.99587300	-2.46147300
H	-1.04501400	1.05094200	-2.48776900
H	-0.95485600	-1.62388400	-2.07278800
N	-1.98331000	-1.58631200	-2.03472500
C	-2.43204400	-3.99425900	-1.98963400
H	-1.39323600	-4.18488400	-1.71224300
H	-3.06902100	-4.67396700	-1.42483700
H	-2.55619600	-4.17236200	-3.06365800
C	-5.05005800	-2.59352300	-2.79697700
H	-4.51002800	-2.44067800	-3.73547900
H	-5.23877100	-3.66328600	-2.66663900
H	-6.00424400	-2.06989200	-2.87589400
C	-8.50260200	-0.29743900	0.66842700
C	-7.34191600	0.01779600	1.36514400
C	-6.14689100	-0.66240500	1.10676600
C	-6.11286900	-1.66146500	0.11695200
C	-7.29489200	-2.01014400	-0.53248900
C	-8.48182200	-1.32728600	-0.26905200
H	-5.05190600	0.39855400	2.66651400
H	-9.42309100	0.23863900	0.87278500
H	-7.35350400	0.79237200	2.12729000
C	-4.96059100	-0.37381000	1.90882100
C	-4.81109500	-2.35150700	-0.21434100
H	-7.29663000	-2.83124400	-1.24274800
H	-9.38985300	-1.60762100	-0.79235000
C	-3.66062100	-2.01890400	0.72763700
C	-3.79019900	-1.02508500	1.77108400
H	-4.96998100	-3.43683800	-0.16315500
H	-2.93120800	-0.78544500	2.38926400
N	-2.60865500	-2.66910900	0.37864500
N	-1.41772700	-2.53152600	1.04708200
C	-0.70593400	-3.69443400	1.22861300
O	-1.12662500	-4.77311600	0.83153100
H	-1.02539200	-1.57973100	1.15324100
C	0.54410700	-3.59783700	2.05017800
C	1.01991600	-4.79824800	2.59014800
C	1.20328200	-2.40199600	2.33803500
C	2.11946500	-4.79742000	3.43736000
H	0.49889000	-5.71745500	2.34503800

C	2.32487200	-2.40984300	3.16485000
H	0.85848900	-1.45884700	1.93100300
C	2.77121600	-3.59939600	3.73075700
H	2.47415900	-5.72972900	3.86605800
H	2.84533600	-1.47898000	3.36585500
H	3.63948900	-3.59878200	4.38156300

IMIV'-2

C	6.06107300	3.67988700	-2.49938600
C	5.06637000	3.31889700	-1.62565900
C	4.74102400	1.95096700	-1.41866000
C	5.45381100	0.96450500	-2.15708800
C	6.48549100	1.36934600	-3.04494700
C	6.78702900	2.69614300	-3.21252900
H	6.29042800	4.72980200	-2.65029400
C	3.69943000	1.53329500	-0.52844800
C	5.12675700	-0.40705300	-1.99165300
H	7.02590600	0.60328000	-3.59393600
H	7.57418100	2.99705800	-3.89593000
C	4.09535500	-0.80650600	-1.17908000
C	3.36382600	0.19608100	-0.48611400
H	5.70789500	-1.15551600	-2.52461200
C	2.95183200	2.47828000	0.34469500
C	3.61388100	3.28239800	1.32834300
C	1.57318700	2.51718500	0.27174700
C	2.83845100	4.16034700	2.13752100
C	5.01527200	3.21301500	1.56277700
C	0.78515600	3.38278300	1.07723500
C	3.48347300	4.96833300	3.11149100
C	1.43007600	4.19524300	1.97724200
C	5.60860700	3.99781800	2.51886400
H	5.61646200	2.52194200	0.98248700
C	4.83924300	4.89556400	3.29733000
H	2.87515700	5.63739600	3.71364000
H	0.84638500	4.87079700	2.59762500
H	6.67851600	3.92531000	2.68554000
H	5.32385500	5.51239500	4.04688300
O	0.92702600	1.72718000	-0.65092700
H	4.50917800	4.08008400	-1.08983400
O	2.29057500	-0.19561900	0.28445300
P	0.80892000	0.10871000	-0.37956300
O	-0.17196600	-0.15884900	0.72668900
O	0.68303900	-0.54314600	-1.71446200
C	3.80633600	-2.25185900	-0.94152400
C	3.09818700	-3.01569800	-1.88592500
C	4.30207600	-2.85102600	0.23436600
C	2.58156300	-2.45033300	-3.09767800
C	2.87473700	-4.41471500	-1.63996900
C	4.08550600	-4.25222500	0.46250800
C	5.03858700	-2.11504600	1.22075000
C	1.90055900	-3.21880900	-3.99450900

