Supplementary Materials

Monoalkylation of Aniline with Trichloroacetimidate Catalyzed by (±)-Camphorsulfonic acid through the S_N1 reaction via dual hydrogen-bonding activation modes

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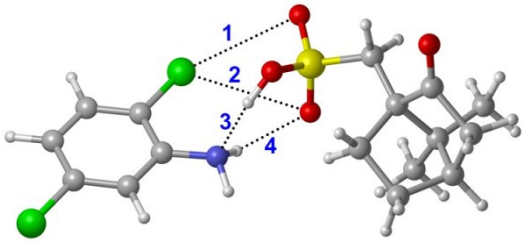
1. QTAIM Analyses

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



(a)

Figure S1 Intermolecular interactions in **COM1-1** 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 **COM1-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COM1-1(a)	1	lp…π	3.47	0.0055	0.0199	0.0040	-0.0030	0.0010
	2	lp…π	3.55	0.0055	0.0195	0.0040	-0.0031	0.0009
	3	O-H…N	1.72	0.0507	0.1019	0.0315	-0.0376	-0.0061
	4	N-H…O	2.16	0.0187	0.0625	0.0157	-0.0157	0.0000

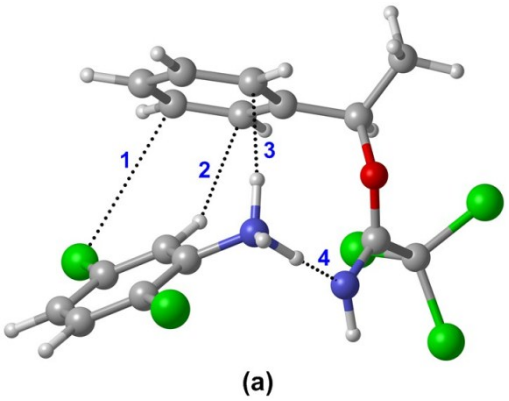


Figure S2 Intermolecular interactions in **COM1-2** and numbers of bond critical points (BCPs No.).

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 **COM1-2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COM1-2 (a)	1	lp…π	3.64	0.0046	0.0142	0.0028	-0.0020	0.0008
	2	C-H…π	2.70	0.0082	0.0252	0.0054	-0.0044	0.0010
	3	N-H…π	2.32	0.0140	0.0389	0.0092	-0.0086	0.0006
	4	N-H…N	1.51	0.0868	0.0701	0.0498	-0.0820	-0.0322

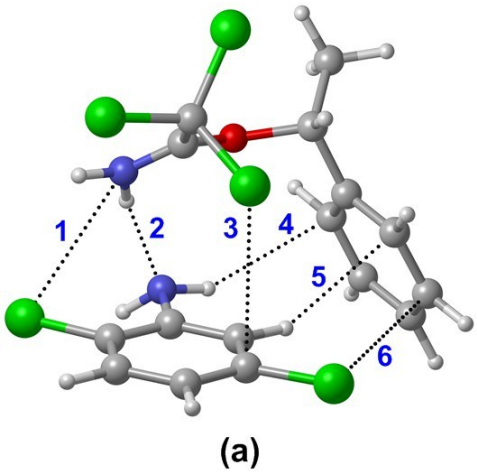


Figure S3 Intermolecular interactions in **COM1-3** and numbers of bond critical points (BCPs No.).

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 **COM1-3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COM1-3 (a)	1	lp…π	3.29	0.0076	0.0296	0.0060	-0.0046	0.0014
	2	N-H…N	1.93	0.0342	0.0806	0.0222	-0.0242	-0.0020
	3	lp…π	3.51	0.0058	0.0188	0.0037	-0.0028	0.0009
	4	N-H…π	2.71	0.0067	0.0218	0.0044	-0.0034	0.0010
	5	lp…π	3.55	0.0056	0.0172	0.0034	-0.0025	0.0009
	6	C-H…π	2.74	0.0079	0.0281	0.0058	-0.0045	0.0013

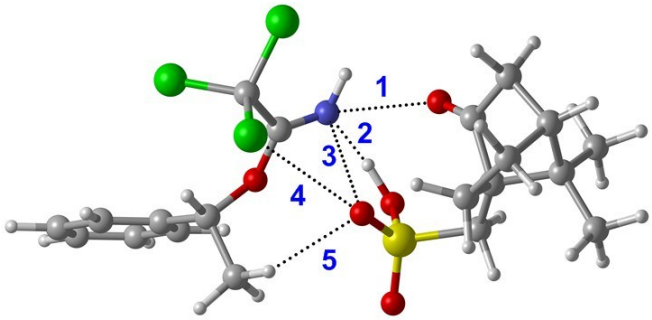


Figure S4 Intermolecular interactions in **COM2-1** and numbers of bond critical points (BCPs No.)

Table S4 Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **COM2-1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
COM2-1 (a)	1	lp…π	2.76	0.0136	0.0595	0.0127	-0.0106	0.0021
	2	O-H…N	1.55	0.0743	0.0943	0.0455	-0.0675	-0.0220
	3	π…π	3.00	0.0115	0.0397	0.0091	-0.0083	0.0008
	4	lp…lp	3.27	0.0068	0.0259	0.0055	-0.0045	0.0010
	5	C-H…O	2.42	0.0116	0.0387	0.0091	-0.0084	0.0007

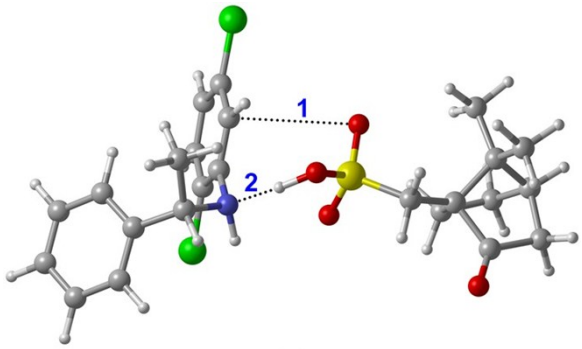


Figure S5 Intermolecular interactions in**IM2** and numbers of bond critical points (BCPs No.).

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 **IM2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IM2(a)	1	π…π	3.38	0.0054	0.0178	0.0037	-0.0029	0.0008
	2	O-H…N	1.54	0.0829	0.0795	0.0490	-0.0782	-0.0292

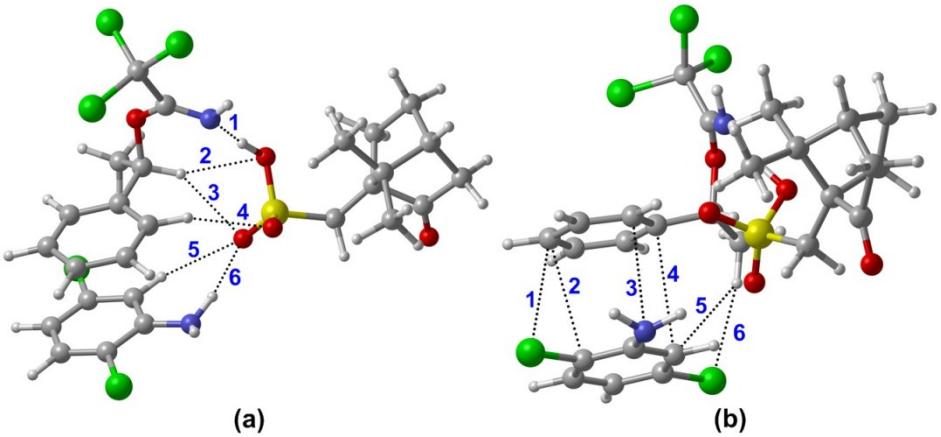


Figure S6 Intermolecular interactions in **IM-BI1** and numbers of bond critical points (BCPs No.).

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 **IM-BI1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IM-BI1 (a)	1	O-H…N	1.50	0.0855	0.0694	0.0509	-0.0845	-0.0336
	2	C-H…π	2.40	0.0122	0.0428	0.0099	-0.0090	0.0009
	3	C-H…π	2.60	0.0087	0.0292	0.0066	-0.0058	0.0008
	4	C-H…O	2.38	0.0123	0.0367	0.0091	-0.0090	0.0001
	5	C-H…O	2.68	0.0056	0.0221	0.0046	-0.0036	0.0010
	6	N-H…O	2.03	0.0211	0.0640	0.0167	-0.0174	-0.0007
IM-BI1 (b)	1	lp…π	3.50	0.0062	0.0204	0.0041	-0.0031	0.0010
	2	π…π	3.33	0.0068	0.0198	0.0042	-0.0034	0.0008
	3	π…π	3.31	0.0070	0.0200	0.0045	-0.0039	0.0006
	4	π…π	3.42	0.0063	0.0168	0.0035	-0.0028	0.0007
	5	C-H…π	2.95	0.0049	0.0168	0.0033	-0.0024	0.0009
	6	C-H…Cl	2.77	0.0085	0.0289	0.0059	-0.0046	0.0013

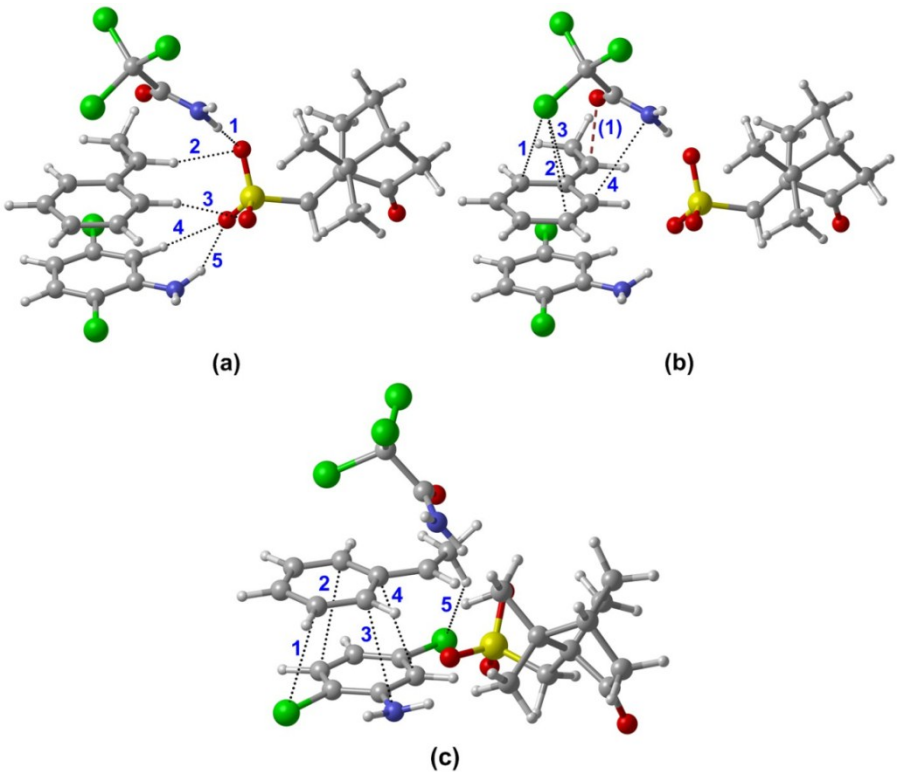


Figure S7 Intermolecular interactions in **TS-BI1** and numbers of bond critical points (BCPs No.).

