Electronic Supporting Information

for

Competition between C−H···S and S–H···Cl H-bonds in $CHCl_3$-H_2S complex: A combined matrix isolation IR spectroscopic and quantum chemical investigation

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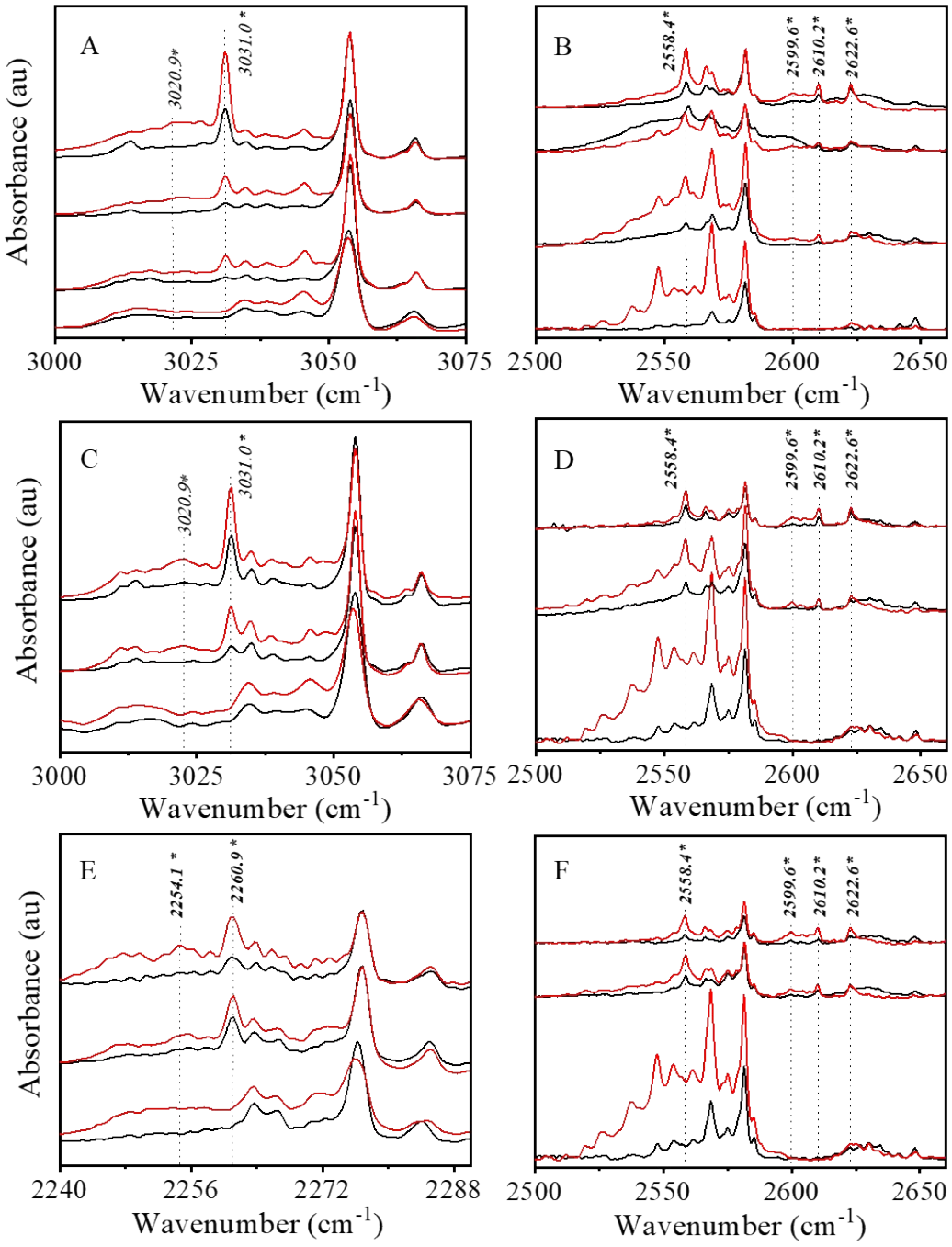

Figure S1: Changes in ν_{C-H} region of $CHCl_3$ (A and C) and ν_{C-D} region of $CDCl_3$ (E) upon addition of H_2S at $CHCl_3$:H_2S:Ar mixing ratios of 5:5:5000; 5:2:5000, 5:1:5000, and 5:0:5000 from top to bottom (A) and $CHCl_3$($CDCl_3$):H_2S:Ar mixing ratios of 2:2:5000, 2:1:5000, and 2:0:5000 from top to bottom (C and E). Changes in ν_{S-H} region of H_2S upon addition of $CHCl_3$ (B and D) and $CDCl_3$ (F) at $CHCl_3$:H_2S:Ar mixing ratios of 5:5:5000; 2:5:5000, and 1:5:5000, and 0:5:5000 from top to bottom (B) and $CHCl_3$($CDCl_3$):H_2S:Ar mixing ratios of 2:2:5000, 1:2:5000, and 0:2:5000 from top to bottom (D and F)

Bar diagrams of the spectral band intensities (absorbance of spectral bands in the experimental spectra) of the newly appearing bands due to formation of $CHCl_3$-H_2S complexes have been plotted against their wavenumbers to quantitatively estimate the variation in population of different complexes with change in $CHCl_3$(CDCl3):H_2S:Ar mixing ratios as well as due to annealing of deposited matrix. As FWHM of the bands are nearly constant at various mixing proportion, the peak height gives idea about the population variation. The band intensity in the pre-annealed spectrum has been shown in solid colour lines, whereas that in the annealed spectrum have been shown with dashed colour lines.