H	2.71953800	-1.39002400	-3.27339500
C	2.14952600	-5.18422300	-2.60594500
C	3.37184200	-4.99890500	-0.47535400
C	4.61021700	-4.85572800	1.64962400
H	5.21396100	-1.05554500	1.06465500
C	5.52174100	-2.72710500	2.34178100
C	1.67950700	-4.60771400	-3.74750200
H	1.51086400	-2.77268100	-4.90378700
H	1.98668300	-6.23950800	-2.40517000
H	3.20415800	-6.05860300	-0.29665900
C	5.30753400	-4.12042400	2.56192300
H	4.43278700	-5.91608900	1.80785800
H	6.07714800	-2.15126300	3.07506000
H	1.13212600	-5.19913600	-4.47458300
H	5.70143700	-4.58737900	3.45895900
C	-0.70194600	3.43922300	0.94625500
C	-1.27795200	4.24129900	-0.05773900
C	-1.51723400	2.77539300	1.88084100
C	-0.48834200	4.91817600	-1.04410500
C	-2.70279100	4.41161100	-0.09935400
C	-2.94448900	2.93345800	1.81531900
C	-0.97695200	1.93587200	2.90951800
C	-1.07119800	5.71399800	-1.98762500
H	0.58933100	4.78964000	-1.02994100
C	-3.27340000	5.26736500	-1.09508800
C	-3.50252200	3.74922900	0.83162400
C	-3.76373700	2.26986700	2.78434800
H	0.09556800	1.78069500	2.94276000
C	-1.79058300	1.32386400	3.81673700
C	-2.48637300	5.90059300	-2.01076100
H	-0.45620500	6.21605600	-2.72754800
H	-4.35242100	5.39763500	-1.10288000
H	-4.58219500	3.87627100	0.79220100
C	-3.20617700	1.49957500	3.76094800
H	-4.84130800	2.40224400	2.72289600
H	-1.36292500	0.68971700	4.58662100
H	-2.92834100	6.54721900	-2.76188400
H	-3.83373500	1.01073800	4.50082000
C	-2.54351100	-0.06036700	-2.28270100
C	-3.92948000	-0.12941300	-2.09621600
C	-4.70737600	1.01383600	-2.21532000
C	-4.07924400	2.23281800	-2.48294400
C	-2.69484500	2.29140600	-2.64154000
C	-1.90459900	1.14682200	-2.54990600

C	-2.90297700	-2.20656900	-1.56595000
C	-4.31648900	-1.58550500	-1.86946700
H	-5.78547500	0.97138200	-2.09458000
H	-4.66750200	3.14208500	-2.55372200
H	-2.21760200	3.24987200	-2.82630500
H	-0.82790300	1.18455700	-2.66854700
H	-0.97292400	-1.39974700	-2.01382900
N	-1.97582000	-1.33513100	-2.20711900
C	-2.66948800	-3.67179700	-1.87060100
H	-1.65990100	-3.94947000	-1.55398600
H	-3.38438300	-4.30447400	-1.33869100
H	-2.75076700	-3.83972600	-2.94538600
C	-4.94804200	-2.19304700	-3.12080400
H	-4.21776100	-2.17498900	-3.93495300
H	-5.26649400	-3.22683900	-2.95597000
H	-5.80687300	-1.60302200	-3.44516300
C	-8.65831900	0.31807700	0.57970300
C	-7.62622300	0.13895300	1.48875400
C	-6.46478400	-0.55281400	1.11895200
C	-6.33377000	-1.05848400	-0.19029700
C	-7.39655100	-0.91314700	-1.07823200
C	-8.54419900	-0.21882800	-0.70215000
H	-5.59516400	-0.38274900	3.10507500
H	-9.55223000	0.85937800	0.86873300
H	-7.70965000	0.52894300	2.49901800
C	-5.41476800	-0.76610800	2.10392600
C	-5.09213100	-1.83622300	-0.54598700
H	-7.33603000	-1.34036400	-2.07271900
H	-9.35366800	-0.10153500	-1.41470600
C	-4.00845700	-1.74799800	0.48138400
C	-4.23724400	-1.37801000	1.83916300
H	-5.37795700	-2.90433200	-0.53412400
H	-3.44504100	-1.46382100	2.57241500
N	-2.86003800	-2.02569000	-0.05793900
N	-1.71335900	-2.27188400	0.65421300
C	-1.71501200	-3.42748400	1.40888000
O	-2.69032500	-4.16419100	1.43977100
H	-1.03840900	-1.45321000	0.72404300
C	-0.46693700	-3.71096900	2.17787200
C	-0.52923100	-4.75203800	3.10801700
C	0.72433300	-3.00177100	2.00031300
C	0.58953100	-5.07791300	3.86546300
H	-1.46306400	-5.29176400	3.22162600
C	1.83900500	-3.32716800	2.76600900

H	0.79783400	-2.19438100	1.28120700
C	1.77473900	-4.36407600	3.69443000
H	0.53743900	-5.88675000	4.58694900
H	2.76314700	-2.77427100	2.62682300
H	2.65489800	-4.61856400	4.27702600

IMIV'-3

C	4.51482500	5.49653400	1.62891000
C	4.06763600	4.40224500	0.93273900
C	2.68106100	4.09077400	0.87790200
C	1.77250400	4.92328900	1.58838100
C	2.26448600	6.05590100	2.29050100
C	3.60476900	6.34141100	2.30881600
H	5.57733000	5.71452200	1.66436600
C	2.17241600	2.95356200	0.17296100
C	0.39047000	4.60770600	1.58387400
H	1.55499500	6.68627100	2.81926900
H	3.97299000	7.20642800	2.85056700
C	-0.09658100	3.48899000	0.95126700
C	0.82863500	2.64635300	0.27800600
H	-0.30088600	5.27077500	2.09825500
C	3.04361000	2.06419200	-0.64035400
C	3.80278200	2.54738100	-1.75516100
C	3.05899900	0.71348100	-0.35427300
C	4.61805400	1.63378500	-2.48031300
C	3.74909300	3.89841800	-2.19742200
C	3.84810800	-0.21415000	-1.08928700
C	5.38664600	2.10021400	-3.58004300
C	4.62566400	0.26366300	-2.11527200
C	4.49388300	4.31746500	-3.27098700
H	3.10150400	4.59908600	-1.68177400
C	5.33265800	3.41381100	-3.96622500
H	6.01014500	1.38904800	-4.11473700
H	5.24370400	-0.42753800	-2.68316800
H	4.43519200	5.35143000	-3.59540200
H	5.91969400	3.76116100	-4.80999400
O	2.30646900	0.25185900	0.70083300
H	4.77499900	3.75498700	0.42550800
O	0.35608600	1.50260900	-0.32584800
P	0.67556400	0.08654100	0.45882600
O	0.47090500	-0.99904400	-0.56654700
O	0.02846000	0.02350400	1.79334200
C	-1.57367100	3.25843300	0.92036500
C	-2.24814200	2.81646300	2.07384200
C	-2.30218200	3.65391000	-0.22049700
C	-1.55049500	2.35435600	3.23846700
C	-3.68524800	2.84106500	2.10954000
C	-3.73824800	3.63630200	-0.18714500
C	-1.66414100	4.12629800	-1.41402900
C	-2.22849100	1.98630700	4.36337500