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 **TS-BI1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TS-BI1 (a)	1	N-H…O	1.68	0.0463	0.1421	0.0366	-0.0376	-0.0010
	2	C-H…O	2.16	0.0189	0.0532	0.0142	-0.0151	-0.0009
	3	C-H…O	2.20	0.0175	0.0475	0.0127	-0.0136	-0.0009
	4	C-H…O	2.39	0.0108	0.0400	0.0090	-0.0080	0.0010
	5	N-H…O	1.95	0.0261	0.0796	0.0208	-0.0217	-0.0009
TS-BI1 (b)	(1)	C…O	2.31	0.0305	0.0939	0.0236	-0.0238	-0.0002
	1	lp…π	3.59	0.0056	0.0181	0.0037	-0.0028	0.0009
	2	lp…π	3.59	0.0057	0.0183	0.0037	-0.0028	0.0009
	3	lp…π	3.60	0.0056	0.0183	0.0037	-0.0028	0.0009
	4	π…π	3.29	0.0072	0.0217	0.0046	-0.0038	0.0008
TS-BI1 (c)	1	lp…π	3.44	0.0073	0.0231	0.0046	-0.0035	0.0011
	2	π…π	3.47	0.0060	0.0161	0.0034	-0.0027	0.0007
	3	π…π	3.24	0.0076	0.0224	0.0049	-0.0043	0.0006
	4	π…π	3.36	0.0076	0.0203	0.0042	-0.0034	0.0008
	5	C-H…Cl	2.66	0.0107	0.0373	0.0078	-0.0062	0.0016

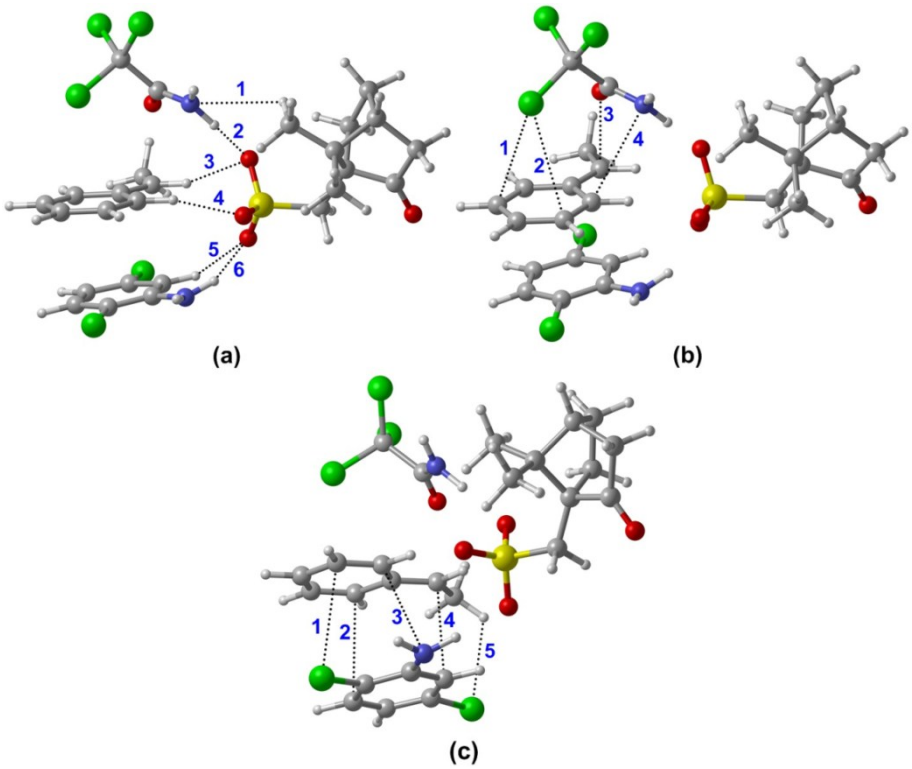


Figure S8 Intermolecular interactions in **IM-BI2** and numbers of bond critical points (BCPs No.)

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 **IM-BI2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IM-BI2 (a)	1	C-H…π	2.84	0.0061	0.0252	0.0049	-0.0035	0.0014
	2	N-H…O	1.71	0.0418	0.1336	0.0334	-0.0334	0.0000
	3	C-H…π	2.22	0.0168	0.0477	0.0126	-0.0132	-0.0006
	4	C-H…O	2.19	0.0180	0.0487	0.0131	-0.0140	-0.0009
	5	C-H…O	2.37	0.0113	0.0417	0.0094	-0.0084	0.0010
	6	N-H…O	1.94	0.0270	0.0828	0.0216	-0.0225	-0.0009
IM-BI2 (b)	1	lp…π	3.53	0.0060	0.0200	0.0040	-0.0030	0.0010
	2	lp…π	3.54	0.0062	0.0202	0.0041	-0.0031	0.0010
	3	lp…π	2.51	0.0199	0.0660	0.0158	-0.0150	0.0008
	4	π…π	3.31	0.0067	0.0201	0.0043	-0.0035	0.0008
IM-BI2 (c)	1	lp…π	3.47	0.0068	0.0211	0.0042	-0.0032	0.0010
	2	π…π	3.36	0.0065	0.0180	0.0037	-0.0030	0.0007
	3	lp…π	3.26	0.0073	0.0216	0.0047	-0.0041	0.0006
	4	π…π	3.08	0.0093	0.0245	0.0050	-0.0039	0.0011
	5	C-H…Cl	2.76	0.0094	0.0350	0.0069	-0.0051	0.0018

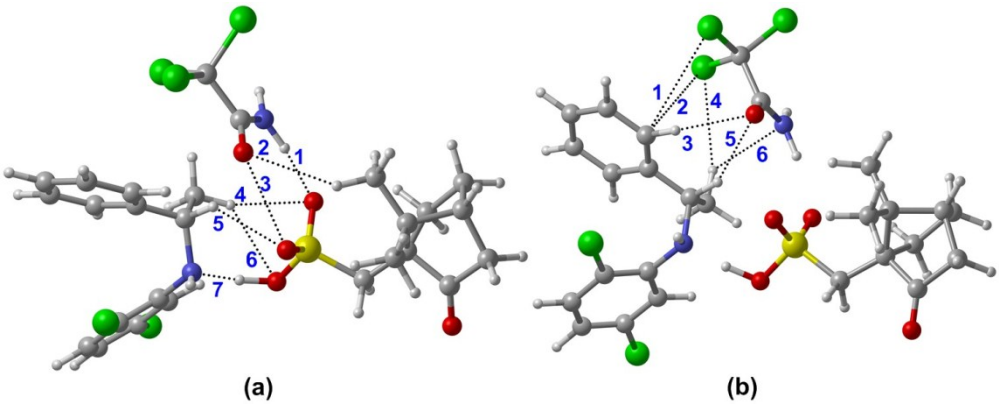


Figure S9 Intermolecular interactions in **IM-BI3** and numbers of bond critical points (BCPs No.).

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 **IM-BI3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IM-BI3 (a)	1	N-H…O	1.89	0.0273	0.0870	0.0218	-0.0219	-0.0001
	2	C-H…O	2.72	0.0057	0.0208	0.0044	-0.0035	0.0009
	3	lp…lp	3.13	0.0064	0.0247	0.0056	-0.0050	0.0006
	4	C-H…π	2.60	3.1275	0.0290	0.0064	-0.0056	0.0008
	5	C-H…O	2.45	0.0117	0.0389	0.0091	-0.0085	0.0006
	6	C-H…π	2.65	0.0080	0.0307	0.0065	-0.0054	0.0011
	7	O-H…N	1.43	0.1104	-0.0275	0.0586	-0.1242	-0.0656
IM-BI3 (b)	1	lp…π	3.65	0.0047	0.0161	0.0031	-0.0022	0.0009
	2	lp…π	3.66	0.0049	0.0144	0.0029	-0.0022	0.0007
	3	C-H…π	2.37	0.0117	0.0394	0.0092	-0.0086	0.0006
	4	C-H…Cl	3.13	0.0044	0.0144	0.0027	-0.0019	0.0008
	5	C-H…π	2.49	0.0095	0.0325	0.0074	-0.0067	0.0007
	6	C-H…π	2.88	0.0063	0.0201	0.0043	-0.0035	0.0008

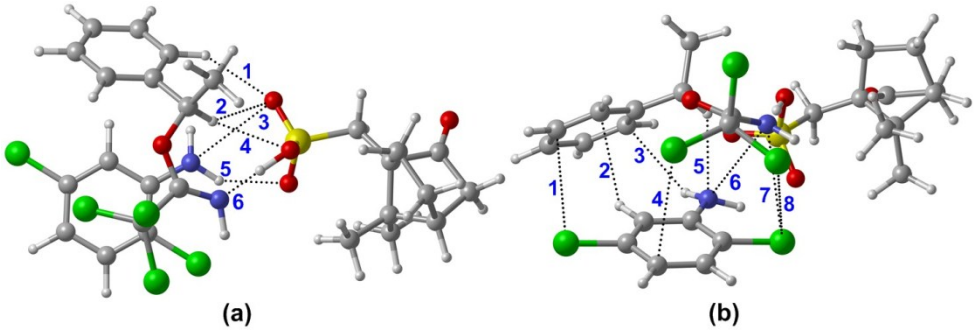


Figure S10 Intermolecular interactions in **IM-BII1** and numbers of bond critical points (BCPs No.).

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 **IM-BII1**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$	G	V	H
IM-BII1 (a)	1	C-H…O	2.41	0.0100	0.0343	0.0079	-0.0073	0.0006
	2	C-H…π	2.51	0.0101	0.0330	0.0077	-0.0072	0.0005
	3	lp…π	3.07	0.0084	0.0300	0.0067	-0.0060	0.0007
	4	C-H…π	2.42	0.0125	0.0491	0.0109	-0.0094	0.0015
	5	N-H…O	2.09	0.0199	0.0628	0.0162	-0.0167	-0.0005
	6	O-H…N	1.49	0.0876	0.0619	0.0516	-0.0878	-0.0362
IM-BII1 (b)	1	lp…π	3.78	0.0036	0.0109	0.0021	-0.0016	0.0005
	2	C-H…π	2.81	0.0077	0.0267	0.0053	-0.0039	0.0014
	3	N-H…π	2.64	0.0078	0.0276	0.0056	-0.0043	0.0013
	4	lp…π	3.39	0.0078	0.0255	0.0052	-0.0040	0.0012
	5	C-H…N	2.47	0.0131	0.0387	0.0091	-0.0085	0.0006
	6	lp…π	3.23	0.0082	0.0227	0.0055	-0.0053	0.0002
	7	lp…π	3.38	0.0072	0.0253	0.0052	-0.0040	0.0012
	8	lp…lp	3.63	0.0062	0.0213	0.0042	-0.0030	0.0012

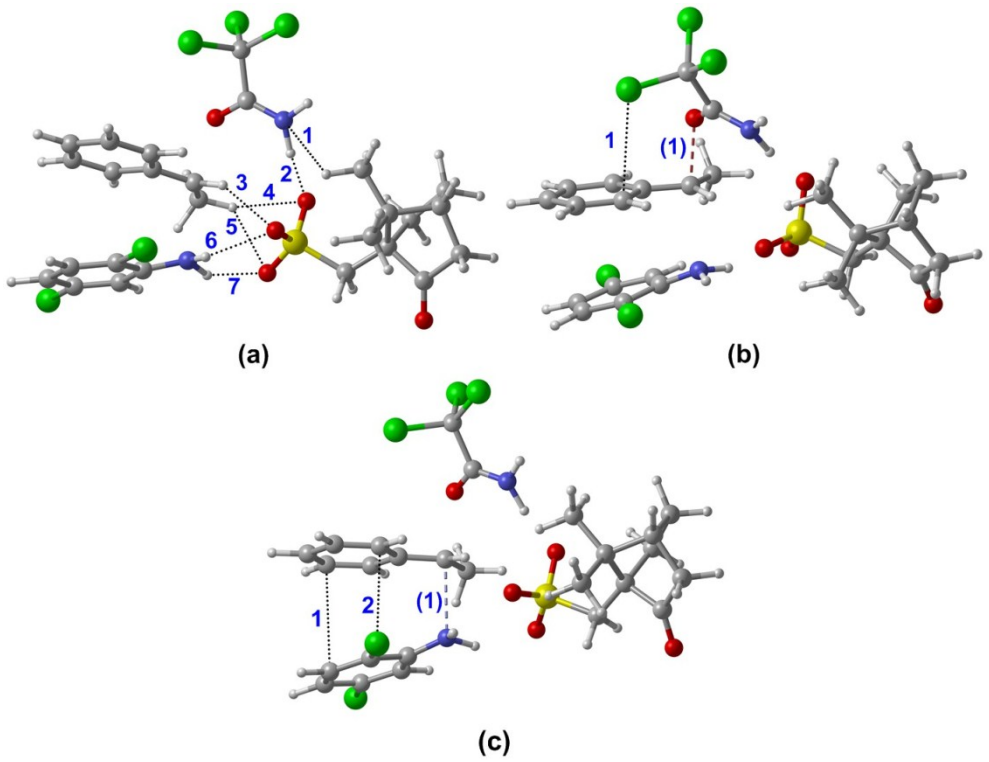


Figure S11 Intermolecular interactions in **TS-BII1** and numbers of bond critical points (BCPs No.).

