Electronic Supplementary Information (ESI)

Characterization of non-covalent contacts in mono- and di-halo substituted acetaldehydes: Probing the substitution effects of electron donating and withdrawing groups

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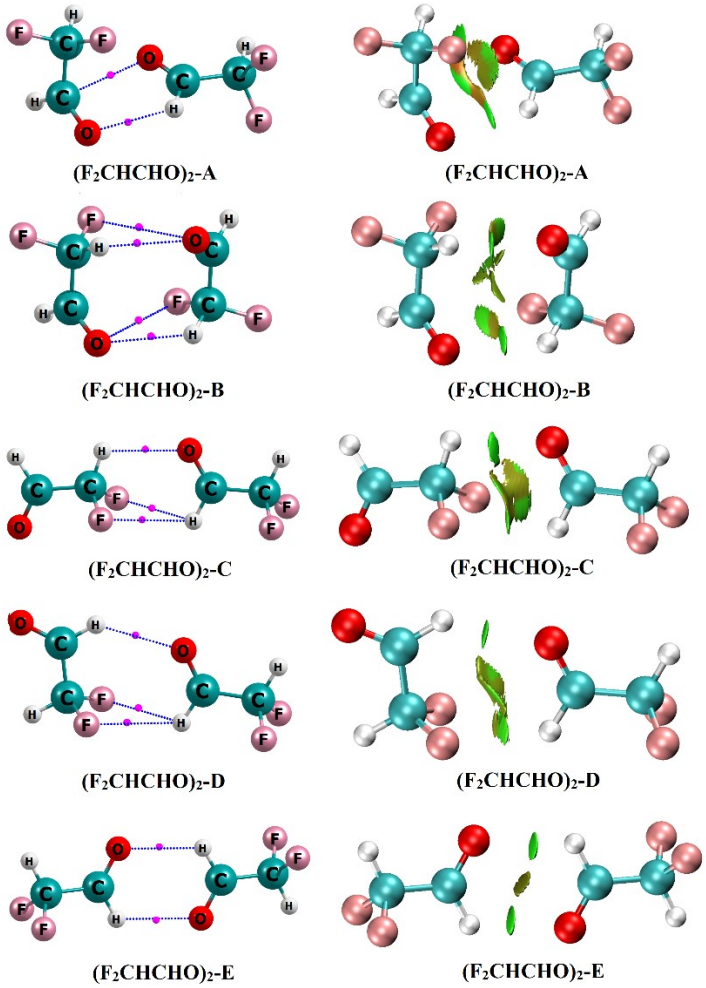

Figure S1. Five most stable conformers of di-fluoroacetaldehyde dimer $(F_2CHCHO)_2$ on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S1: Five most stable conformers of acetaldehyde dimer **$(F_2CHCHO)_2$** along with the stabilisation energy (ΔE), dipole moment (μ), bond path length (R_{ij}), bond angle (θ), molecular electron density (ρ_{BCP}) and Laplacian of electron density ($\nabla^2\rho_{BCP}$), potential energy density (V), kinetic energy density (G), ellipticity (ε) calculated at (3, -1) BCP, MP2/aug-cc-pVTZ level of theory.

Conformers $(FCH_2CHO)_2$	**Contact Type**	θ **(deg.)**	$\mathbf{R_{ij}}$ Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	**V (kJ/mol)**	**G (kJ/mol)**	$\lvert V/G\rvert$	ε	ΔE **(kJ/mol)**
A	O=C…O **(C…O=C)**	91 **(99)**	2.83	0.0736	1.0573	-19.63	24.18	0.81	1.547	-27.84
	C-H…O	119	2.39	0.0709	1.0935	-17.77	23.74	0.75	0.2383	
B	*C-O…F **(C-F … O)**	81**(78)**	3.17	0.0351	0.5432	-9.06	11.91	0.76	1.5209	-18.43
	*C-H…O	121	2.48	0.0553	0.8521	-13.28	18.22	0.73	0.1579	
C	C-H…O	111	2.50	0.0628	0.9463	-15.48	20.61	0.75	0.1502	-17.22
	*C-H…F	110	2.67	0.0334	0.5842	-9.68	12.78	0.76	0.3091	
D	C-H…O	135	2.47	0.0574	0.8352	-13.39	18.04	0.74	0.0328	-16.34
	*C-H…F	115	2.64	0.0351	0.5721	-9.50	12.52	0.76	0.1831	
E	*C-H…O	123	2.49	0.0574	0.857	-13.84	18.56	0.75	0.0291	-16.26

*C-O…F and *C-H…O are the unique interactions while *C-H…F are the unique and bifurcated interactions.

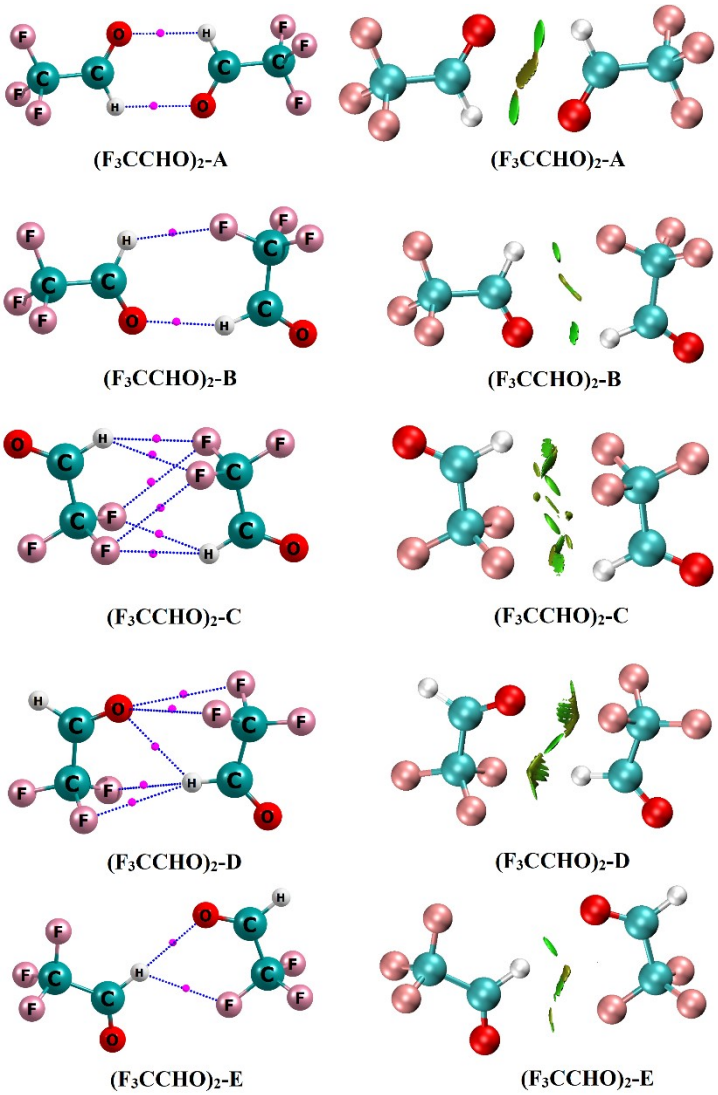

Figure S2. Five most stable conformers of trifluoroacetaldehyde dimer $(\mathbf{F_3CCHO})_2$ on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S2: Five most stable conformers of tri-fluoroacetaldehyde dimer **$(F_3CCHO)_2$**.

Conformers $(F_3CCHO)_2$	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	V (kJ/mol)	G (kJ/mol)	$\lvert V/G\rvert$	ε	ΔE (kJ/mol)
A	*C-H…O	120	2.48	0.0587	0.8884	-14.24	19.21	0.74	0.0610	-17.85
B	C-H…F	119	2.50	0.0405	0.7073	-11.11	15.18	0.73	0.0578	-13.63
	C-H…O	154	2.40	0.0621	0.9076	-14.74	19.7	0.75	0.0037	
C	*C-H…F	130	2.69	0.0297	0.4562	-7.52	9.96	0.76	0.0985	-12.21
	*C-F…F	105	3.04	0.0297	0.4925	-8.99	11.20	0.8	0.0931	
D	*C-O…F **(C-F…O)**	154 **(89)**	3.06	0.0290	0.5118	-8.18	11.06	0.74	0.1205	-12.04
	C-H…O	127	2.57	0.0506	0.6976	-11.50	15.22	0.76	0.0493	
	*C-H…F	156	2.82	0.0202	0.3307	-5.07	7.03	0.72	0.2700	
E	C-H…O	178	2.38	0.0641	0.9366	-15.53	20.49	0.76	0.0054	-11.91
	C-H…F	116	2.60	0.0351	0.5963	-9.58	12.88	0.74	0.3024	

*C-H…O and *C-F…F are the unique interaction and *C-H…F and *C-O…F are the unique and bifurcated interactions.

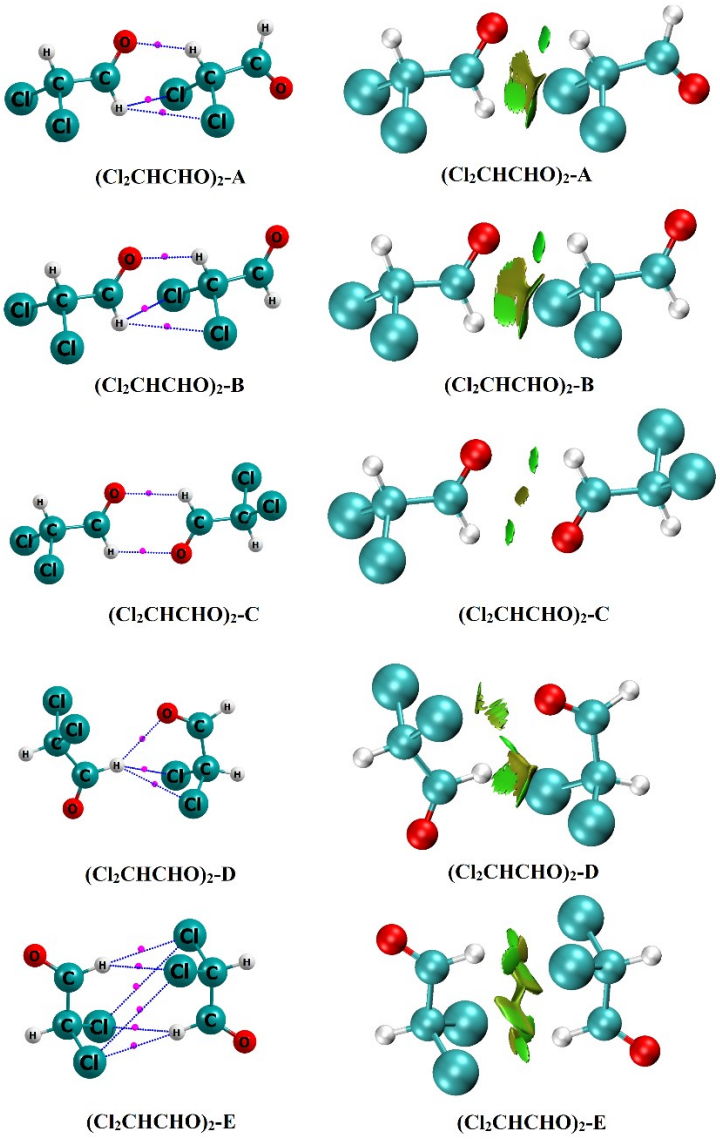

Figure S3. Five most stable conformers of di-chloroacetaldehyde $(Cl_2CHCHO)_2$ on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S3: Five most stable conformers of di-chloroacetaldehyde dimer **$(Cl_2CHCHO)_2$**.

Conformers $(Cl_2CHCHO)_2$	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	V (kJ/mol)	G (kJ/mol)	$\lvert V/G\rvert$	ε	ΔE (kJ/mol)
A	C-H…O	136	2.29	0.0864	1.3036	-22.25	28.83	0.77	0.0464	-22.36
	*C-H…Cl	117	2.97	0.0398	0.5287	-8.40	11.37	0.74	0.1180	
B	C-H…O	125	2.37	0.0749	1.1491	-18.83	25.05	0.75	0.1020	-20.15
	*C-H…Cl	113	2.99	0.0385	0.5238	-8.22	11.24	0.73	0.2063	
C	*C-H…O	124	2.46	0.0614	0.9149	-14.90	19.90	0.75	0.0223	-17.56
D	C-H…O	149	2.43	0.0634	0.8908	-15.20	19.70	0.77	0.0065	-17.35
	*C-H…Cl	133	2.91	0.0405	0.5287	-8.44	11.40	0.74	0.1211	
E	*C-H…Cl	148	2.93	0.0398	0.4900	-7.90	10.60	0.75	0.0874	-16.64
	*C-Cl…Cl	94	4.08	0.0196	0.2221	-3.04	4.53	0.67	0.1354	

*C-H…O are the unique interaction and *C-H…Cl are the unique and bifurcated interactions.

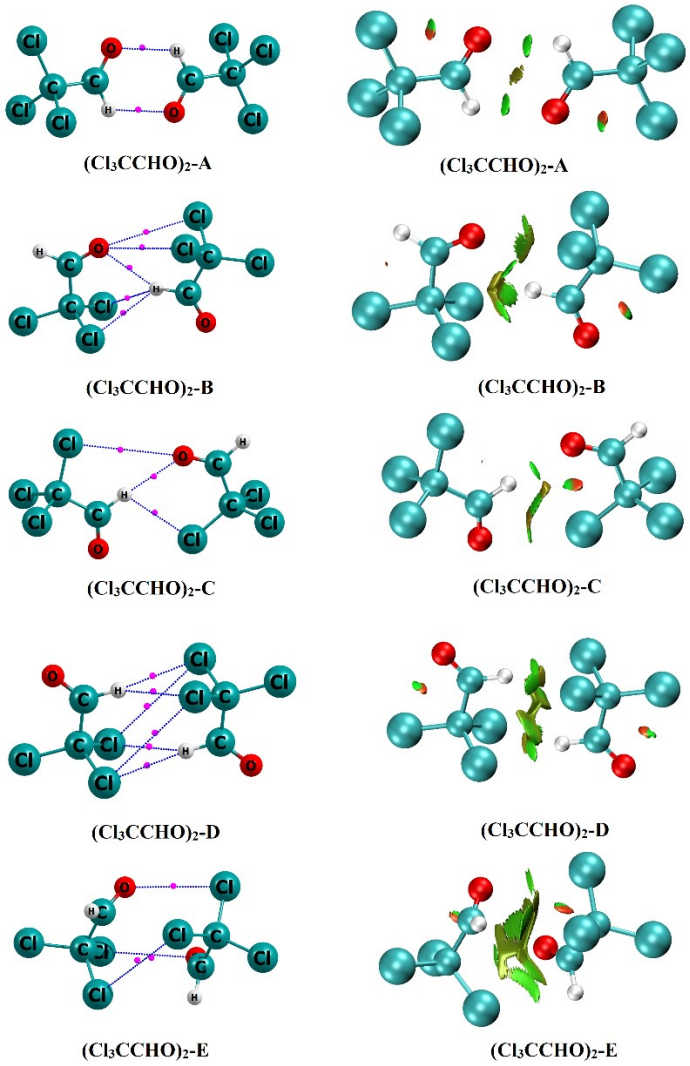

Figure S4. Five most stable conformers of tri-chloroacetaldehyde dimer $(Cl_3CCHO)_2$ on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and Colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S4: Five most stable conformers of tri-chloroacetaldehyde dimer **$(Cl_3CCHO)_2$**.

Conformers $(Cl_3CCHO)_2$	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	V (kJ/mol)	G (kJ/mol)	$\lvert V/G\rvert$	ε	ΔE (kJ/mol)
A	*C-H…O	123	2.44	0.0641	0.9608	-15.63	20.88	0.75	0.0371	-19.60
B	*C-Cl…O **(C-O…Cl)**	81 **(149)**	3.60	0.0439	0.5697	-4.54	6.61	0.69	0.6633	-19.52
	C-H…O	150	2.41	0.0648	0.8208	-15.63	20.27	0.77	0.0183	
	*C-H…Cl	78	2.88	0.0216	0.3186	-9.25	12.36	0.75	0.1195	
C	C-Cl…O **(C-O…Cl)**	92 **(174)**	3.18	0.0499	0.7459	-12.59	17.17	0.73	0.0734	-19.48
	C-H…Cl	108	2.84	0.0506	0.8014	-12.06	16.17	0.75	0.3345	
	C-H…O	178	2.34	0.0675	1.0163	-16.98	22.31	0.76	0.0484	
D	*C-H…Cl	149	2.87	0.0445	0.5504	-9.05	12.00	0.75	0.0814	-17.97
	*C-Cl…Cl	95	4.04	0.0209	0.2462	-3.38	5.02	0.67	0.1180	
E	*C-Cl…O **(C-O…Cl)**	86 **(119)**	3.39	0.0324	0.4804	-6.84	9.94	0.69	0.0226	-17.68
	C-Cl…Cl	93	3.93	0.0324	0.2945	-4.20	6.11	0.69	0.1704	

*C-H…O and *C-Cl…Cl are the unique interaction and *C-H…Cl and *C-Cl…O are the unique and bifurcated interactions.

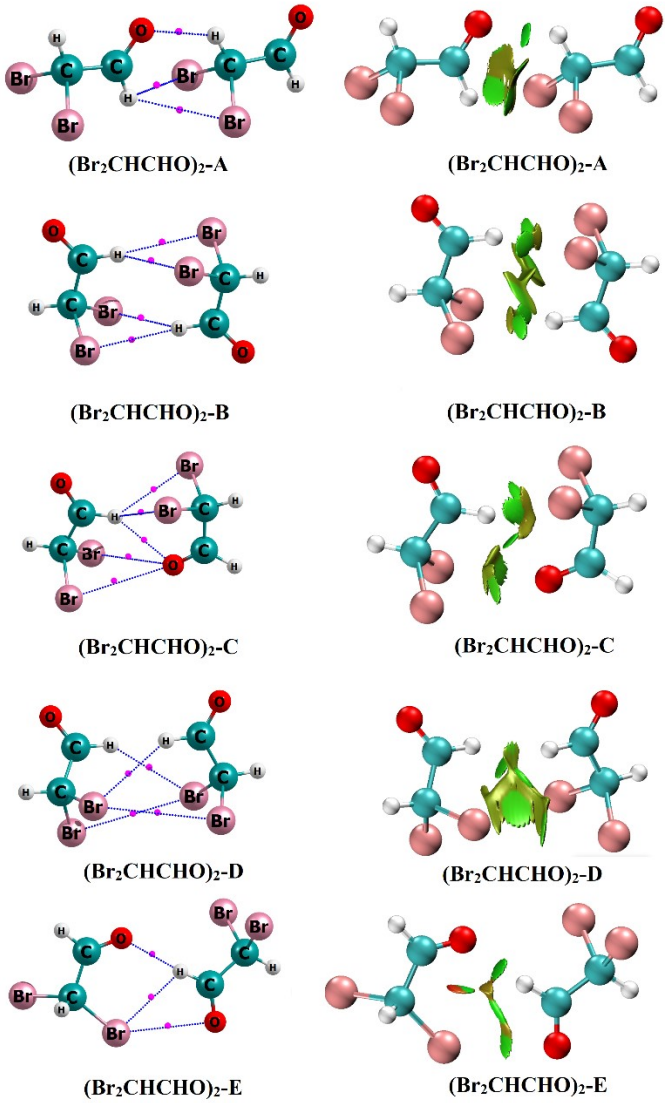

Figure S5. Five most stable conformers of di-bromoacetaldehyde dimer $(Br_2CHCHO)_2$on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S5: Five most stable conformers of di-bromoacetaldehyde dimer **$(Br_2CHCHO)_2$**.

Conformers $(Br_2CHCHO)_2$	**Contact Type**	θ **(deg.)**	R_{ij} Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	**V (kJ/mol)**	**G (kJ/mol)**	$\lvert V/G\rvert$	ε	ΔE **(kJ/mol)**
A	C-H…O	129	2.34	0.079	1.2046	-19.95	26.33	0.76	0.075	-28.17
	*C-H…Br	115	3.04	0.0445	0.5407	-9.35	12.02	0.78	0.1629	
B	*C-H…Br	147	3.10	0.0065	0.4852	-8.52	10.87	0.78	0.0766	-27.92
C	*C-H…Br	136	2.96	0.0472	0.5528	-9.75	12.38	0.79	0.1139	-27.04
	C-H…O	141	2.48	0.0587	0.8183	-13.94	18.11	0.77	0.0220	
	*C-Br…O **(C-O…Br)**	77 **(148)**	3.58	0.0283	0.3959	-5.89	8.34	0.71	0.1605	
D	*C-H…Br	143	3.02	0.0445	0.4828	-8.59	10.88	0.79	0.0599	-23.95
	*C-Br…Br	130	3.98	0.0324	0.3573	-5.81	8.01	0.73	0.1024	
E	C-H…O	175	2.34	0.0682	1.0211	-17.13	22.45	0.76	0.0640	-23.49
	C-H…Br	114	2.86	0.0607	0.7725	-14.03	17.52	0.8	0.1190	
	C-Br…O **(C-O…Br)**	137 **(85)**	3.34	0.0479	0.7001	-11.81	15.41	0.77	0.4008	

*C-H…O and *C-Br…Br are the unique interaction and *C-H…Br and *C-Br…O are the unique and bifurcated interactions.