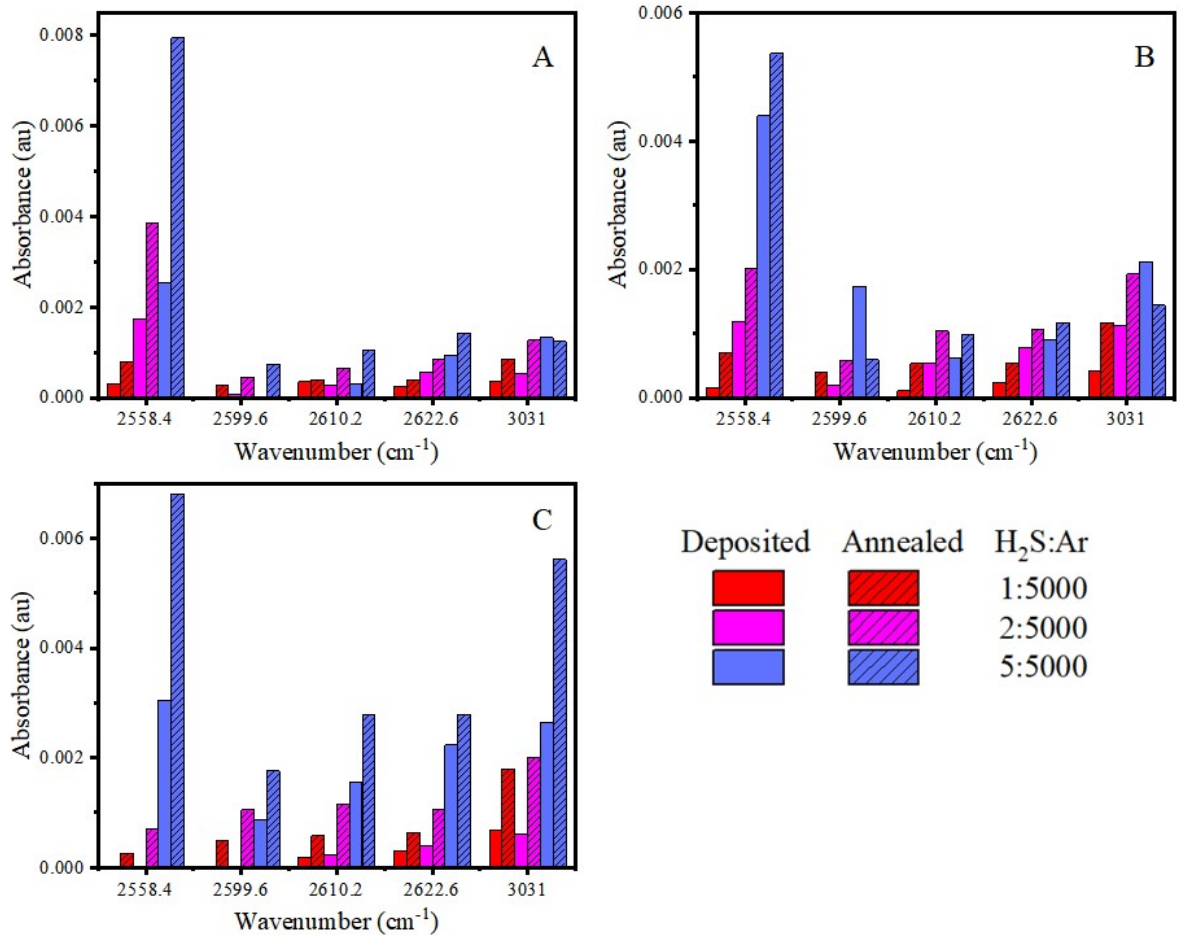

Figure S2: Variation in intensities of ν_{C-H} (divided by 5) and ν_{S-H} band with varying H_2S concentration. $CHCl_3$:Ar mixing ratio is 1:5000 (A) 1:2000 (B) 1:1000 (C)