Table S11 Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms (*d*, in Å), classifications of the intermolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.),the electronic kinetic energy density (*G*, in a.u.), the electronic potential energy density (*V*, in a.u.) and the electronic energy density (*H*, in a.u.) at the BCPs of **TS-BII1**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
TS-BII1 (a)	1	C-H…π	2.73	0.0074	0.0291	0.0058	-0.0043	0.0015
	2	N-H…O	1.64	0.0514	0.1469	0.0395	-0.0424	-0.0029
	3	C-H…O	2.32	0.0145	0.0418	0.0107	-0.0109	-0.0002
	4	C-H…O	2.57	0.0087	0.0309	0.0068	-0.0060	0.0008
	5	C-H…O	2.57	0.0095	0.0342	0.0075	-0.0064	0.0011
	6	N-H…O	2.22	0.0167	0.0586	0.0142	-0.0138	0.0004
	7	N-H…O	1.94	0.0273	0.0857	0.0222	-0.0230	-0.0008
TS-BII1 (b)	(1)	C…O	2.11	0.0471	0.1261	0.0352	-0.0388	-0.0036
	1	lp…π	3.54	0.0053	0.0163	0.0032	-0.0023	0.0009
TS-BII1 (c)	(1)	C…N	2.55	0.0249	0.0646	0.0158	-0.0156	0.0002
	1	π…π	3.68	0.0042	0.0120	0.0025	-0.0020	0.0005
	2	lp…π	3.36	0.0076	0.0250	0.0050	-0.0039	0.0011

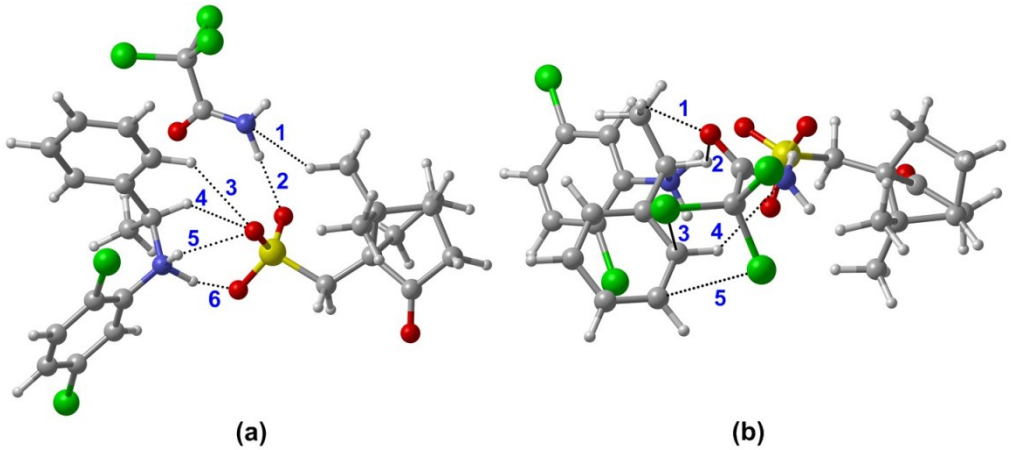
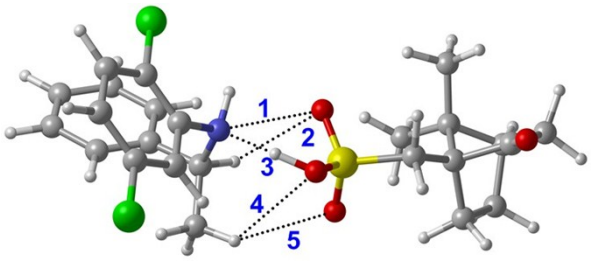


Figure S12 Intermolecular interactions in **IM-BII2** and numbers of bond critical points (BCPs No.).

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 **IM-BII2**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IM-BII2 (a)	1	C-H…π	2.82	0.0056	0.0217	0.0043	-0.0031	0.0012
	2	N-H…O	1.86	0.0299	0.0941	0.0236	-0.0238	-0.0002
	3	C-H…O	2.62	0.0072	0.0257	0.0056	-0.0047	0.0009
	4	C-H…π	2.52	0.0115	0.0413	0.0092	-0.0082	0.0010
	5	N-H…O	2.24	0.0175	0.0646	0.0152	-0.0144	0.0008
	6	N-H…O	1.47	0.0859	0.1419	0.0627	-0.0898	-0.0271
IM-BII2 (b)	1	C-H…O	2.37	0.0114	0.0438	0.0097	-0.0084	0.0013
	2	C-H…π	2.44	0.0120	0.0459	0.0102	-0.0088	0.0014
	3	lp…π	3.63	0.0054	0.0171	0.0035	-0.0027	0.0008
	4	C-H…π	2.89	0.0062	0.0201	0.0042	-0.0033	0.0009
	5	lp…π	3.55	0.0056	0.0177	0.0035	-0.0026	0.0009



(a)

Figure S13 Intermolecular interactions in **IM-BII3** 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 **IM-BII3**.

	BCPs No.	Classification	*d*	ρ	$\nabla^2\rho$	*G*	*V*	*H*
IM-BII3 (a)	1	lp…π	2.96	0.0111	0.0422	0.0097	-0.0088	0.0009
	2	C-H…π	2.52	0.0106	0.0374	0.0084	-0.0074	0.0010
	3	O-H…N	1.53	0.0841	0.0741	0.0492	-0.0798	-0.0306
	4	C-H…O	2.70	0.0071	0.0287	0.0059	-0.0046	0.0013
	5	C-H…O	2.91	0.0048	0.0185	0.0037	-0.0028	0.0009

2. Cartesian Coordinates

R1

C	0.64651600	0.92912700	-0.00841900
C	-0.75222500	1.02592700	-0.00622100
C	-1.53238800	-0.11929100	-0.00086900
C	-0.97376900	-1.39226500	0.00330800
C	0.41214100	-1.49713400	0.00220400
C	1.20501100	-0.35946400	-0.00363500
H	-1.22361500	2.00292400	-0.01584300
H	-1.60374900	-2.27263600	0.00786000
H	0.89009600	-2.47044700	0.00808700
N	1.43330300	2.06026200	-0.06702500
H	0.99956300	2.91504600	0.24549500
H	2.39085000	1.95134500	0.23234700
Cl	2.94442200	-0.52569300	0.00126000
Cl	-3.26900900	0.05101900	0.00303600

R2

C	2.96062400	-1.03738500	0.67749900
C	2.21826600	0.03716600	0.18971500
C	2.81255800	0.93543400	-0.69658000
C	4.13491900	0.75639400	-1.09025000
C	4.87523700	-0.31459600	-0.59659600
C	4.28548400	-1.21203200	0.28931700
H	2.49778100	-1.74367800	1.36276000
H	2.22935500	1.76330500	-1.08630500
H	4.58755300	1.45518300	-1.78652000
H	5.90638700	-0.45270800	-0.90518700
H	4.85358400	-2.05376100	0.67224300
C	0.81009400	0.25021300	0.68901300
C	0.77413100	1.15218900	1.91622700
H	0.36488900	-0.72440800	0.91546700
H	-0.25278100	1.32688500	2.25052400
H	1.33024200	0.68559400	2.73285700
H	1.24507100	2.11052000	1.68009200
O	0.07031500	0.87449100	-0.38621000
C	-1.26282100	1.06468400	-0.26779400
C	-2.13851300	-0.20743100	-0.17841300
Cl	-1.39127900	-1.53630200	-1.09606200
Cl	-2.27040000	-0.67977300	1.55036000
Cl	-3.76380900	0.09062900	-0.80508300
N	-1.82835000	2.18655800	-0.29319400
H	-1.11273300	2.91601700	-0.32338000

CSA

C	2.64162400	0.03681200	0.53721300
C	2.27559200	1.52916500	0.44000100
C	0.44582200	-0.02262900	-0.05080600
C	0.45748100	-0.48555400	1.43640500
C	1.96522300	-0.50260100	1.81034100
H	2.35121600	2.05829600	1.39450900
H	2.86371500	2.08704600	-0.29355400
H	3.71310000	-0.16874900	0.46847900
H	-0.13139200	0.19304000	2.05836000
H	-0.00317200	-1.47290500	1.52340500
H	2.18354400	0.12507400	2.67767000
H	2.30551700	-1.51295200	2.04821200
C	-0.80048900	-0.28975400	-0.87375000
H	-0.89697500	0.45694000	-1.66651700
H	-0.82217100	-1.29709900	-1.29943300
S	-2.29660500	-0.17216500	0.10834200
O	-2.53542900	-1.45244800	0.73657800
O	-2.30358400	1.05575100	0.88056800
O	-3.40605400	0.00311000	-1.05970900
H	-3.72043900	0.92035500	-1.01720600
O	0.14297800	2.37197400	-0.43495800
C	0.82187500	1.46098600	-0.03657000
C	1.78848700	-0.61125700	-0.59492000
C	2.13829900	-0.11640600	-2.00239900
H	3.15676600	-0.41912200	-2.26543500
H	1.46308600	-0.56285800	-2.74025200
H	2.07024000	0.96879300	-2.11473300
C	1.83956100	-2.13919500	-0.60250400
H	2.86788300	-2.47177600	-0.78016400
H	1.49613300	-2.59149400	0.32892800
H	1.22450400	-2.54245100	-1.41364400

CSA⁻

C	-2.47527000	-0.61525200	-0.46955100
C	-2.86385100	0.82140100	-0.09911300
C	-0.45048700	0.32470100	0.04680300
C	-0.41982100	0.14587600	-1.50616200
C	-1.77789600	-0.53335600	-1.83957700
H	-3.34175600	1.37781800	-0.91149600
H	-3.51344200	0.89014500	0.77898000
H	-3.29713800	-1.33703700	-0.41395200
H	-0.27087800	1.10363200	-2.01025100
H	0.43359800	-0.48021600	-1.76730900
H	-2.37564000	0.04290100	-2.55388800
H	-1.62763100	-1.52664000	-2.27040700
C	0.85792200	0.64165200	0.75244400
H	0.97414500	1.72662000	0.83014500
H	0.85612100	0.23419400	1.76858900
S	2.38674800	0.04228500	-0.02573700
O	2.15887300	-1.40593000	-0.25157700
O	2.49854600	0.82159600	-1.27618300
O	3.41537800	0.34625100	0.98519500
O	-1.30579500	2.57126600	0.58389800
C	-1.49335100	1.42974200	0.23782700
C	-1.29175900	-0.91394800	0.49624500
C	-1.68819700	-0.85800500	1.97657500
H	-2.47231900	-1.59500700	2.18716400
H	-0.82653800	-1.10484800	2.60380900
H	-2.05043500	0.12406900	2.29603100
C	-0.63513900	-2.26894400	0.23784800
H	-1.36553700	-3.06636500	0.43112200
H	-0.25067500	-2.37221400	-0.77644400
H	0.23124000	-2.40228500	0.88899400