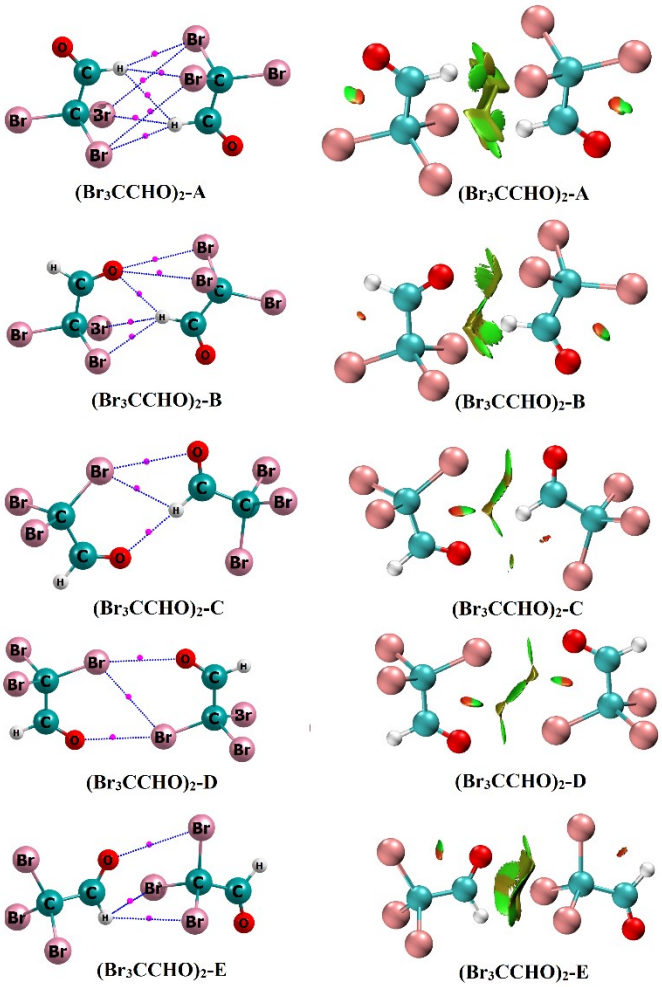

Figure S6. Five most stable conformers of tri-bromoacetaldehyde dimer $(Br_3CCHO)_2$ on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S6: Five most stable conformers of tri-bromoacetaldehyde dimer **$(Br_3CCHO)_2$**.

Conformers $(Br_3CCHO)_2$	**Contact Type**	θ **(deg.)**	**R_{ij} Å**	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	**V (kJ/mol)**	**G (kJ/mol)**	$\lvert V/G\rvert$	ε	ΔE **(kJ/mol)**
A	*C-H…Br	147	2.96	0.0486	0.5383	-9.68	12.16	0.8	0.0709	-32.31
	*C-Br…Br	93	4.20	0.0250	0.2704	-3.77	5.56	0.68	0.0332	
	C-H…H	124	2.72	0.0189	0.2583	-3.99	5.50	0.73	11.8902	
B	*C-Br…O **(C-O…Br)**	80 **(148)**	3.58	0.0283	0.6035	-5.96	8.44	0.71	0.2348	-31.81
	C-H…O	149	2.42	0.0641	0.9077	-15.55	20.12	0.77	0.0238	
	*C-H…Br	130	2.93	0.0513	0.4007	-10.89	13.66	0.8	0.1223	
C	C-Br…O **(C-O…Br)**	139 **(88)**	3.21	0.0607	0.8763	-15.27	19.55	0.78	0.0456	-27.09
	C-H…Br	110	2.87	0.0614	0.8087	-14.73	18.35	0.8	0.2450	
	C-H…O	179	2.37	0.0641	0.9632	-15.96	21.07	0.76	0.0884	
D	*C-Br…O **(C-O…Br)**	161 **(143)**	3.11	0.0580	0.9077	-14.57	19.62	0.74	0.0352	-26.04
	C-Br…Br	108	3.64	0.0567	0.6711	-11.77	15.00	0.78	0.2026	
E	C-Br…O **(C-O…Br)**	78 **(129)**	3.46	0.0385	0.5142	-8.11	11.04	0.73	0.0210	-25.41
	*C-H…Br	112	2.99	0.0506	0.6204	-10.90	13.89	0.78	0.3317	

*C-Br…Br are the unique interaction and *C-H…Br and *C-Br…O are the unique and bifurcated interactions.

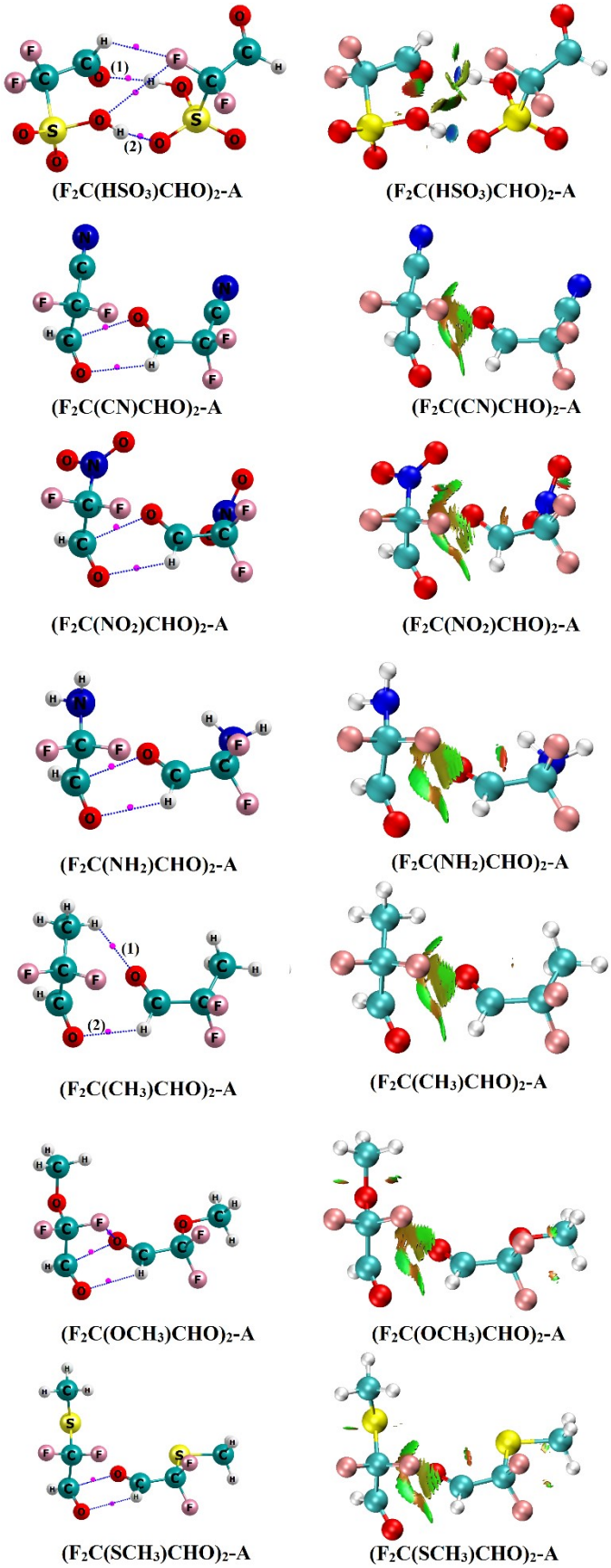

Figure S7. Interacting geometries of substituted di-fluoroacetaldehydes **($F_2C(Y)CHO$)** dimer on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020a.u.

Table S7: Geometrical and topological data for dimers of substituted di-fluoroacetaldehydes **$(F_2C(Y)CHO)_2$-A.**

Conformers	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} $e\text{Å}^{-3}$	$\nabla^2\rho_{BCP}$ $e\text{Å}^{-5}$	V (kJ/mol)	G (kJ/mol)	$\lvert V/G \rvert$	ε	ΔE (kJ/mol)
$(F_2C(HSO_3)CHO)_2$-A	C-H…F	119	2.47	0.0459	0.787	-12.36	16.89	0.73	0.1816	-72.61
	C-O…F **(C-F…O)**	137 **(112)**	3.21	0.0236	0.4128	-6.67	8.94	0.75	0.8894	
	(1) O-H…O	172	1.71	0.2700	2.6192	-108.84	90.02	1.21	0.0064	
	(2)O-H…O	169	1.78	0.2146	2.5154	-83.29	75.83	1.1	0.0277	
$(F_2C(CN)CHO)_2$-A	O=C…O	93	2.71	0.0918	1.2698	-25.22	29.86	0.84	0.6231	-28.17
	C-H…O	114	2.41	0.0688	1.0815	-17.49	23.44	0.75	0.3835	
$(F_2C(NO_2)CHO)_2$-A	O=C…O	94	2.67	0.0985	1.3639	-27.57	32.34	0.85	0.6619	-33.06
	C-H…O	113	2.42	0.0682	1.0742	-17.43	23.33	0.75	0.4298	
$(F_2C(NH_2)CHO)_2$-A	O=C…O	94	2.72	0.0871	1.2022	-23.43	28.07	0.83	0.2731	-22.40
	C-H…O	115	2.45	0.0648	1.0018	-16.21	21.72	0.75	0.4322	
$(F_2C(CH_3)CHO)_2$-A	**(1)**C-H…O	127	2.38	0.0675	1.067	-16.93	22.97	0.74	0.2437	-28.47
	(2)C-H…O	119	2.34	0.0769	1.207	-19.75	26.30	0.75	0.2062	
$((F_2C(OCH_3)CHO)_2$-A	C-O…F **(C-F…O)**	77 **(81)**	2.99	0.0472	0.8135	-13.60	17.87	0.76	3.1892	-25.12
	O=C…O	97	2.66	0.0958	1.3253	-26.52	31.27	0.85	0.1730	
	C-H…O	117	2.41	0.0702	1.0863	-17.72	23.62	0.75	0.3969	
$(F_2C(SCH_3)CHO)_2$-A	O=C…O	94	2.69	0.0925	1.2722	-25.29	29.95	0.84	0.2931	-27.59
	C-H…O	115	2.42	0.0702	1.0815	-17.71	23.56	0.75	0.4112	

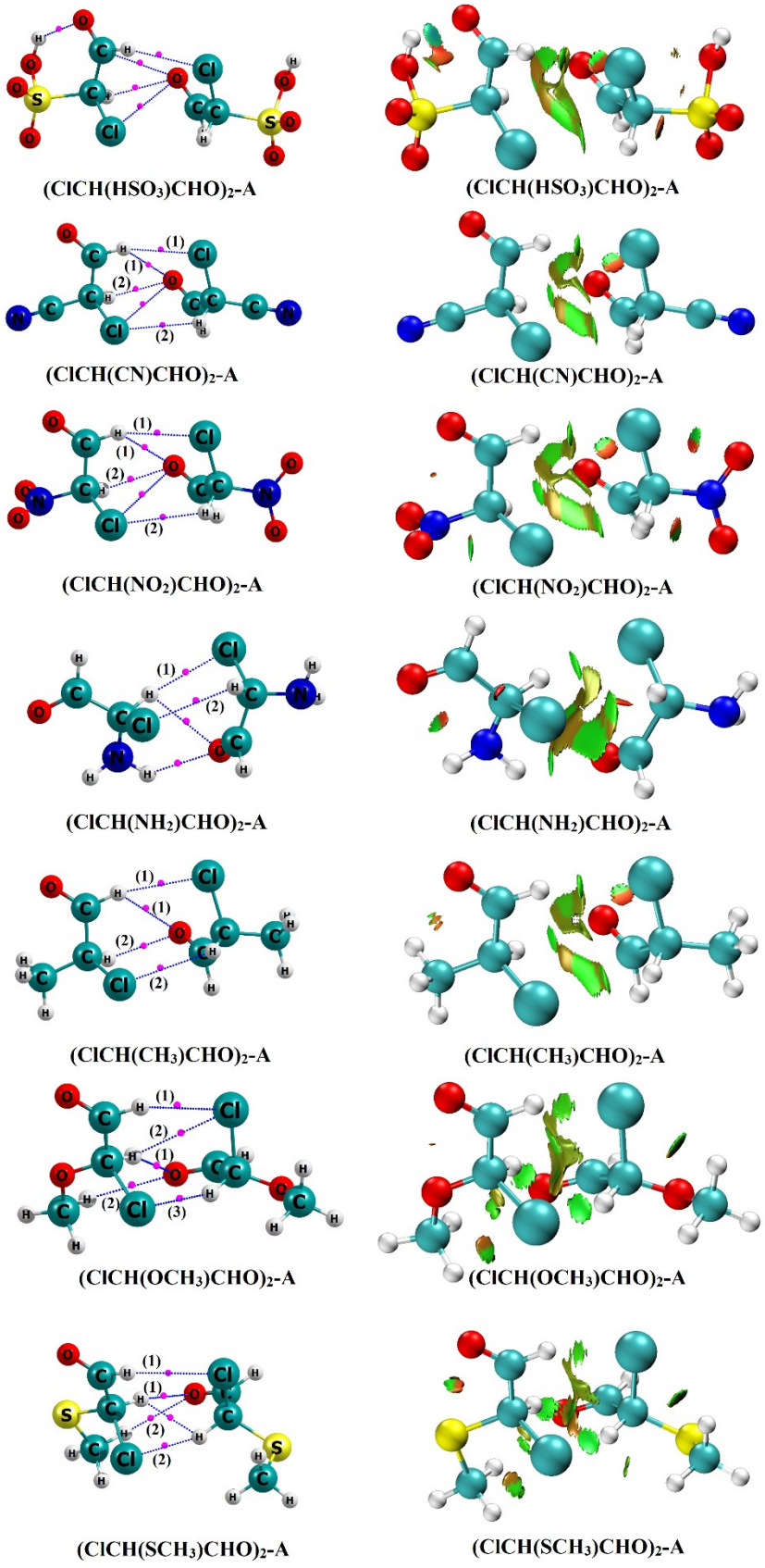

Figure S8. Interacting geometries of substituted chloro-acetaldehyde **(ClCH(Y)CHO)** dimer on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of-0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S8: Geometrical and topological data for dimers of substituted chloro-acetaldehyde **$(ClCH(Y)CHO)_2$-A.**

Conformers	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	V (kJ/mol)	G (kJ/mol)	$\lvert V/G \rvert$	ε	ΔE (kJ/mol)
$(ClCH(HSO_3)CHO)_2$-A	O-H…O(**intra**)	136 **(107)**	1.98	0.162	2.3247	-52.38	57.79	0.91	0.145	-31.64
	C-H…Cl	100	2.8	0.0486	0.6059	-10.12	13.32	0.76	0.0519	
	O=C…O	124	2.93	0.052	0.9004	-14.19	19.33	0.73	3.0210	
	C-H…O	105	2.43	0.0736	1.1853	-19.66	25.95	0.76	0.3618	
	C-Cl…O **(C-O…Cl)**	61 **(78)**	3.35	0.0533	0.6952	-11.83	15.36	0.77	1.214	
$(ClCH(CN)CHO)_2$-A	**(1)**C-H…Cl	163	2.81	0.0486	0.5938	-9.31	12.71	0.73	0.594	-29.22
	(1)C-H…O	103	2.79	0.0371	0.5697	-8.97	12.23	0.73	0.7386	
	(2)C-H…O	121	2.31	0.0796	1.2842	-20.87	27.88	0.75	0.1538	
	C-Cl…O **(C-O…Cl)**	63 **(77)**	3.36	0.0533	0.6735	-11.59	14.94	0.78	0.8153	
	(2)C-H…Cl	113	2.97	0.0439	0.5914	-10.08	13.12	0.77	0.0525	
$(ClCH(NO_2)CHO)_2$-A	**(1)**C-H…Cl	160	2.81	0.0479	0.5914	-9.94	13.01	0.76	0.0505	-27.46
	(1)C-H…O	106	2.73	0.0412	0.6228	-9.93	13.43	0.74	0.4938	
	(2)C-H…O	114	2.37	0.0709	1.166	-18.54	25.14	0.74	0.2015	
	C-Cl…O **(C-O…Cl)**	62 **(81)**	3.37	0.0479	0.6276	-10.27	13.66	0.75	1.1038	
	(2) C-H…Cl	112	2.99	0.0412	0.56	-8.63	11.92	0.72	0.3637	
$(ClCH(NH_2)CHO)_2$-A	**(1)**C-H…Cl	156	2.64	0.0695	0.8642	-16.07	19.77	0.81	0.0152	-45.35
	C-H…O	103	2.63	0.054	0.8497	-14.06	18.59	0.76	0.3519	
	(2)C-H…Cl	110	2.89	0.0567	0.758	-12.72	16.67	0.76	1.1965	
	N-H…O	129	2.23	0.083	1.4025	-22.7	30.42	0.75	0.1416	
$(ClCH(CH_3)CHO)_2$-A	**(1)**C-H…Cl	165	2.79	0.052	0.618	-10.78	13.8	0.78	0.0516	-30.47
	(1)C-H…O	104	2.93	0.029	0.449	-6.9	9.56	0.72	3.4468	
	(2)C-H…O	127	2.35	0.0756	1.1418	-18.88	24.98	0.76	0.1370	
	(2)C-H…Cl	112	3.01	0.0439	0.6011	-9.32	12.83	0.73	4.4532	
$(ClCH(OCH_3)CHO)_2$-A	**(1)**C-H…Cl	120	3.08	0.0337	0.4321	-6.35	8.89	0.71	0.1801	-32.35
	(2)C-H…Cl	123	3.02	0.0364	0.4683	-7.64	10.21	0.75	0.2023	
	(1)C-H…O	157	2.44	0.0628	0.8618	-15.13	19.27	0.79	0.0847	
	(2)C-H…O	144	2.62	0.0391	0.5794	-7.64	10.21	0.75	0.2023	
	(3)C-H…Cl	157	2.58	0.081	0.9656	-19.19	22.73	0.84	0.0221	
$(ClCH(SCH_3)CHO)_2$-A	**(1)**C-H…Cl	121	3.07	0.0337	0.4225	-6.43	8.96	0.72	0.1410	-33.86
	(1) C-H…O	162	2.4	0.0661	0.9173	-16.32	20.63	0.79	0.0899	
	C-H…H	115	2.2	0.0533	0.7749	-13.66	17.37	0.79	1.9720	
	(2) C-H…O	152	2.54	0.0452	0.6663	-10.48	14.3	0.73	0.0873	
	(2)C-H…Cl	156	2.54	0.0864	1.0501	-21.34	24.96	0.86	0.0155	

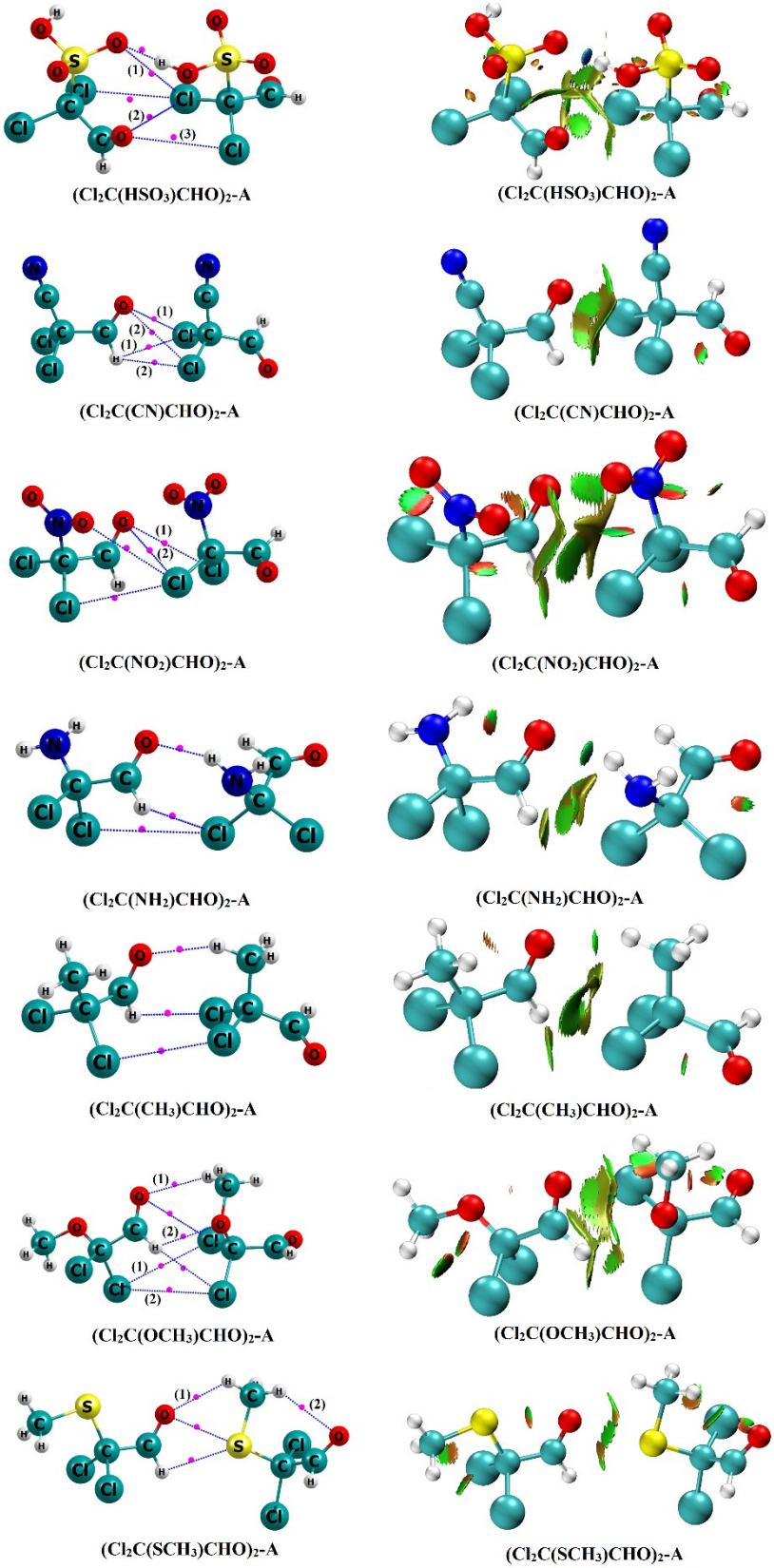

Figure S9. Interacting geometries of substituted di-chloroacetaldehyde **$(Cl_2C(Y)CHO)_2$** dimer on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S9: Geometrical and topological data for dimers of substituted di-chloroacetaldehydes **$(Cl_2C(Y)CHO)_2$-A.**