H	-0.47074900	2.27083300	3.19381800
C	-4.35578800	2.48719200	3.32595400
C	-4.39621700	3.24009400	0.97827400
C	-4.46946900	4.09044800	-1.33095100
H	-0.57982900	4.14460500	-1.45773600
C	-2.39631800	4.55755600	-2.48222300
C	-3.65274000	2.07448300	4.41916100
H	-1.68386800	1.62785700	5.23066900
H	-5.43941200	2.56916700	3.36040500
H	-5.48351000	3.26674800	1.01070800
C	-3.82234300	4.54722300	-2.44080700
H	-5.55500800	4.07429600	-1.28551800
H	-1.89203000	4.91528300	-3.37449100
H	-4.17084300	1.80976600	5.33534700
H	-4.38577600	4.89901600	-3.29926700
C	3.83163100	-1.67014500	-0.76458900
C	4.59623700	-2.15470000	0.31360500
C	3.10033200	-2.55936000	-1.57339400
C	5.37662600	-1.28727900	1.14622400
C	4.61492300	-3.56247600	0.59542600
C	3.09902100	-3.96211600	-1.26299800
C	2.35282300	-2.12118500	-2.71663200
C	6.11630500	-1.78496100	2.18036500
H	5.37350700	-0.22173400	0.94012900
C	5.40476300	-4.04318900	1.68756100
C	3.85319400	-4.43086600	-0.18763400
C	2.33412500	-4.85722000	-2.08110900
H	2.33916000	-1.06321400	-2.95322500
C	1.67266200	-3.00990700	-3.49584300
C	6.13226100	-3.18467200	2.45756500
H	6.70104900	-1.11334100	2.80057800
H	5.40334500	-5.11020200	1.89226500
H	3.85543300	-5.49444800	0.03964600
C	1.64813300	-4.40085600	-3.16642800
H	2.32890100	-5.91233500	-1.82153900
H	1.11754000	-2.65966200	-4.36103300
H	6.72594000	-3.55830100	3.28555500
H	1.07826500	-5.08614700	-3.78594800
C	-1.79479400	-1.31153300	-2.65205300
C	-3.16320300	-1.26215500	-2.37926200
C	-3.87645000	-0.08915900	-2.58937700
C	-3.19399700	1.04038200	-3.04529200
C	-1.82133700	0.98331000	-3.28905700
C	-1.10164600	-0.19474700	-3.10181800

C	-2.22381200	-3.29874100	-1.58356600
C	-3.61711700	-2.62689200	-1.87717600
H	-4.94149000	-0.03828000	-2.38411900
H	-3.72677000	1.97425500	-3.18487300
H	-1.30034800	1.87989000	-3.61094800
H	-0.02888100	-0.23636100	-3.25265100
H	-0.31166500	-2.65590600	-2.15560100
N	-1.29075400	-2.60420900	-2.43144400
C	-2.09734700	-4.80425600	-1.66255900
H	-1.08058000	-5.09021900	-1.37679800
H	-2.79997200	-5.29407400	-0.98315100
H	-2.27699100	-5.13843400	-2.68544400
C	-4.42628700	-3.38580800	-2.92398400
H	-3.80058400	-3.57117100	-3.80184400
H	-4.78868600	-4.34481600	-2.54144700
H	-5.27902700	-2.78949200	-3.25436000
C	-7.52042400	0.12711300	0.44007800
C	-6.36959100	0.13468000	1.21470200
C	-5.30721600	-0.73051100	0.92211400
C	-5.40240500	-1.60752200	-0.17613400
C	-6.58218200	-1.64301300	-0.91580400
C	-7.62802500	-0.77195200	-0.62068300
H	-4.11473400	-0.01373200	2.59736100
H	-8.33687700	0.80319400	0.66869800
H	-6.27886000	0.80536600	2.06375400
C	-4.12522500	-0.72473700	1.77351800
C	-4.25946300	-2.54527800	-0.45958100
H	-6.69234800	-2.35385100	-1.72735100
H	-8.53295300	-0.80082700	-1.21828800
C	-3.05335800	-2.30657300	0.39328300
C	-3.04349800	-1.51645300	1.57854000
H	-4.59865500	-3.56052600	-0.18892200
H	-2.13629700	-1.41908600	2.16567900
N	-2.01714700	-2.86478800	-0.15999500
N	-0.79935400	-3.01190600	0.45281900
C	-0.78656500	-3.80058000	1.58539600
O	-1.75567000	-4.47624700	1.89764000
H	-0.12837600	-2.23966600	0.17658000
C	0.44935400	-3.73173600	2.41993100
C	0.42532100	-4.45279200	3.61766600
C	1.55341400	-2.93289100	2.10758100
C	1.48969300	-4.37014200	4.50598500
H	-0.44467300	-5.06112400	3.83901200
C	2.60378700	-2.83183700	3.01502700