$H_2NCOCCl_3$

C	1.25669600	-0.52462700	-0.08939600
N	2.19335200	0.44678900	-0.07916800
H	1.96372100	1.42692200	-0.08872500
O	1.47784000	-1.70813200	-0.11896400
C	-0.21427400	0.01528600	-0.00404300
Cl	-0.46424800	1.31817600	-1.20506000
Cl	-1.35017600	-1.29188800	-0.29905200
Cl	-0.45341200	0.68006800	1.63640700
H	3.15878300	0.15859700	-0.09376900

P

C	3.21791100	0.63778800	-0.38951300
C	1.94393500	0.96672700	0.07470200
C	1.51929400	0.44459000	1.29852500
C	2.34397600	-0.40544800	2.02967000
C	3.60935900	-0.73339900	1.55284200
C	4.04813100	-0.20482300	0.34157700
H	3.55298600	1.03454600	-1.34439900
H	0.52955000	0.68210300	1.67897200
H	1.99542600	-0.81160800	2.97395700
H	4.25227300	-1.39520100	2.12437100
H	5.03520600	-0.45251900	-0.03592600
C	1.04162300	1.84465900	-0.76844200
H	1.67859500	2.35249200	-1.50136800
C	-0.47544200	-1.17539100	-0.67282400
C	-0.78624100	0.17549700	-0.89800900
C	-2.02845100	0.64046400	-0.45033500
C	-2.90991700	-0.20333500	0.21200200
C	-2.58006900	-1.52879500	0.46191300
C	-1.35574300	-2.00761300	0.01112100
H	-2.30118300	1.67690000	-0.62314700
H	-3.27230300	-2.17677300	0.98655500
H	-1.08166200	-3.04395300	0.17243600
N	0.11277000	1.02518000	-1.59515700
H	-0.42565500	1.66368600	-2.17463500
C	0.32445200	2.91566300	0.05831700
H	1.04927900	3.52253900	0.60719600
H	-0.25408700	3.57815900	-0.59437200
H	-0.36416800	2.47360600	0.78317800
Cl	0.99751700	-1.85958300	-1.28016600
Cl	-4.44813900	0.41959900	0.74746000

COM1-1

C	3.15362900	-1.21596100	-1.28241100
C	1.82557100	-1.64926000	-1.27974200
C	1.45202100	-2.69777500	-0.43314900
C	2.39550800	-3.29679300	0.39464700
C	3.71825700	-2.85851100	0.38527900
C	4.09805500	-1.81771600	-0.45665400
H	3.44244400	-0.38876200	-1.92645800
H	0.41662200	-3.02036100	-0.39144500
H	2.09563700	-4.10410300	1.05474200
H	4.44963000	-3.32434400	1.03773200
H	5.12528100	-1.46858300	-0.46476500
C	0.82076700	-0.92542900	-2.11288000
C	-0.27469000	-1.74130700	-2.75941300
H	1.31298800	-0.25193600	-2.81929400
H	-0.93832600	-1.10094800	-3.34602600
H	0.16795100	-2.48442000	-3.42851700
H	-0.87732000	-2.25775900	-2.00852500
O	-1.35310200	-1.49840000	0.45821800
C	-2.59078000	-1.31809600	0.91036700
C	-3.29319800	-0.03608600	0.41863400
Cl	-2.32200200	1.37799200	0.93580000
Cl	-3.34763800	-0.08020400	-1.37836900
Cl	-4.93090200	0.12365400	1.03739600
N	-3.21874000	-2.09472900	1.67947100
H	-2.61418200	-2.88540900	1.91045300
C	0.88507300	0.98310700	-0.32441300
C	1.32386200	0.53462800	0.92450900
C	2.25004300	1.27778400	1.64076800
C	2.74420000	2.48381800	1.15322400
C	2.30317900	2.94303100	-0.08185400
C	1.39170400	2.19244700	-0.81428600
H	0.93090400	-0.39816900	1.31625200
H	3.46037900	3.05451900	1.73239600
H	2.66976400	3.88037600	-0.48430200
N	-0.02591100	0.17298600	-1.04558500
H	-0.93894300	-0.75978200	-0.12936500
H	-0.56774000	0.75058600	-1.68948900
Cl	0.87206700	2.77244400	-2.37744300
Cl	2.79806700	0.69147900	3.18484600

pR1

C	-0.60443500	0.84017100	0.00003400
C	0.77065500	1.01670900	0.00002800
C	1.57784700	-0.11697600	-0.00008200
C	1.00816400	-1.39111500	-0.00015100
C	-0.37217600	-1.54099200	-0.00018000
C	-1.19560600	-0.41888200	-0.00019100
H	1.21888700	2.00591900	0.00020200
H	1.65051800	-2.26449500	-0.00011200
H	-0.82004900	-2.52838000	-0.00010600
N	-1.47240000	2.03816700	-0.00013600
H	-1.31930800	2.61727900	-0.83465900
H	-2.46166900	1.74537300	0.00471700
Cl	-2.92146000	-0.58515100	0.00017300
Cl	3.28876100	0.06757400	0.00010600
H	-1.31238600	2.62245000	0.82942200

COM1-2

C	2.06336700	0.04234400	0.54290200
C	2.31588200	-0.89070500	-0.45389600
C	3.51859600	-1.58963800	-0.49918700
C	4.48814000	-1.34738500	0.46865400
C	4.25363500	-0.41233200	1.46893400
C	3.04377100	0.27745200	1.49914500
H	1.12050200	0.58267300	0.56894600
H	5.42443000	-1.89245400	0.43184700
H	5.00610800	-0.21819600	2.22463900
N	1.27052500	-1.13199000	-1.43668800
H	1.00362400	-0.24770600	-1.88805500
H	1.58196700	-1.79613000	-2.15095100
H	0.34099600	-1.51212400	-0.91600600
C	-0.52734800	2.67843600	0.14979200
C	-0.75801800	1.98702900	-1.03864300
C	0.25309800	1.93953000	-2.00886700
C	1.48312100	2.54858500	-1.77598200
C	1.70818200	3.23091100	-0.57843000
C	0.69941400	3.30611700	0.37584600
H	-1.31229900	2.73944800	0.89854200
H	0.06077800	1.45714400	-2.96632800
H	2.25800900	2.51476200	-2.53562500
H	2.66379400	3.71211800	-0.39930700
H	0.86525900	3.84698200	1.30124200
C	-2.08051400	1.29611600	-1.27600600
H	-2.75394800	1.50082700	-0.44220200
C	-2.75338400	1.63917300	-2.58822800
H	-2.12769100	1.35237300	-3.43609800
H	-3.70953900	1.12021400	-2.67165400
H	-2.92633500	2.71620300	-2.63417500
O	-1.80201500	-0.15298900	-1.32950900
C	-1.86850500	-0.96798300	-0.28830500
C	-3.12104000	-0.92986600	0.62711100
N	-0.90509800	-1.77628000	-0.10459900
H	-1.05294100	-2.46678500	0.62736200
Cl	-3.39382900	-2.52078000	1.36373600
Cl	-2.77525000	0.25537500	1.91936000
Cl	-4.55983300	-0.46878800	-0.28720400
Cl	3.80947000	-2.75292000	-1.75522000
Cl	2.74914900	1.44745200	2.73955500

COM1-3

C	1.01896900	-1.79345100	0.03279500
C	0.09362100	-2.05585100	-0.97891200
C	-1.08435300	-2.73639400	-0.64633200
C	-1.32775300	-3.17300500	0.64857100
C	-0.40767600	-2.90516800	1.65550600
C	0.75292600	-2.21134500	1.33209100
H	1.94780200	-1.28132100	-0.19833000
H	-2.24109100	-3.71542500	0.86589100
H	-0.58632100	-3.23145300	2.67298100
N	0.27301500	-1.54144100	-2.28488900
H	1.21611500	-1.18715400	-2.41787900
H	0.05534400	-2.22474500	-3.00616500
H	-1.17170000	-0.26805700	-2.19444900
C	2.79139400	1.16474800	0.70408300
C	2.15764400	1.48205900	-0.49431300
C	2.66616500	0.99171500	-1.70321500
C	3.79600300	0.18083900	-1.70451300
C	4.43366000	-0.13003800	-0.50068800
C	3.93553600	0.36590700	0.69959000
H	2.39567200	1.53784800	1.64524000
H	2.17748400	1.24671600	-2.64073700
H	4.19406600	-0.19349100	-2.64221300
H	5.32054100	-0.75438000	-0.50311000
H	4.42653400	0.12404200	1.63577800
C	0.94692300	2.37373600	-0.48858700
H	0.61966800	2.56369800	0.53250700
C	1.10168600	3.65987500	-1.27055800
H	1.37165000	3.45130700	-2.30775200
H	0.18342200	4.24925000	-1.24862100
H	1.90742600	4.24099500	-0.81673200
O	-0.12048100	1.59450100	-1.19655700
C	-1.23367000	1.12134800	-0.77127200
C	-1.88414100	1.56835800	0.55278000
N	-1.78949300	0.20983000	-1.50448600
H	-2.68880200	-0.19406200	-1.26782500
Cl	-3.54077100	0.95774600	0.69353900
Cl	-0.87807600	0.85224700	1.83302200
Cl	-1.91002700	3.33378900	0.63182400
Cl	-2.27395000	-3.02488100	-1.89215200
Cl	1.89163500	-1.83763600	2.59184600

COM2-1

C	3.49413200	0.00337200	1.55570400
C	3.61172800	-0.54380000	0.09887600
C	5.30660400	0.97013600	0.28633000
C	4.69819500	0.97310000	1.69908900
H	2.52910000	0.48426900	1.71341700
H	3.54816300	-0.83117000	2.26159300
H	4.38681300	1.97647300	2.00052400
H	5.41573900	0.62005700	2.44345700
C	5.16024100	-0.51952200	-0.14030100
C	3.20762500	0.62648800	-0.78784600
C	4.30173300	1.68678400	-0.63240600
H	4.70180600	1.93460200	-1.61942500
H	3.89050600	2.60540700	-0.20291200
H	6.32653300	1.35936100	0.22673300
C	5.93913700	-1.49145800	0.74672100
H	5.64406000	-1.45436300	1.79672000
H	5.80445100	-2.52047400	0.39885800
H	7.00945100	-1.26554700	0.69071800
C	5.55604600	-0.78314800	-1.59731100
H	6.61241000	-0.53839100	-1.74794800
H	5.42790200	-1.84147400	-1.84502000
H	4.97105500	-0.20804900	-2.32020500
C	2.92644500	-1.86233000	-0.19118200
H	3.09780400	-2.19435200	-1.21915200
H	3.28452400	-2.63590900	0.49415500
S	1.12854400	-1.89116500	0.02662500
O	0.80109600	-3.20075700	0.56076700
O	0.72119800	-0.70410100	0.77719500
O	0.57980300	-1.80838100	-1.43980500
H	0.16224900	-0.87607000	-1.63750800
O	2.24729900	0.68778400	-1.51696700
C	-5.40975000	-0.37415400	0.92274200
C	-4.28403500	-0.88329100	0.27870600
C	-4.44249700	-1.75758800	-0.79773600
C	-5.71734100	-2.11505500	-1.22261500
C	-6.84125800	-1.60867500	-0.57258400
C	-6.68632200	-0.73825700	0.50176500
H	-5.28667900	0.31473100	1.75534400
H	-3.56245400	-2.14320500	-1.30410800
H	-5.83465500	-2.79221300	-2.06262900
H	-7.83501900	-1.89008200	-0.90576600
H	-7.55790000	-0.33526800	1.00761500
C	-2.90536700	-0.53183100	0.78446600