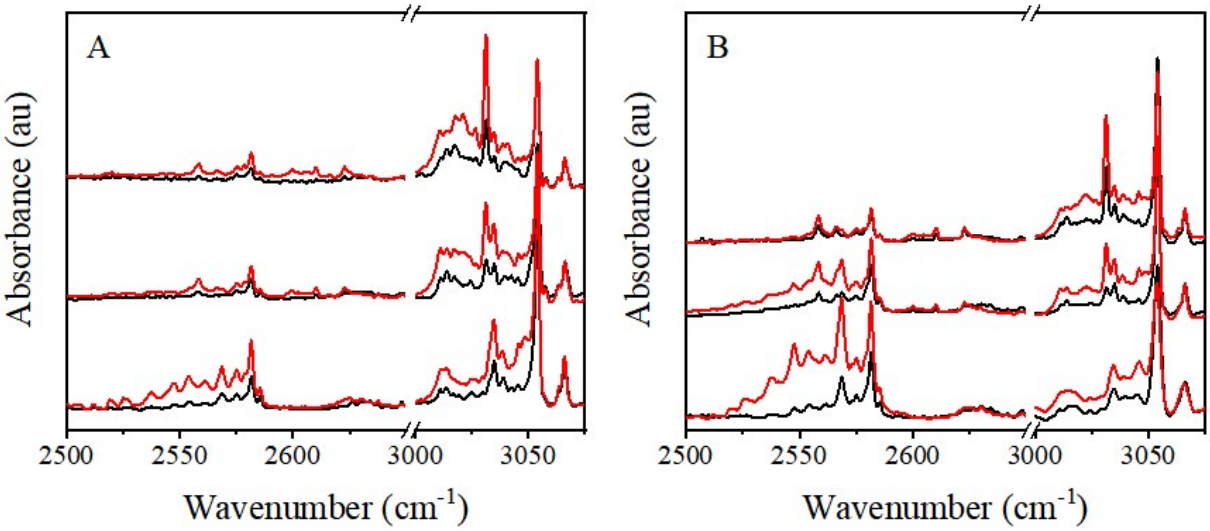

Figure S3: $CHCl_3$: H_2S:Ar (in ν_{C-H} region), and H_2S:$CHCl_3$:Ar (in ν_{S-H} region) in the mixing proportion of 1:2:5000; 1:1:5000, and 1:0:5000 (A); 2:2:5000; 2:1:5000, and 2:0:5000 (B) from top to bottom

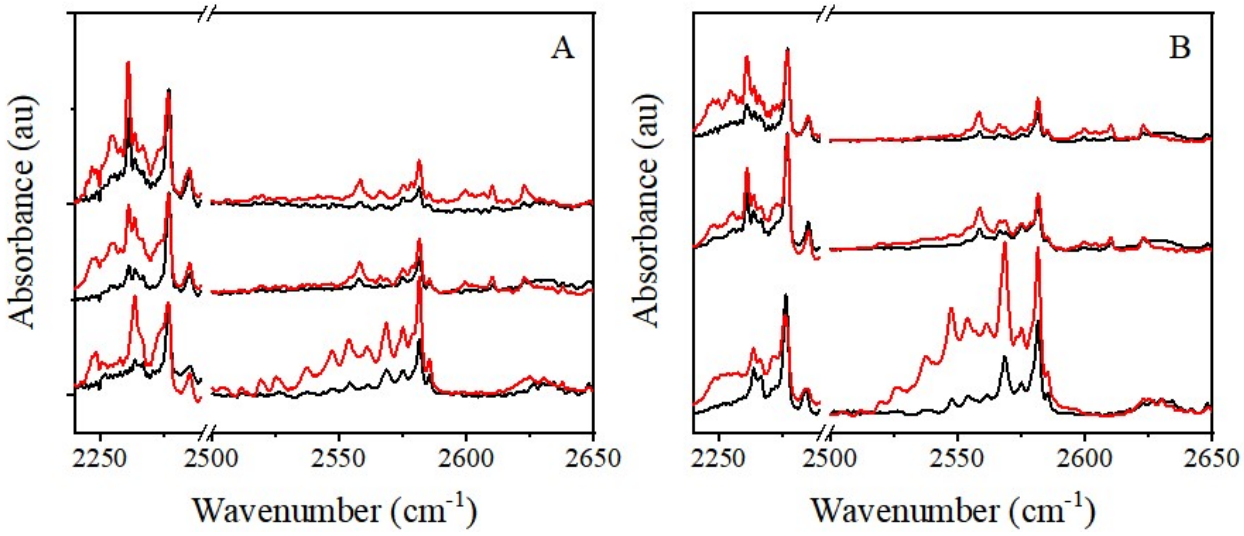

Figure S4: $CDCl_3$: H_2S:Ar (in ν_{C-D} region), and H_2S:$CDCl_3$:Ar (in ν_{S-H} region) in the mixing proportion of 1:2:5000; 1:1:5000, and 1:0:5000 (A); 2:2:5000; 2:1:5000, and 2:0:5000 (B) from top to bottom

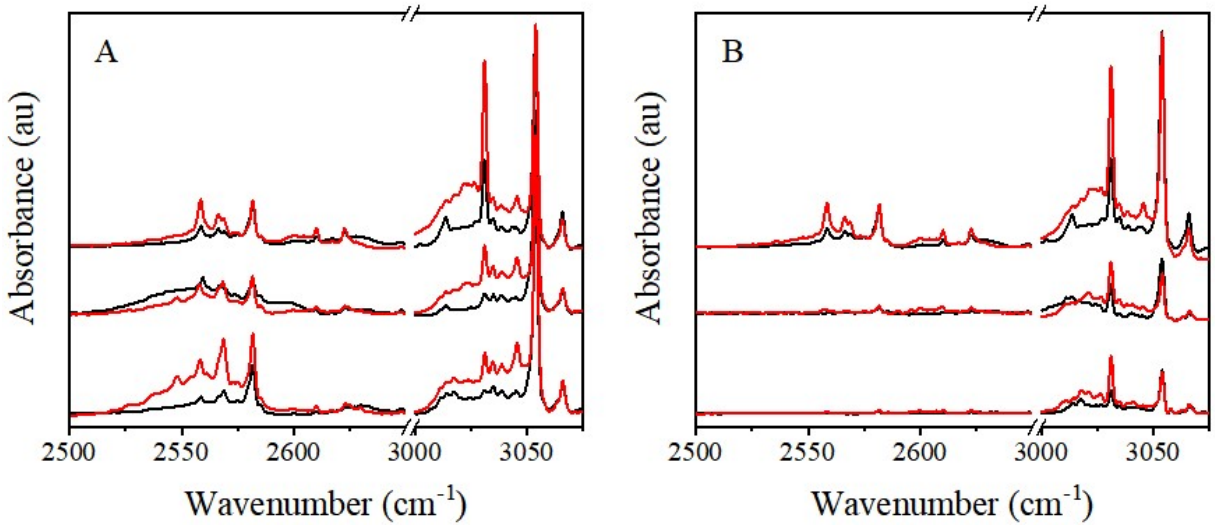

Figure S5: $CHCl_3$: H_2S:Ar (in ν_{C-H} region), and H_2S:$CHCl_3$:Ar (in ν_{S-H} region) in the mixing proportion of 5:5:5000; 5:2:5000, and 5:1:5000 (A) 5:5:5000; 2:5:5000, and 1:5:5000 (B) from top to bottom

