

1) Completion of Reference [20].

M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, O. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, and D.J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2013.

2) Table S1

Measured transitions frequencies (ν) and observed- calculated values ($\Delta\nu$) of the isotopologues of conformer I of $(\text{CH}_2\text{ClF})_2$. F_1 and F are half integer numbers, rounded to the next integer in the Table.

										$^{35}\text{Cl}(2) - ^{35}\text{Cl}(7)$		$^{37}\text{Cl}(2) - ^{35}\text{Cl}(7)$		$^{35}\text{Cl}(2) - ^{37}\text{Cl}(7)$	
J'	K'_{-1}	K'_{+1}	F_1'	F'	J''	K''_{-1}	K''_{+1}	F_1''	F''	ν/MHz	$\Delta\nu/\text{MHz}$	ν/MHz	$\Delta\nu/\text{MHz}$	ν/MHz	$\Delta\nu/\text{MHz}$
4	1	4	6	4	3	1	3	5	3	6825.556	-0.008	6759.511	-0.012	6714.582	-0.008
4	1	4	6	7	3	1	3	5	6	6825.656	0.001	6759.618	-0.001	6714.702	0.001
4	1	4	6	5	3	1	3	5	4	6826.171	-0.004	6760.249	-0.004	6715.028	-0.004
4	1	4	6	6	3	1	3	5	5	6826.626	-0.005	6760.666	-0.007	6715.389	-0.005
4	1	4	5	4	3	1	3	4	3	6826.774	-0.010				
4	1	4	5	5	3	1	3	4	4	6826.849	-0.007	6760.895	-0.009	6715.800	-0.007
4	1	4	5	6	3	1	3	4	5	6826.988	0.002	6760.621	-0.001	6715.970	-0.002
4	1	4	5	3	3	1	3	4	2	6827.021	-0.009				
4	1	4	3	4	3	1	3	2	3	6827.090	-0.002	6760.412	0.002	6716.178	-0.001
4	1	4	4	3	3	1	3	3	2	6827.072	-0.005			6716.156	0.007
4	1	4	4	4	3	1	3	3	3	6827.072	-0.009				
4	1	4	4	5	3	1	3	3	4	6827.325	-0.001	6760.602	-0.001	6716.459	-0.007

4	1	4	3	3	3	1	3	2	2	6827.404	-0.009				
4	0	4	5	6	3	0	3	4	5	6862.669	0.000	6797.298	0.001	6753.334	0.000
4	0	4	6	7	3	0	3	5	6	6863.295	0.000	6796.964	-0.001	6753.828	0.000
4	0	4	5	4	3	0	3	4	3	6863.512	0.000	6797.134	-0.001	6754.052	-0.002
4	0	4	5	5	3	0	3	4	4	6863.570	-0.001	6797.178	-0.001	6754.103	0.001
4	0	4	4	3	3	0	3	3	2	6863.665	0.003			6754.174	0.001
4	0	4	4	2	3	0	3	3	1	6863.693	-0.008				
4	0	4	6	6	3	0	3	5	5	6863.722	-0.001			6754.174	-0.001
4	0	4	3	3	3	0	3	2	2	6863.722	-0.004				
4	0	4	6	5	3	0	3	5	4	6863.748	0.000	6797.551	-0.001	6754.494	-0.001
4	0	4	3	4	3	0	3	2	3	6863.858	0.000			6754.431	-0.004
4	0	4	6	4	3	0	3	5	3	6864.029	0.001	6797.732	0.001	6754.374	0.003
4	0	4	4	5	3	0	3	3	4	6864.168	0.002	6797.566	0.000	6754.358	0.000
4	2	3	6	6	3	2	2	4	5	6864.988	-0.007	6796.432	-0.001		
4	0	4	4	4	3	0	3	3	3	6865.339	0.001	6798.774	0.001	6755.656	-0.001
4	2	3	6	5	3	2	2	5	4	6865.431	-0.008				
4	0	4	5	3	3	0	3	4	2	6866.081	-0.002			6754.374	0.000
4	2	3	5	6	3	2	2	5	5	6866.655	0.002				
4	2	2	4	5	3	2	1	3	4	6867.559	-0.004				
4	2	3	4	4	3	2	2	3	3	6867.713	-0.001				
4	2	3	6	7	3	2	2	5	6					6753.424	-0.003
4	2	2	5	6	3	2	1	4	5	6868.052	-0.003				
4	0	4	5	5	3	0	3	4	5	6868.105	-0.001				
4	2	3	5	5	3	2	1	5	4	6868.735	-0.004				
4	2	2	4	2	3	2	1	2	1	6868.735	-0.005				
4	2	2	6	6	3	2	1	5	5	6869.113	-0.001				
4	2	2	5	4	3	2	1	4	3	6869.512	-0.004				
4	2	2	4	3	3	2	1	3	2	6870.307	-0.007				
4	2	2	4	4	3	2	1	3	3	6870.320	0.002				
4	2	2	5	5	3	2	1	4	4	6870.572	0.002				
4	1	3	3	4	3	1	2	2	3	6901.596	-0.004	6835.329	0.005	6793.871	0.000
4	1	3	6	7	3	1	2	5	6	6901.837	-0.002	6835.312	-0.002	6794.191	0.000