H	-2.96725400	0.37969600	1.37774000
C	-2.26956500	-1.64077900	1.60689800
H	-2.13819400	-2.53474600	0.99129400
H	-1.28908700	-1.32818400	1.97120700
H	-2.92357000	-1.88475800	2.44810200
O	-2.05618800	-0.33931400	-0.37640300
C	-1.33321600	0.70391000	-0.74390800
C	-1.54966800	2.06657800	-0.03799800
N	-0.49966800	0.52311400	-1.67847100
H	0.06444000	1.32639900	-1.93117800
Cl	-0.61727400	3.35707300	-0.83537200
Cl	-3.27573000	2.50316400	-0.10832300
Cl	-0.98723600	1.94596200	1.64716000

pR2

C	2.42537700	-0.78820300	0.99881800
C	2.04717600	0.31085000	0.22784100
C	2.84427700	0.71862500	-0.84553700
C	4.00690700	0.02117500	-1.14825900
C	4.38636000	-1.07358900	-0.37172000
C	3.59997800	-1.47486000	0.70371600
H	1.81002200	-1.09995200	1.83902500
H	2.55492300	1.57645000	-1.44685900
H	4.62263500	0.33423100	-1.98438300
H	5.29841400	-1.61173300	-0.60631000
H	3.89685900	-2.32310900	1.31051800
C	0.81078200	1.07315900	0.59826000
C	1.01275800	2.52467200	0.96485400
H	0.24269300	0.54601500	1.36263200
H	0.06090000	3.01285400	1.18507800
H	1.64279200	2.56024600	1.85648800
H	1.52462200	3.06129400	0.16373100
O	-0.04860600	1.12447300	-0.66142700
C	-1.12673800	0.52618700	-0.96734000
C	-1.96214500	-0.29217100	0.04278200
Cl	-0.97061800	-1.67421000	0.52953400
Cl	-2.34876300	0.77679100	1.40140200
Cl	-3.47038600	-0.87524000	-0.68462500
N	-1.53445700	0.63318200	-2.20291500
H	-0.96360900	1.15818400	-2.85753500
H	-2.40255900	0.21761100	-2.51835600

TS-AI (S_N1)

Value of imaginary frequency = -180.4 cm^{-1}

C	-2.43534300	-0.91470700	-0.87830000
C	-2.27908900	0.35981600	-0.29183200
C	-3.26332000	0.84692300	0.59529500
C	-4.37727100	0.07804100	0.87567300
C	-4.52413300	-1.17772800	0.27579700
C	-3.55886600	-1.67500000	-0.60181200
H	-1.67749900	-1.28274700	-1.56367900
H	-3.14691000	1.81842000	1.06282800
H	-5.13626900	0.44585200	1.55650700
H	-5.40335400	-1.77433100	0.49768300
H	-3.68911100	-2.64758900	-1.06217400
C	-1.13877700	1.13673700	-0.65177900
H	-0.46619500	0.68382300	-1.37753400
C	-1.04631000	2.60421700	-0.50140500
H	-1.46106600	2.96084300	0.44076000
H	-0.01882600	2.94710300	-0.61106200
H	-1.64051200	3.03437600	-1.32032700
O	0.11049400	0.74016200	0.95005400
C	1.19802200	0.19164000	1.14869100
C	2.09942600	-0.20943600	-0.05490400
N	1.63239900	-0.10227700	2.36430700
H	2.53360100	-0.52334900	2.53697000
Cl	3.70455400	-0.77827100	0.42719400
Cl	1.24141900	-1.51630000	-0.90747300
Cl	2.27243300	1.20954200	-1.10497900
H	1.03646000	0.13471000	3.14630200

IM-AI

C	0.50921800	-1.31190900	0.00007600
C	-0.44823900	-0.24849600	0.00012800
C	0.00822300	1.10703800	0.00012200
C	1.35726800	1.37200300	-0.00003300
C	2.27402600	0.30626100	-0.00010000
C	1.85737600	-1.03207800	0.00000400
H	0.15642100	-2.33951400	0.00009700
H	-0.70505800	1.92352600	0.00026700
H	1.71794100	2.39390100	-0.00009200
H	3.33752100	0.52774700	-0.00024100
H	2.58924400	-1.83133300	0.00000200
C	-1.79402800	-0.58451600	-0.00011700
H	-2.02365100	-1.65155200	-0.00020700
C	-2.95932000	0.30686800	-0.00007400
H	-2.73247400	1.36998000	-0.00007900
H	-3.58377300	0.05810900	-0.86946900
H	-3.58331300	0.05811100	0.86968900

IM-AII

C	0.17470100	1.15080600	-1.29201400
C	0.52362500	1.09371400	0.06251000
C	1.48137300	1.97606700	0.55837700
C	2.08255900	2.90542300	-0.28959600
C	1.72146500	2.96572300	-1.63044800
C	0.76262500	2.08530600	-2.13295400
H	-0.55820400	0.45926600	-1.70377900
H	1.77696600	1.94468700	1.60190400
H	2.83088100	3.58331900	0.10682900
H	2.18342900	3.69574700	-2.28663000
H	0.47811700	2.12643600	-3.17900100
C	-0.12292100	0.05809300	0.94672700
H	0.05181400	-0.95652400	0.57747100
O	-1.60639700	0.29611100	0.87330400
C	-2.41204400	-0.40570100	0.18996200
C	-3.86218800	0.12716600	0.20259600
N	-2.10670900	-1.43710600	-0.54638100
H	-2.84693900	-1.93558200	-1.02902600
Cl	-5.00711600	-1.14620700	-0.26268500
Cl	-4.26225900	0.74319700	1.79884000
Cl	-3.85397200	1.42549000	-1.00968900
H	-1.14568900	-1.75177000	-0.68893600
C	2.19535000	-1.65133400	-0.89799200
C	2.41877100	-1.90169000	0.46059500
C	3.39500300	-1.13110900	1.10455800
C	4.09926900	-0.16549500	0.39825400
C	3.88751700	0.04980200	-0.96103600
C	2.92416900	-0.70930100	-1.60995300
H	3.60466600	-1.29294100	2.15760600
H	4.45358800	0.80447500	-1.49278200
H	2.71909400	-0.55766900	-2.66373300
N	1.61351100	-2.79483000	1.17132300
H	1.36868200	-3.62773800	0.64784800
H	1.99868500	-3.04701000	2.07328100
C	0.19784000	0.10310500	2.42150700
H	-0.04569900	1.07895300	2.84599800
H	-0.35532900	-0.67413300	2.95067100
H	1.26603500	-0.08759700	2.54734500
Cl	0.91037600	-2.53172400	-1.71265200
Cl	5.25537000	0.81449700	1.24426500

TS-AII (S_N2)

Value of imaginary frequency = -231.5 cm^{-1}

C	0.56244900	-2.07995000	-0.40711100
C	0.22370200	-0.78592400	0.03952600
C	0.38989100	0.31772000	-0.81946200
C	0.89139300	0.12625600	-2.09834000
C	1.21118800	-1.16160700	-2.53246000
C	1.04527200	-2.26747800	-1.69237200
H	0.45610800	-2.92312500	0.27144000
H	0.14304800	1.31866400	-0.47982000
H	1.03859800	0.97539700	-2.75654100
H	1.60259500	-1.30625200	-3.53468700
H	1.31984400	-3.25944200	-2.03373900
C	-0.28950000	-0.63056700	1.36775500
H	-0.24371300	-1.50382300	2.00877400
O	-2.29970000	-1.01559900	1.13245900
C	-2.90576400	-0.85098700	0.07017800
C	-4.01673300	0.23814400	0.00748500
N	-2.62766700	-1.47223400	-1.06676600
H	-3.17048500	-1.31627800	-1.90490400
Cl	-5.30515700	-0.20145900	-1.12896400
Cl	-4.67649500	0.51831100	1.60725800
Cl	-3.16642700	1.70237900	-0.58247900
H	-1.86677700	-2.13820300	-1.08950000
C	3.61940000	-0.88667300	0.30840700
C	3.03404400	-0.06886800	1.28662100
C	2.99312800	1.31020300	1.05023000
C	3.50290700	1.83241400	-0.13283800
C	4.07941700	1.01653900	-1.09927900
C	4.13989400	-0.35270100	-0.86171200
H	2.58749300	1.98227200	1.80088000
H	4.48672200	1.44404000	-2.00749200
H	4.60192100	-1.01676500	-1.58441400
N	2.41923900	-0.61520700	2.41666000
H	2.78801000	-1.52586200	2.66989100
H	2.43703100	0.00468700	3.21887600
C	-0.52058900	0.68418800	2.01362100
H	-1.09955300	1.35139200	1.37229600
H	-1.02841800	0.56910200	2.96944900
H	0.46014900	1.14680300	2.17331300
Cl	3.72501900	-2.60568100	0.59195600
Cl	3.39855500	3.54468500	-0.40566900

IM1

C	3.21687900	0.66653100	-0.33991900
C	1.93464800	1.00648800	0.09793600
C	1.46937700	0.51707800	1.32237100
C	2.27708400	-0.31624800	2.08866600
C	3.55163200	-0.65859400	1.64253200
C	4.02502800	-0.16300300	0.43015100
H	3.59080700	1.05926200	-1.28300000
H	0.47738500	0.77524900	1.68263900
H	1.91350600	-0.69286700	3.03848000
H	4.18042300	-1.30411700	2.24628200
H	5.02250600	-0.41622600	0.08831000
C	1.06709300	1.85839300	-0.78610200
H	1.68338200	2.32984000	-1.55812600
C	-0.47941900	-1.26419200	-0.65444000
C	-0.79881900	0.06990000	-0.90638500
C	-2.00333100	0.61656400	-0.48108600
C	-2.88577500	-0.18185900	0.23892500
C	-2.57101800	-1.51048400	0.51927400
C	-1.37466900	-2.04943800	0.06490700
H	-2.26512900	1.64559000	-0.70602500
H	-3.26826700	-2.12177100	1.08099300
H	-1.12863900	-3.08681600	0.26105400
N	0.14582800	0.91872000	-1.63924000
H	0.77054000	0.30417600	-2.17864300
H	-0.36983200	1.49588700	-2.31260500
C	0.22355400	2.90943300	-0.09041700
H	0.90447800	3.60623900	0.40233800
H	-0.38300300	3.48028500	-0.80041900
H	-0.42651600	2.48326700	0.67473900
Cl	0.99007700	-1.95780200	-1.25336100
Cl	-4.38043200	0.48765800	0.78043100