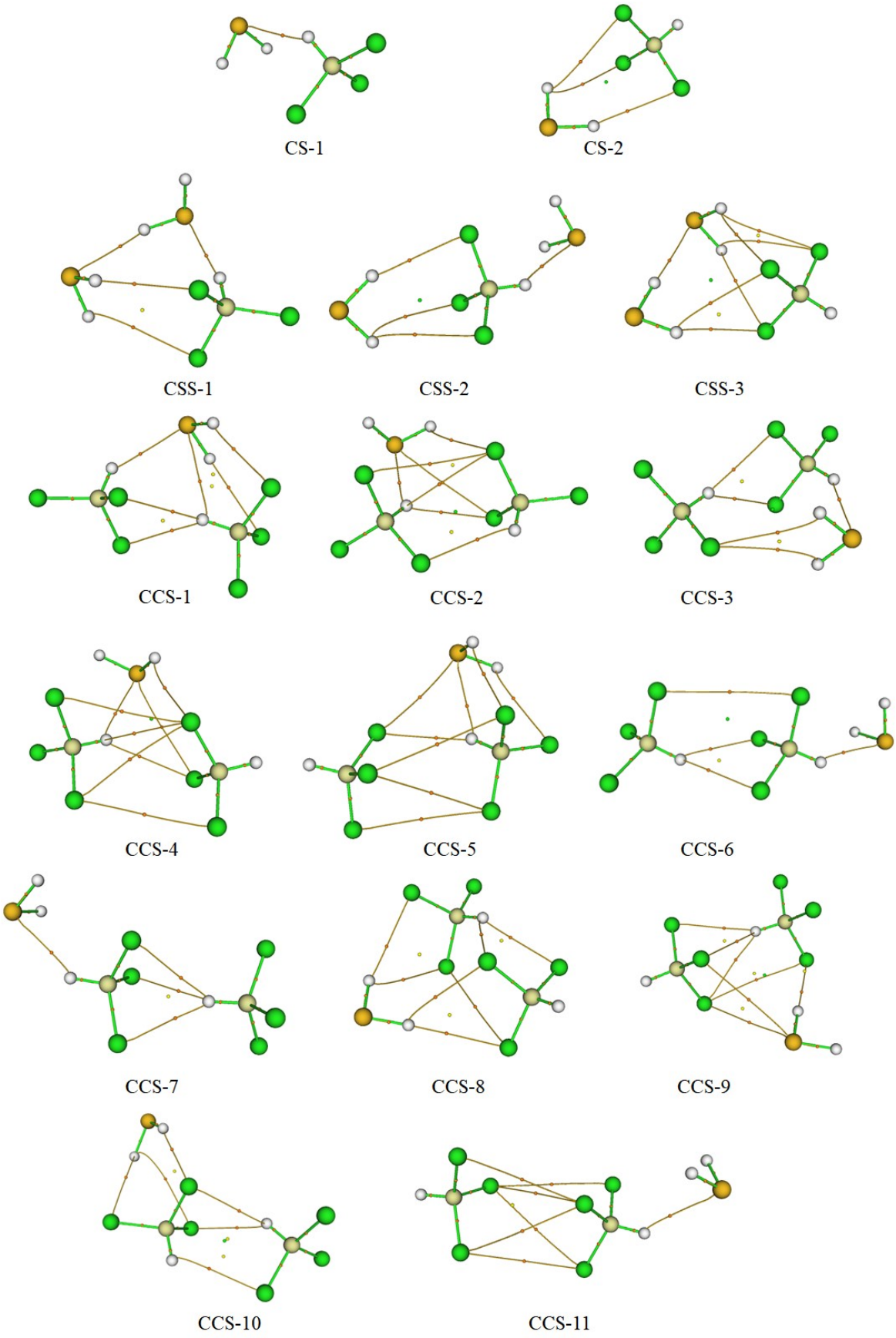

Figure S6: Bond critical points for all the conformers of $(CHCl_3)_X$-$(H_2S)_Y$ (X,Y=1,2) complex, calculated at ωB97X-D/aug-cc-pV(D+d)Z level of theory