4	1	3	6	6	3	1	2	5	5	6902.286	-0.006	6835.670	-0.006	6794.614	-0.004
4	1	3	5	6	3	1	2	4	5	6902.370	-0.002	6835.854	-0.001	6794.733	-0.001
4	1	3	4	3	3	1	2	3	2	6902.570	-0.007	6836.228	-0.006		
4	1	3	4	5	3	1	2	3	4	6902.756	0.000	6836.207	-0.003	6795.010	0.000
4	1	3	6	4	3	1	2	5	3	6902.926	-0.011	6836.099	-0.010	6795.232	-0.006
4	1	3	4	4	3	1	2	4	3	6903.447	-0.005	6836.850	-0.007	6795.556	-0.005
4	1	3	3	2	3	1	2	3	1	6903.610	-0.006				
4	1	3	5	5	3	1	2	4	4	6903.790	-0.006	6837.155	-0.009	6795.853	-0.003
4	1	3	6	5	3	1	2	5	4	6903.926	-0.001	6837.181	0.000	6795.942	0.000
4	1	3	5	3	3	1	2	4	2	6904.190	-0.006				
4	1	3	3	3	3	1	2	2	2	6904.304	0.000				
4	1	3	5	4	3	1	2	3	3	6905.591	-0.001	6838.873	-0.001		
5	1	5	7	5	4	1	4	6	4	8532.026	0.009	8449.462	0.005	8393.285	0.007
5	1	5	7	8	4	1	4	6	7	8532.132	0.001	8449.524	-0.001	8393.394	0.001
5	1	5	4	2	4	1	4	3	1	8532.245	0.007				
5	1	5	7	6	4	1	4	6	5	8532.382	0.002	8449.863	0.001	8393.536	0.001
5	1	5	7	7	4	1	4	6	6	8532.608	0.007	8450.043	0.002	8393.722	0.006
5	1	5	4	3	4	1	4	3	2	8532.660	0.005	8449.996	0.000	8393.907	0.004
5	1	5	6	5	4	1	4	5	4	8532.703	0.002			8393.867	0.002
5	1	5	6	6	4	1	4	5	5	8532.761	0.001	8450.210	0.004	8393.961	0.000
5	1	5	6	7	4	1	4	5	6	8532.794	0.000	8450.018	-0.001	8394.022	-0.001
5	1	5	4	5	4	1	4	3	4	8532.814	0.005	8449.835	0.002	8394.164	0.003
5	1	5	5	3	4	1	4	4	2	8532.883	-0.001	8450.043	0.005	8394.227	0.005
5	1	5	5	4	4	1	4	4	3	8533.006	0.000	8450.243	0.000	8394.282	-0.002
5	1	5	5	5	4	1	4	4	4	8533.093	0.011	8450.349	0.003	8394.351	0.001
5	1	5	5	6	4	1	4	4	5	8533.082	-0.005	8450.063	-0.001	8394.428	0.001
5	1	5	4	4	4	1	4	3	3	8533.179	0.006			8394.351	0.002
5	1	5	6	4	4	1	4	5	3			8450.087	0.005	8393.939	0.006
5	0	5	6	6	4	0	4	5	5	8575.277	-0.001	8500.719	0.001	8440.352	-0.001
5	0	5	4	2	4	0	4	3	1	8576.343	0.002				
5	0	5	6	5	4	0	4	5	4	8576.509	-0.001	8500.072	0.001	8440.785	-0.002
5	0	5	4	4	4	0	4	3	3	8576.519	0.001	8501.567	-0.001	8441.687	0.002

5	0	5	5	3	4	0	4	4	2	8576.620	-0.002	8502.980	0.000		
5	0	5	4	5	4	0	4	3	4	8577.131	0.001	8502.175	0.001	8440.995	0.002
5	0	5	7	7	4	0	4	6	6	8577.168	0.000	8497.189	-0.001	8441.060	-0.003
5	0	5	7	5	4	0	4	6	4	8577.233	-0.001	8504.582	0.002	8441.223	-0.001
5	0	5	6	7	4	0	4	5	6	8577.288	0.000	8498.919	0.001	8440.766	0.000
5	0	5	5	4	4	0	4	4	3	8577.880	-0.001	8498.720	-0.001	8441.411	-0.002
5	0	5	7	6	4	0	4	6	5	8578.186	-0.002	8497.819	-0.001	8441.578	0.004
5	0	5	7	8	4	0	4	6	7	8578.286	0.001	8495.342	0.000	8441.332	0.001
5	0	5	6	4	4	0	4	5	3	8578.331	0.003	8501.797	0.000	8441.165	-0.002
5	2	4	4	5	4	2	3	3	4	8578.415	0.000			8442.190	0.000
5	0	5	5	5	4	0	4	4	4	8578.513	0.001	8498.804	0.000	8441.968	-0.001
5	2	4	7	8	4	2	3	6	7	8578.568	-0.001	8497.315	0.004	8442.422	0.001
5	0	5	5	6	4	0	4	4	5	8578.684	0.000	8496.527	-0.002	8441.620	-0.002
5	2	4	7	5	4	2	3	6	4	8578.960	0.001	8495.885	0.001		
5	0	5	4	3	4	0	4	3	2	8579.026	0.001	8504.113	0.000	8442.467	-0.007
5	2	3	6	7	4	2	2	6	6	8579.757	0.000	8505.475	-0.001	8446.922	-0.002
5	2	4	4	3	4	2	3	3	2	8580.034	0.007				
5	2	4	7	7	4	2	3	6	6					8443.712	0.000
5	2	4	7	6	4	2	3	6	5	8580.056	-0.001	8498.225	-0.003	8443.517	-0.002
5	2	4	5	6	4	2	3	4	5	8580.121	0.000			8443.765	0.002
5	2	4	5	3	4	2	3	4	2	8580.210	0.002				
5	2	3	7	8	4	2	2	6	7	8580.322	-0.001	8503.495	-0.004	8444.802	0.002
5	2	3	4	4	4	2	2	5	3					8446.655	-0.002
5	2	3	5	3	4	2	2	4	2	8580.374	-0.001				
5	2	4	6	7	4	2	3	6	6	8580.399	0.000			8444.353	0.000
5	2	3	5	6	4	2	2	6	5	8580.470	-0.004			8445.579	-0.001
5	2	4	6	5	4	2	3	5	4					8445.258	-0.001
5	2	4	6	4	4	2	3	5	3	8580.575	-0.002	8497.173	-0.006		
5	2	4	6	6	4	2	3	5	5					8445.548	0.002
5	2	3	7	5	4	2	2	6	4	8580.600	0.000			8444.696	0.002
5	2	4	4	4	4	2	3	3	3	8580.671	-0.003	8497.944	-0.002		
5	0	5	6	6	4	0	4	5	6	8580.715	0.001				