H	1.62133200	-2.39153700	1.16696500
C	2.57543700	-3.54755400	4.20896900
H	1.46725300	-4.93385600	5.43278300
H	3.44784600	-2.19099800	2.78306500
H	3.40395700	-3.46543700	4.90579700

IMIV'-4

C	7.55635300	1.46333500	1.32553400
C	6.51137900	0.83620900	0.69478500
C	5.32561000	1.54745800	0.36017500
C	5.23312400	2.91584900	0.74551100
C	6.33630200	3.53967100	1.38719900
C	7.47825500	2.83503500	1.66491500
H	8.44965700	0.89955600	1.57425100
C	4.21182200	0.93719100	-0.30661000
C	4.02209100	3.62363100	0.53493100
H	6.24895900	4.58682300	1.66337700
H	8.31488300	3.31851300	2.15825400
C	2.93081800	3.02166200	-0.03964000
C	3.05977600	1.67690600	-0.47935700
H	3.94885000	4.65345600	0.87563600
C	4.21173500	-0.49868600	-0.69967700
C	5.19906600	-1.07290400	-1.56518700
C	3.22093900	-1.31934300	-0.19416700
C	5.19909100	-2.47978300	-1.78064000
C	6.16220800	-0.28367400	-2.25051700
C	3.24945500	-2.73469800	-0.34420600
C	6.17591800	-3.05419800	-2.63658400
C	4.23357800	-3.28748600	-1.12403800
C	7.08691200	-0.86617500	-3.08036000
H	6.15037300	0.79305800	-2.11755100
C	7.10266000	-2.26832500	-3.27133600
H	6.16773100	-4.13069600	-2.78300300
H	4.28263100	-4.36736300	-1.23993900
H	7.80959500	-0.24619900	-3.60101100
H	7.84205600	-2.71472900	-3.92802300
O	2.19514500	-0.77440500	0.54154700
H	6.58261200	-0.21849900	0.45429600
O	1.99416800	1.10824300	-1.12982200
P	1.03421900	0.04947900	-0.30766900
O	0.44645800	-0.82746500	-1.37016400
O	0.19428300	0.74361400	0.70700300
C	1.61731100	3.72202200	-0.13344200
C	0.83574700	3.86201700	1.02964900
C	1.16835400	4.23804400	-1.36226600
C	1.21976900	3.29311300	2.28833000
C	-0.40947900	4.57395900	0.96315600
C	-0.07605500	4.95244400	-1.41808300
C	1.91516000	4.08451700	-2.57520600
C	0.43088300	3.42859200	3.39214100

H	2.14123200	2.72469900	2.34468100
C	-1.20583400	4.69969200	2.14625300
C	-0.82584400	5.11747500	-0.25280000
C	-0.52200000	5.47579600	-2.67377300
H	2.85918500	3.54968500	-2.54258600
C	1.45402500	4.59325200	-3.75387000
C	-0.80209000	4.14354100	3.32303600
H	0.73470300	2.97893300	4.33204700
H	-2.14850800	5.23607900	2.07911400
H	-1.76038000	5.67359400	-0.29494200
C	0.21502000	5.29973800	-3.80702900
H	-1.46378500	6.01832000	-2.70005600
H	2.03037000	4.46197100	-4.66392300
H	-1.42101600	4.23371600	4.21056200
H	-0.13369900	5.69699700	-4.75474800
C	2.31178400	-3.58586200	0.44895300
C	2.63806300	-3.86063800	1.79294800
C	1.13783700	-4.10947500	-0.11766200
C	3.81958300	-3.34196400	2.41808000
C	1.76876100	-4.69046300	2.57910500
C	0.26556700	-4.92621200	0.68273100
C	0.74990400	-3.82453600	-1.46729500
C	4.11054000	-3.62757400	3.72008700
H	4.48721500	-2.71334500	1.83795100
C	2.11243200	-4.96889200	3.94034100
C	0.60398600	-5.20410900	2.00610100
C	-0.96147000	-5.39930800	0.11390200
H	1.39443100	-3.19510800	-2.06955600
C	-0.42867800	-4.28814400	-1.97233500
C	3.24594300	-4.45494000	4.49628900
H	5.00957800	-3.22316900	4.17379200
H	1.44493700	-5.60023500	4.52041200
H	-0.05773600	-5.82298200	2.60818200
C	-1.30452100	-5.08015400	-1.16735600
H	-1.61470300	-6.00754200	0.73400500
H	-0.72926400	-4.02781300	-2.97989200
H	3.49674000	-4.67154700	5.52962400
H	-2.24105800	-5.43387800	-1.58967500
C	-4.97477400	-1.96584500	0.78495900
C	-4.88802800	-0.68867100	1.36046000
C	-6.04884300	0.02139300	1.62965500
C	-7.28609200	-0.54343700	1.30270700
C	-7.35121500	-1.81527900	0.73883000
C	-6.19504500	-2.54890800	0.47431100