IM2

C	4.65286000	-2.65723100	-0.58759500
C	4.24922000	-1.36411900	-0.92308300
C	5.05461700	-0.28593400	-0.54357100
C	6.22857500	-0.50094400	0.17109300
C	6.61813500	-1.79512300	0.50666100
C	5.82992500	-2.87550300	0.12122200
H	4.03373600	-3.50240000	-0.87946100
H	4.75763700	0.72976100	-0.79046700
H	6.84030500	0.34549100	0.46620300
H	7.53501700	-1.96082300	1.06300000
H	6.12921100	-3.88746800	0.37430000
C	2.92267800	-1.15340100	-1.62489400
H	2.58513600	-2.12238600	-2.00854500
C	2.50241100	0.43293600	1.40142000
C	2.04106800	0.44678500	0.08022000
C	1.73090000	1.67314200	-0.50962000
C	1.93082700	2.85170100	0.19674300
C	2.41272000	2.83806400	1.49963500
C	2.68558700	1.61722200	2.10416500
H	1.29978900	1.70003300	-1.50448800
H	2.55516900	3.76792000	2.03735500
H	3.04326000	1.57657800	3.12649600
N	1.83354300	-0.75384900	-0.67213600
H	1.67188900	-1.51620800	-0.01334800
H	0.47762600	-0.55855700	-1.37103000
C	2.99319200	-0.18293900	-2.79757800
H	3.69705400	-0.56579100	-3.53965500
H	2.00984100	-0.07579700	-3.26459700
H	3.33814800	0.80621800	-2.48879000
Cl	2.83496200	-1.07682100	2.19879200
Cl	1.54960300	4.37028900	-0.56186600
C	-6.06865800	-0.07900600	0.85557600
C	-6.26456300	-1.57761100	0.58450400
C	-4.04914200	-0.68135600	-0.00455400
C	-3.75603900	-0.42430100	1.50661700
C	-5.13214400	0.02351900	2.07415500
H	-6.49420100	-2.16671100	1.47683500
H	-7.03475900	-1.79308800	-0.16170400
H	-6.99815600	0.48916300	0.94576300
H	-3.34946800	-1.31612600	1.98989400
H	-3.00866700	0.36339100	1.61632300
H	-5.47228100	-0.61562300	2.89335900
H	-5.08396400	1.04459900	2.45821900

C	-2.87478200	-0.85237300	-0.95446400
H	-2.60468100	-1.91105700	-1.02344800
H	-3.10790100	-0.48792700	-1.95961300
S	-1.37915500	-0.00990700	-0.46716700
O	-1.63473900	1.41892900	-0.36578700
O	-0.78574200	-0.69476600	0.68015600
O	-0.47760800	-0.30956700	-1.73275600
O	-4.54085000	-3.05998700	-0.33274000
C	-4.89647600	-1.96447300	0.02193300
C	-5.15315300	0.37408600	-0.32035600
C	-5.78717500	0.17600400	-1.70201200
H	-6.71771000	0.74829100	-1.77426000
H	-5.11852400	0.54658300	-2.48538900
H	-6.01440900	-0.86853800	-1.93427100
C	-4.70239500	1.83028200	-0.20830400
H	-5.57792000	2.48603400	-0.27600800
H	-4.17741000	2.05218700	0.72156800
H	-4.01734300	2.08530800	-1.02082400

IM-BI1

C	1.60987200	0.33492800	-1.11580600
C	2.21346000	0.68635800	0.09484300
C	3.60053600	0.84116900	0.14974500
C	4.37114300	0.66460900	-0.99340400
C	3.76277100	0.33893500	-2.20382700
C	2.38359200	0.16623900	-2.26130500
H	0.53534100	0.17665400	-1.16319800
H	4.08667700	1.08788200	1.08834600
H	5.44953500	0.77324300	-0.93742000
H	4.36562600	0.19208600	-3.09453600
H	1.90833900	-0.11341800	-3.19664100
C	1.34296300	0.98564300	1.29062800
H	0.41037100	0.42560000	1.22977500
O	1.02093900	2.43006500	1.21842300
C	0.09268500	2.84957300	0.39554700
C	0.44750000	4.26787700	-0.11307300
N	-0.92756600	2.18578100	0.02865500
H	-1.51939300	2.67994300	-0.63314500
Cl	0.77493300	5.32508600	1.27212600
Cl	1.89515500	4.09358500	-1.12531500
Cl	-0.87679000	4.96488300	-1.07646500
H	-1.50120600	0.93302400	0.61894600
C	3.90666700	-2.82103000	-1.14819900
C	2.72054100	-2.76583500	-0.39494400
C	2.84802700	-2.55164000	0.98984900
C	4.10344200	-2.41144200	1.55652400
C	5.27220000	-2.45827000	0.80391100
C	5.15431500	-2.66824600	-0.56520100
H	1.94898000	-2.50999000	1.59761700
H	6.24002600	-2.34372900	1.27525000
H	6.03805500	-2.71507800	-1.19244200
N	1.48877200	-2.96448400	-0.96063400
H	1.41471600	-2.76037300	-1.94624300
H	0.69715400	-2.66064000	-0.40590900
C	1.96155800	0.78876100	2.65507200
H	2.30731600	-0.24224200	2.75071500
H	2.80990200	1.45968400	2.80462300
H	1.22081900	0.98909100	3.43120800
Cl	3.79503900	-3.09392700	-2.87215800
Cl	4.22736800	-2.15989600	3.28555200
C	-6.36205100	-0.41918900	-0.47008100
C	-6.86998900	-1.84715600	-0.24205700
C	-4.52849800	-1.43890100	0.40495200

C	-5.02190900	-0.50405100	1.54741500
C	-6.23627100	0.23649300	0.92007200
H	-7.70983600	-1.91816800	0.45487200
H	-7.15737100	-2.36555900	-1.16099100
H	-6.94500200	0.15778700	-1.19271000
H	-5.29246900	-1.08663000	2.43361300
H	-4.22338700	0.18057800	1.83735500
H	-7.14995600	0.10977900	1.50655100
H	-6.04783800	1.30915100	0.83960800
C	-3.20058500	-2.14304700	0.63781400
H	-3.13104700	-2.49071000	1.67246700
H	-3.10341200	-3.02657800	-0.00224300
S	-1.69780400	-1.23694800	0.33551200
O	-1.54120800	-0.97674400	-1.09541500
O	-1.96875500	0.11005100	1.09373000
O	-0.60224500	-1.95298300	0.98728500
O	-5.50702300	-3.66188600	0.68833600
C	-5.62705500	-2.51434200	0.34157900
C	-4.87102500	-0.62053000	-0.88442300
C	-4.67659400	-1.42641400	-2.17229500
H	-5.13617400	-0.90272400	-3.01709200
H	-3.60823700	-1.53383800	-2.38160900
H	-5.11070200	-2.42957800	-2.12443700
C	-4.16992800	0.73524300	-1.05130400
H	-4.76693700	1.35446800	-1.73090300
H	-4.05925400	1.27834000	-0.10969500
H	-3.17905800	0.60617500	-1.49073800

TS-BI1 (S_N1)

Value of imaginary frequency = -80.9 cm^{-1}

C	1.53548700	0.26821600	-1.06340300
C	2.23877000	0.38890200	0.16076800
C	3.60364800	0.75604800	0.15564700
C	4.24475000	0.99826800	-1.04479800
C	3.53823700	0.87769600	-2.24626700
C	2.19096600	0.51518700	-2.25790000
H	0.49211900	-0.04208900	-1.06433300
H	4.14744800	0.84739200	1.08883000
H	5.29296800	1.27522500	-1.05690000
H	4.05132800	1.05642500	-3.18629900
H	1.66223800	0.41136700	-3.19879800
C	1.52123400	0.15317200	1.36025300
H	0.47823000	-0.14763700	1.26799300
O	0.75440500	2.31211000	1.62538500
C	0.14295900	2.82336800	0.69255600
C	0.66237300	4.20742100	0.18266300
N	-0.84523100	2.26323400	0.01321600
H	-1.31062100	2.74987700	-0.73729800
Cl	1.20073700	5.18045600	1.55268500
Cl	2.04468600	3.82473200	-0.88035900
Cl	-0.56360400	5.11433000	-0.74079200
H	-1.20464500	1.33800700	0.33168000
C	3.67364500	-2.55182200	-1.28263100
C	2.44771700	-2.79781900	-0.63128000
C	2.48058500	-2.91017100	0.77657600
C	3.68331000	-2.78076700	1.45183900
C	4.88365900	-2.50220900	0.80551300
C	4.85892100	-2.39719000	-0.58190100
H	1.55364100	-3.11528600	1.30300100
H	5.80703400	-2.40804500	1.36251200
H	5.77274000	-2.20393300	-1.13376900
N	1.27830700	-2.94783800	-1.30536500
H	1.23892800	-2.65278100	-2.26796300
H	0.42169100	-2.86494300	-0.76413200
C	2.06417400	0.09424400	2.72225800
H	2.00526000	-0.95757400	3.03438800
H	3.09015300	0.44090900	2.82720100
H	1.39783400	0.65406900	3.38216400
Cl	3.69873600	-2.47331900	-3.03010500
Cl	3.70115000	-2.99522900	3.18976300
C	-6.15768600	0.05007900	-0.45036300
C	-6.85086300	-1.30937300	-0.30869700

C	-4.46131300	-1.27080400	0.29600100
C	-4.79075300	-0.35770200	1.51220300
C	-5.91537100	0.57581700	0.98022300
H	-7.68406300	-1.31686200	0.39969100
H	-7.21599800	-1.71706800	-1.25556100
H	-6.67120000	0.75321900	-1.11167100
H	-5.10770700	-0.95608600	2.37206900
H	-3.89329800	0.18995900	1.80520900
H	-6.82472900	0.51966900	1.58454100
H	-5.59520500	1.62003800	0.97374000
C	-3.22927500	-2.15037500	0.42421400
H	-3.21399000	-2.62228400	1.41046400
H	-3.24170100	-2.95488900	-0.31716500
S	-1.63159000	-1.37082300	0.23315100
O	-1.42772400	-1.10663900	-1.21060300
O	-1.66952100	-0.10822200	1.03916700
O	-0.64055700	-2.32642700	0.78125200
O	-5.74309100	-3.34750500	0.48335400
C	-5.69973100	-2.17621700	0.20151900
C	-4.71737700	-0.32214100	-0.91981100
C	-4.65057600	-1.05502300	-2.26273400
H	-5.03218200	-0.41440600	-3.06503500
H	-3.60811000	-1.30009600	-2.48702500
H	-5.22398000	-1.98681500	-2.27593000
C	-3.83526100	0.92995100	-1.01355200
H	-4.33497500	1.66106100	-1.66075700
H	-3.65677200	1.39808500	-0.04304000
H	-2.86899500	0.67731400	-1.45526600

IM-BI2

C	1.50358400	0.25764400	-1.09788600
C	2.27825300	0.34415900	0.08855700
C	3.62633200	0.77152600	0.02052900
C	4.17845200	1.10734600	-1.20095400
C	3.40380000	1.01089400	-2.36259100
C	2.07370900	0.59052000	-2.31389800
H	0.47194300	-0.08788500	-1.05011900
H	4.22171800	0.83792700	0.92395700
H	5.20978300	1.43638200	-1.26215900
H	3.85018500	1.25967700	-3.32099000
H	1.49176800	0.51437200	-3.22560300
C	1.65510000	-0.00729800	1.30383500
H	0.60797200	-0.31171900	1.25633200
O	0.72474500	2.29944200	1.67118500
C	0.12485100	2.82247400	0.74572100
C	0.64322300	4.21214400	0.24383200
N	-0.86309400	2.27053000	0.05056400
H	-1.33746600	2.76648000	-0.68730000
Cl	1.28116700	5.13668600	1.60517400
Cl	1.95732700	3.83370700	-0.90638500
Cl	-0.61347700	5.16740200	-0.58380300
H	-1.19934000	1.33530300	0.34687400
C	3.63113500	-2.51580100	-1.27728200
C	2.41500800	-2.81318300	-0.62782300
C	2.45233700	-2.93785700	0.78030700
C	3.65410600	-2.78245100	1.45659200
C	4.83880800	-2.44105400	0.81346300
C	4.80722500	-2.31777200	-0.57411800
H	1.53498300	-3.18542500	1.30517000
H	5.76043000	-2.32251300	1.36893400
H	5.71202200	-2.07923300	-1.12332300
N	1.25280800	-2.98940200	-1.30204400
H	1.20167000	-2.69415200	-2.26403800
H	0.39259800	-2.95046800	-0.76074200
C	2.25172000	-0.00518100	2.64417900
H	1.93864700	-0.90702200	3.17798200
H	3.33661300	0.08403300	2.66487400
H	1.79457700	0.84506100	3.16711900
Cl	3.65365900	-2.42024000	-3.02353700
Cl	3.68726500	-3.04465800	3.18576900
C	-6.09515500	0.10886900	-0.45238600
C	-6.82700200	-1.22990100	-0.31155000
C	-4.43893700	-1.25914500	0.29932300