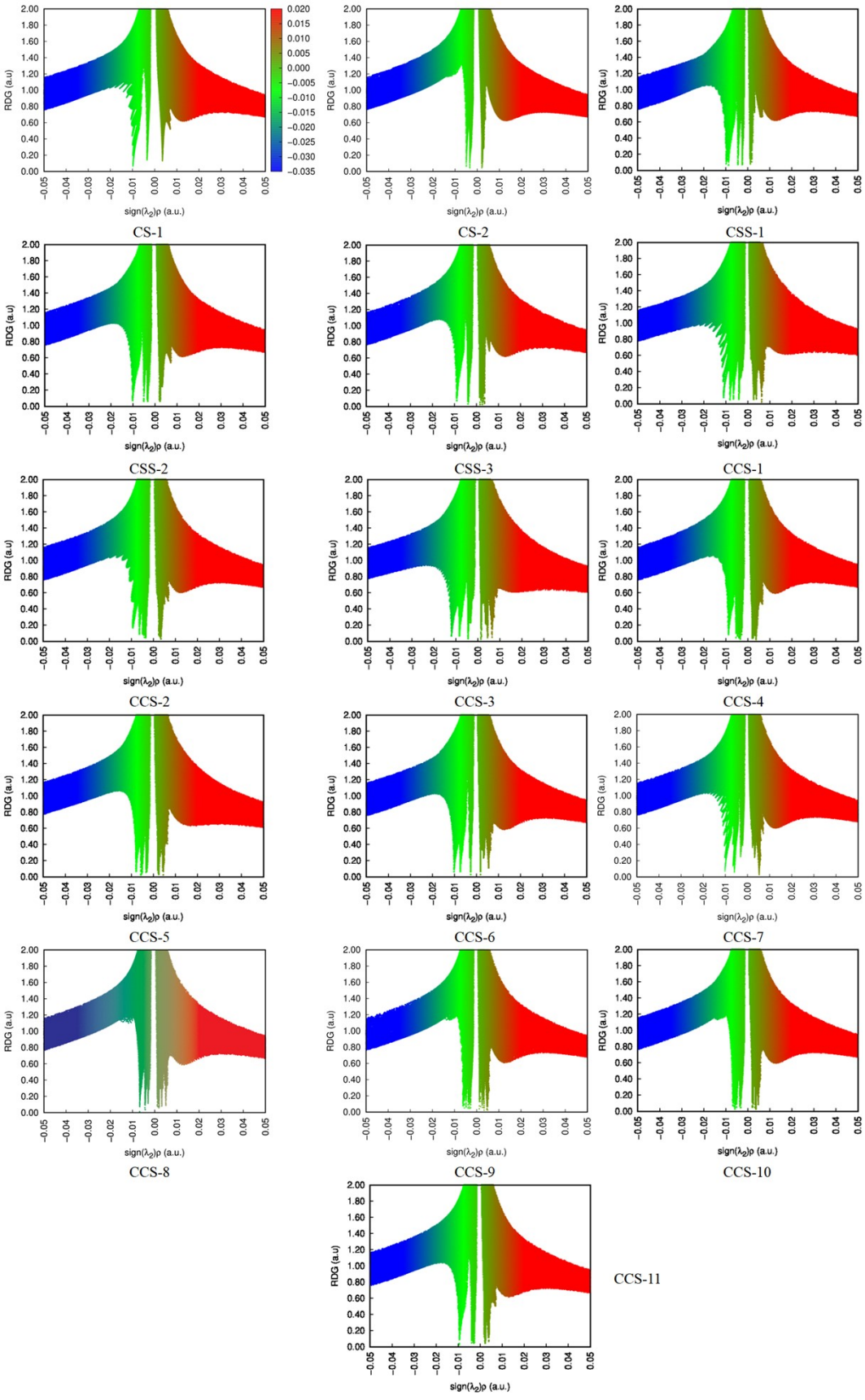

Figure S7: Reduced density gradient plot for different conformers of $(CHCl_3)_X$-$(H_2S)_Y$ (X,Y=1,2)

Table S1: ν_{C-H}, ν_{S-H}^{asym} and the spectral shifts in them for CS-2 conformer, calculated at different level of theories

aug-cc-pV(Q+d)Z						
Method	ν_{C-H}^{mono}	$\nu_{C-H}^{complex}$	$\Delta\nu_{C-H}$	ν_{S-H}^{asym}		$\Delta\nu_{S-H}^{asym}$
MP2	3193.0	3178.3	**-14.7**	2798.6	2789.5	**-9.1**

aug-cc-pV(T+d)Z						
Methods	ν_{C-H}^{mono}	$\nu_{C-H}^{complex}$	$\Delta\nu_{C-H}$	ν_{S-H}^{asym}		$\Delta\nu_{S-H}^{asym}$
B3LYP	3177.46	3177.77	**0.31**	2695.98	2696.67	**0.69**
B3PW91	3174.23	3174.51	**0.28**	2719.48	2719.77	**0.29**
B97D3	3123.38	3124.61	**1.23**	2664.34	2666.84	**2.5**
BLYP	3103.43	3103.72	**0.29**	2609.38	2611.18	**1.8**
HSEh1PBE	3183.52	3183.73	**0.21**	2732.78	2731.03	**-1.75**
M062X	3201.63	3202.59	**0.96**	2749.86	2745.01	**-4.85**
Mpw1pw91	3190.97	3191.35	**0.38**	2739.82	2740.09	**0.27**
PBEPBE	3094.56	3095.11	**0.55**	2643.11	2638.18	**-4.93**
TPSSh	3173.73	3174.2	**0.47**	2711.4	2711.73	**0.33**

Def2tzvpp						
Methods	ν_{C-H}^{mono}	$\nu_{C-H}^{complex}$	$\Delta\nu_{C-H}$	ν_{S-H}^{asym}		$\Delta\nu_{S-H}^{asym}$
B3LYP	3173.46	3173.56	**0.1**	2700.13	2700.29	**0.16**
B3PW91	3170.46	3170.8	**0.34**	2723.51	2724.39	**0.88**
B97D3	3115.92	3116.65	**0.73**	2667.19	2667.99	**0.8**
BLYP	3098.11	3098.17	**0.06**	2613.34	2615.4	**2.06**
HSEh1PBE	3179.35	3179.35	**0**	2737.58	2734.85	**-2.73**
M062X	3199.56	3196.51	**-3.05**	2755.28	2749.07	**-6.21**
Mpw1pw91	3187.12	3187.18	**0.06**	2743.75	2743.6	**-0.15**
PBEPBE	3090.07	3090.27	**0.2**	2647	2642.41	**-4.59**
TPSSh	3169.49	3169.52	**0.03**	2714.96	2714.87	**-0.09**