C	-2.72309400	-1.48987500	0.81151300
C	-3.42555200	-0.40728500	1.70143000
H	-6.00692700	1.00478700	2.08575400
H	-8.19785600	0.01084800	1.49729600
H	-8.31694100	-2.24385800	0.48823800
H	-6.24416200	-3.53496800	0.02503100
H	-3.50370200	-3.31118800	0.05639500
N	-3.69932200	-2.51087600	0.64415500
C	-1.36848600	-2.01917500	1.22963600
H	-0.92473200	-2.56518300	0.39131700
H	-0.69800300	-1.20085400	1.49965300
H	-1.49085000	-2.70595200	2.06954400
C	-3.16570600	-0.65751400	3.18804600
H	-3.38753300	-1.70233200	3.42447100
H	-2.12532100	-0.44873900	3.45246500
H	-3.81959500	-0.03971500	3.80597800
C	-4.83121400	4.73132900	1.59655000
C	-4.24010000	4.37714200	0.39283200
C	-3.58345000	3.14632600	0.25687500
C	-3.54192600	2.24542100	1.33944200
C	-4.08119400	2.64200600	2.56143200
C	-4.73306500	3.86659700	2.68696100
H	-2.88199200	3.60197100	-1.75640500
H	-5.34572100	5.68088800	1.69449700
H	-4.27749200	5.05184100	-0.45837100
C	-2.91476100	2.82411400	-0.99704400
C	-2.83005900	0.92515600	1.16080600
H	-4.00831500	1.98882100	3.42374600
H	-5.16754800	4.14482600	3.64148600
C	-2.53999000	0.61155600	-0.26718500
C	-2.36788600	1.61589900	-1.26794700
H	-1.81419800	1.04113400	1.58586200
H	-1.91630300	1.36766100	-2.22068300
N	-2.53956300	-0.67482700	-0.46989900
N	-2.15017500	-1.25219000	-1.65358100
C	-2.99185300	-1.86942600	-2.55257900
O	-2.50071200	-2.53701900	-3.44923800
H	-1.11329300	-1.30278800	-1.74972700
C	-4.47767600	-1.69267800	-2.46678900
C	-5.25107200	-2.78419500	-2.87255600
C	-5.10311600	-0.48531200	-2.14448900
C	-6.63565900	-2.67766700	-2.93639900
H	-4.74959900	-3.70578000	-3.15047100
C	-6.48816100	-0.37760600	-2.22410300

H	-4.52043600	0.38789700	-1.87583300
C	-7.25503700	-1.47138200	-2.61613200
H	-7.22970600	-3.53158000	-3.24516200
H	-6.96689600	0.56490100	-1.98001800
H	-8.33548500	-1.38335700	-2.67224100

TSIV'-3

Value of imaginary frequency = -1071.2 cm^{-1}

C	7.48302500	-0.48668000	1.64912400
C	6.30922400	-0.82437900	1.02398900
C	5.40173700	0.17986900	0.58696600
C	5.72381600	1.53991300	0.85155400
C	6.95283600	1.85904300	1.48908800
C	7.81874700	0.87000400	1.87517200
H	8.15901300	-1.26806000	1.98102600
C	4.16685600	-0.12250300	-0.07387100
C	4.79864000	2.55419700	0.50530300
H	7.18415600	2.90428100	1.67378800
H	8.75323100	1.11984200	2.36644600
C	3.57593000	2.26608600	-0.05495800
C	3.28058700	0.90406300	-0.33350000
H	5.05256100	3.58959300	0.71831000
C	3.79016500	-1.51797300	-0.42189400
C	4.60754000	-2.34838800	-1.25634600
C	2.60168900	-2.02868200	0.05759500
C	4.21902800	-3.69959500	-1.47366900
C	5.77326000	-1.86642700	-1.91203000
C	2.20855600	-3.38025600	-0.13035300
C	5.02329100	-4.53544500	-2.29404000
C	3.03008400	-4.18996600	-0.87692200
C	6.52256600	-2.69381600	-2.70983300
H	6.06095400	-0.82851400	-1.78559100
C	6.15318200	-4.04730000	-2.89666700
H	4.71666600	-5.56729400	-2.44043100
H	2.75621500	-5.23094700	-1.02986700
H	7.40545500	-2.30563300	-3.20730900
H	6.76032200	-4.68980700	-3.52565200
O	1.76119100	-1.20085000	0.77951900
H	6.06119800	-1.86846100	0.86893800
O	2.08124900	0.61419900	-0.94957300
P	0.89202900	-0.13905000	-0.11803400
O	0.01489700	-0.81926800	-1.10629200
O	0.30801000	0.81551300	0.91436300
C	2.61617500	3.37209000	-0.33377100
C	2.14807400	4.15659200	0.74254400
C	2.25816000	3.69762600	-1.65809500
C	2.40161100	3.82374300	2.11540700
C	1.37742400	5.33833400	0.47397500
C	1.44587000	4.85589800	-1.90803300
C	2.70195000	2.93636500	-2.78886400

C	1.95909800	4.62322400	3.12848000
H	2.94014700	2.91105700	2.34328900
C	0.95230500	6.16205000	1.56464200
C	1.05558200	5.66580700	-0.84197700
C	1.07120500	5.17243900	-3.25342700
H	3.34649400	2.07931500	-2.62728700
C	2.32374700	3.26935900	-4.05640300
C	1.23594200	5.82119700	2.85261000
H	2.15511200	4.34509100	4.15906400
H	0.38904000	7.06287000	1.33662800
H	0.47788500	6.56627800	-1.03893200
C	1.48617900	4.39910800	-4.29625700
H	0.45345200	6.05079600	-3.42280800
H	2.66457600	2.67257300	-4.89618800
H	0.90563100	6.44915900	3.67382400
H	1.19637800	4.64494100	-5.31271300
C	0.97282800	-3.93129400	0.49586800
C	0.91758300	-4.10428200	1.89474800
C	-0.09891700	-4.34772800	-0.31535600
C	1.97457900	-3.68337600	2.76617000
C	-0.22577500	-4.74242600	2.48408700
C	-1.22689700	-5.00805800	0.28414200
C	-0.13641700	-4.09939500	-1.72877500
C	1.88617800	-3.85786100	4.11650300
H	2.85778900	-3.22016700	2.33918100
C	-0.27984700	-4.90670800	3.90483400
C	-1.25987800	-5.19806800	1.66425500
C	-2.31866100	-5.42033900	-0.54802700
H	0.68669600	-3.56150100	-2.18535500
C	-1.20390300	-4.48989500	-2.48081600
C	0.73981500	-4.47423100	4.69926500
H	2.69666700	-3.52721700	4.75786300
H	-1.15576600	-5.38569500	4.33360900
H	-2.11786500	-5.69223000	2.11475400
C	-2.30971700	-5.17119600	-1.88614600
H	-3.15940600	-5.92340600	-0.07799800
H	-1.23334300	-4.26460600	-3.54107700
H	0.68889700	-4.60127200	5.77570600
H	-3.14936700	-5.46241500	-2.50772100
C	-5.19865600	-0.40120900	1.41299400
C	-4.56651800	0.83226500	1.61706900
C	-5.32724600	1.97741000	1.79594200
C	-6.72272700	1.88050800	1.75514800
C	-7.33575400	0.64468600	1.55838900