Conformers	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	V (kJ/mol)	G (kJ/mol)	$\lvert V/G\rvert$	ε	ΔE (kJ/mol)
$(Cl_2C(HSO_3)CHO)_2$-A	O-H…O	178	1.76	0.2308	2.5347	-91.23	80.07	1.14	0.0225	-54.47
	C-Cl…O **(S-O…Cl)**	101 **(117)**	3.49	0.0317	0.4321	-6.65	9.19	0.72	0.1473	
	C-Cl…Cl	154	3.42	0.0499	0.717	-10.75	15.10	0.71	0.1351	
	C-Cl…O **(C-O…Cl)**	92 **(74)**	3.48	0.0452	0.5649	-9.08	12.23	0.74	0.4125	
	C-Cl…O **(C-O…Cl)**	84 **(111)**	3.70	0.0196	0.2511	-3.60	5.20	0.69	0.2237	
$(Cl_2C(CN)CHO)_2$-A	**(1)**C-Cl…O **(C-O…Cl)**	74 **(87)**	3.31	0.0452	0.6663	-10.7	14.41	0.74	0.3923	-16.39
	(2)C-Cl…O **(C-O…Cl)**	72 **(84)**	3.35	0.0425	0.6276	-10.05	13.57	0.74	0.6092	
	(1) C-H…Cl	103	3.04	0.0378	0.5866	-8.88	12.41	0.72	3.4924	
	(2)C-H…Cl	107	2.97	0.0432	0.6107	-9.63	13.12	0.73	0.6033	
$(Cl_2C(NO_2)CHO)_2$-A	**(1)**C-Cl…O **(C-O…Cl)**	68 **(72)**	3.30	0.0452	0.6711	-11.15	14.55	0.77	0.8169	-25.87
	(2)C-Cl…O **(C-O…Cl)**	73 **(89)**	3.45	0.0513	0.6614	-10.71	14.47	0.74	0.0406	
	C-Cl…O **(N-O…Cl)**	110 **(116)**	3.59	0.0243	0.3331	-5.04	7.05	0.71	0.0898	
	C-Cl…Cl	130	3.71	0.0317	0.4225	-5.79	8.63	0.67	0.0271	
$(Cl_2C(NH_2)CHO)_2$-A	N-H…O	152	2.06	0.1309	1.8974	-40.39	46.00	0.88	0.0254	-30.05
	C-H…Cl	101	3.03	0.0432	0.6011	-9.32	12.84	0.73	0.8673	
	C-Cl…Cl	94	3.93	0.0223	0.2752	-3.71	5.62	0.66	0.3676	
$(Cl_2C(CH_3)CHO)_2$-A	C-H…O	156	2.35	0.0695	1.0308	-17.05	22.54	0.76	0.0284	-21.95
	C-H…Cl	92	2.89	0.0439	0.5625	-9.17	12.23	0.75	0.0227	
	C-Cl…Cl	133	3.8	0.0277	0.3573	-4.87	7.28	0.67	0.0200	
$(Cl_2C(OCH_3)CHO)_2$-A	**(1)**C-H…O	109	2.63	0.0479	0.7411	-11.89	16.01	0.74	0.1973	-25.58
	C-Cl…O **(C-O…Cl)**	83 **(75)**	3.65	0.0304	0.4152	-5.87	8.59	0.68	1.0811	
	(1)C-Cl…Cl	93	3.87	0.0263	0.3186	-4.37	6.53	0.67	0.0700	
	(2)C-H…O	109	2.63	0.0634	0.968	-15.99	21.16	0.76	0.2073	
	C-H…Cl	140	2.98	0.0344	0.4683	-7.18	9.94	0.72	0.6956	
	(2)C-Cl…Cl	98	4.05	0.0189	0.2269	-3.01	4.60	0.65	0.1282	
$(Cl_2C(SCH_3)CHO)_2$-A	**(1)**C-H…O	124	2.57	0.0499	0.7604	-14.4	18.57	0.78	6.111	-19.65
	(2)C-H…O	122	2.61	0.058	0.8352	-11.85	16.25	0.73	0.7387	
	C-S…O (C-O…S)	178**(94)**	3.03	0.0682	1.0332	-17.83	22.96	0.78	0.1142	
	C-H…S	102	2.92	0.0493	0.7387	-12.24	16.17	0.76	1.4021	

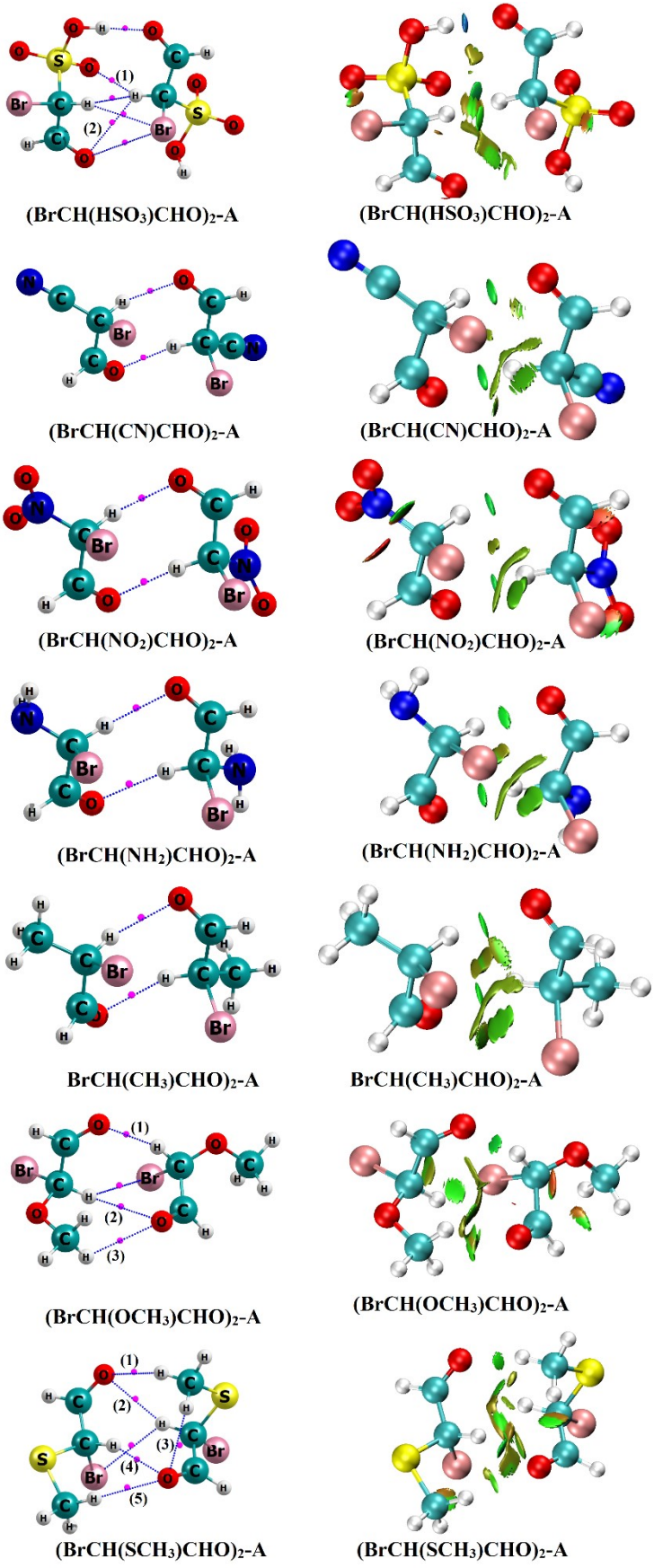

Figure S10. Interacting geometries for substituted bromo-acetaldehyde **(BrCH(Y)CHO)$_2$** dimer on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S10: Geometrical and topological data for dimers of substituted bromo-acetaldehydes **$(BrCH(Y)CHO)_2$-A.**

Conformers	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} $e\text{Å}^{-3}$	$\nabla^2\rho_{BCP}$ $e\text{Å}^{-5}$	V (kJ/mol)	G (kJ/mol)	$\lvert V/G \rvert$	ε	ΔE (kJ/mol)
$(BrCH(HSO_3)CHO)_2$-A	O-H…O=S	174	1.77	0.2308	2.6071	-89.57	78.52	1.14	0.0152	-69.93
	(1)C-H…O=S	152	2.11	0.1242	1.7839	-35.57	42.02	0.85	0.0093	
	C-H…H	107	2.35	0.0425	0.6156	-10.22	13.49	0.76	3.6902	
	C-H…Br	153	2.79	0.0634	0.7121	-14.01	16.69	0.84	0.0406	
	(2)C-H…O=C	124	2.89	0.0297	0.4297	-6.97	9.34	0.75	0.3272	
	C-Br…O **(C-O…Br)**	73 **(109)**	3.59	0.0324	0.4200	-6.86	9.13	0.75	0.0857	
$(BrCH(CN)CHO)_2$-A	*C-H…O	152	2.17	0.1019	1.5329	-27.92	34.79	0.8	0.0286	-37.12
$(BrCH(NO_2)CHO)_2$-A	*C-H…O	159	2.12	0.1154	1.6898	-32.65	39.28	0.83	0.018	-40.00
$(BrCH(NH_2)CHO)_2$-A	*C-H…O	163	2.25	0.0898	1.2939	-23.58	29.39	0.8	0.0218	-32.65
$(BrCH(CH_3)CHO)_2$-A	*C-H…O	152	2.27	0.0857	1.2625	-22.27	28.28	0.79	0.0706	-34.11
$(BrCH(OCH_3)CHO)_2$-A	**(1)**C-H…O	162	2.21	0.0958	1.4267	-25.88	32.33	0.8	0.006	-36.28
	C-H…Br	140	2.89	0.0553	0.6180	-11.61	14.21	0.82	0.0682	
	(2)C-H…O	132	2.75	0.0351	0.4707	-7.87	10.33	-0.76	0.2595	
	(3) C-H…O	110	2.66	0.0432	0.6952	-10.40	14.64	0.71	0.6968	
$(BrCH(SCH_3)CHO)_2$-A	**(1)** C-H…O	156	2.44	0.0594	0.8570	-14.16	18.74	0.76	0.0442	-47.03
	(2) C-H…O	154	2.55	0.0486	0.6711	-11.58	14.9	0.78	0.1167	
	C-H…Br	64	2.99	0.0479	0.5842	-10.51	13.19	0.8	0.3162	
	(3) C-H…O	117	2.64	0.056	0.8135	-13.65	17.89	0.76	3.1703	
	(4) C-H…O	151	2.18	0.1093	1.5908	-30.19	36.71	0.82	0.0301	
	(5) C-H…O	131	2.72	0.0304	0.4756	-7.12	10.01	0.71	0.3144	

*C-H…O are the unique interaction.

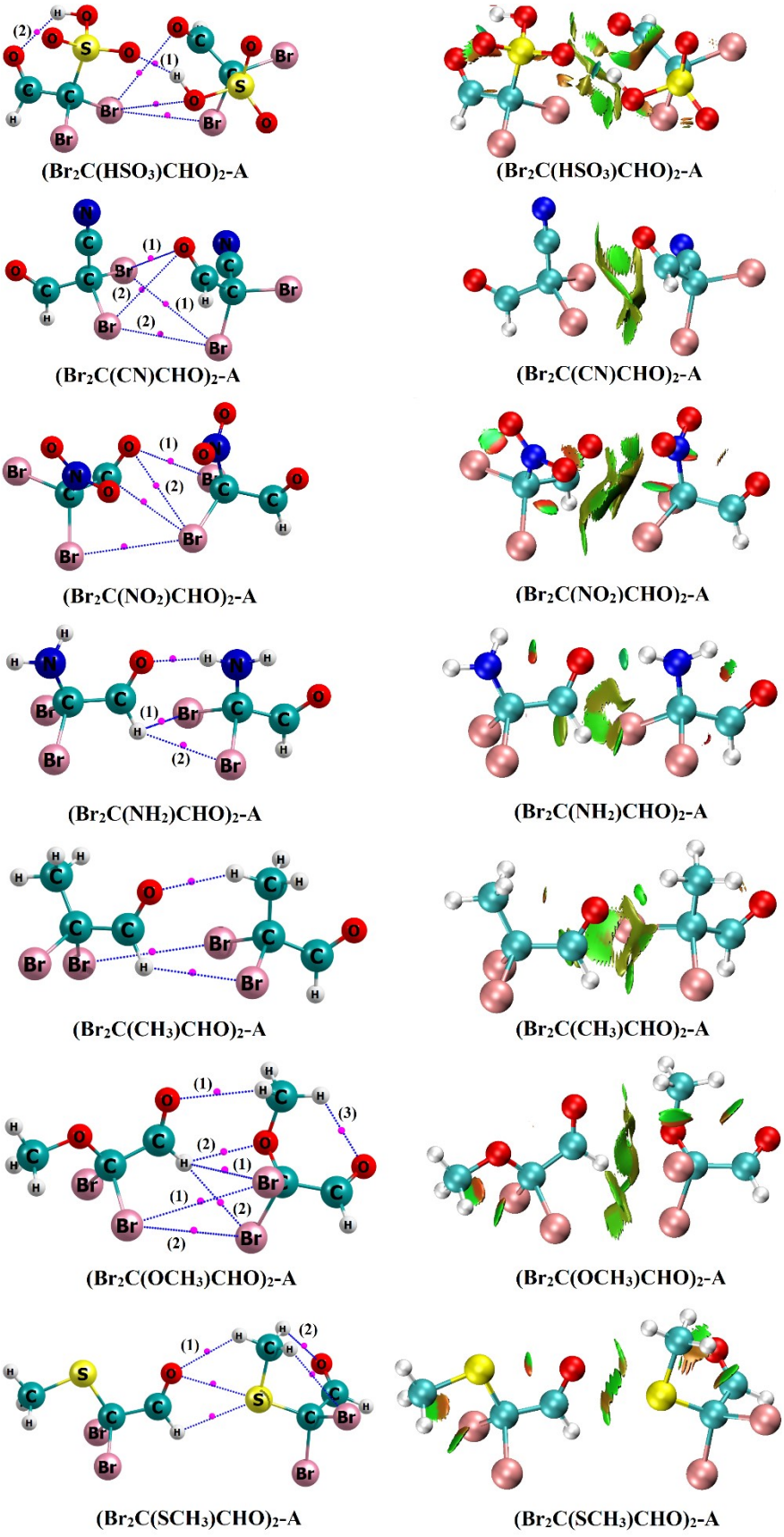

Figure S11. Interacting geometries of substituted di-bromoacetaldehyde **$(Br_2C(Y)CHO)_2$** dimer on the basis of stabilisation energy (ΔE) along with non-covalent interaction (NCI) Plots with RDG isosurface value 0.5 a.u. and colour is plotted in the range of -0.035<ρ* sign (λ_2) < 0.020 a.u.

Table S11: Geometrical and topological data for dimers of substituted di-bromoacetaldehyde **$(Br_2C(Y)CHO)_2$-A.**

Conformers	Contact Type	θ (deg.)	R_{ij} Å	ρ_{BCP} eÅ^{-3}	$\nabla^2\rho_{BCP}$ eÅ^{-5}	V (kJ/mol)	G (kJ/mol)	$\lvert V/G \rvert$	ε	ΔE (kJ/mol)
$(Br_2C(HSO_3)CHO)_2$-A	**(1)**O-H…O	131	2.04	0.1417	2.1654	-43.64	51.25	0.85	0.2127	-47.65
	C-Br…O **(C-O…Br)**	100 **(94)**	3.5	0.0385	0.4876	-7.77	10.53	0.74	0.1618	
	(2)O-H…O	149	1.86	0.1714	2.3947	-62.14	63.63	0.98	0.0426	
	C-Br…O **(S-O…Br)**	97 **(130)**	3.33	0.0513	0.7314	-11.86	15.87	0.75	0.1849	
	C-Br…Br	152	3.62	0.0526	0.618	-10.68	13.73	0.78	0.1641	
$(Br_2C(CN)CHO)_2$-A	**(1)**C-Br…O **(C-O…Br)**	76 **(99)**	3.37	0.0472	0.6252	-10.44	13.72	0.76	0.1638	-31.52
	(2)C-Br…O **(C-O…Br)**	70 **(78)**	3.6	0.0405	0.5021	-8.08	10.87	0.74	1.093	
	(1)C-Br…Br	99	4.11	0.0256	0.2969	-4.28	6.20	0.69	0.2322	
	(2)C-Br…Br	101	4.02	0.031	0.3476	-5.13	7.30	0.7	0.1262	
$((Br_2C(NO_2)CHO)_2$-A	**(1)**C-Br…O **(C-O…Br)**	68 **(92)**	3.41	0.0459	0.6204	-10.53	13.69	0.77	0.1366	-35.74
	(2)C-Br…O **(C-O…Br)**	66 **(74)**	3.48	0.0553	0.6518	-11.97	14.85	0.81	0.7839	
	C-Br…O **(N-O…Br)**	104 **(119)**	3.59	0.0304	0.4031	-6.34	8.65	0.73	0.0781	
	C-Br…Br	82	3.84	0.0398	0.4587	-7.32	9.90	0.74	0.0575	
$(Br_2C(NH_2)CHO)_2$-A	N-H…O	161	2.03	0.1357	1.9384	-42.81	47.76	0.9	0.0064	-41.76
	(1)C-H…Br	110	3.08	0.0439	0.5504	-9.27	12.11	0.77	0.3775	
	(2)C-H…Br	135	2.84	0.0614	0.6832	-13.07	15.83	0.83	0.0453	
$(Br_2C(CH_3)CHO)_2$-A	C-H…O	149	2.38	0.0648	0.9704	-15.70	21.05	0.75	0.0234	-30.26
	C-Br…Br	131	3.88	0.0385	0.4369	-6.86	9.35	0.73	0.0749	
	C-H…Br	122	2.99	0.0466	0.548	-9.65	12.29	0.79	0.052	
$((Br_2C(OCH_3)CHO)_2$-A	**(1)** C-H…O	117	2.68	0.0425	0.618	-10.11	13.47	0.75	0.1399	-36.12
	(2)C-H…O	115	2.42	0.0769	1.2118	-20.6	26.78	0.77	0.237	
	(3)C-H…O	125	2.38	0.0756	1.1418	-19.36	25.21	0.77	0.0303	
	(1)C-H…Br	102	3.23	0.0533	0.4828	-7.46	10.29	0.73	1.1433	
	(2)C-H…Br	160	2.86	0.0351	0.6301	-11.75	14.46	0.81	0.1910	
	(1)C-Br…Br	91	4.11	0.0265	0.2959	-4.14	6.09	0.68	0.0794	
	(2)C-Br…Br	89	4.24	0.0215	0.2410	-3.19	4.87	0.66	0.3544	
$(Br_2C(SCH_3)CHO)_2$-A	**(1)**C-H…O	125	2.54	0.052	0.8039	-12.48	17.07	0.73	0.5765	-20.73
	(2)C-H…O	118	2.49	0.0641	0.9922	-16.36	21.65	0.76	0.4575	
	C-H…Br	111	2.87	0.0675	0.9053	-16.83	20.73	0.81	4.9829	
	C-S…O (C-O…S)	177 **(92)**	3.03	0.0675	1.0404	-17.87	23.08	0.77	0.0868	
	C-H…S	104	2.86	0.054	0.7797	-13.23	17.22	0.77	0.4667	

Table S12: Cartesian Coordinates of acetaldehydes monomers, dimers and their derivatives optimized at MP2/aug-cc-pVDZ level.