Table S2: NBO analysis showing the charge transfer interaction energy (in kcal mol^{-1}) between different orbitals in the conformers of $(CHCl_3)_X$-$(H_2S)_Y$ (X,Y=1,2), calculated at ωB97X-D/aug-cc-pV(D+d)Z level of theory

	n(S)→σ*(C−H)	**n(Cl)→σ*(S−H)**	**n(S)→σ*(S−H)**	**n(Cl)→σ*(C−H)**
CS-1	4.49	-	-	-
CS-2	-	1.66	-	-
CSS-1	6.93	1.22	5.28	-
CSS-2	5.35	0.12 1.81	-	-
CSS-3	-	0.73 1.50	5.39	-
CCS-1	5.95 0.40	2.92	-	5.08
CCS-2	4.32	0.12	-	1.52 2.34 0.62
CCS-3	6.00	0.14	-	6.21 0.52
CCS-4	4.38	0.40 0.23	-	2.64
CCS-5	2.25	0.09	-	1.19 2.55
CCS-6	5.70	0.12	-	4.57
CCS-7	5.2	0.12	-	3.88
CCS-8	-	1.52 1.34	-	3.90
CCS-9	-	0.58 2.09	-	3.72
CCS-10	-	1.82	-	1.14 3.33
CCS-11	4.11	-	-	0.44

Table S3: ρ_c and $\nabla^2\rho_c$ (in a.u.) at bond critical points for conformers $(CHCl_3)_X$-$(H_2S)_Y$ (X,Y=1,2), calculated at ωB97X-D/aug-cc-pV(D+d)Z level of theory

Conformer	ρ_{CP}	$\nabla^2\rho_{CP}$	ρ_{CP}	$\nabla^2\rho_{CP}$	ρ_{CP}	$\nabla^2\rho_{CP}$
CS-1	**C−H···S**					
	0.0098	0.0311				
CS-2	**S−H···Cl**		**S−H···Cl**		**S−H···Cl**	
	0.0034	0.0120	0.0034	0.0119	0.0050	0.0172
CSS-1	**S−H···Cl**		**S−H···Cl**		**S−H···S**	
	0.0045	0.0160	0.0025	0.0093	0.0088	0.0277
	C−H···S					
	0.0098	0.0322				
CSS-2	**S−H···Cl**		**S−H···Cl**		**S−H···Cl**	
	0.0051	0.0174	0.0033	0.0115	0.0035	0.0123
	C−H···S					
	0.0102	0.0330				
CSS-3	**S−H···Cl**		**S−H···Cl**		**S−H···Cl**	
	0.0039	0.0139	0.0039	0.0138	0.0039	0.0140
	S−H···Cl		**S−H···Cl**		**S−H···Cl**	
	0.0038	0.0136	0.0036	0.0127	0.0036	0.0127
	S−H···S					
	0.0090	0.0278				
CCS-1	**C−H···Cl**		**C−H···Cl**		**C−H···S**	
	0.0081	0.0245	0.0081	0.0245	0.0041	0.0125
	S−H···Cl		**C−H···S**		**S−H···Cl**	
	0.0066	0.0189	0.0110	0.0265	0.0066	0.0188
CCS-2	**C−H···Cl**		**C−H···Cl**		**C−H···Cl**	
	0.0064	0.0232	0.0044	0.0157	0.0049	0.0172
	C−H···Cl		**C−H···S**		**Cl···Cl**	
	0.0042	0.0152	0.0094	0.0297	0.0035	0.0115
	S···Cl					
	0.0041	0.0112				
CCS-3	**C−H···Cl**		**C−H···Cl**		**C−H···S**	
	0.0084	0.0253	0.0084	0.0253	0.0120	0.0280
	S−H···Cl		**S−H···Cl**			
	0.0045	0.0138	0.0044	0.0137		
CCS-4	**C−H···Cl**		**C−H···Cl**		**C−H···Cl**	
	0.0047	0.0169	0.0054	0.0187	0.0034	0.0123
	C−H···S		**Cl···Cl**		**Cl···Cl**	
	0.0089	0.0277	0.0028	0.0088	0.0034	0.0113
	Cl···Cl		**S···Cl**			
	0.0038	0.0123				
CCS-5	**C−H···Cl**		**S−H···Cl**		**S−H···Cl**	
	0.0079	0.0245	0.0051	0.0154	0.0052	0.0157
	C−H···S		**Cl···Cl**		**Cl···Cl**	
	0.0079	0.0203	0.0033	0.0090	0.0031	0.0084
	Cl···Cl		**S···Cl**			
	0.0028	0.0077	0.0057	0.0152		
CCS-6	**C−H···Cl**		**C−H···Cl**		**C−H···S**	
	0.0074	0.0253	0.0074	0.0254	0.0102	0.0330
	Cl···Cl					
	0.0026	0.0081				
CCS-7	**C−H···Cl**		**C−H···Cl**		**C−H···Cl**	