C	-6.58180100	-0.51718200	1.39183200
C	-2.96443000	-0.82497000	1.04395700
C	-3.05585400	0.61362000	1.67182900
H	-4.85247300	2.94107800	1.95411700
H	-7.32779400	2.77232000	1.87947500
H	-8.41926800	0.58129000	1.52503800
H	-7.05743200	-1.47759700	1.22140100
H	-4.48704200	-2.25220600	0.77338300
N	-4.24951000	-1.42316000	1.30709400
C	-1.82482100	-1.71858800	1.49474200
H	-1.70193800	-2.54650300	0.79303200
H	-0.88650500	-1.16854100	1.55628000
H	-2.05783200	-2.13002900	2.47844100
C	-2.54827100	0.63807100	3.11543900
H	-2.98770700	-0.19476400	3.67248200
H	-1.45826500	0.55840500	3.15449000
H	-2.85417400	1.55708100	3.61826700
C	-2.16982000	5.75158600	0.34419700
C	-2.01677600	4.95574000	-0.77271200
C	-2.03904500	3.55354600	-0.66108200
C	-2.23364300	2.94444900	0.60381700
C	-2.32325700	3.77080300	1.73397200
C	-2.30542200	5.15016400	1.60278600
H	-1.65189000	3.24115700	-2.77232600
H	-2.16199300	6.83282100	0.25356300
H	-1.87839500	5.39861400	-1.75565400
C	-1.88454000	2.73550200	-1.83786500
C	-2.26045900	1.47336900	0.66332100
H	-2.42326800	3.33037800	2.71861700
H	-2.39281000	5.77022200	2.48943600
C	-2.37881900	0.78555200	-0.58702600
C	-2.03934300	1.38375600	-1.83209400
H	-1.00151100	1.17001500	0.80160700
H	-1.95604900	0.77991100	-2.72714400
N	-2.80481700	-0.46345900	-0.40982700
N	-2.69964100	-1.41743800	-1.38748300
C	-3.75481700	-1.83299700	-2.16655900
O	-3.57899800	-2.68653300	-3.01920100
H	-1.74751500	-1.72999000	-1.59434000
C	-5.12073800	-1.24923600	-1.93770700
C	-6.18259200	-2.15709100	-1.90600400
C	-5.38236900	0.12360300	-1.90438400
C	-7.49327900	-1.69945300	-1.81716900
H	-5.96881100	-3.21993100	-1.96560400

C	-6.69646400	0.57751200	-1.84405600
H	-4.57279800	0.84334200	-1.96302100
C	-7.75096400	-0.33035500	-1.79451200
H	-8.31241000	-2.41027300	-1.78103400
H	-6.89474400	1.64407700	-1.82937300
H	-8.77339800	0.02939500	-1.73647800

IMIV'-5

C	-7.00908000	-0.67587400	-2.66603300
C	-6.00401700	-0.96311800	-1.77706500
C	-5.28633200	0.08033600	-1.13226700
C	-5.60981900	1.42794200	-1.45696100
C	-6.66447600	1.69220200	-2.37109800
C	-7.35412600	0.66496200	-2.95970600
H	-7.54133300	-1.48527700	-3.15471300
C	-4.22680400	-0.16735400	-0.19787100
C	-4.86765100	2.48887400	-0.87879500
H	-6.90504100	2.72651300	-2.59928700
H	-8.15550900	0.87380400	-3.66042500
C	-3.80712800	2.25647700	-0.03620100
C	-3.50396400	0.90488300	0.26682300
H	-5.13576500	3.51320400	-1.12465500
C	-3.87221700	-1.54196100	0.24456300
C	-4.84380300	-2.39378700	0.86752400
C	-2.59161200	-2.02314700	0.06642800
C	-4.49493200	-3.74125800	1.15745200
C	-6.13509000	-1.93330300	1.24339400
C	-2.24326300	-3.38336600	0.28794700
C	-5.44815800	-4.59590900	1.77179500
C	-3.20235100	-4.21101300	0.81806500
C	-7.03052700	-2.77806100	1.84915500
H	-6.40383700	-0.89830200	1.06251100
C	-6.69104000	-4.12768700	2.10833400
H	-5.16694300	-5.62475700	1.97689600
H	-2.96297800	-5.25847400	0.98142700
H	-8.00775100	-2.40660400	2.13948800
H	-7.41340600	-4.78386500	2.58211500
O	-1.60216200	-1.17201600	-0.43373600
H	-5.74278600	-1.99503400	-1.56997100
O	-2.43034300	0.66151200	1.11808100
P	-1.08854700	0.05499900	0.47512200
O	-0.11442100	-0.22771300	1.54056800
O	-0.62733500	1.03584900	-0.67931900
C	-3.03368200	3.38335500	0.55701600
C	-2.30499000	4.24830100	-0.28358700
C	-3.10099300	3.62407100	1.94557700
C	-2.15225900	4.01723400	-1.69216200
C	-1.67580700	5.41275500	0.27797700
C	-2.42165800	4.76134400	2.49956900
C	-3.84777400	2.78992500	2.84029500
C	-1.49010800	4.90908900	-2.48344000