CH_3CHO

C	-0.227067000	0.405111000	-0.000488000
O	-1.244515000	-0.278443000	0.000124000
H	-0.304708000	1.519270000	0.000966000
C	1.173874000	-0.152241000	0.000062000
H	1.152723000	-1.250049000	-0.000219000
H	1.714035000	0.220776000	-0.886119000
H	1.713225000	0.220320000	0.886936000

FCH_2CHO

C	0.700328000	-0.374753000	0.000080000
O	1.836020000	0.079210000	-0.000092000
H	0.494379000	-1.469498000	0.000292000
C	-0.523787000	0.524200000	0.000082000
F	-1.687318000	-0.263846000	-0.000094000
H	-0.528033000	1.156780000	0.900930000
H	-0.527889000	1.156972000	-0.900619000

F_2CHCHO

C	0.946151458	-0.001888634	0.393723219
O	2.006653358	0.000043393	-0.211804781
H	0.880115959	-0.004439268	1.503761930
C	-0.397184039	-0.000040747	-0.332844552
H	-0.304557911	0.000430221	-1.427130714
F	-1.108351694	-1.110531375	0.069051281
F	-1.105269236	1.112224213	0.070119690

F_3CCHO

C	1.065732816	-0.581496474	-0.000196854
O	2.059851017	0.118461090	-0.000116419
H	1.089866474	-1.692002449	0.000107423
C	-0.357814839	0.005301298	-0.000062972
F	-0.370695013	1.344092750	-0.002264349
F	-1.027611417	-0.440504076	-1.095601168
F	-1.025713787	-0.436757501	1.098130635

$ClCH_2CHO$

C	-1.157330504	-0.328212905	0.198947359
O	-2.278456795	-0.068347161	-0.213634175
H	-0.911006755	-1.311627239	0.659871260
C	-0.020631431	0.680248077	0.133747571
Cl	1.549955188	-0.168355946	-0.077775620
H	-0.172835941	1.369785522	-0.705888821
H	0.030030469	1.238459065	1.081106918

Cl_2CHCHO

C	1.353315251	-0.001593882	0.386822219
O	2.438212221	-0.002454324	-0.170909964
H	1.234295879	-0.001809257	1.492998994
C	0.043737558	-0.000367249	-0.396953847
H	0.220325594	-0.000465147	-1.478668345
Cl	-0.864855016	-1.477593586	0.041579044
Cl	-0.861182526	1.479574826	0.041582219

Cl_3CCHO

C	0.875790464	-0.004755187	-1.271301244
O	2.086793019	-0.005840529	-1.208864679
H	0.299019542	-0.006972439	-2.222434906
C	-0.050254376	0.000009525	-0.028879319
Cl	0.858793820	0.003857702	1.481080864
Cl	-1.073156115	1.465126170	-0.165363128
Cl	-1.076613230	-1.464150896	-0.157221736

$BrCH_2CHO$

C	-1.699362008	-0.203637431	0.343924057
O	-2.727716426	-0.251039905	-0.317089947
H	-1.506546688	-0.915620074	1.178469103
C	-0.612574668	0.822327427	0.090835907
Br	1.100651419	-0.104639383	-0.038385993
H	-0.793857797	1.359001916	-0.848072324
H	-0.529043617	1.515175828	0.941272756

Br_2CHCHO

C	0.000361957	1.734093736	-0.382990976
O	0.000928177	2.831520566	0.151339931
H	-0.000296868	1.593061649	-1.486899168
C	0.000032280	0.445896921	0.427663061
H	0.000080964	0.643423971	1.505823076
Br	-1.610467347	-0.542145267	-0.021385111
Br	1.610193763	-0.542671798	-0.021405749

Br_3CCHO

C	-0.132236632	-0.000620196	1.808870186
O	-1.185947070	-0.001857941	2.410939484
H	0.865093146	0.000195796	2.303060352
C	-0.017707329	-0.000058209	0.268001818
Br	-1.736820587	-0.000818637	-0.589388095
Br	1.003406320	1.597590877	-0.191452624
Br	1.005475932	-1.596236713	-0.192068058

FCH(HSO_3)CHO

C	1.691995569	-0.700068162	-0.290550590
O	2.725369197	-0.502561750	0.322505487
H	1.404447532	-1.695829988	-0.692304603
C	0.696924320	0.425039929	-0.586535300
H	0.510128456	0.540754060	-1.668327588
F	1.095793788	1.614534074	-0.035904147
S	-0.942502781	0.003576180	0.147041953
O	-1.299623339	-1.197169861	-0.962912089
O	-0.760574289	-0.654571619	1.461757957
O	-1.860520531	1.131362966	-0.068188722
H	-1.467403749	-1.999259693	-0.431685337

FCH(CN)CHO

C	1.223369427	-0.119425780	-0.348216622
O	1.919452355	-0.988738585	0.145197770
H	1.419832302	0.337311337	-1.342995236
C	-0.016800319	0.435864250	0.375633295
F	-0.259011096	1.733045965	-0.090251709
H	0.171438083	0.473992000	1.459315804
C	-1.187466867	-0.417508149	0.088068324
N	-2.104343182	-1.127484097	-0.165507064

FCH(NO_2)CHO

C	-1.405898536	0.061106214	0.429483960
O	-2.197213260	-0.819881829	0.143295378
H	-1.460557783	0.661621318	1.364197252
C	-0.232564934	0.434589991	-0.488165483
F	0.038942683	1.770703806	-0.351229228
H	-0.403206076	0.163305157	-1.536951398
N	0.971937207	-0.359465343	-0.017751780
O	1.058989511	-1.498028824	-0.489579445
O	1.705786987	0.165512885	0.822554703

FCH(NH_2)CHO

C	-0.944041099	-0.504638771	0.268323558
O	-1.813111012	0.163461265	-0.272015627
H	-1.136148845	-1.537064113	0.632536149
C	0.498594508	-0.020532077	0.427109012
F	1.235292849	-0.975808668	-0.387314883
H	0.882992037	-0.186731834	1.444303045
N	0.646645073	1.313775127	0.032629598
H	0.175170370	1.522250325	-0.844543076
H	1.611404520	1.630732190	0.028660240

$FCH(CH_3)CHO$

C	-0.953492205	-0.477627447	-0.191312392
O	-1.983683890	0.124173558	0.080850346
H	-0.941393626	-1.361994287	-0.869038162
C	0.402015956	-0.056518776	0.358146633
F	1.350226443	-1.021244356	-0.056137239
H	0.369278406	-0.086699871	1.459491491
C	0.812380212	1.315521412	-0.151489688
H	0.059445126	2.053437389	0.163814755
H	1.791626945	1.593898278	0.262300462
H	0.873049326	1.310917570	-1.250201359

$FCH(OCH_3)CHO$

C	-0.953492205	-0.477627447	-0.191312392
O	-1.983683890	0.124173558	0.080850346
H	-0.941393626	-1.361994287	-0.869038162
C	0.402015956	-0.056518776	0.358146633
F	1.350226443	-1.021244356	-0.056137239
H	0.369278406	-0.086699871	1.459491491
C	0.812380212	1.315521412	-0.151489688
H	0.059445126	2.053437389	0.163814755
H	1.791626945	1.593898278	0.262300462
H	0.873049326	1.310917570	-1.250201359

$FCH(SCH_3)CHO$

C	1.742492838	-0.019470548	-0.203582955
O	2.444087676	-0.797167425	0.425194449
H	2.064430517	0.438644547	-1.165549933
C	0.353363400	0.399297573	0.266216374
F	0.133277524	1.725867147	-0.169918285
H	0.291839136	0.399790237	1.365469394
S	-0.865979518	-0.732016709	-0.440900429
C	-2.325731363	-0.098506874	0.456481524
H	-2.192012506	-0.227606014	1.540382583
H	-2.497349366	0.956461419	0.205226579
H	-3.184185981	-0.698411837	0.121900213

ClCH(HSO_3)CHO

C	1.279265891	-1.318099034	-0.296016461
O	2.314887463	-1.361093627	0.341604023
H	0.757406634	-2.223351441	-0.671329075
C	0.579451204	0.000921827	-0.673187016
H	0.478389992	0.077728200	-1.769811084
Cl	1.399080616	1.431127061	-0.040980545
S	-1.157214333	-0.062233361	-0.076370331
O	-0.899812465	-0.275586515	1.543514254
O	-1.813286699	1.241533436	-0.291557085
O	-1.705221296	-1.342474526	-0.563696539
H	-0.829574240	0.616229023	1.936038887

ClCH(CN)CHO

C	-0.583865072	-1.345214605	0.121876929
O	-1.724798209	-1.406511323	-0.296160927
H	0.069794246	-2.237170905	0.244600012
C	0.089657972	-0.026109605	0.543092494
Cl	1.743974005	0.001113918	-0.182141751
H	0.231297025	-0.032488308	1.636684905
C	-0.677408263	1.155929491	0.139740894
N	-1.302939693	2.113597434	-0.177692958

ClCH(NO_2)CHO

C	-0.061469758	1.575911015	-0.112614740
O	-1.069567235	1.860083960	0.506584026
H	0.719864683	2.318431892	-0.385895630
C	0.257241528	0.144200800	-0.576134321
Cl	1.873704453	-0.294363841	0.004548808
H	0.227273162	0.054169229	-1.670222571
N	-0.814161423	-0.772909411	-0.040019029
O	-1.788139667	-0.894393161	-0.792861510
O	-0.676744146	-1.250531037	1.085204422

ClCH(NH_2)CHO

C	1.381758528	0.182418510	0.197968384
O	1.807097442	-0.861980525	-0.262884674
H	2.057189785	1.016454243	0.499250159
C	-0.095830825	0.528666593	0.421800306
H	-0.249375308	0.672861572	1.502978748
Cl	-1.154196435	-0.886026869	-0.028976159
N	-0.384978565	1.753920949	-0.261487646
H	-1.312003441	2.101534838	-0.021398870
H	-0.351967959	1.623495162	-1.273354981

ClCH(CH_3)CHO

C	-1.045683878	-0.795597885	0.191217141
O	-2.136045662	-0.524200866	-0.291508930
H	-0.760116021	-1.841961227	0.444154870
C	0.011590569	0.260610799	0.495807332
Cl	1.579146404	-0.393354383	-0.150243475
H	0.150359365	0.302831206	1.589227760
C	-0.298852851	1.624839801	-0.093025127
H	-1.251860859	1.989233372	0.319990307
H	0.500648245	2.336761534	0.154287448
H	-0.398478406	1.554650260	-1.185444352

ClCH(OCH_3)CHO

C	1.601754444	-0.018538137	0.288590517
O	2.232863402	-0.860772943	-0.324764545
H	2.084466755	0.853355465	0.785150339
C	0.081614478	-0.055528685	0.450206011
Cl	-0.493542453	1.597100859	-0.155583403
H	-0.201397982	-0.047429098	1.520004497
O	-0.461384881	-1.097315702	-0.247836990
C	-1.859019784	-1.295548145	0.033236035
H	-2.017670299	-1.412751910	1.119230520
H	-2.449488988	-0.445568302	-0.341846386
H	-2.143612367	-2.215922851	-0.488996291

ClCH(SCH_3)CHO

C	-1.653681020	-0.555536626	-0.253430922
O	-2.474751910	-1.122637363	0.451018828
H	-1.813356550	-0.386918000	-1.342267088
C	-0.335362906	-0.022123842	0.296038687
H	-0.319663805	-0.103662119	1.391934077
Cl	-0.285683746	1.754349054	-0.098057073
S	1.022523377	-0.955731683	-0.455382952
C	2.390786298	-0.221320447	0.501227165
H	2.257246302	-0.418138399	1.574866419
H	3.313242257	-0.707079232	0.151757981
H	2.446343559	0.858558336	0.305643783

$BrCH(HSO_3)CHO$

C	-0.319936331	1.858510716	0.342779855
O	-0.398276260	2.929793543	-0.235384920
H	-0.381437311	1.755242305	1.447728410
C	-0.159525244	0.544809145	-0.428814021
H	-0.101606265	0.713963828	-1.513315167
Br	-1.668575772	-0.595405369	-0.012524038
S	1.404839123	-0.248258215	0.088228135
O	1.404652852	-1.612492509	-0.846297299
O	1.299253974	-0.645107813	1.509617276
O	2.482814455	0.606728704	-0.437708962
H	0.974976801	-2.309179757	-0.313324791

BrCH(CN)CHO

C	1.300840976	-1.040711729	-0.391949946
O	1.841184394	-2.001581723	0.127257603
H	1.263920809	-0.883923389	-1.492512680
C	0.596399693	0.039375021	0.441439132
H	0.685514200	-0.193734437	1.511103206
Br	-1.306066602	-0.062066141	-0.028806822
C	1.111144162	1.373396469	0.127661365
N	1.569015835	2.432894519	-0.155902497

$BrCH(NO_2)CHO$

C	0.628018563	1.570504411	0.378864981
O	0.832138633	2.633674422	-0.183323404
H	0.596988668	1.451638500	1.482450375
C	0.364896289	0.290828408	-0.421679653
Br	-1.436823125	-0.287795164	-0.025068185
H	0.478732369	0.438170404	-1.501045134
N	1.332892713	-0.781164576	0.004774237
O	2.010578265	-1.298788298	-0.891804955
O	1.397951881	-1.024489271	1.215059228

$BrCH(NH_2)CHO$

C	-1.591076705	-0.393077623	0.380653071
O	-2.459764552	-1.041072627	-0.186468304
H	-1.473598298	-0.380184749	1.487760668
C	-0.596466370	0.484632167	-0.367742204
Br	1.169846323	-0.276712075	0.011474150
H	-0.736974042	0.374394491	-1.454732070
N	-0.645331126	1.828788947	0.182218481
H	0.112045874	2.396152155	-0.201084709
H	-1.525398929	2.272292928	-0.094789933

$BrCH(CH_3)CHO$

C	-1.571587107	-0.468028701	0.368382508
O	-2.516324075	-1.025185668	-0.173872827
H	-1.379041203	-0.569324339	1.462681900
C	-0.601863978	0.430694188	-0.377189076
H	-0.754209345	0.317425385	-1.458749584
Br	1.195000764	-0.265858121	0.007887916
C	-0.713836825	1.877993964	0.091240212
H	-1.715833946	2.265015153	-0.158534095
H	-0.564118823	1.946760018	1.179955196
H	0.042490816	2.502691940	-0.405055550

$BrCH(OCH_3)CHO$

C	1.302470313	-0.958223050	-0.391062516
O	1.889977712	-1.966835945	-0.025031671
H	1.264669065	-0.654052496	-1.460426018
C	0.554104672	-0.069763553	0.601492495
Br	-1.342419491	-0.143467361	-0.054107845
H	0.535631095	-0.533186296	1.595067231
O	1.016673852	1.224240453	0.741163538
C	1.184575972	1.967179910	-0.484421554
H	0.270427566	1.909533986	-1.095770505
H	1.361402667	3.003614828	-0.175442896
H	2.052443594	1.601051697	-1.054758739

$BrCH(SCH_3)CHO$

C	-0.569150240	1.455072861	-0.418564387
O	-1.291886239	2.316634277	0.066717080
H	-0.202420352	1.497187961	-1.468764264
C	-0.179506448	0.204821758	0.345290801
H	-0.351461537	0.321082000	1.425210330
Br	1.708055570	-0.158393863	0.054192513
S	-1.154121292	-1.180380126	-0.342107800
C	-2.771558433	-0.679630808	0.349005625
H	-2.741681615	-0.701305379	1.448108359
H	-3.063844724	0.319392337	-0.005380674
H	-3.500210105	-1.421143603	-0.010312606

$F_2C(HSO_3)CHO$

C	1.704051285	-0.452040140	0.564886130
O	2.314722889	-1.201945157	-0.173246281
H	1.811672179	-0.431456732	1.669320853
C	0.692657564	0.571205564	0.011496905
F	0.590313626	1.625503390	0.866419793
F	1.037904972	1.012050430	-1.218765585
S	-1.017336382	-0.175900634	-0.146559873
O	-1.035858115	-0.863934777	1.374701420
O	-1.998638439	0.915926441	-0.171155502
O	-0.964257258	-1.272512531	-1.134605765
H	-1.096261581	-1.827375514	1.222901105

$F_2C(CN)CHO$

C	-1.091754578	-0.551412748	-0.580561418
O	-1.988995242	-0.986540383	0.112085033
H	-1.001315012	-0.731285387	-1.673650053
C	0.041042458	0.331217861	0.003496803
F	-0.284779382	0.766908011	1.246366412
F	0.170981403	1.426149620	-0.823653805
C	1.330861202	-0.401687337	0.041080030
N	2.322365796	-1.054658724	0.026924009

$F_2C(NO_2)CHO$

C	1.428917746	0.633089669	-0.000968924
O	1.131320632	1.811558406	-0.037811831
H	2.472047285	0.251828044	0.028636956
C	0.364355470	-0.482309078	0.004730845
F	0.502296103	-1.260576409	-1.090539058
F	0.501583301	-1.251757670	1.106900160
N	-1.031224639	0.130180249	0.004109591
O	-1.486672151	0.413348287	1.112897326
O	-1.525651347	0.342996817	-1.103488555

$F_2C(NH_2)CHO$

C	1.059993889	-0.581983318	0.150020163
O	2.072160738	0.026389540	-0.141509405
H	1.076251273	-1.617022795	0.563419250
C	-0.351186894	0.004698036	-0.011078855
F	-0.316156418	1.241928732	-0.571923658
F	-0.833820887	0.190430254	1.302435387
N	-1.167950281	-0.839563519	-0.791246990
H	-2.073765733	-0.403834738	-0.964259375
H	-1.307169407	-1.740835454	-0.336609648

$F_2C(CH_3)CHO$

C	-1.086202980	-0.564137873	-0.000865205
O	-2.068829039	0.159797241	-0.000287872
H	-1.152186620	-1.674461281	-0.001612932
C	0.349141095	-0.020262197	-0.000135999
F	0.972931002	-0.579727435	-1.109072433
F	0.970873561	-0.580150777	1.109922821
C	0.502815755	1.473631107	0.000237071
H	0.020792962	1.890553457	-0.894116930
H	0.020028830	1.890346019	0.894268275
H	1.573232849	1.718699970	0.000694281

$F_2C(OCH_3)CHO$

C	-1.583919054	0.070949969	-0.001080580
O	-2.118637318	-1.021209430	-0.000013229
H	-2.147072657	1.029629699	-0.002647474
C	-0.058785242	0.269588820	-0.000134940
F	0.257722550	1.064519413	-1.096691802
F	0.256332930	1.061822197	1.098906938
O	0.603857917	-0.896280736	-0.001181124
C	2.050867704	-0.766383597	-0.000131236
H	2.383569908	-0.238276344	-0.903556394
H	2.382298824	-0.238063086	0.903628362
H	2.423955128	-1.795370874	0.000276760

$F_2C(SCH_3)CHO$

C	-1.674585638	-0.241114322	-0.496601098
O	-2.490337239	-0.684185965	0.290828408
H	-1.829819784	-0.215909609	-1.597243737
C	-0.314187350	0.318492736	-0.045645242
F	-0.405502176	0.855763222	1.212080489
F	0.006068076	1.375434331	-0.887175183
S	0.927288935	-0.991164334	-0.138321112
C	2.394884776	0.051651933	0.180510297
H	2.525213723	0.783762836	-0.625959005
H	2.297773342	0.546528442	1.155564359
H	3.251149128	-0.637233656	0.200416887

$Cl_2C(HSO_3)CHO$

C	1.287617366	-0.414375949	-1.275563767
O	2.146426532	-1.269912154	-1.214630065
H	0.945011611	0.061485105	-2.219292652
C	0.567736278	0.149039597	-0.019337195
Cl	1.161885381	-0.567687594	1.475604409
Cl	0.743206162	1.918267528	-0.048966358
S	-1.244262932	-0.276292438	-0.219321215
O	-1.348687596	-1.745099035	-0.096220828
O	-1.742467966	0.481493616	-1.378161710
O	-1.896851724	0.434827062	1.114928309
H	-1.822831469	-0.219126478	1.837659016

$Cl_2C(CN)CHO$

C	-0.667769829	-0.004759949	-1.382939651
O	-1.875185091	-0.005204987	-1.506932760
H	0.054555528	-0.007747684	-2.228543199
C	0.033564125	0.000122240	-0.002435803
Cl	1.058503197	-1.474096254	0.056919363
Cl	1.059038195	1.474121125	0.046833774
C	-0.909129160	0.004029685	1.117592187
N	-1.684466435	0.007516434	2.018128037

$Cl_2C(NO_2)CHO$

C	0.151658495	0.011205328	1.592935176
O	1.312523093	-0.009007655	1.948720091
H	-0.719783190	0.035139486	2.282549442
C	-0.260623499	0.003468228	0.100623054
Cl	-1.212936698	-1.453310171	-0.205598591
Cl	-1.192088702	1.468782785	-0.230884267
N	1.045425639	-0.010575607	-0.726589468
O	1.547802177	1.089179073	-0.950665340
O	1.507302126	-1.119194006	-0.990249915

$Cl_2C(NH_2)CHO$

C	1.166483402	-0.436097617	-0.738877493
O	2.303837713	-0.614311814	-0.339245480
H	0.873062555	-0.469604062	-1.809066511
C	0.018345517	-0.103879611	0.227998134
Cl	-0.321968901	1.685775620	-0.165427687
Cl	-1.443080646	-1.022531844	-0.262144355
N	0.365128598	-0.369901247	1.555097944
H	-0.289390104	0.021504705	2.228578654
H	1.326600796	-0.083377167	1.742763776

$Cl_2C(HSO_3)CHO$

C	1.287617366	-0.414375949	-1.275563767
O	2.146426532	-1.269912154	-1.214630065
H	0.945011611	0.061485105	-2.219292652
C	0.567736278	0.149039597	-0.019337195
Cl	1.161885381	-0.567687594	1.475604409
Cl	0.743206162	1.918267528	-0.048966358
S	-1.244262932	-0.276292438	-0.219321215
O	-1.348687596	-1.745099035	-0.096220828
O	-1.742467966	0.481493616	-1.378161710
O	-1.896851724	0.434827062	1.114928309
H	-1.822831469	-0.219126478	1.837659016

$Cl_2C(CN)CHO$

C	-0.667769829	-0.004759949	-1.382939651
O	-1.875185091	-0.005204987	-1.506932760
H	0.054555528	-0.007747684	-2.228543199
C	0.033564125	0.000122240	-0.002435803
Cl	1.058503197	-1.474096254	0.056919363
Cl	1.059038195	1.474121125	0.046833774
C	-0.909129160	0.004029685	1.117592187
N	-1.684466435	0.007516434	2.018128037

$Cl_2C(NO_2)CHO$

C	0.151658495	0.011205328	1.592935176
O	1.312523093	-0.009007655	1.948720091
H	-0.719783190	0.035139486	2.282549442
C	-0.260623499	0.003468228	0.100623054
Cl	-1.212936698	-1.453310171	-0.205598591
Cl	-1.192088702	1.468782785	-0.230884267
N	1.045425639	-0.010575607	-0.726589468
O	1.547802177	1.089179073	-0.950665340
O	1.507302126	-1.119194006	-0.990249915

$Cl_2C(NH_2)CHO$

C	1.166483402	-0.436097617	-0.738877493
O	2.303837713	-0.614311814	-0.339245480
H	0.873062555	-0.469604062	-1.809066511
C	0.018345517	-0.103879611	0.227998134
Cl	-0.321968901	1.685775620	-0.165427687
Cl	-1.443080646	-1.022531844	-0.262144355
N	0.365128598	-0.369901247	1.555097944
H	-0.289390104	0.021504705	2.228578654
H	1.326600796	-0.083377167	1.742763776

$Cl_2C(CH_3)CHO$

C	-0.760569526	-1.280094582	0.025443900
O	-1.904699952	-1.271137199	-0.386376652
H	-0.218566608	-2.221343213	0.277428581
C	0.090456501	-0.024449576	0.287825856
Cl	1.643799164	-0.315819332	-0.599022825
Cl	-0.711684661	1.432079580	-0.349714723
C	0.380174694	0.125522960	1.776253817
H	-0.564059026	0.309413642	2.311707108
H	0.851678502	-0.793524039	2.157753042
H	1.062225959	0.972254714	1.935518706

$Cl_2C(OCH_3)CHO$

C	0.184466426	1.027025088	-1.072937035
O	0.698344103	2.084803312	-0.766908011
H	-0.099092144	0.760399660	-2.116774614
C	-0.138100974	-0.127334334	-0.090017283
Cl	0.244214771	0.345808865	1.600237293
Cl	-1.897824881	-0.422098233	-0.254609929
O	0.485562460	-1.299747167	-0.482174667
C	1.933385592	-1.237019025	-0.422694086
H	2.317720149	-0.355450475	-0.961044623
H	2.268305578	-1.210088666	0.623438005
H	2.274683222	-2.154427163	-0.914733676

$Cl_2C(SCH_3)CHO$

C	-0.066375761	0.803212746	-1.340172605
O	0.567302882	1.842635928	-1.374811489
H	-0.448476660	0.283329966	-2.246579676
C	-0.342172359	0.011535535	-0.050760798
Cl	-0.232616793	1.051280986	1.391035005
Cl	-1.975917685	-0.717401363	-0.186214299
S	0.841951166	-1.382012004	-0.046891984
C	2.387596946	-0.439803974	0.191720388
H	2.507017435	0.331446466	-0.582872864
H	2.406380093	0.010720602	1.192428963
H	3.196227938	-1.180014464	0.099113840