5	2	3	5	6	4	2	2	4	5	8580.956	-0.001			8445.710	0.001
5	2	4	7	6	4	2	3	6	5	8580.055	-0.002			8445.908	0.001
5	2	4	5	6	4	2	3	4	5	8580.120	0.000				
5	2	4	6	6	4	2	3	5	5			8499.673	0.003		
5	2	3	6	6	4	2	2	5	5			8502.515	0.000	8448.368	0.000
5	2	3	7	7	4	2	2	5	6					8445.731	0.002
5	2	3	6	4	4	2	2	3	3					8446.670	0.001
5	2	3	7	8	4	2	2	6	7	8580.321	-0.003				
5	2	4	7	7	4	2	3	5	6	8581.097	0.001	8499.168	0.001		
5	2	3	4	5	4	2	2	3	4	8581.209	-0.004	8499.277	0.007	8445.082	0.000
5	2	4	5	5	4	2	2	4	4			8499.125	-0.003		
5	2	3	5	5	4	2	2	5	4			8503.137	0.001		
5	1	4	7	8	4	1	3	6	7	8627.672	0.000	8544.456	-0.001	8492.976	0.000
5	1	4	4	5	4	1	3	3	4	8627.708	-0.002	8544.606	-0.002	8492.949	0.001
5	1	4	7	7	4	1	3	6	6	8627.771	0.000	8544.516	0.002	8493.090	0.002
5	1	4	6	7	4	1	3	5	6	8628.001	0.000	8544.781	-0.001	8493.314	0.001
5	1	4	5	6	4	1	3	4	5	8628.247	0.000	8545.005	0.000	8493.498	0.000
5	1	4	5	4	4	1	3	4	3	8628.405	0.003	8545.317	0.000	8493.553	0.001
5	1	4	7	5	4	1	3	6	4	8628.514	0.006	8545.141	0.007	8493.721	0.006
5	1	4	5	5	4	1	3	4	4	8628.638	0.001	8545.374	0.003	8493.802	0.001
5	1	4	6	6	4	1	3	5	5	8628.649	0.005	8545.366	0.001	8493.817	0.005
5	1	4	4	3	4	1	3	3	2	8628.789	0.000	8545.469	0.001	8493.899	-0.001
5	1	4	7	6	4	1	3	6	5	8628.926	0.002	8545.596	0.001	8494.018	0.001
5	1	4	6	4	4	1	3	5	3	8629.035	0.004	8545.690	0.005	8494.227	0.006
5	1	4	4	4	4	1	3	3	3	8629.143	0.000	8545.732	0.004	8494.227	0.001
5	1	4	6	5	4	1	3	5	4	8629.846	0.003	8546.496	0.000	8494.799	0.001
6	1	6	8	6	5	1	5	7	5	10238.147	0.001	10139.025	-0.002	10071.618	0.001
6	1	6	8	9	5	1	5	7	8	10238.212	0.001	10139.049	-0.001	10071.686	0.001
6	1	6	8	7	5	1	5	7	6	10238.344	0.001	10139.255	0.002	10071.748	-0.001
6	1	6	8	8	5	1	5	7	7	10238.463	0.002	10139.341	0.008	10071.852	0.001
6	1	6	7	6	5	1	5	6	5	10238.522	-0.001	10139.398	-0.005	10071.941	0.000
6	1	6	7	7	5	1	5	6	6	10238.566	-0.002	10139.421	-0.001	10072.017	-0.002