H	-2.56489100	3.11194400	-2.12323900
C	-1.00777000	6.33413800	-0.59175700
C	-1.73836200	5.63500500	1.65280400
C	-2.48392100	4.99681300	3.90999000
H	-4.39492700	1.94185500	2.44192800
C	-3.88548300	3.04876600	4.17921000
C	-0.93346000	6.10157500	-1.93212400
H	-1.37831900	4.71248100	-3.54476200
H	-0.56503700	7.22488400	-0.15413500
H	-1.25417000	6.51350900	2.07321700
C	-3.18786200	4.16512800	4.72803900
H	-1.95792900	5.85919800	4.30996200
H	-4.45636100	2.40185900	4.83730300
H	-0.43041000	6.80722000	-2.58605100
H	-3.22942300	4.35050600	5.79620100
C	-0.93473400	-3.96199400	-0.14104400
C	-0.85330600	-4.56747300	-1.41140700
C	0.17326200	-3.95831000	0.72071100
C	-1.94864000	-4.57069600	-2.33632100
C	0.36876000	-5.20897000	-1.80986700
C	1.39911500	-4.57997600	0.30090200
C	0.14922200	-3.29242100	1.98923100
C	-1.83571400	-5.16973800	-3.55712000
H	-2.87684500	-4.08443100	-2.05420200
C	0.44304200	-5.83016400	-3.09696000
C	1.46264200	-5.20649700	-0.94232600
C	2.55245500	-4.48241400	1.14402800
H	-0.77104400	-2.82005600	2.31665600
C	1.27564300	-3.19702900	2.75183500
C	-0.62333900	-5.81319000	-3.94569400
H	-2.67580300	-5.15785700	-4.24389400
H	1.37359500	-6.31357300	-3.38110700
H	2.39111400	-5.67934600	-1.25464100
C	2.50037000	-3.79345200	2.32056400
H	3.47496200	-4.94945700	0.80841200
H	1.26832800	-2.63757600	3.68006300
H	-0.55592000	-6.28517000	-4.92038300
H	3.38303400	-3.69268700	2.94504500
C	5.47338800	-1.16366800	-0.69481400
C	5.21258800	-0.04530600	-1.49806800
C	6.24868500	0.74686000	-1.96001700
C	7.56269200	0.41356000	-1.61168600
C	7.81154400	-0.70284800	-0.81521600
C	6.77227600	-1.50740900	-0.34396800

C	3.19983900	-0.88527800	-0.59236800
C	3.71238300	0.04320900	-1.74946400
H	6.04050900	1.62216700	-2.57117700
H	8.38772500	1.02826400	-1.95598100
H	8.83324400	-0.94612900	-0.53853800
H	6.97143500	-2.35941400	0.29821700
H	4.23582100	-2.35278100	0.48794800
N	4.27735400	-1.82558800	-0.37942000
C	1.85194000	-1.53952000	-0.81817300
H	1.46620400	-1.92832500	0.12636200
H	1.14487100	-0.79604300	-1.19988100
H	1.92227800	-2.36196900	-1.53267600
C	3.36184900	-0.52703200	-3.12790600
H	3.58727200	-1.59788400	-3.13995700
H	2.30350400	-0.38576800	-3.36416400
H	3.96283700	-0.06368200	-3.91183400
C	2.56492300	5.05676900	-3.43507500
C	2.13838400	4.91540400	-2.14108100
C	2.29151500	3.68612700	-1.44646700
C	2.91865900	2.57971900	-2.10785900
C	3.35214900	2.76348200	-3.45361600
C	3.17871200	3.96261700	-4.09470500
H	1.35447200	4.40003700	0.36548900
H	2.44536400	6.00306200	-3.95240900
H	1.67764000	5.74544600	-1.61527600
C	1.85662200	3.55636700	-0.10179400
C	3.09456200	1.38449300	-1.37583900
H	3.84151500	1.94680800	-3.96961200
H	3.52480300	4.07919200	-5.11690200
C	2.72508400	1.33303500	-0.04136200
C	2.07421800	2.39930500	0.61677400
H	0.08252500	1.64751600	-0.40255800
H	1.76720400	2.29679100	1.65298500
N	3.10335500	0.11563500	0.50924700
N	2.70662500	-0.26301600	1.76468800
C	3.59806500	-0.55342900	2.76150400
O	3.20431200	-1.06873600	3.80173800
H	1.72279600	-0.48978800	1.92490000
C	5.05211200	-0.23583400	2.56673800
C	5.96033600	-1.11743600	3.15750300
C	5.52222800	0.91833900	1.93158300
C	7.32768800	-0.86748200	3.09199700
H	5.57915800	-1.99131700	3.67691900
C	6.88791300	1.17570900	1.88607100

H	4.82621700	1.62391400	1.49198900
C	7.79157200	0.28170100	2.45742600
H	8.02787900	-1.56388800	3.54214700
H	7.24808700	2.07306000	1.39355900
H	8.85738800	0.48203200	2.40636900