$Br_2C(HSO_3)CHO$

C	-0.027659566	0.092075783	1.846749752
O	-1.115927395	0.083350708	2.401370901
H	0.931936699	0.164594762	2.401601093
C	0.150575799	0.029208467	0.319831554
Br	0.604309306	1.819460081	-0.253347841
Br	1.554877277	-1.239027782	-0.078194405
S	-1.396208771	-0.563053060	-0.539202512
O	-2.463736557	0.553197663	0.014580950
O	-1.274303266	-0.322397535	-1.982837206
O	-1.691084855	-1.885287085	0.048341400
H	-2.541218160	0.370510859	0.978497418

$Br_2C(CN)CHO$

C	-0.000701160	1.123931730	-1.370018731
O	-0.001400732	2.334764419	-1.463667228
H	-0.000635542	0.424932506	-2.235238350
C	0.000027517	0.392055253	-0.010228467
Br	-1.606844071	-0.718791512	0.014749757
Br	1.607249420	-0.718117340	0.014266089
C	0.000013229	1.296491669	1.133873383
N	0.000229663	2.044840905	2.058180934

$Br_2C(NO_2)CHO$

C	0.000382066	0.741989584	1.601464455
O	0.000519652	1.933053798	1.842253333
H	0.000534469	-0.056985510	2.374299251
C	-0.000016404	0.189484614	0.159202446
Br	1.594493603	-0.867911544	-0.070611295
Br	-1.594882019	-0.867260127	-0.070280030
N	0.000220667	1.407919463	-0.787307265
O	-1.103177928	1.867282358	-1.077789062
O	1.103823524	1.867627382	-1.076459768

$Br_2C(NH_2)CHO$

C	0.228523607	1.550235334	-0.780148026
O	0.612550712	2.670270733	-0.486917683
H	0.056800828	1.207445425	-1.822018124
C	-0.021800515	0.487627839	0.295679905
Br	-1.682849270	-0.450530926	-0.114318690
Br	1.497844670	-0.811403880	-0.069150237
N	-0.051209541	1.037672134	1.576456596
H	0.663751257	1.758414723	1.686119585
H	-0.027660624	0.348810888	2.324261309

$Br_2C(CH_3)CHO$

C	0.000083081	1.543820648	-0.803867867
O	0.000127532	2.728954373	-0.513120424
H	-0.000050272	1.174531130	-1.853359175
C	0.000076731	0.444535877	0.261467537
Br	-1.601106731	-0.627058636	-0.100182249
Br	1.600981316	-0.627216860	-0.100252101
C	0.000249772	0.952589429	1.688502470
H	-0.895088500	1.570146687	1.853902640
H	0.000623371	0.107084308	2.389617874
H	0.895422940	1.570568441	1.853390926

$Br_2C(OCH_3)CHO$

C	-0.086315159	1.101367612	1.314792735
O	-0.316093975	2.294478684	1.403144168
H	0.101410470	0.440072796	2.189043293
C	-0.009300819	0.373235064	-0.041046692
Br	1.823756471	-0.283216722	-0.169153624
Br	-1.243643795	-1.193130122	0.167999489
O	-0.249679056	1.108226279	-1.157527606
C	-1.596815633	1.640088573	-1.288101034
H	-2.295090942	0.813095660	-1.481022655
H	-1.887127563	2.201580031	-0.391334513
H	-1.542372819	2.307601222	-2.155089693

$Br_2C(SCH_3)CHO$

C	0.182221127	-0.566088420	1.622434691
O	0.803794312	-1.533565193	2.021280875
H	-0.322627727	0.158565317	2.300419757
C	0.015306981	-0.218158083	0.130053776
Br	-1.912651899	-0.232187102	-0.189921715
Br	0.687595455	1.639041331	-0.007904850
S	0.747916898	-1.356679760	-1.052555774
C	2.508669526	-1.196868760	-0.600066892
H	2.821239710	-0.146251891	-0.683156716
H	2.690455670	-1.592884904	0.406662661
H	3.053709392	-1.797243103	-1.343871024

$(CH_3CHO)_2$-A

C	-0.279496000	1.750807000	0.000193000
O	0.939964000	1.584937000	-0.003914000
H	-0.955435000	0.866808000	0.002195000
C	-0.939964000	3.105167000	0.002873000
H	-0.188344000	3.905465000	0.000457000
H	-1.594504000	3.190335000	-0.880661000
H	-1.588351000	3.189823000	0.890933000
C	0.279496000	-1.750807000	0.000193000
O	-0.939964000	-1.584937000	-0.003914000
H	0.955435000	-0.866808000	0.002195000
C	0.939964000	-3.105167000	0.002873000
H	1.588351000	-3.189823000	0.890933000
H	0.188344000	-3.905465000	0.000457000
H	1.594504000	-3.190335000	-0.880661000

$(CH_3CHO)_2$-B

C	0.198756000	2.356319000	0.000000000
O	1.209176000	1.657902000	0.000000000
H	0.301214000	3.467927000	0.000000000
C	-1.209176000	1.825105000	0.000000000
H	-1.223723000	0.726866000	0.000000000
H	-1.737618000	2.218860000	0.884804000
H	-1.737618000	2.218860000	-0.884804000
C	-0.198756000	-2.356319000	0.000000000
O	-1.209176000	-1.657902000	0.000000000
H	-0.301214000	-3.467927000	0.000000000
C	1.209176000	-1.825105000	0.000000000
H	1.737618000	-2.218860000	0.884804000
H	1.737618000	-2.218860000	-0.884804000
H	1.223723000	-0.726866000	0.000000000

$(CH_3CHO)_2$-C

C	-1.097003000	1.104543000	0.000000000
O	-1.881760000	0.156974000	0.000000000
H	0.000000000	0.915953000	0.000000000
C	-1.528161000	2.549059000	0.000000000
H	-2.623144000	2.629648000	0.000000000
H	-1.105768000	3.052600000	0.885656000
H	-1.105768000	3.052600000	-0.885656000
C	1.948823000	-1.475447000	0.000000000
O	2.098454000	-0.256009000	0.000000000
H	2.847411000	-2.135475000	0.000000000
C	0.595953000	-2.149353000	0.000000000
H	0.021513000	-1.826017000	0.881750000
H	0.021513000	-1.826017000	-0.881750000
H	0.693028000	-3.243821000	0.000000000

$(CH_3CHO)_2$-D

C	0.593615000	2.256897000	0.000000000
O	-0.593615000	1.943374000	0.000000000
H	0.874964000	3.336733000	0.000000000
C	1.721847000	1.251013000	0.000000000
H	2.701667000	1.748820000	0.000000000
H	1.632478000	0.597474000	0.881088000
H	1.632478000	0.597474000	-0.881088000
C	-0.593615000	-2.256897000	0.000000000
O	0.593615000	-1.943374000	0.000000000
H	-0.874964000	-3.336733000	0.000000000
C	-1.721847000	-1.251013000	0.000000000
H	-1.632478000	-0.597474000	-0.881088000
H	-2.701667000	-1.748820000	0.000000000
H	-1.632478000	-0.597474000	0.881088000

$(CH_3CHO)_2$-E

C	-1.401805000	-1.964179000	0.000000000
O	-0.216002000	-1.646883000	0.000000000
H	-1.685170000	-3.041897000	0.000000000
C	-2.527159000	-0.951801000	0.000000000
H	-3.512048000	-1.438851000	0.000000000
H	-2.436241000	-0.308544000	0.889381000
H	-2.436241000	-0.308544000	-0.889381000
C	1.010349000	1.496080000	0.000000000
O	1.125296000	2.718991000	0.000000000
H	0.000000000	1.027313000	0.000000000
C	2.167416000	0.531643000	0.000000000
H	2.090602000	-0.126101000	-0.880895000
H	3.121340000	1.075399000	0.000000000
H	2.090602000	-0.126101000	0.880895000

$(FCH_2CHO)_2$-A

C	1.642195000	0.493815000	0.854291000
O	0.735477000	0.002021000	1.509285000
H	2.143541000	1.440967000	1.166858000
C	2.198548000	-0.086373000	-0.426324000
H	2.057904000	0.647080000	-1.237495000
H	3.276992000	-0.281910000	-0.297086000
F	1.565802000	-1.277139000	-0.775468000
C	-1.716955000	-0.562845000	-0.151430000
O	-2.704378000	-1.118436000	0.311797000
H	-0.870550000	-1.118325000	-0.606494000
C	-1.592723000	0.951531000	-0.123151000
F	-0.466145000	1.361213000	-0.875711000
H	-2.484320000	1.416833000	-0.567178000
H	-1.455660000	1.293246000	0.913035000

$(FCH_2CHO)_2$-B

C	-1.425106000	1.180662000	0.223753000
O	-0.526967000	1.350926000	-0.591813000
H	-1.595199000	1.883672000	1.070066000
C	-2.365789000	-0.005086000	0.159120000
H	-2.754368000	-0.132646000	-0.862167000
H	-1.829552000	-0.910532000	0.480614000
F	-3.446907000	0.213488000	1.031681000
C	1.425106000	-1.180662000	-0.223753000
O	0.526967000	-1.350926000	0.591813000
H	1.595199000	-1.883672000	-1.070066000
C	2.365789000	0.005086000	-0.159120000
H	1.829552000	0.910532000	-0.480614000
H	2.754368000	0.132646000	0.862167000
F	3.446907000	-0.213488000	-1.031681000

$(FCH_2CHO)_2$-C

C	-0.795188000	1.622418000	-0.067785000
O	-1.315063000	0.738233000	-0.740038000
H	0.113123000	1.437554000	0.544008000
C	-1.369325000	3.026971000	-0.035244000
H	-2.398956000	3.005154000	0.353844000
F	-0.590135000	3.839672000	0.804819000
H	-1.363830000	3.460751000	-1.047080000
C	0.795188000	-1.622418000	0.067785000
O	1.315063000	-0.738233000	0.740038000
H	-0.113123000	-1.437554000	-0.544008000
C	1.369325000	-3.026971000	0.035244000
F	0.590135000	-3.839672000	-0.804819000
H	2.398956000	-3.005154000	-0.353844000
H	1.363830000	-3.460751000	1.047080000

$(FCH_2CHO)_2$-D

C	0.329805000	1.522712000	-0.044591000
O	-0.329805000	1.842596000	-1.025407000
H	-0.101551000	1.517438000	0.982753000
C	1.785935000	1.106573000	-0.149766000
H	2.415357000	1.987510000	-0.352252000
F	2.189292000	0.545186000	1.075770000
H	1.915138000	0.356386000	-0.943040000
C	-0.329805000	-1.522712000	-0.044591000
O	0.329805000	-1.842596000	-1.025407000
H	0.101551000	-1.517438000	0.982753000
C	-1.785935000	-1.106573000	-0.149766000
H	-1.915138000	-0.356386000	-0.943040000
H	-2.415357000	-1.987510000	-0.352252000
F	-2.189292000	-0.545186000	1.075770000

$(FCH_2CHO)_2$-E

C	1.105296000	1.174275000	0.000000000
O	1.646848000	0.074619000	0.000000000
H	0.000000000	1.288923000	0.000000000
C	1.916625000	2.456434000	0.000000000
F	1.052011000	3.563240000	0.000000000
H	2.548361000	2.503594000	0.900349000
H	2.548361000	2.503594000	-0.900349000
C	-0.799303000	-2.388319000	0.000000000
O	-0.776054000	-3.613244000	0.000000000
H	0.121921000	-1.765355000	0.000000000
C	-2.118378000	-1.633018000	0.000000000
H	-2.699841000	-1.881058000	-0.900726000
H	-2.699841000	-1.881058000	0.900726000
F	-1.875427000	-0.242781000	0.000000000

$(F_2CHCHO)_2$-A

C	-1.939917000	1.100679000	0.019585000
O	-1.346018000	1.482887000	-0.974863000
H	-2.358706000	1.801629000	0.774092000
C	-2.222348000	-0.376811000	0.311017000
F	-1.630615000	-1.178109000	-0.623057000
H	-1.903384000	-0.690900000	1.313846000
F	-3.595297000	-0.546876000	0.220163000
C	1.186713000	0.213720000	0.222817000
O	0.472279000	0.240634000	1.217314000
H	0.815278000	0.486547000	-0.786542000
C	2.652674000	-0.199080000	0.312584000
H	2.974941000	-0.465041000	1.328251000
F	2.850273000	-1.270752000	-0.528431000
F	3.419977000	0.845576000	-0.153706000

$(F_2CHCHO)_2$-B

C	0.991104000	1.666188000	-0.121427000
O	1.540545000	1.019615000	-1.001024000
H	1.547516000	2.154218000	0.707409000
C	-0.524162000	1.857836000	-0.086165000
F	-0.991104000	1.301196000	1.088674000
F	-0.784239000	3.209670000	-0.034923000
H	-1.050649000	1.408235000	-0.937437000
C	-0.991104000	-1.666188000	-0.121427000
O	-1.540545000	-1.019615000	-1.001024000
H	-1.547516000	-2.154218000	0.707409000
C	0.524162000	-1.857836000	-0.086165000
F	0.784239000	-3.209670000	-0.034923000
H	1.050649000	-1.408235000	-0.937437000
F	0.991104000	-1.301196000	1.088674000

$(F_2CHCHO)_2$-C

C	0.390642000	-1.439092000	0.000000000
O	1.454603000	-0.835395000	0.000000000
H	-0.593981000	-0.928025000	0.000000000
C	0.341302000	-2.964597000	0.000000000
H	1.332281000	-3.437709000	0.000000000
F	-0.363107000	-3.373187000	1.111620000
F	-0.363107000	-3.373187000	-1.111620000
C	0.088091000	3.534280000	0.000000000
O	-1.018974000	4.045122000	0.000000000
H	1.023086000	4.137532000	0.000000000
C	0.266170000	2.005076000	0.000000000
F	-0.363107000	1.488561000	1.111382000
F	-0.363107000	1.488561000	-1.111382000
H	1.308218000	1.659629000	0.000000000

$(F_2CHCHO)_2$-D

C	-1.297239000	0.289676000	0.000512000
O	-0.586303000	1.284920000	-0.001568000
H	-0.890842000	-0.742129000	0.003554000
C	-2.819749000	0.398453000	-0.000998000
F	-3.297533000	-0.263332000	-1.111479000
F	-3.299567000	-0.257999000	1.111665000
H	-3.188463000	1.432765000	-0.003839000
C	2.705433000	0.700033000	-0.000981000
O	3.888825000	1.008208000	-0.001792000
H	1.874389000	1.433835000	-0.001250000
C	2.277986000	-0.767681000	0.000742000
H	3.123449000	-1.468543000	0.001316000
F	1.491518000	-1.000351000	1.112587000
F	1.490328000	-1.003190000	-1.109279000

$(F_2CHCHO)_2$-E

C	0.097305000	1.799300000	0.000000000
O	-1.016589000	1.291655000	0.000000000
H	1.028541000	1.197110000	0.000000000
C	0.278674000	3.314860000	0.000000000
H	-0.666960000	3.873113000	0.000000000
F	1.016589000	3.660930000	1.111719000
F	1.016589000	3.660930000	-1.111719000
C	-0.097305000	-1.799300000	0.000000000
O	1.016589000	-1.291655000	0.000000000
H	-1.028541000	-1.197110000	0.000000000
C	-0.278674000	-3.314860000	0.000000000
F	-1.016589000	-3.660930000	-1.111719000
H	0.666960000	-3.873113000	0.000000000
F	-1.016589000	-3.660930000	1.111719000

$(F_3CCHO)_2$-A

C	0.081873000	1.789306000	0.000000000
O	-1.011611000	1.251631000	0.000000000
H	1.037465000	1.228648000	0.000000000
C	0.234592000	3.320514000	0.000000000
F	-0.940148000	3.963628000	0.000000000
F	0.940148000	3.700291000	1.096960000
F	0.940148000	3.700291000	-1.096960000
C	-0.081873000	-1.789306000	0.000000000
O	1.011611000	-1.251631000	0.000000000
H	-1.037465000	-1.228648000	0.000000000
C	-0.234592000	-3.320514000	0.000000000
F	-0.940148000	-3.700291000	-1.096960000
F	0.940148000	-3.963628000	0.000000000
F	-0.940148000	-3.700291000	1.096960000

$(F_3CCHO)_2$-B

C	-0.314301000	1.519204000	0.000000000
O	0.849088000	1.158740000	0.000000000
H	-1.177596000	0.823943000	0.000000000
C	-0.667893000	3.021149000	0.000000000
F	-2.012953000	3.184453000	0.000000000
F	-0.165573000	3.629699000	1.095280000
F	-0.165573000	3.629699000	-1.095280000
C	1.552651000	-2.197633000	0.000000000
O	2.471837000	-2.996052000	0.000000000
H	1.670979000	-1.095586000	0.000000000
C	0.092054000	-2.701143000	0.000000000
F	-0.165573000	-3.447293000	-1.094662000
F	-0.165573000	-3.447293000	1.094662000
F	-0.773182000	-1.646969000	0.000000000

$(F_3CCHO)_2$-C

C	0.997552000	2.109597000	0.000000000
O	1.518075000	3.208515000	0.000000000
H	-0.097725000	1.937126000	0.000000000
C	1.832926000	0.813959000	0.000000000
F	3.149908000	1.039616000	0.000000000
F	1.518075000	0.068057000	1.095702000
F	1.518075000	0.068057000	-1.095702000
C	-0.997552000	-2.109597000	0.000000000
O	-1.518075000	-3.208515000	0.000000000
H	0.097725000	-1.937126000	0.000000000
C	-1.832926000	-0.813959000	0.000000000
F	-1.518075000	-0.068057000	-1.095702000
F	-3.149908000	-1.039616000	0.000000000
F	-1.518075000	-0.068057000	1.095702000

$(F_3CCHO)_2$-D

C	-1.952423000	1.302207000	0.000000000
O	-1.612368000	0.133300000	0.000000000
H	-3.007123000	1.645007000	0.000000000
C	-0.886442000	2.418574000	0.000000000
F	-1.469229000	3.638323000	0.000000000
F	-0.097393000	2.319641000	1.094042000
F	-0.097393000	2.319641000	-1.094042000
C	1.550317000	-0.987893000	0.000000000
O	2.767036000	-1.017785000	0.000000000
H	0.948822000	-0.057828000	0.000000000
C	0.701737000	-2.274249000	0.000000000
F	-0.097393000	-2.293429000	-1.097646000
F	1.452337000	-3.386652000	0.000000000
F	-0.097393000	-2.293429000	1.097646000

$(F_3CCHO)_2$-E

C	1.400566000	2.370082000	0.000000000
O	1.711612000	1.193057000	0.000000000
H	2.135280000	3.201340000	0.000000000
C	-0.069444000	2.827732000	0.000000000
F	-0.926305000	1.796984000	0.000000000
F	-0.302282000	3.591739000	1.096830000
F	-0.302282000	3.591739000	-1.096830000
C	-0.583393000	-1.429120000	0.000000000
O	-1.796258000	-1.315305000	0.000000000
H	0.124302000	-0.576387000	0.000000000
C	0.065242000	-2.830008000	0.000000000
F	-0.302282000	-3.532399000	1.095124000
F	-0.302282000	-3.532399000	-1.095124000
F	1.417629000	-2.724451000	0.000000000

$(ClCH_2CHO)_2$-A

C	-1.358147000	-0.917048000	1.093655000
O	-0.668704000	-0.119423000	1.710567000
H	-1.430419000	-1.985124000	1.407778000
C	-2.194627000	-0.606255000	-0.131323000
H	-1.848641000	-1.245005000	-0.958556000
H	-3.246083000	-0.851212000	0.088334000
Cl	-2.101103000	1.098375000	-0.642541000
C	1.713175000	1.089760000	0.020818000
O	2.540329000	1.980334000	0.164077000
H	0.676829000	1.288569000	-0.324084000
C	2.052664000	-0.359062000	0.338129000
Cl	1.205116000	-1.463254000	-0.812386000
H	3.132456000	-0.528627000	0.247128000
H	1.696254000	-0.607312000	1.348329000

$(ClCH_2CHO)_2$-B

C	2.621779000	-0.595700000	-0.445776000
O	3.613773000	-1.289978000	-0.285803000
H	1.972650000	-0.683359000	-1.344688000
C	2.211678000	0.440651000	0.593677000
H	3.099269000	0.951446000	0.987710000
Cl	1.123240000	1.679669000	-0.133981000
H	1.661680000	-0.055839000	1.405280000
C	-0.951059000	-0.808495000	-0.123670000
O	-0.090759000	-1.478885000	0.434849000
H	-0.982250000	-0.696675000	-1.229761000
C	-2.026133000	-0.070805000	0.652406000
H	-1.693732000	0.963692000	0.825980000
Cl	-3.544104000	-0.005794000	-0.307287000
H	-2.224639000	-0.578131000	1.604855000

$(ClCH_2CHO)_2$-C

C	-1.642704000	1.567839000	0.313888000
O	-0.499432000	1.886510000	0.009294000
H	-2.366746000	2.314419000	0.710004000
C	-2.159874000	0.150039000	0.160764000
H	-2.724007000	0.067925000	-0.781375000
H	-1.333059000	-0.571385000	0.182108000
Cl	-3.302284000	-0.217889000	1.501923000
C	1.642704000	-1.567839000	-0.313888000
O	0.499432000	-1.886510000	-0.009294000
H	2.366746000	-2.314419000	-0.710004000
C	2.159874000	-0.150039000	-0.160764000
H	1.333059000	0.571385000	-0.182108000
H	2.724007000	-0.067925000	0.781375000
Cl	3.302284000	0.217889000	-1.501923000

$(ClCH_2CHO)_2$-D

C	-0.862847000	1.573525000	0.046458000
O	-1.571172000	0.596325000	-0.169866000
H	0.202206000	1.463714000	0.340115000
C	-1.390806000	2.989874000	-0.099200000
H	-2.485989000	3.000207000	-0.040185000
Cl	-0.720192000	4.021835000	1.213457000
H	-1.050595000	3.414968000	-1.055941000
C	0.862847000	-1.573525000	-0.046458000
O	1.571172000	-0.596325000	0.169866000
H	-0.202206000	-1.463714000	-0.340115000
C	1.390806000	-2.989874000	0.099200000
Cl	0.720192000	-4.021835000	-1.213457000
H	2.485989000	-3.000207000	0.040185000
H	1.050595000	-3.414968000	1.055941000