6	1	6	7	8	5	1	5	6	7	10238.586	0.001	10139.321	0.000	10072.044	-0.001
6	1	6	5	6	5	1	5	4	5	10238.623	0.002	10139.230	-0.002	10072.171	0.002
6	1	6	5	4	5	1	5	4	3					10072.071	-0.001
6	1	6	6	4	5	1	5	5	3	10238.738	0.000				
6	1	6	6	5	5	1	5	5	4	10238.778	-0.002	10139.519	0.003	10072.272	0.000
6	1	6	6	7	5	1	5	5	6	10238.820	-0.003	10139.398	0.000	10072.348	-0.001
6	1	6	6	6	5	1	5	5	5	10238.835	-0.001	10139.562	0.000	10072.324	-0.001
6	1	6	5	5	5	1	5	4	4	10238.855	-0.002			10072.295	0.001
6	0	6	8	9	5	0	5	7	8	10292.470	0.001	10192.927	0.009	10127.975	0.001
6	0	6	7	8	5	0	5	6	7	10292.597	0.000	10189.719	-0.001	10127.994	0.000
6	0	6	6	7	5	0	5	5	6	10292.909	-0.001	10192.294	0.001	10128.439	0.000
6	0	6	8	7	5	0	5	7	6	10292.955	0.000	10190.937	-0.001	10128.126	0.001
6	0	6	6	5	5	0	5	5	4	10293.571	-0.001	10190.076	-0.001	10128.566	0.000
6	0	6	6	6	5	0	5	5	5	10293.765	-0.001	10188.289	-0.001	10128.726	-0.001
6	0	6	8	8	5	0	5	7	7	10294.103	0.002	10190.305	0.002	10128.539	0.000
6	0	6	5	6	5	0	5	4	5	10294.376	0.001	10186.657	0.003	10129.086	0.000
6	0	6	7	6	5	0	5	6	5	10294.443	0.000	10190.766	0.000	10128.778	-0.004
6	0	6	8	6	5	0	5	7	5	10294.465	0.003	10184.644	0.001	10128.791	0.002
6	0	6	7	5	5	0	5	6	4	10294.544	0.001			10129.131	-0.002
6	0	6	6	4	5	0	5	5	3	10294.654	-0.001				
6	0	6	5	5	5	0	5	4	4	10294.731	0.002				
6	0	6	5	4	5	0	5	4	3	10294.925	0.004			10129.548	0.004
6	2	5	8	6	5	2	4	7	5	10295.399	0.005			10131.383	0.004
6	2	5	5	6	5	2	4	4	5	10295.405	0.001			10131.383	0.000
6	2	5	5	3	5	2	4	4	2	10295.427	0.004				
6	2	5	8	9	5	2	4	7	8	10295.434	0.000	10195.958	-0.001	10131.416	0.005
6	0	6	7	7	5	0	5	6	6	10295.495	0.000	10187.475	-0.002	10129.032	0.000
6	2	5	7	8	5	2	4	6	7	10296.326	0.001	10196.682	-0.002	10132.299	-0.001
6	2	5	6	7	5	2	4	5	6	10296.335	0.000	10196.655	0.002	10132.284	-0.003
6	2	5	5	5	5	2	4	4	4	10296.390	0.003				
6	2	5	8	7	5	2	4	7	6	10296.390	0.000	10196.935	0.003	10132.195	0.005
6	2	5	5	4	5	2	4	4	3	10296.412	0.002				

6	2	5	6	4	5	2	4	5	3	10296.412	0.001				
6	2	5	8	8	5	2	4	7	7	10296.425	0.003	10196.919	0.000	10132.195	0.000
6	2	5	7	5	5	2	4	6	4	10296.466	-0.003			10132.299	0.001
6	0	6	5	3	5	0	5	4	2	10296.638	0.004				
6	2	5	6	5	5	2	4	5	4	10297.207	-0.001				
6	2	5	7	6	5	2	4	6	5	10297.269	0.003				
6	2	5	7	7	5	2	4	6	6	10297.349	0.004	10197.673	0.000		
6	2	5	6	6	5	2	4	5	5	10297.436	0.002	10197.616	0.004	10133.197	-0.002
6	2	4	8	6	5	2	3	7	5	10299.669	0.005				
6	2	4	5	6	5	2	3	4	5	10299.686	0.000	10200.225	-0.007		
6	2	4	8	9	5	2	3	7	8	10299.736	0.000	10200.278	0.001	10136.171	0.001
6	2	4	7	8	5	2	3	6	7	10300.674	0.003	10201.060	0.001		
6	2	4	7	5	5	2	3	6	4	10300.707	0.005				
6	2	4	8	8	5	2	3	7	7	10300.917	0.005				
6	2	4	8	7	5	2	3	7	6	10300.930	0.002				
6	2	4	5	5	5	2	3	4	4	10300.960	0.004				
6	2	4	6	5	5	2	3	5	4	10301.727	0.001	10202.084	-0.002		
6	2	4	6	6	5	2	3	6	5	10301.806	0.004	10202.174	0.002		
6	2	4	7	7	5	2	3	6	6	10301.892	0.002	10202.250	0.005		
6	2	4	7	6	5	2	3	5	5	10301.957	0.002				
6	1	5	8	8	5	1	4	7	7	10353.010	0.001	10253.104	0.000	10191.293	-0.006
6	1	5	8	9	5	1	4	7	8	10353.021	0.000	10253.135	0.000	10191.293	-0.001
6	1	5	5	6	5	1	4	4	5	10353.130	0.008	10253.294	-0.001	10191.345	0.002
6	1	5	7	8	5	1	4	6	7	10353.237	-0.001	10253.343	0.001	10191.521	0.003
6	1	5	6	7	5	1	4	5	6	10353.415	0.000	10253.506	0.000	10191.655	0.000
6	1	5	7	7	5	1	4	6	6	10353.549	0.000	10253.622	0.001	10191.752	-0.001
6	1	5	6	6	5	1	4	5	5	10353.632	-0.007	10253.718	-0.001	10191.818	-0.004
6	1	5	8	6	5	1	4	7	5	10353.660	0.001	10253.675	0.002	10191.842	0.001
6	1	5	6	5	5	1	4	5	4	10353.751	0.001	10253.913	0.002	10191.882	-0.002
6	1	5	5	4	5	1	4	4	3	10353.816	0.004	10253.856	-0.003		
6	1	5	5	5	5	1	4	4	4	10353.833	0.002	10253.856	0.003	10191.973	-0.001
6	1	5	8	7	5	1	4	7	6	10353.846	0.001	10253.890	0.000	10191.973	0.000