$P1_{C2}$

C	-1.47152000	2.47038500	-0.62309100
C	-1.88450200	1.75665800	0.50868200
C	-3.02413600	2.14245400	1.19549500
C	-3.78435300	3.21295700	0.71460000
C	-3.38520500	3.89000700	-0.43564400
C	-2.21764500	3.53574500	-1.11534000
C	0.36722000	1.17724300	-0.03524900
C	-0.87505500	0.66017500	0.78557500
H	-3.31795800	1.63862500	2.11247100
H	-4.67923100	3.52131100	1.24398000
H	-3.97859700	4.72192300	-0.80205200
H	-1.89235800	4.08634600	-1.99227400
H	0.35440400	2.68267800	-1.50888300
N	-0.25440400	1.97300000	-1.11363100
C	1.39069400	1.99131600	0.73447200
H	1.85930200	1.39353100	1.51918700
H	2.17665000	2.34093400	0.05624100
H	0.90908300	2.86731100	1.17868100
C	-0.59171700	0.41600100	2.26847400
H	-1.46881800	-0.02507900	2.75051700
H	0.24120100	-0.28400100	2.38649500
H	-0.35035500	1.34934500	2.78417900
C	-4.43381700	-3.35542500	0.16366100
C	-3.32822600	-3.63269300	-0.59830900
C	-2.22139500	-2.74378800	-0.63425700
C	-2.26972000	-1.53742800	0.13377800
C	-3.43038800	-1.28212100	0.91442500
C	-4.47974800	-2.16543500	0.92953700
H	-1.06337200	-3.95900400	-1.99607600
H	-5.27348000	-4.04209100	0.18283800
H	-3.28004300	-4.54313300	-1.18982600
C	-1.07359900	-3.03902500	-1.41865600
C	-1.15725200	-0.66182100	0.06445100
H	-3.48356900	-0.37259500	1.49892700
H	-5.35623900	-1.94906400	1.53206100
C	-0.06507400	-1.00688600	-0.69575900
C	0.00441800	-2.19140100	-1.45677500
H	0.88381100	-2.40705300	-2.05449900
N	0.96588100	-0.05717300	-0.56429000
N	1.80576600	0.08912300	-1.64967400
C	3.17043300	0.18401800	-1.53722100
O	3.82332000	0.62027100	-2.47383100
H	1.40822900	0.49120200	-2.49732900

C	3.82277800	-0.25076500	-0.25966100
C	3.37110200	-1.31040200	0.53317500
C	4.98273200	0.43946700	0.09844100
C	4.07346900	-1.65870400	1.68325100
H	2.48329300	-1.86494900	0.25040300
C	5.67056400	0.10175900	1.25892000
H	5.33035100	1.24319100	-0.54229400
C	5.21470800	-0.94792000	2.05313400
H	3.72875500	-2.48748800	2.29286300
H	6.56191800	0.65256600	1.54027100
H	5.75116400	-1.21756500	2.95726800

ent-**P1**$_{C2}$

C	1.47152000	2.47038500	-0.62309100
C	1.88450200	1.75665800	0.50868200
C	3.02413600	2.14245400	1.19549500
C	3.78435300	3.21295700	0.71460000
C	3.38520500	3.89000700	-0.43564400
C	2.21764500	3.53574500	-1.11534000
C	-0.36722000	1.17724300	-0.03524900
C	0.87505500	0.66017500	0.78557500
H	3.31795800	1.63862500	2.11247100
H	4.67923100	3.52131100	1.24398000
H	3.97859700	4.72192300	-0.80205200
H	1.89235800	4.08634600	-1.99227400
H	-0.35440400	2.68267800	-1.50888300
N	0.25440400	1.97300000	-1.11363100
C	-1.39069400	1.99131600	0.73447200
H	-1.85930200	1.39353100	1.51918700
H	-2.17665000	2.34093400	0.05624100
H	-0.90908300	2.86731100	1.17868100
C	0.59171700	0.41600100	2.26847400
H	1.46881800	-0.02507900	2.75051700
H	-0.24120100	-0.28400100	2.38649500
H	0.35035500	1.34934500	2.78417900
C	4.43381700	-3.35542500	0.16366100
C	3.32822600	-3.63269300	-0.59830900
C	2.22139500	-2.74378800	-0.63425700
C	2.26972000	-1.53742800	0.13377800
C	3.43038800	-1.28212100	0.91442500
C	4.47974800	-2.16543500	0.92953700
H	1.06337200	-3.95900400	-1.99607600
H	5.27348000	-4.04209100	0.18283800
H	3.28004300	-4.54313300	-1.18982600
C	1.07359900	-3.03902500	-1.41865600
C	1.15725200	-0.66182100	0.06445100
H	3.48356900	-0.37259500	1.49892700
H	5.35623900	-1.94906400	1.53206100
C	0.06507400	-1.00688600	-0.69575900
C	-0.00441800	-2.19140100	-1.45677500
H	-0.88381100	-2.40705300	-2.05449900
N	-0.96588100	-0.05717300	-0.56429000
N	-1.80576600	0.08912300	-1.64967400
C	-3.17043300	0.18401800	-1.53722100
O	-3.82332000	0.62027100	-2.47383100
H	-1.40822900	0.49120200	-2.49732900

C	-3.82277800	-0.25076500	-0.25966100
C	-3.37110200	-1.31040200	0.53317500
C	-4.98273200	0.43946700	0.09844100
C	-4.07346900	-1.65870400	1.68325100
H	-2.48329300	-1.86494900	0.25040300
C	-5.67056400	0.10175900	1.25892000
H	-5.33035100	1.24319100	-0.54229400
C	-5.21470800	-0.94792000	2.05313400
H	-3.72875500	-2.48748800	2.29286300
H	-6.56191800	0.65256600	1.54027100
H	-5.75116400	-1.21756500	2.95726800

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