	0.0059	0.0198	0.0059	0.0197	0.0065	0.0214
	C−H···S					
	0.0101	0.0329				
CCS-8	**C−H···Cl**		**C−H···Cl**		**S−H···Cl**	
	0.0068	0.0235	0.0068	0.0240	0.0044	0.0152
	S−H···Cl		**S−H···Cl**		**S−H···Cl**	
	0.0043	0.0151	0.0044	0.0154	0.0043	0.0154
	Cl···Cl					
	0.0030	0.0090				
CCS-9	**C−H···Cl**		**C−H···Cl**		**C−H···Cl**	
	0.0063	0.0206	0.0056	0.0188	0.0048	0.0161
	S−H···Cl		**Cl···Cl**		**S···Cl**	
	0.0061	0.0206	0.0034	0.0104	0.0039	0.0111
	S···Cl					
	0.0032	0.0111				
CCS-10	**C−H···Cl**		**C−H···Cl**		**C−H···Cl**	
	0.0058	0.0211	0.0062	0.0216	0.0069	0.0238
	S−H···Cl		**S−H···Cl**		**S−H···Cl**	
	0.0034	0.0122	0.0051	0.0177	0.0033	0.0109
CCS-11	**C−H···S**		**Cl···Cl**		**Cl···Cl**	
	0.0095	0.0301	0.0029	0.0090	0.0032	0.0100
	Cl···Cl		**Cl···Cl**		**Cl···Cl**	
	0.0028	0.0083	0.0036	0.0109	0.0031	0.0094
	Cl···Cl					
	0.0032	0.0100				

Table S4: Cartesian coordinates and normal mode frequencies of all the optimized geometries of conformers calculated at ωB97X-D/aug-cc-pV(D+d)Z level of theory

Conformer		Coordinates (Å)			Frequencies (cm^{-1})		
	C	-0.00003800	0.00001400	0.45807100			
	H	-0.00001600	0.00001900	1.54950800	265.7745	266.0740	374.2014
$CHCl_3$	Cl	1.42391200	-0.90074400	-0.08432500	682.7769	784.1662	785.6653
	Cl	0.06812800	1.68349100	-0.08427400	1227.1065	1227.3114	3183.1590
	Cl	-1.49202600	-0.78275300	-0.08422000			
	H	0.00000000	0.97424600	-0.82756600			
H_2S	H	0.00000000	-0.97424600	-0.82756600	1197.9721	2745.6311	2761.5041
	S	0.00000000	0.00000000	0.10344600			
	H	-2.79424900	-0.99739700	-0.30896400			
	H	-2.77862400	0.94999500	-0.36213400	30.3131	35.0620	57.6573
	S	-3.04686700	0.00276300	0.55931000	74.9307	178.7199	196.4571
CS-1	C	0.57511500	-0.00006500	0.14366800	266.1704	266.8238	375.0038
	H	-0.29722200	-0.00025700	0.80229900	679.7311	778.5123	789.4248
	Cl	0.48985000	1.46311400	-0.85372700	1199.6232	1229.6780	1251.4815
	Cl	0.48132500	-1.45433900	-0.86601100	2733.3918	2751.1742	3161.9590
	Cl	2.03878200	-0.00854900	1.13490500			
	C	1.35386000	-0.07019700	-0.00057400			
	H	2.44093800	-0.16402500	-0.00136000	35.8697	37.1866	58.8168
	Cl	0.73831800	-0.86236600	1.45700900	107.6981	118.8350	141.9701
CS-2	Cl	0.73674200	-0.85596900	-1.46094300	265.6543	266.6288	375.7966
	Cl	0.96156800	1.65827200	0.00343700	682.9571	781.3851	786.5011
	H	-1.93051300	0.93593700	0.00211700	1203.6170	1226.2413	1226.5305
	H	-2.20148400	-0.98832700	-0.00066000	2728.3579	2745.2211	3187.5559
	S	-2.99092400	0.10366700	0.00073800			
	H	-1.69717600	2.71651200	1.20812300			
	H	-2.34672800	1.38002200	-0.05168400	16.3888	22.1031	42.2872
	S	-1.62650600	2.51992500	-0.11863200	58.9335	68.5735	89.5123
	C	1.18787500	0.00747400	-0.00872900	106.1124	140.9890	188.2226
	H	0.51802900	0.86256600	-0.04533000	192.7888	225.4641	266.6125
CSS-1	Cl	0.86686000	-0.99737400	-1.44465000	266.9237	338.0380	375.5274
	Cl	0.82978900	-0.89550800	1.48848200	677.6285	774.0933	787.5723
	Cl	2.86048900	0.60076800	-0.00585700	1198.5854	1206.3316	1253.2506
	S	-3.15553300	-1.26994000	0.03315700	1260.9615	2654.9874	2722.8899
	H	-2.49777800	-1.51872400	-1.11156300	2742.8968	2746.2330	3133.2263
	H	-2.06234000	-1.51902600	0.77485100			
	H	3.53291700	-0.93960200	-1.07775800			
	H	3.44403900	-1.25395400	0.84331100	20.0484	20.6696	40.7511
	S	3.94457400	-0.29831000	0.03446700	41.7398	51.1497	55.4042
	C	0.38078400	0.46780800	0.04574500	78.9295	119.5911	129.6186
	H	1.43149100	0.76094500	0.11684600	163.5741	170.7204	182.7814
CSS-2	Cl	0.06663900	-0.71642000	1.32552300	265.8926	266.5753	376.3476
	Cl	0.14195100	-0.25974800	-1.55555500	679.7981	775.7684	788.2971
	Cl	-0.63063400	1.90406200	0.24534700	1199.5920	1201.2731	1234.6412
	S	-3.79857700	-0.72345800	-0.06424900	1252.6046	2731.6772	2731.8010
	H	-3.15006000	-0.05660200	0.91068500	2747.8015	2748.2338	3161.7428
	H	-2.70429300	-0.74355700	-0.85138600			
	C	-1.57725300	-0.87090800	0.00174700	23.8326	36.3462	36.9211
CSS-3	H	-2.27453700	-1.71028700	0.00346400	42.6782	63.9018	77.6409
	Cl	-0.57675800	-0.99007900	1.45751800	97.2404	109.5432	115.2699