6	1	5	7	5	5	1	4	6	4	10353.927	0.000	10253.931	-0.003	10192.123	0.003
6	1	5	5	3	5	1	4	4	2	10354.015	0.000				
6	1	5	7	6	5	1	4	6	5	10354.392	0.002	10254.416	0.005	10192.444	-0.001
6	1	5	6	4	5	1	4	5	3	10354.484	0.001	10254.538	-0.003		
7	1	7	9	7	6	1	6	8	6	11943.874	-0.002	11828.211	0.010	11749.546	-0.002
7	1	7	9	10	6	1	6	8	9	11943.919	0.001	11828.211	0.002	11749.591	-0.004
7	1	7	9	8	6	1	6	8	7	11943.979	0.002	11828.324	-0.002	11749.609	0.002
7	1	7	9	9	6	1	6	8	8	11944.047	0.002	11828.368	0.004	11749.672	0.002
7	1	7	8	7	6	1	6	7	6	11944.082	-0.002	11828.409	0.002	11749.729	-0.002
7	1	7	8	8	6	1	6	7	7	11944.125	-0.001	11828.409	-0.001	11749.809	-0.004
7	1	7	8	6	6	1	6	7	5	11944.133	0.000	11828.409	0.010	11749.780	-0.001
7	1	7	8	9	6	1	6	7	8	11944.149	-0.001	11828.368	-0.002	11749.823	0.000
7	1	7	6	7	6	1	6	5	6	11944.197	0.001			11749.937	0.009
7	1	7	7	6	6	1	6	6	5	11944.288	-0.003	11828.508	-0.004	11749.990	0.002
7	1	7	7	5	6	1	6	6	4	11944.288	-0.007				
7	1	7	7	8	6	1	6	6	7	11944.328	-0.002	11828.448	0.000	11750.027	-0.007
7	1	7	7	7	6	1	6	6	6	11944.328	-0.001	11828.530	0.002	11750.027	0.000
7	1	7	6	6	6	1	6	5	5	11944.328	0.000	11828.530	0.004	11749.990	0.000
7	0	7	9	9	6	0	6	8	8			11889.200	-0.002	11813.562	0.002
7	0	7	8	8	6	0	6	7	7			11889.299	0.005	11813.439	0.000
7	0	7	7	7	6	0	6	6	6			11889.423	0.006	11813.835	-0.003
7	0	7	6	6	6	0	6	5	5			11889.577	0.011	11813.684	-0.006
7	0	7	9	10	6	0	6	8	9			11889.577	0.005	11813.634	0.002
7	0	7	6	5	6	0	6	5	4			11889.593	-0.001		
7	0	7	9	8	6	0	6	8	7			11889.593	-0.009	11813.603	0.002
7	0	7	8	9	6	0	6	7	8			11889.616	-0.002	11813.464	-0.001
7	0	7	7	6	6	0	6	6	5			11889.657	0.000		
7	0	7	7	8	6	0	6	6	7			11889.714	0.006	11813.898	-0.001
7	0	7	6	7	6	0	6	5	6			11889.714	0.000	11813.804	0.002
7	0	7	8	7	6	0	6	7	6			11889.724	0.000		
7	0	7	9	7	6	0	6	8	6			11889.815	0.000		
7	0	7	8	6	6	0	6	7	5			11889.896	-0.002	11813.961	0.006

7	0	7	7	5	6	0	6	6	4		11890.265	0.000	11813.804	-0.001	
7	1	6	9	9	6	1	5	8	8	12077.876	-0.003	11961.327	0.003	11889.131	0.000
7	1	6	9	10	6	1	5	8	9	12077.941	0.001	11961.397	0.005	11889.176	0.001
7	1	6	6	7	6	1	5	5	6	12078.045	0.000	11961.527	-0.007	11889.239	-0.001
7	1	6	8	9	6	1	5	7	8	12078.091	0.002	11961.527	-0.001	11889.336	0.003
7	1	6	7	8	6	1	5	6	7	12078.223	0.000	11961.655	0.001	11889.433	-0.004
7	1	6	8	8	6	1	5	7	7	12078.233	0.002	11961.655	0.001	11889.433	0.000
7	1	6	7	7	6	1	5	6	6	12078.340	-0.001	11961.778	0.006	11889.516	-0.003
7	1	6	6	6	6	1	5	5	5	12078.373	-0.004	11961.802	-0.003	11889.530	-0.002
7	1	6	9	7	6	1	5	8	6	12078.432	0.003	11961.821	0.007	11889.589	-0.002
7	1	6	9	8	6	1	5	8	7	12078.504	-0.001	11961.909	-0.005	11889.638	-0.001
7	1	6	6	5	6	1	5	5	4	12078.519	0.004	11961.928	0.003	11889.638	-0.005
7	1	6	7	6	6	1	5	6	5	12078.580	-0.001	11962.032	0.001	11889.704	-0.001
7	1	6	8	6	6	1	5	7	5	12078.592	0.005	11961.954	0.001	11889.775	0.010
7	1	6	6	4	6	1	5	5	3	12078.686	-0.003	11962.110	-0.002		
7	1	6	8	7	6	1	5	7	6	12078.851	0.002	11962.233	0.001	11889.942	-0.001
7	1	6	7	5	6	1	5	6	4	12078.986	0.002	11962.390	0.003	11890.064	0.005
9	1	9	11	9	8	1	8	10	8	15354.111	0.004	15205.334	0.001	15104.142	0.002
9	1	9	11	10	8	1	8	10	9	15354.111	0.001	15205.358	0.000	15104.119	-0.005
9	1	9	11	12	8	1	8	10	11	15354.130	-0.001	15205.334	-0.001	15104.167	0.000
9	1	9	11	11	8	1	8	10	10	15354.130	-0.001	15205.358	0.000	15104.151	0.002
9	1	9	10	9	8	1	8	9	8	15354.149	-0.002	15205.378	0.001	15104.184	-0.001
9	1	9	10	8	8	1	8	9	7	15354.216	-0.006	15205.400	-0.002	15104.254	0.000
9	1	9	10	10	8	1	8	9	9	15354.216	-0.009	15205.358	-0.004	15104.323	-0.004
9	1	9	8	6	8	1	8	7	5	15354.236	0.005				
9	1	9	10	11	8	1	8	9	10	15354.236	0.001	15205.391	-0.004	15104.278	-0.001
9	1	9	8	7	8	1	8	7	6	15354.244	-0.004	15205.445	0.001	15104.278	-0.007
9	1	9	8	9	8	1	8	7	8	15354.289	0.007	15205.400	-0.006	15104.354	0.002
9	1	9	8	8	8	1	8	7	7	15354.289	-0.002	15205.445	-0.002		
9	1	9	9	8	8	1	8	8	7	15354.289	-0.006	15205.460	-0.004	15104.354	-0.003
9	1	9	9	10	8	1	8	8	9	15354.311	0.007	15205.460	-0.002	15104.323	0.002
9	1	9	9	9	8	1	8	8	8	15354.311	0.005	15205.445	-0.001	15104.374	0.000