C	-4.74251500	-0.33335100	1.51225300
C	-5.84227000	0.62841100	0.97865900
H	-7.66280600	-1.21246100	0.39370100
H	-7.19998900	-1.62847000	-1.25933500
H	-6.58672200	0.82587400	-1.11578100
H	-5.07357300	-0.91956600	2.37527900
H	-3.82948900	0.19064600	1.80213200
H	-6.75385400	0.59460800	1.58135300
H	-5.49702400	1.66466100	0.97388800
C	-3.23293100	-2.17225000	0.43277000
H	-3.23171500	-2.63883700	1.42186900
H	-3.26998700	-2.98065900	-0.30372500
S	-1.61041900	-1.44698900	0.23667000
O	-1.40123000	-1.20273500	-1.21070500
O	-1.59466800	-0.18206000	1.03411700
O	-0.65754000	-2.44173500	0.78503400
O	-5.78108000	-3.29710800	0.48857300
C	-5.70289000	-2.12826400	0.20421000
C	-4.66532600	-0.30552100	-0.91852300
C	-4.61821300	-1.04197600	-2.25978800
H	-4.98168700	-0.39218300	-3.06331700
H	-3.58278200	-1.31674300	-2.48278100
H	-5.21774300	-1.95739800	-2.27154300
C	-3.74581200	0.91804800	-1.01113200
H	-4.21657800	1.65937100	-1.66879000
H	-3.56552300	1.38750100	-0.04156700
H	-2.78226700	0.63487600	-1.44081300

IM-BI3

C	-2.46774800	1.82112200	1.28184500
C	-2.71128600	0.87476100	0.28352500
C	-4.00804000	0.73210600	-0.21864000
C	-5.04445900	1.51737400	0.27597600
C	-4.79401800	2.45949200	1.27081800
C	-3.50361800	2.61317600	1.76902600
H	-1.45728900	1.94801800	1.66429400
H	-4.21498800	-0.00042100	-0.99452300
H	-6.04796300	1.39631900	-0.11946200
H	-5.60209700	3.07663700	1.65042300
H	-3.29829200	3.35489300	2.53449000
C	-1.57325500	0.00414700	-0.20264400
H	-0.63125000	0.45612000	0.12807800
C	-3.75679200	-2.24108400	1.24858500
C	-2.71308000	-2.16939900	0.31940700
C	-2.77535500	-2.96146800	-0.82861500
C	-3.88262300	-3.76647900	-1.05587400
C	-4.92873700	-3.82458500	-0.14167400
C	-4.85284000	-3.06595000	1.01930000
H	-1.94621500	-2.95296100	-1.52846300
H	-5.78301300	-4.46365000	-0.33144700
H	-5.64825300	-3.10560800	1.75471000
N	-1.56106700	-1.34067100	0.50345800
H	-1.42482500	-1.14738900	1.49716900
H	-0.39125800	-2.01721300	0.04934300
C	-1.53557900	-0.17215800	-1.71522400
H	-0.66275500	-0.75632200	-2.01964200
H	-2.43910500	-0.65207600	-2.09869700
H	-1.46320500	0.81792900	-2.17144800
Cl	-3.68934200	-1.31792100	2.71979500
Cl	-3.95030900	-4.73167300	-2.50043000
C	6.24084200	-0.35897800	0.39434700
C	6.74320600	-1.73362600	0.85082600
C	4.42526100	-1.67238700	0.02882800
C	4.94275800	-1.34648500	-1.40096900
C	6.15341900	-0.40396900	-1.14489200
H	7.60438500	-2.10676000	0.28908600
H	6.99522900	-1.77834500	1.91421300
H	6.81049200	0.48529300	0.79137800
H	5.22124700	-2.26250500	-1.93165700
H	4.15195200	-0.86016400	-1.97509400
H	7.07808800	-0.78379200	-1.58760700
H	5.97519200	0.58920100	-1.56223600

C	3.09262400	-2.39746500	0.11870000
H	3.04058500	-3.19587200	-0.62707400
H	2.94798700	-2.85188200	1.10286100
S	1.65950500	-1.37607900	-0.14009900
O	1.34747900	-0.62568400	1.07549300
O	1.85298100	-0.59224500	-1.36930900
O	0.54220100	-2.44107200	-0.36520500
O	5.39417400	-3.78317500	0.78748000
C	5.51221800	-2.59945700	0.59215500
C	4.73874100	-0.35635200	0.81680400
C	4.50303000	-0.49948400	2.32333700
H	4.94210100	0.35088300	2.85537400
H	3.42795600	-0.50226300	2.52593100
H	4.92760600	-1.41606900	2.74485100
C	4.03905800	0.92361300	0.33731700
H	4.62576500	1.78591600	0.67493400
H	3.95156300	0.98343300	-0.74936000
H	3.03706400	1.01982500	0.76256900
C	0.57006400	2.81772600	-0.29928100
N	0.96355800	2.16679100	-1.40378200
H	0.80938300	2.54743700	-2.32390100
O	0.70913200	2.42880000	0.83865200
C	-0.14357400	4.18871500	-0.58683800
Cl	-1.58197700	3.89167600	-1.60667800
Cl	-0.63125000	4.95055500	0.92208400
Cl	0.98941000	5.25702300	-1.46529900
H	1.38432900	1.24115600	-1.31005300

IM-BI4

C	-2.10520400	3.16760600	-0.41397000
C	-2.54210700	1.92751800	-0.88374300
C	-3.90353600	1.74194400	-1.13966700
C	-4.80901500	2.77491000	-0.91695100
C	-4.36362300	4.00702000	-0.44491600
C	-3.00785300	4.20381500	-0.19715400
H	-1.04671800	3.31410600	-0.21103200
H	-4.26390100	0.78297000	-1.50274300
H	-5.86457300	2.61723300	-1.11425000
H	-5.07171200	4.81161300	-0.27458500
H	-2.65284400	5.16302700	0.16562900
C	-1.54011000	0.80362200	-1.04043700
H	-0.53611000	1.23865600	-1.01591700
C	-3.66314800	-0.30199000	1.44577100
C	-2.78247300	-0.76255800	0.45920500
C	-3.11518300	-1.92172300	-0.24518300
C	-4.31879100	-2.56672400	0.00379400
C	-5.19917000	-2.09884500	0.97315400
C	-4.85682600	-0.96741700	1.70226200
H	-2.41848800	-2.31936500	-0.97510600
H	-6.13171200	-2.61771300	1.16042700
H	-5.51975100	-0.58807300	2.47132500
N	-1.54857900	-0.11287100	0.16211500
H	-1.24593000	0.44688500	0.96111500
H	-0.35767800	-1.05214900	-0.05056700
C	-1.67504900	0.01756200	-2.33719100
H	-2.65607600	-0.45235300	-2.44180900
H	-1.54194900	0.70424900	-3.17584700
H	-0.89761000	-0.74922600	-2.39806200
Cl	-3.27070700	1.10825800	2.38385900
Cl	-4.72015800	-3.99713300	-0.90091200
C	6.21886700	0.78089400	0.06291100
C	6.72279500	-0.45874800	0.81081800
C	4.41333700	-0.59219800	-0.02537900
C	4.94596000	-0.58400700	-1.48735100
C	6.14687300	0.40225000	-1.43094100
H	7.58850200	-0.94131300	0.34802700
H	6.96939000	-0.27011500	1.85952900
H	6.78117200	1.69464000	0.27223700
H	5.23765300	-1.59180200	-1.79944600
H	4.15976900	-0.24421800	-2.16419000
H	7.07849100	-0.05601300	-1.77352800
H	5.96597800	1.27953100	-2.05552800

C	3.07936100	-1.27726400	0.21582000
H	3.05341400	-2.24493500	-0.29348500
H	2.90762500	-1.45872900	1.28053500
S	1.64353200	-0.38577200	-0.34724400
O	1.27603500	0.64352200	0.63185700
O	1.82441200	0.03891400	-1.72995700
O	0.56062500	-1.52925300	-0.26792800
O	5.38218500	-2.47920400	1.19056100
C	5.49705400	-1.36728300	0.73927200
C	4.71230100	0.86335000	0.45832700
C	4.45543600	1.05017600	1.95607900
H	4.85925300	2.01084800	2.29216600
H	3.37714200	1.05501500	2.14409600
H	4.89913700	0.26395400	2.57481400
C	4.00425000	1.99274700	-0.30133100
H	4.57558000	2.91851800	-0.16585100
H	3.91045600	1.80276600	-1.37166900
H	2.99880300	2.15554200	0.08924800

IM-BII1

C	-3.39553900	-2.05608600	-1.63432800
C	-2.04724600	-2.24016500	-1.32962600
C	-1.63734500	-3.39592600	-0.66001600
C	-2.57589900	-4.35432100	-0.28637800
C	-3.92540300	-4.16267200	-0.57829700
C	-4.33111500	-3.01557800	-1.25607400
H	-3.71513900	-1.14565300	-2.13104000
H	-0.58357000	-3.52524500	-0.41804400
H	-2.25465300	-5.24547600	0.24352000
H	-4.65864500	-4.90188800	-0.27243900
H	-5.38196400	-2.85606400	-1.47428100
C	-1.00098000	-1.21146900	-1.67971300
H	-0.27818500	-1.18067900	-0.86768400
O	-1.67950900	0.07344100	-1.73675200
C	-1.14406500	1.13620800	-1.19293000
C	-2.11793100	2.32983700	-1.35139400
N	0.02271000	1.21608200	-0.69592500
H	0.22429000	2.12027100	-0.27667500
Cl	-1.99523400	2.84249900	-3.05924100
Cl	-3.77129600	1.83389400	-0.98345400
Cl	-1.65485300	3.68199500	-0.29881500
H	1.15851400	0.25276600	-0.73550400
C	-2.02589000	1.04425200	2.24264500
C	-2.02625800	-0.28491200	1.77886200
C	-3.27607900	-0.88416200	1.53900300
C	-4.44069100	-0.17602500	1.77869500
C	-4.43544700	1.12778800	2.26581800
C	-3.20531100	1.73217900	2.49351200
H	-3.32035700	-1.90634900	1.17469100
H	-5.36368100	1.65392100	2.44954800
H	-3.15100600	2.74813000	2.86938400
N	-0.85869900	-0.95694300	1.52718600
H	-0.00396500	-0.62162300	1.95739200
H	-0.91204300	-1.96187600	1.43757700
C	-0.30838000	-1.44598300	-3.00946400
H	0.20269100	-2.41114900	-2.97543400
H	-1.03752800	-1.45638000	-3.82335500
H	0.43839200	-0.66852200	-3.19172400
Cl	-0.49220200	1.81249200	2.58677900
Cl	-5.97165500	-0.94840500	1.44391700
C	6.29754800	1.27222500	-0.06281800
C	7.29109200	0.14743300	0.24754100
C	4.95439900	-0.56169400	-0.08151300