$(ClCH_2CHO)_2$-E

C	-0.699430000	-2.704543000	0.000000000
O	-1.155348000	-1.572383000	0.000000000
H	-1.369424000	-3.597461000	0.000000000
C	0.774527000	-3.064634000	0.000000000
Cl	1.841485000	-1.639783000	0.000000000
H	0.987507000	-3.675192000	0.892386000
H	0.987507000	-3.675192000	-0.892386000
C	0.485781000	1.550118000	0.000000000
O	1.703171000	1.687077000	0.000000000
H	0.000000000	0.550999000	0.000000000
C	-0.422385000	2.775492000	0.000000000
H	-0.226536000	3.379471000	0.896999000
H	-0.226536000	3.379471000	-0.896999000
Cl	-2.157136000	2.309298000	0.000000000

$(Cl_2CHCHO)_2$-A

C	0.552905000	-1.236874000	0.000000000
O	1.646223000	-0.689018000	0.000000000
H	-0.406184000	-0.677986000	0.000000000
C	0.419798000	-2.753952000	0.000000000
H	1.397144000	-3.249784000	0.000000000
Cl	-0.469362000	-3.224133000	1.478338000
Cl	-0.469362000	-3.224133000	-1.478338000
C	0.873077000	3.738251000	0.000000000
O	0.066435000	4.650048000	0.000000000
H	1.971929000	3.917712000	0.000000000
C	0.473074000	2.252762000	0.000000000
Cl	-0.469362000	1.892952000	1.478415000
Cl	-0.469362000	1.892952000	-1.478415000
H	1.339339000	1.580852000	0.000000000

$(Cl_2CHCHO)_2$-B

C	0.599827000	3.836157000	0.000000000
O	1.718098000	4.323266000	0.000000000
H	-0.331365000	4.445236000	0.000000000
C	0.377813000	2.326826000	0.000000000
H	1.311023000	1.753754000	0.000000000
Cl	-0.546726000	1.905649000	1.476008000
Cl	-0.546726000	1.905649000	-1.476008000
C	0.386480000	-1.208215000	0.000000000
O	1.452496000	-0.610850000	0.000000000
H	-0.597896000	-0.694277000	0.000000000
C	0.321111000	-2.730122000	0.000000000
Cl	-0.546726000	-3.240054000	1.478155000
Cl	-0.546726000	-3.240054000	-1.478155000
H	1.319456000	-3.182145000	0.000000000

$(Cl_2CHCHO)_2$-C

C	-0.317801000	1.754397000	0.000000000
O	-1.295034000	1.019255000	0.000000000
H	0.723483000	1.371458000	0.000000000
C	-0.467435000	3.271805000	0.000000000
H	-1.519715000	3.577800000	0.000000000
Cl	0.317801000	3.903163000	1.478007000
Cl	0.317801000	3.903163000	-1.478007000
C	0.317801000	-1.754397000	0.000000000
O	1.295034000	-1.019255000	0.000000000
H	-0.723483000	-1.371458000	0.000000000
C	0.467435000	-3.271805000	0.000000000
Cl	-0.317801000	-3.903163000	-1.478007000
H	1.519715000	-3.577800000	0.000000000
Cl	-0.317801000	-3.903163000	1.478007000

$(Cl_2CHCHO)_2$-D

C	-2.116509000	-1.358250000	-0.757206000
O	-0.903707000	-1.427493000	-0.671823000
H	-2.752928000	-2.246831000	-0.965017000
C	-2.923247000	-0.063942000	-0.592443000
Cl	-1.903556000	1.318410000	-0.176267000
H	-3.465880000	0.165711000	-1.521173000
Cl	-4.170570000	-0.397296000	0.660729000
C	1.480021000	0.936763000	0.138233000
O	1.247433000	2.122286000	0.327177000
H	0.695727000	0.191409000	-0.108458000
C	2.900051000	0.385801000	0.229545000
H	3.626762000	1.167195000	0.479307000
Cl	2.929832000	-0.861183000	1.512640000
Cl	3.326919000	-0.309229000	-1.363941000

$(Cl_2CHCHO)_2$-E

C	0.753348000	2.089049000	0.000000000
O	0.801062000	3.308735000	0.000000000
H	-0.196277000	1.512628000	0.000000000
C	2.025201000	1.243158000	0.000000000
H	2.926491000	1.866854000	0.000000000
Cl	2.025201000	0.231220000	1.477577000
Cl	2.025201000	0.231220000	-1.477577000
C	-0.753348000	-2.089049000	0.000000000
O	-0.801062000	-3.308735000	0.000000000
H	0.196277000	-1.512628000	0.000000000
C	-2.025201000	-1.243158000	0.000000000
Cl	-2.025201000	-0.231220000	-1.477577000
H	-2.926491000	-1.866854000	0.000000000
Cl	-2.025201000	-0.231220000	1.477577000

$(Cl_3CCHO)_2$-A

C	-0.015295000	1.765740000	0.000000000
O	-1.097094000	1.210883000	0.000000000
H	0.952868000	1.223909000	0.000000000
C	0.148405000	3.304337000	0.000000000
Cl	-1.402003000	4.145253000	0.000000000
Cl	1.097094000	3.710571000	1.464777000
Cl	1.097094000	3.710571000	-1.464777000
C	0.015295000	-1.765740000	0.000000000
O	1.097094000	-1.210883000	0.000000000
H	-0.952868000	-1.223909000	0.000000000
C	-0.148405000	-3.304337000	0.000000000
Cl	-1.097094000	-3.710571000	-1.464777000
Cl	1.402003000	-4.145253000	0.000000000
Cl	-1.097094000	-3.710571000	1.464777000

$(Cl_3CCHO)_2$-B

C	-2.172465000	1.331124000	0.000000000
O	-1.889222000	0.150532000	0.000000000
H	-3.212369000	1.721915000	0.000000000
C	-1.071300000	2.434357000	0.000000000
Cl	-1.848694000	4.038308000	0.000000000
Cl	-0.069092000	2.232500000	1.463151000
Cl	-0.069092000	2.232500000	-1.463151000
C	1.372681000	-0.864877000	0.000000000
O	2.532811000	-0.505533000	0.000000000
H	0.500849000	-0.181096000	0.000000000
C	0.936450000	-2.350905000	0.000000000
Cl	-0.069092000	-2.581459000	-1.465292000
Cl	2.311568000	-3.457977000	0.000000000
Cl	-0.069092000	-2.581459000	1.465292000

$(Cl_3CCHO)_2$-C

C	1.311472000	2.445300000	0.000000000
O	1.569605000	1.258342000	0.000000000
H	2.082229000	3.245654000	0.000000000
C	-0.128440000	3.012433000	0.000000000
Cl	-1.343837000	1.736967000	0.000000000
Cl	-0.263885000	4.034773000	1.465302000
Cl	-0.263885000	4.034773000	-1.465302000
C	-0.480929000	-1.515101000	0.000000000
O	-1.692632000	-1.423323000	0.000000000
H	0.209565000	-0.645962000	0.000000000
C	0.227406000	-2.903912000	0.000000000
Cl	-0.263885000	-3.799091000	1.463505000
Cl	-0.263885000	-3.799091000	-1.463505000
Cl	1.994397000	-2.650222000	0.000000000

$(Cl_3CCHO)_2$-D

C	0.642455000	2.108360000	0.000000000
O	0.556657000	3.318486000	0.000000000
H	-0.229409000	1.419618000	0.000000000
C	1.993976000	1.348045000	0.000000000
Cl	3.377701000	2.436810000	0.000000000
Cl	1.993976000	0.310478000	1.465053000
Cl	1.993976000	0.310478000	-1.465053000
C	-0.642455000	-2.108360000	0.000000000
O	-0.556657000	-3.318486000	0.000000000
H	0.229409000	-1.419618000	0.000000000
C	-1.993976000	-1.348045000	0.000000000
Cl	-1.993976000	-0.310478000	-1.465053000
Cl	-3.377701000	-2.436810000	0.000000000
Cl	-1.993976000	-0.310478000	1.465053000

$(Cl_3CCHO)_2$-E

C	1.390630000	0.141157000	-1.198648000
O	0.832672000	1.189018000	-1.447852000
H	1.276485000	-0.787225000	-1.799676000
C	2.359329000	-0.050878000	-0.004276000
Cl	1.712729000	-1.418542000	0.966731000
Cl	3.935284000	-0.528211000	-0.715229000
Cl	2.517885000	1.401105000	0.974088000
C	-1.392174000	0.136889000	1.200409000
O	-0.829130000	1.181872000	1.450194000
H	-1.284711000	-0.791797000	1.802273000
C	-2.359407000	-0.050604000	0.004109000
Cl	-3.938249000	-0.524690000	0.713015000
Cl	-2.512743000	1.403161000	-0.972200000
Cl	-1.715517000	-1.417969000	-0.968222000

$(BrCH_2CHO)_2$-A

C	-0.459005000	1.964412000	0.869939000
O	0.459005000	1.983198000	1.681362000
H	-0.497466000	2.680320000	0.018704000
C	-1.613893000	0.989663000	0.976729000
H	-2.521966000	1.521805000	1.298345000
Br	-2.003881000	0.250205000	-0.785871000
H	-1.378502000	0.161793000	1.657545000
C	0.459005000	-1.964412000	0.869939000
O	-0.459005000	-1.983198000	1.681362000
H	0.497466000	-2.680320000	0.018704000
C	1.613893000	-0.989663000	0.976729000
H	1.378502000	-0.161793000	1.657545000
H	2.521966000	-1.521805000	1.298345000
Br	2.003881000	-0.250205000	-0.785871000

$(BrCH_2CHO)_2$-B

C	1.843265000	1.592070000	-0.861476000
O	0.698426000	2.032478000	-0.856179000
H	2.464215000	1.613496000	-1.784798000
C	2.492668000	0.965733000	0.351738000
H	3.484454000	1.398407000	0.543425000
H	1.842652000	1.000859000	1.233711000
Br	2.787051000	-0.915696000	-0.101608000
C	-0.784250000	0.267698000	0.890928000
O	-0.333514000	0.499757000	2.006709000
H	-0.277837000	-0.438040000	0.195388000
C	-2.046200000	0.913755000	0.367415000
Br	-3.218162000	-0.492542000	-0.314558000
H	-2.572760000	1.452603000	1.163853000
H	-1.804054000	1.567577000	-0.481638000

$(BrCH_2CHO)_2$-C

C	-1.648209000	1.587253000	0.287919000
O	-0.469488000	1.914110000	0.200975000
H	-2.437007000	2.338615000	0.515708000
C	-2.124218000	0.164476000	0.102340000
H	-2.833468000	0.099660000	-0.735938000
H	-1.286305000	-0.534413000	-0.010722000
Br	-3.125075000	-0.328570000	1.707600000
C	1.648209000	-1.587253000	-0.287919000
O	0.469488000	-1.914110000	-0.200975000
H	2.437007000	-2.338615000	-0.515708000
C	2.124218000	-0.164476000	-0.102340000
H	1.286305000	0.534413000	0.010722000
H	2.833468000	-0.099660000	0.735938000
Br	3.125075000	0.328570000	-1.707600000

$(BrCH_2CHO)_2$-D

C	-0.106528000	-2.896083000	0.000000000
O	-0.745290000	-1.855585000	0.000000000
H	-0.622341000	-3.886141000	0.000000000
C	1.405141000	-3.012819000	0.000000000
Br	2.298268000	-1.300591000	0.000000000
H	1.718901000	-3.576840000	0.892730000
H	1.718901000	-3.576840000	-0.892730000
C	0.267999000	1.556784000	0.000000000
O	1.432340000	1.938528000	0.000000000
H	0.000000000	0.478650000	0.000000000
C	-0.868118000	2.573577000	0.000000000
H	-0.803493000	3.204134000	0.897505000
H	-0.803493000	3.204134000	-0.897505000
Br	-2.609578000	1.705179000	0.000000000

$(BrCH_2CHO)_2$-E

C	-0.865774000	1.552115000	0.069260000
O	-1.607002000	0.574167000	0.063706000
H	0.228980000	1.444542000	0.219192000
C	-1.387230000	2.958255000	-0.138001000
H	-2.483319000	2.973832000	-0.159768000
Br	-0.777484000	4.057150000	1.357458000
H	-0.955620000	3.403151000	-1.046608000
C	0.865774000	-1.552115000	-0.069260000
O	1.607002000	-0.574167000	-0.063706000
H	-0.228980000	-1.444542000	-0.219192000
C	1.387230000	-2.958255000	0.138001000
Br	0.777484000	-4.057150000	-1.357458000
H	2.483319000	-2.973832000	0.159768000
H	0.955620000	-3.403151000	1.046608000

$(Br_2CHCHO)_2$-A

C	0.937347000	4.080209000	0.000000000
O	2.077053000	4.517013000	0.000000000
H	0.035750000	4.732819000	0.000000000
C	0.650492000	2.586025000	0.000000000
H	1.555495000	1.968020000	0.000000000
Br	-0.362245000	2.172437000	1.608424000
Br	-0.362245000	2.172437000	-1.608424000
C	0.682514000	-0.936433000	0.000000000
O	1.761384000	-0.360255000	0.000000000
H	-0.290269000	-0.400730000	0.000000000
C	0.585385000	-2.451371000	0.000000000
Br	-0.362245000	-2.976649000	1.611462000
Br	-0.362245000	-2.976649000	-1.611462000
H	1.571402000	-2.929942000	0.000000000

$(Br_2CHCHO)_2$-B

C	0.859432000	2.019000000	0.000000000
O	0.909677000	3.239426000	0.000000000
H	-0.093970000	1.448409000	0.000000000
C	2.125802000	1.173123000	0.000000000
H	3.030783000	1.791769000	0.000000000
Br	2.125802000	0.082626000	1.609677000
Br	2.125802000	0.082626000	-1.609677000
C	-0.859432000	-2.019000000	0.000000000
O	-0.909677000	-3.239426000	0.000000000
H	0.093970000	-1.448409000	0.000000000
C	-2.125802000	-1.173123000	0.000000000
Br	-2.125802000	-0.082626000	-1.609677000
H	-3.030783000	-1.791769000	0.000000000
Br	-2.125802000	-0.082626000	1.609677000

$(Br_2CHCHO)_2$-C

C	2.103962000	-1.349761000	0.000000000
O	1.790585000	-0.171516000	0.000000000
H	3.167940000	-1.677568000	0.000000000
C	1.084367000	-2.494822000	0.000000000
H	1.572030000	-3.477190000	0.000000000
Br	0.007594000	-2.393331000	1.613049000
Br	0.007594000	-2.393331000	-1.613049000
C	-1.498818000	0.733916000	0.000000000
O	-2.686217000	0.441598000	0.000000000
H	-0.680958000	-0.012603000	0.000000000
C	-1.036061000	2.182981000	0.000000000
Br	0.007594000	2.474584000	-1.613210000
H	-1.877782000	2.885138000	0.000000000
Br	0.007594000	2.474584000	1.613210000

$(Br_2CHCHO)_2$-D

C	-0.012343000	2.113953000	1.712549000
O	-0.224323000	2.765422000	2.723353000
H	0.680703000	1.244721000	1.677729000
C	-0.691176000	2.444497000	0.390805000
Br	-1.771874000	0.913933000	-0.129341000
H	-1.347022000	3.318569000	0.478434000
Br	0.691176000	2.839497000	-0.915319000
C	0.012343000	-2.113953000	1.712549000
O	0.224323000	-2.765422000	2.723353000
H	-0.680703000	-1.244721000	1.677729000
C	0.691176000	-2.444497000	0.390805000
H	1.347022000	-3.318569000	0.478434000
Br	-0.691176000	-2.839497000	-0.915319000
Br	1.771874000	-0.913933000	-0.129341000

$(Br_2CHCHO)_2$-E

C	-1.963996000	0.187421000	1.698203000
O	-0.759206000	0.302696000	1.554906000
H	-2.494909000	0.579868000	2.594420000
C	-2.901042000	-0.486804000	0.695802000
Br	-1.973373000	-1.199726000	-0.826987000
H	-3.459710000	-1.300656000	1.180103000
Br	-4.232488000	0.863152000	0.217696000
C	1.440751000	-0.635833000	-0.930409000
O	1.177329000	-1.282809000	-1.935365000
H	0.680247000	-0.346518000	-0.175845000
C	2.860278000	-0.173437000	-0.638934000
H	3.566340000	-0.483217000	-1.417949000
Br	2.846377000	1.767220000	-0.552498000
Br	3.409400000	-0.972264000	1.045074000

$(Br_3CCHO)_2$-A

C	0.730484000	2.054198000	0.000000000
O	0.617821000	3.263185000	0.000000000
H	-0.131501000	1.352096000	0.000000000
C	2.089516000	1.318558000	0.000000000
Br	3.579708000	2.529555000	0.000000000
Br	2.089516000	0.192330000	1.595909000
Br	2.089516000	0.192330000	-1.595909000
C	-0.730484000	-2.054198000	0.000000000
O	-0.617821000	-3.263185000	0.000000000
H	0.131501000	-1.352096000	0.000000000
C	-2.089516000	-1.318558000	0.000000000
Br	-2.089516000	-0.192330000	-1.595909000
Br	-3.579708000	-2.529555000	0.000000000
Br	-2.089516000	-0.192330000	1.595909000

$(Br_3CCHO)_2$-B

C	-2.223813000	1.248206000	0.000000000
O	-1.893826000	0.078976000	0.000000000
H	-3.281143000	1.591223000	0.000000000
C	-1.178004000	2.399309000	0.000000000
Br	-2.105523000	4.104864000	0.000000000
Br	-0.082175000	2.221155000	1.596617000
Br	-0.082175000	2.221155000	-1.596617000
C	1.405604000	-0.816525000	0.000000000
O	2.555017000	-0.420966000	0.000000000
H	0.516038000	-0.155718000	0.000000000
C	1.007280000	-2.306917000	0.000000000
Br	-0.082175000	-2.560211000	-1.598661000
Br	2.531627000	-3.479437000	0.000000000
Br	-0.082175000	-2.560211000	1.598661000

$(Br_3CCHO)_2$-C

C	1.300943000	2.476111000	0.000000000
O	1.540042000	1.283969000	0.000000000
H	2.089453000	3.260057000	0.000000000
C	-0.122088000	3.072367000	0.000000000
Br	-1.473972000	1.710497000	0.000000000
Br	-0.226621000	4.187043000	1.597755000
Br	-0.226621000	4.187043000	-1.597755000
C	-0.485915000	-1.540310000	0.000000000
O	-1.700980000	-1.488699000	0.000000000
H	0.169287000	-0.643316000	0.000000000
C	0.277002000	-2.895318000	0.000000000
Br	-0.226621000	-3.882854000	1.597156000
Br	-0.226621000	-3.882854000	-1.597156000
Br	2.186430000	-2.537618000	0.000000000

$(Br_3CCHO)_2$-D

C	1.610343000	2.610812000	0.000000000
O	2.004070000	1.460628000	0.000000000
H	2.289253000	3.491999000	0.000000000
C	0.120754000	3.015362000	0.000000000
Br	-1.041266000	1.493713000	0.000000000
Br	-0.120754000	4.112768000	1.598362000
Br	-0.120754000	4.112768000	-1.598362000
C	-1.610343000	-2.610812000	0.000000000
O	-2.004070000	-1.460628000	0.000000000
H	-2.289253000	-3.491999000	0.000000000
C	-0.120754000	-3.015362000	0.000000000
Br	0.120754000	-4.112768000	1.598362000
Br	0.120754000	-4.112768000	-1.598362000
Br	1.041266000	-1.493713000	0.000000000

$(Br_3CCHO)_2$-E

C	0.240751000	-0.912104000	0.000000000
O	1.273065000	-0.272685000	0.000000000
H	-0.769858000	-0.450294000	0.000000000
C	0.178957000	-2.452125000	0.000000000
Br	1.922443000	-3.258618000	0.000000000
Br	-0.830417000	-2.938140000	1.597671000
Br	-0.830417000	-2.938140000	-1.597671000
C	-0.849068000	4.424465000	0.000000000
O	-2.048332000	4.606242000	0.000000000
H	-0.098168000	5.244945000	0.000000000
C	-0.218584000	2.998505000	0.000000000
Br	-0.830417000	2.076072000	1.601330000
Br	-0.830417000	2.076072000	-1.601330000
Br	1.712306000	3.159451000	0.000000000

$(FCH(HSO_3)CHO)_2$-A

C	1.450620000	0.285948000	-1.266979000
O	0.613420000	1.168544000	-1.359020000
H	1.922332000	-0.192653000	-2.150244000
C	1.899794000	-0.256614000	0.088913000
H	1.639988000	-1.321277000	0.212898000
F	1.388588000	0.487904000	1.122853000
C	-1.618357000	1.449016000	0.528908000
O	-2.066306000	2.542388000	0.230079000
H	-1.003258000	1.252661000	1.430458000
C	-1.910155000	0.214884000	-0.330725000
F	-1.022109000	-0.817211000	-0.022866000
H	-1.893282000	0.433106000	-1.407736000
S	3.736624000	-0.167211000	0.215514000
O	4.011618000	-1.420402000	-0.857014000
O	4.229587000	1.075422000	-0.422670000
O	4.138199000	-0.594290000	1.562887000
H	4.624844000	-1.061776000	-1.527445000
S	-3.588223000	-0.407843000	0.088263000
O	-3.591045000	-1.808399000	-0.800915000
O	-3.584354000	-0.771456000	1.523399000
O	-4.576301000	0.484102000	-0.532439000
H	-3.293274000	-2.512095000	-0.193391000