9	1	9	9	7	8	1	8	8	6		15205.472	0.001	15104.410	-0.002	
9	0	9	10	10	8	0	8	9	9	15428.623	0.001	15279.233	-0.004	15181.177	-0.001
9	0	9	10	11	8	0	8	9	10	15428.710	0.002	15279.586	0.000	15181.388	0.001
9	0	9	10	9	8	0	8	9	8	15428.742	0.001	15279.477	0.000	15181.297	0.001
9	0	9	11	10	8	0	8	10	9	15428.803	-0.001	15279.468	-0.003	15181.240	-0.001
9	0	9	8	8	8	0	8	7	7	15428.821	0.002	15279.427	-0.002		
9	0	9	11	11	8	0	8	10	10	15428.864	-0.001	15279.233	0.000	15181.200	0.000
9	0	9	9	9	8	0	8	8	8	15428.874	0.002	15279.327	-0.002	15181.376	-0.004
9	0	9	9	8	8	0	8	8	7	15428.907	-0.004	15279.497	-0.003	15181.431	0.004
9	0	9	11	12	8	0	8	10	11	15428.978	0.006	15279.602	0.001	15181.431	0.001
9	0	9	9	7	8	0	8	8	6	15428.978	0.002	15279.959	0.000	15181.626	0.000
9	0	9	8	9	8	0	8	7	8	15429.095	0.003	15279.701	0.000	15181.549	0.001
9	0	9	9	10	8	0	8	8	9	15429.106	0.003	15279.651	-0.001	15181.639	0.001
9	0	9	11	9	8	0	8	10	8	15429.143	-0.002	15279.771	-0.001	15181.568	0.001
9	0	9	10	8	8	0	8	9	7	15429.157	0.005	15279.751	-0.003	15181.686	0.001
9	0	9	8	7	8	0	8	7	6	15429.308	0.006	15279.503	-0.001	15181.568	-0.011
9	0	9	8	6	8	0	8	7	5	15429.308	-0.008	15279.913	-0.004	15181.733	0.002
9	1	8	11	11	8	1	7	10	10	15526.292	0.000	15376.443	0.001	15283.423	0.001
9	1	8	11	12	8	1	7	10	11	15526.407	0.000	15376.555	0.003	15283.518	0.002
9	1	8	10	10	8	1	7	9	9	15526.447	-0.001	15376.579	0.002	15283.567	0.000
9	1	8	10	11	8	1	7	9	10	15526.475	0.000	15376.604	0.002	15283.601	0.002
9	1	8	8	9	8	1	7	7	8	15526.475	-0.003	15376.646	0.003	15283.567	0.005
9	1	8	8	8	8	1	7	7	7	15526.508	-0.004	15376.678	0.002	15283.582	-0.009
9	1	8	9	9	8	1	7	8	8	15526.558	-0.001	15376.689	-0.001	15283.655	0.000
9	1	8	9	10	8	1	7	8	9	15526.573	-0.002	15376.700	0.003	15283.681	0.003
9	1	8	11	10	8	1	7	10	9	15526.687	-0.001	15376.817	0.001	15283.742	0.000
9	1	8	11	9	8	1	7	10	8	15526.705	0.000	15376.817	0.009	15283.768	-0.002
9	1	8	8	7	8	1	7	7	6	15526.705	-0.005				
9	1	8	10	8	8	1	7	9	7	15526.771	0.001			15283.857	0.002
9	1	8	9	8	8	1	7	8	7	15526.819	0.000	15376.945	0.008	15283.875	0.009
9	1	8	10	9	8	1	7	9	8	15526.837	-0.002	15376.945	0.003	15283.887	0.000
9	1	8	8	6	8	1	7	7	5	15526.837	-0.007	15376.970	0.000		