C	5.05429600	-0.15020400	-1.57921000
C	5.92421300	1.13755500	-1.55249000
H	8.08943600	0.03684500	-0.49187600
H	7.75969300	0.23293900	1.23187500
H	6.63728300	2.26869900	0.23128000
H	5.50336400	-0.95357000	-2.17206200
H	4.05491700	0.03244700	-1.97760200
H	6.81377400	1.05217800	-2.18210900
H	5.36047100	2.00463700	-1.90312000
C	3.97696900	-1.68180600	0.23932500
H	4.02344400	-2.45581100	-0.53194300
H	4.22652100	-2.16361300	1.19047200
S	2.25084400	-1.28116700	0.41505700
O	2.05506900	-0.48768700	1.63062700
O	2.00227800	-0.38597200	-0.85139200
O	1.48370900	-2.51898600	0.30774500
O	6.67722200	-2.21978100	0.43438500
C	6.37181600	-1.07125300	0.23392300
C	4.98942000	0.81799800	0.65792800
C	5.12726200	0.67797900	2.17682800
H	5.37229500	1.64788300	2.62249200
H	4.17866200	0.33966000	2.60260100
H	5.90193900	-0.03395300	2.47738200
C	3.84242800	1.79403100	0.36312300
H	4.17639000	2.80785100	0.61287700
H	3.53145300	1.78801600	-0.68347700
H	2.96939500	1.56472100	0.97677100

TS-BII1 (S_N2)

Value of imaginary frequency = -292.8 cm^{-1}

C	-2.37450700	1.11150000	1.27765300
C	-2.50416700	0.78014200	-0.07924000
C	-3.77214300	0.79883300	-0.68123900
C	-4.88942500	1.14058000	0.06679600
C	-4.74661200	1.47704100	1.41333400
C	-3.49077700	1.46662900	2.01986100
H	-1.39124000	1.06912900	1.74045900
H	-3.88125300	0.53611500	-1.72855600
H	-5.87105400	1.14060100	-0.39431100
H	-5.62271700	1.74423600	1.99600500
H	-3.38799900	1.71560400	3.07043000
C	-1.32483200	0.38120300	-0.81155700
H	-0.41562900	0.21965900	-0.23863300
O	-0.66160500	2.35147000	-1.19940600
C	0.35222400	2.78425700	-0.64170300
C	0.26554800	4.27160700	-0.16819800
N	1.46139900	2.11477600	-0.41417800
H	2.23024300	2.54460500	0.07763600
Cl	0.03844100	5.27364900	-1.61533000
Cl	-1.14181800	4.41043900	0.90261500
Cl	1.71957700	4.82479400	0.70437500
H	1.60504800	1.15592400	-0.82268400
C	-3.45269700	-2.10001300	1.48327800
C	-2.84159300	-2.25722200	0.22456100
C	-3.67609000	-2.55164200	-0.86696000
C	-5.05001600	-2.62808600	-0.69563100
C	-5.64895200	-2.43822100	0.54378400
C	-4.82684000	-2.18571200	1.63805600
H	-3.23860000	-2.72741100	-1.84440000
H	-6.72419800	-2.50538200	0.65359300
H	-5.25335100	-2.05643200	2.62673700
N	-1.50567900	-2.01634200	0.03169200
H	-0.89076100	-1.98100500	0.83927200
H	-1.01912600	-2.42935400	-0.76432200
C	-1.35718600	-0.01176200	-2.24489200
H	-2.02762100	-0.86847500	-2.36714000
H	-1.76406300	0.81439800	-2.83250800
H	-0.36111400	-0.27770500	-2.59601600
Cl	-2.44828100	-1.83222500	2.88695200
Cl	-6.05062900	-2.95780900	-2.08600500
C	6.11303100	-0.72816000	0.81938300
C	6.63610500	-2.16786700	0.76972100

C	4.44679100	-1.79926900	-0.30141500
C	5.13315100	-0.92673800	-1.39105900
C	6.23889300	-0.16108300	-0.61030900
H	7.58843100	-2.28167800	0.24397100
H	6.74348000	-2.62959700	1.75525200
H	6.56891000	-0.10760000	1.59589100
H	5.53666500	-1.55295600	-2.19293200
H	4.39257900	-0.25996800	-1.83809100
H	7.23658600	-0.33609900	-1.02169400
H	6.06731000	0.91761000	-0.63041500
C	3.16196800	-2.49623600	-0.70878800
H	3.29299000	-2.95955800	-1.69045900
H	2.91217100	-3.29912700	-0.00847200
S	1.65770300	-1.53138300	-0.83476000
O	1.19079900	-1.25414800	0.54991900
O	1.99013900	-0.25897000	-1.55260100
O	0.72949900	-2.38314000	-1.60703200
O	5.45703000	-4.02964100	-0.30318000
C	5.51009300	-2.86593900	0.00644000
C	4.57175100	-0.90917600	0.97588900
C	4.13619000	-1.64019200	2.24822700
H	4.41826800	-1.06240000	3.13495000
H	3.04752200	-1.75166600	2.24422300
H	4.57437200	-2.63821700	2.34434100
C	3.85041200	0.44156600	0.93145200
H	4.28378000	1.09975800	1.69491100
H	3.94598300	0.93196700	-0.04072600
H	2.78835400	0.30689600	1.14667400

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C	-1.44697600	1.52890600	1.30030600
C	-2.29156500	1.01247900	0.31170100
C	-3.64007700	1.36232600	0.30854100
C	-4.14389700	2.20851700	1.29412500
C	-3.30473700	2.70590400	2.28631000
C	-1.95226500	2.36917900	2.28559200
H	-0.39250400	1.25243700	1.29170800
H	-4.30279300	0.97942400	-0.46141200
H	-5.19511800	2.47841700	1.28592900
H	-3.70042800	3.36503100	3.05224400
H	-1.28933900	2.76880200	3.04620300
C	-1.70555900	0.03205300	-0.67273400
H	-0.66199900	0.30271700	-0.84770300
O	-0.64505800	2.44796900	-2.01233900
C	0.15476900	2.88382400	-1.21169500
C	-0.09583400	4.31209600	-0.60976600
N	1.28520100	2.28358700	-0.82533300
H	1.89445900	2.68806200	-0.13315500
Cl	0.70583200	5.46917000	-1.70704700
Cl	-1.82865500	4.62984000	-0.54866300
Cl	0.59910700	4.49936400	1.03118800
H	1.52800000	1.37379200	-1.23007400
C	-3.53485000	-2.10735800	1.34501300
C	-2.78675400	-2.11839500	0.16620800
C	-3.17772200	-2.92538000	-0.89956000
C	-4.33603100	-3.68207400	-0.79558200
C	-5.10257700	-3.65857900	0.36574900
C	-4.69135600	-2.87708900	1.43660900
H	-2.56977400	-2.96198600	-1.79758200
H	-6.00334800	-4.25737200	0.43223900
H	-5.26224800	-2.86222600	2.35770800
N	-1.58126600	-1.34028000	0.01068400
H	-1.11357400	-1.17566500	0.91131600
H	-0.80734300	-1.87533400	-0.57082500
C	-2.39687500	-0.09053900	-2.01468800
H	-3.42930200	-0.43880300	-1.93416000
H	-2.38313100	0.89810900	-2.47514800
H	-1.83647800	-0.77286300	-2.66033500
Cl	-3.01501300	-1.19706200	2.72639800
Cl	-4.82582600	-4.67646900	-2.13058700
C	6.00947200	-0.82575200	0.80219000
C	6.35478200	-2.29658600	1.06218600
C	4.22117500	-1.90072000	-0.10214000

C	4.99886500	-1.36244800	-1.33657100
C	6.19304300	-0.58655700	-0.71090400
H	7.28154400	-2.63091100	0.58702800
H	6.41404200	-2.55305500	2.12381800
H	6.54169700	-0.11658400	1.44191900
H	5.31936100	-2.18580800	-1.98269400
H	4.34281000	-0.71831000	-1.92556600
H	7.16009900	-0.95882400	-1.05933900
H	6.14792700	0.47661400	-0.95694600
C	2.85845200	-2.51248700	-0.37633100
H	2.91416300	-3.16950600	-1.24886800
H	2.52171400	-3.12194500	0.46724700
S	1.51502800	-1.38335900	-0.70199800
O	1.07561000	-0.80703200	0.59511500
O	1.98432400	-0.37427000	-1.67107200
O	0.42417300	-2.26138500	-1.26540300
O	4.94250800	-4.18538400	0.39147100
C	5.14640000	-2.99831000	0.44408400
C	4.45890200	-0.78198300	0.96444800
C	3.95310100	-1.17497700	2.35508300
H	4.31654100	-0.46448800	3.10523000
H	2.85928600	-1.14801300	2.36197400
H	4.26588900	-2.17745100	2.66303800
C	3.90875600	0.61092300	0.63193800
H	4.44395400	1.35275200	1.23713100
H	4.02271500	0.87858100	-0.42055000
H	2.84632900	0.66164600	0.87934400

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C	-2.10520400	3.16760600	-0.41397000
C	-2.54210700	1.92751800	-0.88374300
C	-3.90353600	1.74194400	-1.13966700
C	-4.80901500	2.77491000	-0.91695100
C	-4.36362300	4.00702000	-0.44491600
C	-3.00785300	4.20381500	-0.19715400
H	-1.04671800	3.31410600	-0.21103200
H	-4.26390100	0.78297000	-1.50274300
H	-5.86457300	2.61723300	-1.11425000
H	-5.07171200	4.81161300	-0.27458500
H	-2.65284400	5.16302700	0.16562900
C	-1.54011000	0.80362200	-1.04043700
H	-0.53611000	1.23865600	-1.01591700
C	-3.66314800	-0.30199000	1.44577100
C	-2.78247300	-0.76255800	0.45920500
C	-3.11518300	-1.92172300	-0.24518300
C	-4.31879100	-2.56672400	0.00379400
C	-5.19917000	-2.09884500	0.97315400
C	-4.85682600	-0.96741700	1.70226200
H	-2.41848800	-2.31936500	-0.97510600
H	-6.13171200	-2.61771300	1.16042700
H	-5.51975100	-0.58807300	2.47132500
N	-1.54857900	-0.11287100	0.16211500
H	-1.24593000	0.44688500	0.96111500
H	-0.35767800	-1.05214900	-0.05056700
C	-1.67504900	0.01756200	-2.33719100
H	-2.65607600	-0.45235300	-2.44180900
H	-1.54194900	0.70424900	-3.17584700
H	-0.89761000	-0.74922600	-2.39806200
Cl	-3.27070700	1.10825800	2.38385900
Cl	-4.72015800	-3.99713300	-0.90091200
C	6.21886700	0.78089400	0.06291100
C	6.72279500	-0.45874800	0.81081800
C	4.41333700	-0.59219800	-0.02537900
C	4.94596000	-0.58400700	-1.48735100
C	6.14687300	0.40225000	-1.43094100
H	7.58850200	-0.94131300	0.34802700
H	6.96939000	-0.27011500	1.85952900
H	6.78117200	1.69464000	0.27223700
H	5.23765300	-1.59180200	-1.79944600
H	4.15976900	-0.24421800	-2.16419000
H	7.07849100	-0.05601300	-1.77352800
H	5.96597800	1.27953100	-2.05552800

C	3.07936100	-1.27726400	0.21582000
H	3.05341400	-2.24493500	-0.29348500
H	2.90762500	-1.45872900	1.28053500
S	1.64353200	-0.38577200	-0.34724400
O	1.27603500	0.64352200	0.63185700
O	1.82441200	0.03891400	-1.72995700
O	0.56062500	-1.52925300	-0.26792800
O	5.38218500	-2.47920400	1.19056100
C	5.49705400	-1.36728300	0.73927200
C	4.71230100	0.86335000	0.45832700
C	4.45543600	1.05017600	1.95607900
H	4.85925300	2.01084800	2.29216600
H	3.37714200	1.05501500	2.14409600
H	4.89913700	0.26395400	2.57481400
C	4.00425000	1.99274700	-0.30133100
H	4.57558000	2.91851800	-0.16585100
H	3.91045600	1.80276600	-1.37166900
H	2.99880300	2.15554200	0.08924800