$(FCH(CN)CHO)_2$-A

C	-1.535935000	-0.007282000	1.173097000
O	-0.663220000	0.824490000	1.346406000
H	-2.013450000	-0.565913000	2.008300000
C	-2.050345000	-0.389391000	-0.223532000
H	-1.707539000	-1.415639000	-0.444779000
F	-1.535013000	0.466991000	-1.184969000
C	1.645303000	1.081873000	-0.444704000
O	2.346555000	2.042210000	-0.184191000
H	0.841652000	1.083020000	-1.208886000
C	1.832643000	-0.256039000	0.299506000
F	0.851717000	-1.171857000	-0.130529000
H	1.696928000	-0.086295000	1.378371000
C	-3.527708000	-0.346443000	-0.241004000
N	-4.713414000	-0.319766000	-0.197227000
C	3.165134000	-0.826360000	0.032051000
N	4.240676000	-1.272109000	-0.197591000

$(FCH(NO_2)CHO)_2$-A

C	-1.539671000	0.253085000	1.226160000
O	-0.601663000	1.027920000	1.300161000
H	-2.120894000	-0.091808000	2.106465000
C	-1.989182000	-0.332598000	-0.123176000
H	-1.717558000	-1.395231000	-0.207285000
F	-1.485742000	0.380793000	-1.163928000
C	1.656647000	1.161911000	-0.495586000
O	2.312410000	2.162689000	-0.272201000
H	0.899551000	1.075439000	-1.301454000
C	1.853139000	-0.121081000	0.333882000
F	0.906571000	-1.060606000	-0.016819000
H	1.839656000	0.063658000	1.414150000
N	3.217188000	-0.677780000	-0.002691000
O	4.139075000	-0.281434000	0.717653000
O	3.297843000	-1.414093000	-0.989755000
N	-3.504646000	-0.289427000	-0.151154000
O	-4.029390000	-1.054671000	0.667255000
O	-4.063478000	0.493190000	-0.917604000

$(FCH(NH_2)CHO)_2$-A

C	-1.546658000	-1.030474000	0.354887000
O	-1.053523000	-0.946118000	1.469698000
H	-1.701001000	-2.007384000	-0.153275000
C	-2.048058000	0.165543000	-0.452219000
H	-1.578104000	0.153162000	-1.446892000
F	-1.616972000	1.360412000	0.181640000
C	1.708346000	0.954992000	0.375438000
O	2.643546000	1.707262000	0.133778000
H	0.731323000	1.318321000	0.750817000
C	1.789293000	-0.549911000	0.104898000
F	0.813773000	-0.706201000	-0.996508000
H	1.354068000	-1.150973000	0.913687000
N	-3.461377000	0.069402000	-0.578602000
H	-3.924856000	0.151325000	0.325756000
H	-3.836065000	0.774044000	-1.209738000
N	3.080517000	-0.954952000	-0.223071000
H	3.550003000	-0.327241000	-0.870929000
H	3.161724000	-1.930349000	-0.489736000

$(FCH(CH_3)CHO)_2$-A

C	-1.461829000	-0.548717000	0.923245000
O	-0.779162000	0.201812000	1.605012000
H	-1.682379000	-1.593295000	1.249116000
C	-2.105350000	-0.174383000	-0.399042000
H	-1.739289000	-0.881570000	-1.163035000
F	-1.694789000	1.110465000	-0.783378000
C	1.662780000	0.981068000	-0.156187000
O	2.538292000	1.783028000	0.144521000
H	0.715095000	1.286249000	-0.647744000
C	1.812269000	-0.507926000	0.134912000
F	0.788480000	-1.190636000	-0.586783000
H	1.602641000	-0.674954000	1.203763000
C	3.165263000	-1.057024000	-0.273076000
H	3.946258000	-0.498888000	0.263628000
H	3.237855000	-2.123505000	-0.018731000
H	3.318064000	-0.928624000	-1.354758000
C	-3.625272000	-0.207922000	-0.294125000
H	-4.070274000	0.030665000	-1.269810000
H	-3.963642000	-1.211207000	0.009273000
H	-3.967758000	0.527373000	0.449131000

$(FCH(OCH_3)CHO)_2$-A

C	-1.404425000	0.342285000	1.416144000
O	-0.408439000	1.047690000	1.443171000
H	-1.933701000	0.019317000	2.339405000
C	-2.017753000	-0.184937000	0.116971000
H	-1.563476000	-1.149239000	-0.176775000
F	-1.726446000	0.709915000	-0.924018000
C	1.522240000	1.188676000	-0.669235000
O	2.094732000	2.244767000	-0.454327000
H	0.706488000	1.076501000	-1.412469000
C	1.931084000	-0.087805000	0.070911000
F	0.902469000	-1.058872000	-0.111783000
H	2.006215000	0.071510000	1.159923000
O	-3.379858000	-0.282325000	0.326276000
C	-4.061581000	-0.933936000	-0.763071000
H	-4.015132000	-0.317486000	-1.672264000
H	-3.607853000	-1.921408000	-0.954867000
H	-5.102620000	-1.055830000	-0.442985000
O	3.104950000	-0.538181000	-0.491417000
C	3.703184000	-1.612662000	0.258600000
H	3.862696000	-1.299500000	1.304303000
H	3.068126000	-2.510384000	0.226687000
H	4.667477000	-1.818196000	-0.220294000

$(FCH(SCH_3)CHO)_2$-A

C	-1.186047000	-0.172299000	1.296839000
O	-0.513494000	0.750852000	1.729366000
H	-1.266431000	-1.149632000	1.823304000
C	-1.987562000	-0.102199000	0.004956000
H	-1.660554000	-0.918464000	-0.662274000
F	-1.748098000	1.104880000	-0.657167000
C	1.580928000	1.520813000	-0.353324000
O	2.309177000	2.473705000	-0.124447000
H	0.611294000	1.610257000	-0.885901000
C	1.937121000	0.098293000	0.085988000
F	0.927205000	-0.775520000	-0.415251000
H	1.898870000	0.014555000	1.183751000
S	-3.740394000	-0.320980000	0.401155000
C	-4.324409000	-0.734630000	-1.280036000
H	-4.125740000	0.100754000	-1.964730000
H	-3.844181000	-1.657441000	-1.636331000
H	-5.409616000	-0.894897000	-1.206960000
S	3.560879000	-0.368095000	-0.535368000
C	3.712848000	-1.950786000	0.363168000
H	3.661777000	-1.776828000	1.448397000
H	2.932360000	-2.654492000	0.044496000
H	4.699748000	-2.364452000	0.110524000

$(F_2C(HSO_3)CHO)_2$-A

C	-3.814783000	0.956330000	-0.627598000
O	-3.772795000	2.157055000	-0.438520000
H	-4.746793000	0.357326000	-0.672792000
C	-2.524008000	0.138132000	-0.831988000
F	-1.457326000	0.931100000	-1.113579000
F	-2.694137000	-0.760170000	-1.841971000
C	1.200160000	1.343470000	0.548165000
O	0.701590000	0.998730000	1.612987000
H	0.649500000	1.884215000	-0.244342000
C	2.650567000	0.980295000	0.218854000
F	3.112330000	1.782959000	-0.774969000
F	3.457983000	1.073859000	1.299112000
S	2.695886000	-0.802714000	-0.389684000
O	1.275379000	-0.744696000	-1.223977000
O	3.781126000	-0.916858000	-1.371745000
O	2.534269000	-1.666633000	0.793772000
H	0.573754000	-1.134056000	-0.641847000
S	-2.095866000	-0.844675000	0.690368000
O	-1.925891000	0.371914000	1.745592000
O	-3.302274000	-1.594915000	1.062846000
O	-0.784450000	-1.501946000	0.449337000
H	-0.973682000	0.670434000	1.743767000

$(F_2C(CN)CHO)_2$-A

C	-2.039191000	-0.817553000	-1.044744000
O	-1.563262000	-1.931505000	-0.934225000
H	-2.289827000	-0.343540000	-2.016181000
C	-2.437307000	0.006966000	0.206808000
F	-1.776961000	-0.454320000	1.305701000
F	-3.786251000	-0.216359000	0.398154000
C	1.003280000	-0.502987000	-0.168389000
O	0.353160000	0.394834000	-0.677664000
H	0.582852000	-1.499030000	0.083932000
C	2.494812000	-0.343275000	0.180043000
F	2.625945000	-0.552989000	1.530492000
F	3.177758000	-1.346380000	-0.462623000
C	3.065350000	0.970246000	-0.186116000
N	3.502343000	2.029533000	-0.493885000
C	-2.221081000	1.464263000	0.052439000
N	-2.069744000	2.627667000	-0.128744000

$(F_2C(NO_2)CHO)_2$-A

C	**-2.061499000**	**-1.093762000**	**-1.000243000**
O	-1.602786000	-2.205753000	-0.808599000
H	-2.242255000	-0.651198000	-1.997571000
C	-2.525689000	-0.232233000	0.198516000
F	-2.013548000	-0.666896000	1.354660000
F	-3.886892000	-0.275331000	0.259737000
C	0.907261000	-0.706250000	0.003065000
O	0.255188000	0.162082000	-0.553043000
H	0.500482000	-1.702503000	0.274060000
C	2.369414000	-0.459995000	0.410472000
F	2.425023000	-0.076406000	1.698890000
F	3.103497000	-1.584500000	0.247697000
N	-2.171072000	1.241713000	0.016509000
O	-2.532703000	1.700461000	-1.072191000
O	-1.589820000	1.822455000	0.931272000
N	2.985729000	0.622167000	-0.470719000
O	3.073467000	0.294917000	-1.656655000
O	3.302845000	1.686860000	0.057124000

$(F_2C(NH_2)CHO)_2$-A

C	-1.967978000	1.004194000	0.640306000
O	-1.551567000	1.978369000	0.039494000
H	-2.191655000	1.015972000	1.729279000
C	-2.296614000	-0.315525000	-0.083961000
F	-1.502037000	-0.474269000	-1.186428000
F	-3.599157000	-0.138213000	-0.596850000
C	1.119765000	0.444974000	0.227734000
O	0.514505000	0.061474000	1.218305000
H	0.681152000	1.140194000	-0.516398000
C	2.538899000	-0.045552000	-0.085271000
F	2.397589000	-0.928045000	-1.173475000
F	3.268813000	1.004664000	-0.604172000
N	-2.175870000	-1.442957000	0.745176000
H	-2.465030000	-2.287499000	0.252543000
H	-2.726520000	-1.339107000	1.595705000
N	3.180240000	-0.596414000	1.022718000
H	3.992308000	-1.151685000	0.763338000
H	2.524337000	-1.126804000	1.593356000

$(F_2C(CH_3)CHO)_2$-A

C	2.013376000	0.943469000	-0.766428000
O	1.434317000	1.928331000	-0.340665000
H	2.364156000	0.867349000	-1.819165000
C	2.397099000	-0.250218000	0.129508000
F	1.613911000	-0.238410000	1.259710000
F	3.702233000	0.027918000	0.544770000
C	-1.134091000	0.316536000	-0.251539000
O	-0.492233000	-0.343733000	-1.057724000
H	-0.708530000	1.201551000	0.264896000
C	-2.584346000	-0.022782000	0.112376000
F	-2.618609000	-0.133073000	1.495050000
F	-3.329615000	1.106003000	-0.203883000
C	2.371239000	-1.606694000	-0.526688000
H	1.347301000	-1.851880000	-0.835846000
H	3.030079000	-1.600500000	-1.407123000
H	2.738162000	-2.350666000	0.193447000
C	-3.174902000	-1.244832000	-0.532112000
H	-4.211830000	-1.357233000	-0.188910000
H	-3.149703000	-1.131780000	-1.624111000
H	-2.587832000	-2.128430000	-0.247601000

$(F_2C(OCH_3)CHO)_2$-A

C	-2.016901000	-1.272252000	-0.775869000
O	-1.588796000	-2.286326000	-0.251781000
H	-2.173522000	-1.157480000	-1.866927000
C	-2.461517000	-0.060722000	0.064340000
F	-1.659843000	0.084799000	1.174044000
F	-3.724595000	-0.343862000	0.576836000
C	0.977679000	-0.605222000	-0.212760000
O	0.324347000	-0.029877000	-1.065940000
H	0.585432000	-1.463067000	0.372494000
C	2.416163000	-0.206923000	0.145562000
F	2.451482000	0.040589000	1.511808000
F	3.212366000	-1.332935000	-0.023601000
O	2.845994000	0.839725000	-0.577245000
C	4.205449000	1.256194000	-0.279106000
H	4.282282000	1.573422000	0.769335000
H	4.906547000	0.437823000	-0.489855000
H	4.392602000	2.101376000	-0.948968000
O	-2.480097000	1.044433000	-0.713178000
C	-2.864008000	2.261789000	-0.023892000
H	-3.862069000	2.148687000	0.420349000
H	-2.121635000	2.507025000	0.747019000
H	-2.877088000	3.034083000	-0.799735000

$(F_2C(SCH_3)CHO)_2$-A

C	-2.090438000	-1.459157000	-0.842855000
O	-1.642345000	-2.500723000	-0.396558000
H	-2.295928000	-1.291057000	-1.919801000
C	-2.518221000	-0.306223000	0.094582000
F	-1.864283000	-0.416366000	1.299924000
F	-3.862003000	-0.531764000	0.382498000
C	0.906592000	-0.831686000	-0.169624000
O	0.330233000	-0.308559000	-1.110804000
H	0.456463000	-1.643654000	0.439684000
C	2.316508000	-0.414661000	0.267834000
F	2.248053000	-0.095558000	1.615957000
F	3.113871000	-1.549085000	0.213037000
S	2.970718000	0.931436000	-0.721821000
C	4.579229000	1.059356000	0.139683000
H	4.428884000	1.323612000	1.194277000
H	5.140792000	0.121291000	0.043122000
H	5.125244000	1.867539000	-0.366959000
S	-2.288330000	1.316006000	-0.656491000
C	-3.185118000	2.284234000	0.609056000
H	-4.245186000	2.003131000	0.629151000
H	-2.718826000	2.142469000	1.592929000
H	-3.084806000	3.335644000	0.304692000

$(ClCH(HSO_3)CHO)_2$-A

C	-1.361678000	-0.452934000	0.977492000
O	-0.554107000	0.338476000	1.436525000
H	-1.570555000	-1.437794000	1.442650000
C	-2.168191000	-0.183995000	-0.299428000
H	-1.931248000	-0.949087000	-1.058973000
Cl	-1.911061000	1.430480000	-0.969278000
C	1.774020000	1.424295000	0.028103000
O	2.535635000	2.260434000	0.496983000
H	0.846001000	1.699963000	-0.508474000
C	2.038326000	-0.083115000	0.153564000
Cl	1.163790000	-0.978543000	-1.117584000
H	1.726287000	-0.457352000	1.140665000
S	3.839254000	-0.448186000	0.005516000
O	4.336605000	0.341142000	1.360284000
O	4.063472000	-1.877326000	0.271376000
O	4.337416000	0.233874000	-1.205916000
H	4.103229000	1.286937000	1.207870000
S	-3.951257000	-0.453301000	0.066565000
O	-4.159002000	0.643751000	1.287233000
O	-4.770379000	-0.046055000	-1.089790000
O	-4.027799000	-1.781736000	0.702004000
H	-4.467650000	1.472231000	0.871626000

$(ClCH(CN)CHO)_2$-A

C	-1.443298000	-0.784017000	1.014444000
O	-0.641311000	-0.111884000	1.636314000
H	-1.667326000	-1.842208000	1.274340000
C	-2.228395000	-0.275905000	-0.210187000
H	-1.838431000	-0.815401000	-1.090848000
Cl	-1.981526000	1.470182000	-0.493592000
C	1.849114000	1.268935000	0.112572000
O	2.768808000	2.060207000	0.211922000
H	0.796180000	1.565816000	-0.074077000
C	2.047266000	-0.252577000	0.263389000
Cl	1.119711000	-1.069700000	-1.064805000
H	1.580498000	-0.575959000	1.207485000
C	3.454897000	-0.653299000	0.217821000
N	4.595734000	-0.980219000	0.189747000
C	-3.654864000	-0.590264000	-0.042152000
N	-4.794070000	-0.877535000	0.132344000

$(ClCH(NO_2)CHO)_2$-A

C	-1.493867000	-0.602202000	1.099543000
O	-0.608191000	0.037331000	1.636994000
H	-1.850698000	-1.583890000	1.477327000
C	-2.203099000	-0.135795000	-0.188331000
H	-1.853331000	-0.748723000	-1.031584000
Cl	-1.954905000	1.564248000	-0.534083000
C	1.869059000	1.329843000	0.055069000
O	2.824170000	2.084118000	0.021846000
H	0.814042000	1.658113000	-0.040338000
C	2.030702000	-0.191796000	0.231472000
Cl	1.124672000	-1.019625000	-1.059038000
H	1.657752000	-0.528930000	1.206483000
N	3.499033000	-0.523361000	0.180531000
O	4.055162000	-0.488026000	1.284840000
O	4.026290000	-0.721527000	-0.913787000
N	-3.674273000	-0.495791000	-0.023680000
O	-3.873555000	-1.717571000	-0.051127000
O	-4.504364000	0.390501000	0.169573000

$(ClCH(NH_2)CHO)_2$-A

C	1.521111000	-1.236407000	-0.143101000
O	0.982980000	-1.299232000	-1.238233000
H	1.604577000	-2.120672000	0.524950000
C	2.203138000	0.004247000	0.440097000
H	1.788777000	0.185386000	1.441433000
Cl	1.750862000	1.489769000	-0.538473000
C	-2.793702000	0.939626000	0.053639000
O	-3.953859000	0.611874000	-0.155647000
H	-2.524326000	1.879146000	0.580215000
C	-1.621103000	0.065207000	-0.356681000
Cl	-1.028116000	-0.440334000	1.460460000
H	-0.732257000	0.613526000	-0.686093000
N	-1.971590000	-0.973893000	-1.181429000
H	-2.846650000	-1.435958000	-0.950492000
H	-1.214202000	-1.582357000	-1.476235000
N	3.603657000	-0.261307000	0.526515000
H	4.092265000	0.453943000	1.061884000
H	4.031034000	-0.324180000	-0.397726000

$(ClCH(CH_3)CHO)_2$-A

C	-1.376655000	-0.899670000	0.902293000
O	-0.750980000	-0.239056000	1.718139000
H	-1.406076000	-2.013622000	0.963671000
C	-2.205907000	-0.354726000	-0.249480000
H	-1.788200000	-0.776207000	-1.178268000
Cl	-2.055089000	1.429121000	-0.379084000
C	1.790011000	1.178061000	0.021996000
O	2.684995000	2.013502000	0.012037000
H	0.728839000	1.444751000	-0.169487000
C	2.055411000	-0.295684000	0.315669000
Cl	1.183456000	-1.232538000	-0.986665000
H	1.529981000	-0.560230000	1.246870000
C	3.526578000	-0.663866000	0.350603000
H	4.016683000	-0.090474000	1.152170000
H	3.646960000	-1.738028000	0.548263000
H	4.012165000	-0.409850000	-0.602163000
C	-3.671979000	-0.763223000	-0.082960000
H	-4.255345000	-0.432540000	-0.953147000
H	-3.749606000	-1.860201000	-0.004770000
H	-4.094510000	-0.306428000	0.824453000

$(ClCH(OCH_3)CHO)_2$-A

C	-1.755556000	1.560460000	-0.946540000
O	-0.691615000	2.161012000	-1.018419000
H	-2.658064000	1.860801000	-1.521451000
C	-1.935176000	0.334780000	-0.065359000
H	-1.152606000	0.243062000	0.704645000
Cl	-1.625179000	-1.094230000	-1.206726000
C	2.064436000	-1.467080000	-0.610420000
O	3.146427000	-1.781076000	-1.076264000
H	1.196351000	-2.160759000	-0.575140000
C	1.774396000	-0.085093000	-0.025544000
Cl	1.125723000	-0.456568000	1.694194000
H	0.910602000	0.397787000	-0.513920000
O	2.892482000	0.690507000	0.000113000
C	2.614475000	2.067230000	0.334460000
H	1.813735000	2.462445000	-0.310253000
H	2.318662000	2.143603000	1.392254000
H	3.550759000	2.610261000	0.163703000
O	-3.217661000	0.335928000	0.430063000
C	-3.434101000	-0.685983000	1.425823000
H	-2.677639000	-0.602993000	2.223387000
H	-4.435916000	-0.505679000	1.831071000
H	-3.383054000	-1.681831000	0.960279000

$(ClCH(SCH_3)CHO)_2$-A

C	-1.497471000	1.223427000	-1.520057000
O	-0.447842000	1.851950000	-1.575556000
H	-2.279459000	1.307196000	-2.306769000
C	-1.801983000	0.260382000	-0.383735000
H	-1.025532000	0.306577000	0.391779000
Cl	-1.676348000	-1.411853000	-1.115956000
C	2.022849000	-1.710188000	-0.470848000
O	3.108797000	-2.068566000	-0.898601000
H	1.147617000	-2.393520000	-0.411783000
C	1.747894000	-0.295424000	0.034908000
Cl	0.992779000	-0.517784000	1.699850000
H	0.957482000	0.184130000	-0.563822000
S	3.232610000	0.713432000	0.032902000
C	2.423031000	2.293398000	0.465968000
H	1.618024000	2.516737000	-0.248481000
H	2.032558000	2.252364000	1.492649000
H	3.199313000	3.069305000	0.401959000
S	-3.426100000	0.623589000	0.310520000
C	-3.290405000	-0.456548000	1.776654000
H	-2.434809000	-0.151292000	2.395736000
H	-4.222547000	-0.334322000	2.346287000
H	-3.187278000	-1.503052000	1.457400000

$(Cl_2C(HSO_3)CHO)_2$-A

C	-1.520078000	-1.008996000	1.287460000
O	-0.880087000	-0.156196000	1.872024000
C	-2.530355000	-0.653328000	0.173328000
Cl	-2.160020000	-1.588917000	-1.292288000
Cl	-4.161863000	-0.994777000	0.775352000
C	3.933699000	-1.015585000	-0.597548000
O	3.969267000	-1.765269000	-1.552814000
H	4.833180000	-0.592192000	-0.103120000
C	2.610041000	-0.564270000	0.073503000
Cl	1.196884000	-1.310637000	-0.675324000
Cl	2.736081000	-0.936767000	1.808802000
S	2.509569000	1.296177000	-0.140378000
O	2.211402000	1.532045000	-1.568616000
O	3.704199000	1.840406000	0.530828000
O	1.233037000	1.671963000	0.785615000
H	0.414415000	1.570606000	0.234528000
S	-2.380867000	1.173833000	-0.206043000
O	-2.934872000	1.940029000	0.911782000
O	-1.017774000	1.384435000	-0.767051000
O	-3.442542000	1.305676000	-1.451900000
H	-2.932146000	1.156458000	-2.272266000
H	-1.463939000	-2.097994000	1.502986000