9	1	8	9	7	8	1	7	8	6	15527.008	0.003	15377.105	0.000	15284.035	0.000
10	1	10	12	12	9	1	9	11	11	17058.503	-0.003	16893.177	-0.003	16780.703	0.003
10	1	10	11	10	9	1	9	10	9	17058.519	0.006	16893.198	0.000	16780.716	-0.003
10	1	10	12	10	9	1	9	11	9	17058.519	0.001	16893.183	-0.002	16780.716	-0.006
10	1	10	12	11	9	1	9	11	10	17058.519	0.000	16893.228	0.007	16780.695	0.001
10	1	10	12	13	9	1	9	11	12	17058.565	-0.002	16893.233	0.004	16780.757	0.002
10	1	10	11	9	9	1	9	10	8	17058.574	-0.001			16780.786	-0.004
10	1	10	9	7	9	1	9	8	6	17058.574	-0.002	16893.218	0.011		
10	1	10	11	11	9	1	9	9	10	17058.601	0.008	16893.141	-0.005	16780.794	-0.002
10	1	10	9	8	9	1	9	8	7	17058.597	-0.005	16893.273	0.003		
10	1	10	9	9	9	1	9	8	8	17058.601	-0.005	16893.233	0.002	16780.828	0.001
10	1	10	11	12	9	1	9	10	11	17058.614	-0.003	16893.243	-0.004	16780.828	0.006
10	1	10	9	10	9	1	9	8	9	17058.643	-0.002	16893.251	-0.001	16780.873	0.001
10	1	10	10	11	9	1	9	10	10	17058.643	-0.007	16893.318	-0.004	16780.898	-0.004
10	1	10	10	10	9	1	9	9	9	17058.651	0.001	16893.251	0.002	16780.884	-0.003
10	1	10	10	9	9	1	9	9	8	17058.667	0.000	16893.283	-0.004	16780.884	-0.001
10	1	10	10	8	9	1	9	9	7	17058.699	-0.005	16893.283	-0.004		
10	0	10	11	11	9	0	9	10	10	17138.319	0.002	16972.320	0.000	16863.028	0.003
10	0	10	11	10	9	0	9	10	9	17138.428	0.001	16972.512	-0.002	16863.134	-0.001
10	0	10	9	9	9	0	9	8	8	17138.443	0.000	16972.498	0.003		
10	0	10	12	11	9	0	9	11	10	17138.460	0.001	16972.537	0.000	16863.064	0.004
10	0	10	11	12	9	0	9	10	11	17138.501	-0.001	16972.688	0.003	16863.311	0.003
10	0	10	12	12	9	0	9	11	11	17138.507	0.000	16972.350	0.001	16863.016	0.004
10	0	10	10	10	9	0	9	9	9	17138.510	0.001			16863.179	0.001
10	0	10	10	9	9	0	9	9	8	17138.566	0.001	16972.552	0.005	16863.241	0.002
10	0	10	12	13	9	0	9	11	12	17138.709	0.000	16972.731	0.002	16863.311	0.003
10	0	10	10	8	9	0	9	9	7	17138.724	0.001	16972.988	0.003	16863.504	-0.010
10	0	10	9	10	9	0	9	8	9	17138.809	0.001	16972.812	0.001	16863.408	0.005
10	0	10	10	11	9	0	9	9	10	17138.829	0.001	16972.752	0.001	16863.504	0.004
10	0	10	12	10	9	0	9	11	9	17138.857	0.002	16972.874	0.002	16863.426	0.000
10	0	10	9	8	9	0	9	8	7	17138.870	0.005	16972.580	0.000	16863.311	0.001
10	0	10	11	9	9	0	9	10	8	17138.889	0.002	16972.832	0.000	16863.542	0.002

10	0	10	9	7	9	0	9	8	6	17138.989	-0.003	16972.988	0.000		
10	1	9	12	12	9	1	8	11	11	17249.816	-0.004	17083.318	-0.001	16979.818	-0.004
10	1	9	12	13	9	1	8	11	12	17249.865	-0.002	17083.362	0.001	16979.873	0.000
10	1	9	10	11	9	1	8	9	10	17250.009	0.000	17083.476	0.000	16980.018	0.000
10	1	9	11	12	9	1	8	10	11	17250.042	0.002	17083.466	0.001	16980.084	-0.003
10	1	9	12	11	9	1	8	11	10	17250.064	-0.003	17083.551	-0.003	16980.030	-0.002
10	1	9	9	10	9	1	8	8	9	17250.078	0.001	17083.525	0.001	16980.084	-0.008
10	1	9	10	10	9	1	8	9	9	17250.092	0.005	17083.544	-0.005	16980.067	-0.001
10	1	9	11	11	9	1	8	10	10	17250.092	-0.005	17083.509	-0.003	16980.112	-0.005
10	1	9	9	9	9	1	8	8	8	17250.107	-0.003	17083.568	-0.001	16980.112	0.009
10	1	9	10	9	9	1	8	9	8	17250.204	-0.002	17083.664	-0.004	16980.166	-0.001
10	1	9	9	8	9	1	8	8	7	17250.245	-0.001	17083.673	-0.002	16980.222	-0.005
10	1	9	12	10	9	1	8	11	9	17250.274	0.003	17083.707	-0.003	16980.207	-0.001
10	1	9	11	10	9	1	8	10	9	17250.274	-0.002	17083.692	0.000	16980.262	-0.002
10	1	9	11	9	9	1	8	10	8	17250.376	0.000	17083.754	-0.003	16980.361	0.001
10	1	9	10	8	9	1	8	9	7	17250.457	0.001				
10	1	9	9	7	9	1	8	8	6	17250.542	0.000				
10	2	8	12	13	9	2	7	11	12	17176.221	0.001				
10	2	8	11	9	9	2	7	10	8	17176.474	0.000				
10	2	8	11	12	9	2	7	10	11	17176.474	-0.001				
10	2	8	10	11	9	2	7	9	10	17176.474	-0.002				
10	2	8	12	12	9	2	7	11	11	17176.705	0.000				
10	2	8	9	8	9	2	7	8	7	17176.805	0.000				
10	2	8	12	11	9	2	7	11	10	17176.839	0.000				
10	2	8	9	9	9	2	7	8	8	17176.868	0.000				
10	2	8	11	11	9	2	7	10	10	17176.972	0.000				
10	2	8	10	10	9	2	7	9	9	17177.021	0.000				
10	2	8	11	10	9	2	7	10	9	17177.071	-0.001				
10	2	8	10	9	9	2	7	9	8	17177.081	0.002				