$(Cl_2C(CN)CHO)_2$-A

C	1.126743000	0.032066000	-0.005515000
O	0.510464000	1.062189000	-0.193314000
H	0.654465000	-0.953457000	0.193987000
C	2.670243000	-0.034102000	-0.020836000
Cl	3.167982000	-0.648952000	1.592538000
Cl	3.116864000	-1.211952000	-1.301356000
C	-4.161468000	-0.140275000	0.241577000
O	-4.780872000	-0.987405000	-0.362955000
H	-4.605807000	0.532904000	1.007102000
C	-2.633276000	0.114505000	0.043065000
Cl	-1.906586000	-0.217535000	1.664540000
Cl	-1.965134000	-0.962559000	-1.198751000
C	3.299340000	1.260965000	-0.283253000
N	3.797468000	2.318700000	-0.496576000
C	-2.425436000	1.523066000	-0.310005000
N	-2.392526000	2.678712000	-0.590516000

$(Cl_2C(NO_2)CHO)_2$-A

C	1.089141000	0.102054000	0.972278000
O	0.505680000	1.162707000	0.858105000
H	0.792048000	-0.706963000	1.673146000
C	2.364597000	-0.215906000	0.160336000
Cl	3.744112000	0.038374000	1.232627000
Cl	2.307346000	-1.880747000	-0.438857000
C	-3.877959000	-0.299413000	-0.260889000
O	-4.278070000	-1.131610000	-1.046288000
H	-4.527689000	0.424711000	0.276564000
C	-2.373627000	-0.140053000	0.114990000
Cl	-2.274835000	-0.295684000	1.883346000
Cl	-1.348740000	-1.284026000	-0.715836000
N	2.397994000	0.755322000	-1.043767000
O	1.522113000	0.534861000	-1.880282000
O	3.221264000	1.667320000	-1.029881000
N	-2.017719000	1.323671000	-0.287060000
O	-2.538985000	2.185404000	0.422908000
O	-1.358652000	1.484394000	-1.311559000

$(Cl_2C(NH_2)CHO)_2$-A

C	1.421795000	0.503375000	-0.560596000
O	0.843660000	1.577518000	-0.463918000
H	0.962088000	-0.397306000	-1.013601000
C	2.839263000	0.313325000	-0.012073000
Cl	2.534046000	-0.790992000	1.455518000
Cl	3.794508000	-0.640508000	-1.191184000
C	-2.983094000	1.209813000	0.600544000
O	-4.147362000	1.488257000	0.813355000
H	-2.132711000	1.844994000	0.946139000
C	-2.489034000	0.000728000	-0.223964000
Cl	-1.352391000	-0.871734000	0.891953000
Cl	-3.845649000	-1.051119000	-0.682466000
N	3.461268000	1.533750000	0.271984000
H	4.329700000	1.425242000	0.791857000
H	2.816759000	2.169555000	0.742978000
N	-1.756304000	0.385531000	-1.400143000
H	-1.033780000	1.073620000	-1.156570000
H	-2.399504000	0.783288000	-2.087585000

$(Cl_2C(CH_3)CHO)_2$-A

C	1.290186000	-0.693202000	0.293181000
O	0.863918000	-1.162715000	1.337002000
H	0.762162000	-0.794735000	-0.677659000
C	2.613023000	0.079684000	0.231055000
Cl	3.662372000	-0.879420000	-0.885023000
Cl	2.230669000	1.664958000	-0.538132000
C	-3.993357000	0.147874000	-0.181237000
O	-4.416778000	1.277765000	-0.332738000
H	-4.640174000	-0.755401000	-0.274368000
C	-2.542022000	-0.205472000	0.189654000
Cl	-2.031842000	-1.437069000	-1.043543000
Cl	-1.494155000	1.233485000	0.078288000
C	3.288728000	0.276279000	1.570852000
H	2.620363000	0.847628000	2.231182000
H	3.488855000	-0.705297000	2.023410000
H	4.231174000	0.823154000	1.433259000
C	-2.473651000	-0.824220000	1.579473000
H	-2.776056000	-0.069679000	2.322064000
H	-3.154308000	-1.688394000	1.631266000
H	-1.446327000	-1.156539000	1.781833000

$(Cl_2C(OCH_3)CHO)_2$-A

C	1.075994000	0.827826000	-0.541065000
O	0.820314000	1.993362000	-0.303794000
H	0.428360000	0.163332000	-1.148036000
C	2.353229000	0.140308000	-0.020666000
Cl	1.801514000	-1.359088000	0.856615000
Cl	3.243996000	-0.407777000	-1.524211000
C	-3.951150000	-0.213021000	-0.138548000
O	-4.637358000	-0.063919000	0.852811000
H	-4.368740000	-0.403411000	-1.153590000
C	-2.403083000	-0.139513000	-0.172022000
Cl	-1.736864000	0.095456000	1.479237000
Cl	-1.858682000	-1.721971000	-0.825835000
O	3.071199000	0.983635000	0.747721000
C	4.302906000	0.463485000	1.299588000
H	4.089592000	-0.389058000	1.959802000
H	4.982100000	0.164635000	0.488481000
H	4.727959000	1.296055000	1.870256000
O	-1.971176000	0.812805000	-1.077313000
C	-2.313467000	2.174885000	-0.700627000
H	-3.390738000	2.263008000	-0.486296000
H	-1.720310000	2.482345000	0.169492000
H	-2.048019000	2.779681000	-1.574156000

$(Cl_2C(SCH_3)CHO)_2$-A

C	1.565554000	-0.132939000	-0.020851000
O	1.115566000	-1.265503000	-0.031157000
H	0.929786000	0.778789000	-0.023824000
C	3.075596000	0.159085000	-0.002717000
Cl	3.386108000	1.195880000	-1.454963000
Cl	3.353087000	1.175718000	1.471033000
C	-4.110191000	-0.263000000	1.352392000
O	-4.863324000	-1.218627000	1.404323000
H	-3.737200000	0.277193000	2.250932000
C	-3.489739000	0.270228000	0.050646000
Cl	-4.448544000	-0.206589000	-1.373238000
Cl	-3.392715000	2.059326000	0.178813000
S	4.008868000	-1.380049000	-0.002601000
C	5.689685000	-0.675250000	0.019807000
H	5.865179000	-0.070640000	-0.880500000
H	5.845185000	-0.080928000	0.930588000
H	6.371587000	-1.538142000	0.022475000
S	-1.765620000	-0.331450000	0.018315000
C	-2.081502000	-2.114773000	-0.197636000
H	-2.735283000	-2.499828000	0.598012000
H	-2.521991000	-2.303045000	-1.185255000
H	-1.088486000	-2.580188000	-0.126996000

$(BrCH(HSO_3)CHO)_2$-A

C	1.549465000	-0.518183000	1.845746000
O	0.450947000	-0.915469000	2.205656000
H	2.389533000	-0.331501000	2.548290000
C	1.841541000	-0.253305000	0.368809000
Br	3.522989000	-1.043111000	-0.139775000
H	1.038532000	-0.665464000	-0.259258000
C	-1.817165000	0.804826000	-1.765822000
O	-0.857992000	1.371954000	-2.278868000
H	-2.782995000	0.708435000	-2.302010000
C	-1.734627000	0.152846000	-0.392934000
H	-0.910454000	0.551933000	0.217391000
Br	-1.497430000	-1.748001000	-0.694725000
S	1.842056000	1.567517000	0.113276000
O	1.777843000	1.674386000	-1.510949000
O	0.539278000	2.010857000	0.682262000
O	3.125317000	2.137921000	0.546052000
H	0.817630000	1.623333000	-1.762499000
S	-3.276775000	0.488404000	0.523873000
O	-2.861283000	-0.039933000	2.025928000
O	-4.373423000	-0.351875000	-0.004079000
O	-3.350234000	1.958144000	0.603298000
H	-3.130243000	-0.977512000	2.082025000

$(BrCH(CN)CHO)_2$-A

C	0.227653000	2.190114000	0.730923000
O	1.188768000	1.552786000	1.135173000
H	0.323397000	3.217759000	0.319255000
C	-1.188768000	1.611239000	0.735874000
Br	-1.640275000	1.335141000	-1.155512000
H	-1.210066000	0.619496000	1.210059000
C	-0.227653000	-2.190114000	0.730923000
O	-1.188768000	-1.552786000	1.135173000
H	-0.323397000	-3.217759000	0.319255000
C	1.188768000	-1.611239000	0.735874000
H	1.210066000	-0.619496000	1.210059000
Br	1.640275000	-1.335141000	-1.155512000
C	-2.141523000	2.540384000	1.342440000
N	-2.872553000	3.325678000	1.853830000
C	2.141523000	-2.540384000	1.342440000
N	2.872553000	-3.325678000	1.853830000

$(BrCH(NO_2)CHO)_2$-A

C	1.523870000	0.627331000	1.623439000
O	0.384314000	0.935135000	1.942663000
H	2.309895000	0.392182000	2.370923000
C	1.939729000	0.482406000	0.163376000
Br	2.140819000	-1.396610000	-0.211442000
H	1.199750000	0.898485000	-0.536586000
C	-1.528763000	0.637111000	-1.620427000
O	-0.389798000	0.948907000	-1.937861000
H	-2.314210000	0.404398000	-2.369293000
C	-1.944546000	0.483486000	-0.161188000
H	-1.208862000	0.903780000	0.540757000
Br	-2.128716000	-1.398530000	0.206771000
N	3.233760000	1.238169000	-0.043777000
O	4.032900000	0.871769000	-0.902524000
O	3.332053000	2.237935000	0.686208000
N	-3.245302000	1.227358000	0.047206000
O	-3.347392000	2.232957000	-0.674150000
O	-4.045971000	0.847094000	0.898476000

$(BrCH(NH_2)CHO)_2$-A

C	1.634265000	0.917983000	1.572762000
O	0.577182000	1.352329000	2.017405000
H	2.453343000	0.553978000	2.232064000
C	1.942694000	0.852324000	0.085928000
Br	2.069907000	-1.062399000	-0.315901000
H	1.098999000	1.217017000	-0.518505000
C	-1.633826000	0.918646000	-1.572491000
O	-0.576798000	1.353550000	-2.016721000
H	-2.452680000	0.554726000	-2.232110000
C	-1.942469000	0.852318000	-0.085719000
H	-1.098804000	1.216863000	0.518846000
Br	-2.070205000	-1.062354000	0.315582000
N	3.243264000	1.461267000	-0.155481000
H	3.546175000	1.255823000	-1.109153000
H	3.144763000	2.478739000	-0.092709000
N	-3.242983000	1.461614000	0.155663000
H	-3.143918000	2.479114000	0.094164000
H	-3.546483000	1.255234000	1.108952000

$(BrCH(CH_3)CHO)_2$-A

C	-1.367335000	0.718994000	-1.641158000
O	-0.409685000	1.363783000	-2.054388000
H	-1.935525000	0.030348000	-2.308854000
C	-1.884627000	0.827755000	-0.221454000
Br	-1.987735000	-1.009500000	0.466301000
H	-1.158176000	1.349537000	0.415545000
C	1.368633000	0.717316000	1.641964000
O	0.410462000	1.360833000	2.055945000
H	1.937696000	0.028701000	2.308964000
C	1.885591000	0.827369000	0.222243000
H	1.159535000	1.350413000	-0.414171000
Br	1.986633000	-1.009412000	-0.467251000
C	-3.265552000	1.476527000	-0.190574000
H	-3.972340000	0.928095000	-0.832731000
H	-3.657818000	1.483778000	0.836261000
H	-3.185877000	2.516546000	-0.548779000
C	3.267183000	1.474668000	0.191628000
H	3.188739000	2.514419000	0.550890000
H	3.973557000	0.924844000	0.833051000
H	3.659200000	1.482537000	-0.835297000

$(BrCH(OCH_3)CHO)_2$-A

C	-2.085211000	1.429797000	-0.665285000
O	-1.225658000	2.303623000	-0.702709000
H	-2.844890000	1.327594000	-1.470546000
C	-2.129905000	0.407478000	0.461596000
Br	-1.485690000	-1.251789000	-0.495901000
H	-1.356188000	0.604258000	1.213681000
C	1.681353000	0.847758000	1.567729000
O	0.612958000	0.891947000	2.164900000
H	2.656024000	1.032188000	2.072928000
C	1.802588000	0.561356000	0.076465000
H	0.817452000	0.492200000	-0.411236000
Br	2.614895000	-1.213641000	-0.032085000
O	-3.337067000	0.219480000	1.097598000
C	-4.480525000	-0.017496000	0.249941000
H	-4.249222000	-0.794238000	-0.495692000
H	-5.272562000	-0.369297000	0.920734000
H	-4.806406000	0.908895000	-0.247527000
O	2.670975000	1.472925000	-0.540026000
C	1.948197000	2.636390000	-1.004078000
H	1.426504000	3.142054000	-0.175380000
H	2.706857000	3.301688000	-1.432925000
H	1.211627000	2.349202000	-1.770810000

$(BrCH(SCH_3)CHO)_2$-A

C	-1.697460000	0.628066000	-1.889276000
O	-0.726297000	1.258983000	-2.291056000
H	-2.457554000	0.210120000	-2.586244000
C	-1.925880000	0.349445000	-0.416819000
Br	-1.498445000	-1.583506000	-0.212737000
H	-1.190325000	0.862069000	0.217652000
C	1.237013000	0.455647000	1.626670000
O	0.136858000	0.901116000	1.945071000
H	2.016359000	0.206283000	2.379692000
C	1.667016000	0.304711000	0.184623000
H	0.824408000	0.276809000	-0.518246000
Br	2.689106000	-1.332695000	-0.013786000
S	-3.606382000	0.780866000	0.060694000
C	-3.394314000	0.546545000	1.859097000
H	-3.210225000	-0.516224000	2.071630000
H	-2.560855000	1.161853000	2.225853000
H	-4.334453000	0.863761000	2.332140000
S	2.756985000	1.732405000	-0.163402000
C	1.438632000	3.001439000	-0.212733000
H	0.699405000	2.737922000	-0.981983000
H	0.959436000	3.111620000	0.771352000
H	1.936476000	3.944589000	-0.481712000

$(Br_2C(HSO_3)CHO)_2$-A

C	-3.927950000	-0.770669000	-1.306529000
O	-4.203161000	-0.126107000	-2.307266000
H	-4.357526000	-1.772667000	-1.094671000
C	-2.934926000	-0.289357000	-0.235364000
Br	-3.683383000	-0.628903000	1.512331000
Br	-1.290189000	-1.265549000	-0.522017000
C	1.862940000	0.633844000	-1.420284000
O	0.895149000	1.360620000	-1.278974000
H	2.248924000	0.309243000	-2.412007000
C	2.662732000	0.059795000	-0.239941000
Br	2.270927000	-1.839700000	-0.166122000
Br	4.539873000	0.386028000	-0.574494000
S	-2.637942000	1.546216000	-0.363672000
O	-2.096531000	1.648505000	-1.901119000
O	-3.958930000	2.185513000	-0.229809000
O	-1.495589000	1.919577000	0.491699000
H	-2.877323000	1.416365000	-2.455337000
S	2.235932000	0.876439000	1.384088000
O	0.653164000	0.512149000	1.493547000
O	2.896868000	0.116157000	2.455636000
O	2.434369000	2.323565000	1.172481000
H	0.135621000	1.147391000	0.939115000

$(Br_2C(CN)CHO)_2$-A

C	4.020448000	0.132673000	-0.495722000
O	5.075283000	-0.252912000	-0.034478000
H	3.919365000	0.705758000	-1.443595000
C	2.659570000	-0.135265000	0.186694000
Br	1.880104000	1.629477000	0.529996000
Br	1.589543000	-1.126968000	-1.108555000
C	-1.120798000	-0.093835000	1.271823000
O	-0.354545000	-0.960508000	1.643501000
H	-1.241068000	0.894968000	1.765964000
C	-2.056917000	-0.273513000	0.057230000
Br	-3.870039000	-0.241030000	0.790358000
Br	-1.770320000	1.248069000	-1.131566000
C	-1.838977000	-1.519447000	-0.668915000
N	-1.648752000	-2.531615000	-1.264509000
C	2.776792000	-0.880350000	1.433524000
N	2.918751000	-1.483970000	2.448722000

$(Br_2C(NO_2)CHO)_2$-A

C	-4.086430000	0.568580000	0.144171000
O	-4.756636000	0.454209000	1.150992000
H	-4.431843000	1.064756000	-0.788651000
C	-2.639030000	0.034948000	0.046598000
Br	-2.553365000	-1.188781000	-1.442567000
Br	-1.484346000	1.557494000	-0.214530000
C	0.881963000	-0.817700000	-0.262173000
O	0.196098000	-1.392220000	0.562296000
H	0.659575000	-0.786503000	-1.350556000
C	2.186887000	-0.098943000	0.132737000
Br	3.625142000	-1.277775000	-0.364736000
Br	2.316612000	1.599895000	-0.774204000
N	2.137376000	0.142273000	1.656500000
O	2.887729000	-0.511729000	2.377381000
O	1.274805000	0.951664000	1.999773000
N	-2.331188000	-0.685563000	1.375451000
O	-1.788889000	-0.014754000	2.251333000
O	-2.759718000	-1.834130000	1.459327000

$(Br_2C(NH_2)CHO)_2$-A

C	4.238142000	0.101065000	-0.022083000
O	5.116256000	-0.091726000	0.802521000
H	4.429054000	0.273870000	-1.101798000
C	2.759324000	0.088333000	0.376817000
Br	1.825047000	1.542205000	-0.530726000
Br	2.156443000	-1.650692000	-0.571264000
C	-0.952595000	-0.253939000	0.891824000
O	-0.422784000	-0.089782000	1.984230000
H	-0.392932000	-0.528512000	-0.023023000
C	-2.454545000	-0.054063000	0.710543000
Br	-2.465995000	1.631460000	-0.427432000
Br	-3.152585000	-1.498745000	-0.393813000
N	-3.133143000	0.030499000	1.926196000
H	-4.103391000	0.322919000	1.836116000
H	-2.619181000	0.599590000	2.600285000
N	2.567044000	0.125992000	1.742133000
H	3.256624000	-0.433806000	2.243439000
H	1.600948000	-0.013786000	2.043278000

$(Br_2C(CH_3)CHO)_2$-A

C	4.206486000	0.343308000	-0.289755000
O	5.220421000	0.420764000	0.384485000
H	4.183426000	0.558306000	-1.381152000
C	2.857252000	-0.059906000	0.311846000
Br	1.654694000	1.440095000	-0.084427000
Br	2.290931000	-1.636021000	-0.712847000
C	-1.013462000	-0.636496000	0.618811000
O	-0.443278000	-0.878743000	1.672070000
H	-0.594953000	-0.912750000	-0.372033000
C	-2.372123000	0.062973000	0.582679000
Br	-2.178972000	1.577973000	-0.643504000
Br	-3.584656000	-1.262781000	-0.206779000
C	-2.879020000	0.522178000	1.934060000
H	-2.165598000	1.243524000	2.360625000
H	-3.863388000	0.997407000	1.825930000
H	-2.957064000	-0.344644000	2.606664000
C	2.885227000	-0.359110000	1.795251000
H	3.228067000	0.535916000	2.335592000
H	1.882479000	-0.646034000	2.137186000
H	3.593816000	-1.179917000	1.981920000

$(Br_2C(OCH_3)CHO)_2$-A

C	4.057182000	0.346085000	-0.022122000
O	4.826795000	0.714299000	0.847015000
H	4.370096000	0.072550000	-1.053633000
C	2.538953000	0.234995000	0.215905000
Br	1.722095000	1.506524000	-1.027706000
Br	2.078452000	-1.625082000	-0.369099000
C	-0.927793000	-0.334721000	1.201978000
O	-0.714622000	-1.048017000	2.165759000
H	-0.187908000	0.372669000	0.779102000
C	-2.272184000	-0.331899000	0.458153000
Br	-2.854460000	1.574530000	0.482786000
Br	-1.815794000	-0.797684000	-1.423019000
O	-3.150760000	-1.174696000	1.029978000
C	-4.458463000	-1.267143000	0.421798000
H	-4.950783000	-0.283903000	0.444723000
H	-4.363845000	-1.627748000	-0.612843000
H	-5.006151000	-1.989676000	1.036327000
O	2.082469000	0.547197000	1.455848000
C	2.485736000	-0.355176000	2.528941000
H	1.943708000	-1.303404000	2.418736000
H	3.572884000	-0.502021000	2.523747000
H	2.170089000	0.158332000	3.443461000

$(Br_2C(SCH_3)CHO)_2$-A

C	-4.215013000	0.048109000	1.586832000
O	-3.822382000	0.516496000	2.639482000
H	-5.232541000	-0.383348000	1.451564000
C	-3.356177000	-0.006688000	0.308347000
Br	-3.210301000	-1.908453000	-0.127882000
Br	-4.471661000	0.891656000	-1.059523000
C	1.617024000	0.541175000	0.190489000
O	1.175276000	1.641066000	0.478469000
H	0.975352000	-0.350667000	0.023684000
C	3.119332000	0.276390000	0.027368000
Br	3.518153000	-1.175829000	1.301379000
Br	3.309832000	-0.445087000	-1.798955000
S	4.056554000	1.778283000	0.318360000
C	5.734230000	1.122020000	0.051083000
H	5.956419000	0.331882000	0.781994000
H	5.838716000	0.746910000	-0.976681000
H	6.414677000	1.972098000	0.206186000
S	-1.680254000	0.627268000	0.426534000
C	-2.021809000	2.373094000	0.826082000
H	-2.646289000	2.819320000	0.039182000
H	-2.494637000	2.459270000	1.812263000
H	-1.031976000	2.850584000	0.833030000