3) Table S2. Theoretical principal axis coordinates of the two most stable conformers of (CH₂ClF)₂: (a) MP2/aug-cc-pVTZ, (b) MP2(BSSE)/aug-cc-pVTZ, (c) MP2/6-311++G(d,p), (d) MP2(BSSE)/6-311++G(d,p).

Conformer I

(a)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å	(b)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å	(c)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å	(d)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å
C	-1.9197	-0.7931	0.1525	C	-1.9561	-0.7943	0.1534	C	-1.9471	-0.7882	0.2562	C	-2.0446	-0.6791	0.4905
Cl	-2.0546	0.8425	-0.5060	Cl	-2.0899	0.8447	-0.4961	Cl	-2.1707	0.7603	-0.5583	Cl	-2.3206	0.5378	-0.7547
F	-1.2325	-0.7577	1.3367	F	-1.2629	-0.7677	1.3341	F	-1.1450	-0.6215	1.3582	F	-1.2694	-0.1543	1.4948
H	-2.9216	-1.1634	0.3392	H	-2.9581	-1.1630	0.3430	H	-2.9173	-1.1496	0.5897	H	-3.0040	-0.9678	0.9140
H	-1.3633	-1.3940	-0.5576	H	-1.4058	-1.3938	-0.5628	H	-1.4517	-1.4726	-0.4281	H	-1.5091	-1.5153	0.0468
C	1.5028	0.3731	0.5373	C	1.5397	0.3816	0.5293	C	1.5325	0.4290	0.4885	C	1.6588	0.5663	0.3123
Cl	1.4650	-0.8002	-0.7933	Cl	1.4802	-0.7727	-0.8163	Cl	1.5303	-0.8707	-0.7133	Cl	1.6321	-1.0093	-0.4896
F	2.6972	1.0330	0.5332	F	2.7653	0.9807	0.5665	F	2.7029	1.1333	0.4108	F	2.8938	1.1390	0.1736
H	1.3974	-0.1769	1.4652	H	1.3809	-0.1725	1.4472	H	1.4542	-0.0182	1.4759	H	1.4573	0.4167	1.3700
H	0.6974	1.0800	0.3738	H	0.7759	1.1310	0.3543	H	0.7034	1.0963	0.2692	H	0.9202	1.2066	-0.1645

Conformer II

(a)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å	(b)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å	(c)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å	(d)	<i>a</i> /Å	<i>b</i> /Å	<i>c</i> /Å
C	-2.1313	0.7003	0.4196	C	-2.1923	0.6605	0.3714	C	-2.1333	0.7156	0.4392	C	-2.2224	0.6850	0.4117
Cl	-2.2170	-0.9603	-0.1874	Cl	-2.2287	-1.0513	-0.0711	Cl	-2.2892	-0.9247	-0.1958	Cl	-2.4532	-0.9851	-0.1073
F	-1.4899	1.4913	-0.4944	F	-1.5596	1.3767	-0.6097	F	-1.4190	1.4889	-0.4411	F	-1.5628	1.3907	-0.5636
H	-1.5583	0.6891	1.3391	H	-1.6305	0.7554	1.2927	H	-1.5882	0.6725	1.3778	H	-1.6094	0.6871	1.3092
H	-3.1459	1.0609	0.5468	H	-3.2164	1.0066	0.4532	H	-3.1286	1.1427	0.5410	H	-3.1994	1.1392	0.5612
C	1.2315	-0.2867	-0.1338	C	1.3088	0.2158	-0.2507	C	1.2722	-0.2689	-0.2214	C	1.4199	0.1262	-0.2473
Cl	2.9772	-0.0548	-0.2730	Cl	3.0009	-0.2891	-0.2032	Cl	3.0216	-0.0511	-0.2156	Cl	3.1409	-0.2519	-0.2162
F	0.8152	0.0755	1.1219	F	0.8487	0.4130	1.0257	F	0.7655	-0.0259	1.0330	F	0.9440	0.2567	1.0351
H	1.0148	-1.3384	-0.2826	H	0.7294	-0.5752	-0.7125	H	1.0492	-1.3004	-0.4843	H	0.8892	-0.6932	-0.7265
H	0.7422	0.3509	-0.8607	H	1.2472	1.1518	-0.7933	H	0.8298	0.4447	-0.9111	H	1.2762	1.0723	-0.7630