	Cl	-2.52606200	0.62434600	0.00429700	186.7642	196.6134	266.6863
	Cl	-0.58517500	-0.99000900	-1.46026000	267.2392	303.1761	375.4440
	H	2.18255600	-1.63002000	-0.01698800	682.9925	784.2406	784.5103
	H	2.57274700	0.28207400	0.00880600	1200.5304	1204.5501	1226.3979
	S	3.29069800	-0.86403300	0.00091400	1227.4794	2687.9816	2739.1165
	S	1.03044900	2.56878700	-0.00290400	2746.4236	2755.4979	3185.0762
	H	0.26366200	2.04178900	0.97237400			
	H	0.27664200	2.01344100	-0.97271400			
	H	0.68581200	2.52924600	-0.97375900			
	H	0.68290200	2.52786900	0.97529400	16.6025	24.7106	27.1585
	S	-0.12238500	2.99593400	-0.00008700	36.4522	45.2668	56.9162
	C	-2.26923500	0.00127600	-0.00075500	62.7627	68.6885	82.4643
	H	-2.08820700	1.07877700	-0.00012200	128.9396	227.2849	240.5957
	Cl	-1.50672400	-0.66427600	1.45677200	265.4802	267.0063	267.9410
CCS-1	Cl	-1.51064500	-0.66156300	-1.46164400	270.3606	374.9835	377.5775
	Cl	-4.00991900	-0.29320300	0.00129800	677.4124	685.4223	770.3410
	C	1.88863300	-0.37458600	-0.00092100	784.3033	790.3636	792.9777
	H	0.81734700	-0.16336900	-0.00600900	1202.4257	1229.4841	1230.3255
	Cl	2.59206500	0.35670200	-1.45571400	1250.2618	1251.2053	2723.8355
	Cl	2.10146400	-2.12596800	-0.00428900	2738.6935	3167.6301	3192.3087
	Cl	2.57751900	0.34903800	1.46452100			
	C	1.77266700	-0.57978600	0.06446700			
	H	1.05708400	0.22249400	0.26415600	9.7504	21.3282	28.6595
	Cl	2.27105300	-0.45278300	-1.63040700	36.6935	39.3790	41.5274
	Cl	3.15032100	-0.35847200	1.14826900	55.0221	57.1375	65.2846
	Cl	0.97716100	-2.13865600	0.36909200	79.8303	135.0661	212.7783
	C	-2.23949000	-0.43464100	0.07572400	265.9609	266.8240	268.4096
CCS-2	H	-1.85026500	-1.44640000	0.20231500	268.6395	374.5136	377.9311
	Cl	-4.00339200	-0.51497300	0.01593400	680.3928	685.0960	772.7339
	Cl	-1.69078200	0.52922600	1.45692400	779.7115	788.3999	791.0686
	Cl	-1.57920300	0.20293800	-1.44164300	1200.2430	1226.7781	1230.7721
	S	1.04479800	3.00671200	0.10428500	1235.9589	1243.4640	2735.3294
	H	-0.08372100	2.81955100	-0.60883400	2752.5480	3178.3852	3188.4584
	H	1.83338300	2.83976300	-0.97624600			
	H	0.70238600	2.71574100	0.97992400			
	H	0.69917900	2.72331400	-0.96455200	12.6703	17.4920	23.2827
	S	1.52260200	3.16415200	0.00806600	31.1362	39.7985	48.7104
	C	2.23922400	-0.39600800	-0.00388900	57.3379	61.0718	85.2140
	H	2.52615300	0.65927800	0.00107400	168.5860	219.0019	236.7661
	Cl	1.27627000	-0.67600000	-1.46933300	265.7244	266.4695	268.3805
CCS-3	Cl	1.26344900	-0.68670400	1.45065100	270.5586	375.9694	377.1648
	Cl	3.69433800	-1.39405700	-0.00136000	678.7158	685.1480	772.1740
	C	-2.11294000	-0.28151500	-0.00473200	778.9972	793.7888	794.2242
	H	-1.07778900	-0.62609500	-0.02498300	1201.0259	1231.2945	1235.8437
	Cl	-2.08764200	1.49367500	0.00175800	1240.2484	1256.6718	2735.2051
	Cl	-2.86918600	-0.90462700	1.46684500	2750.3425	3159.2966	3199.7508
	Cl	-2.92247900	-0.89308400	-1.45260700			
	C	2.60823600	0.51360800	0.03465600	19.5251	26.3597	35.3842
	H	3.40834900	1.24652700	0.15015400	37.0949	38.5772	45.3138
	Cl	1.58286900	0.60205200	1.47935400	50.8239	52.1639	63.1232
CCS-4	Cl	1.69007300	0.93933300	-1.41823800	82.4096	161.0761	191.8472
	Cl	3.34762600	-1.08326900	-0.12029200	265.9999	266.2087	267.4317
	C	-1.53719500	-0.73820200	-0.06611900	268.2378	375.6873	376.3150
	H	-0.93554500	0.14480600	-0.29615200	681.0804	683.3343	772.3341

	Cl	-0.53788000	-2.17879300	-0.28868900	783.4961	787.6966	790.9093
	Cl	-2.07734100	-0.59518600	1.61880100	1197.2813	1225.8274	1228.9011
	Cl	-2.92291700	-0.74648100	-1.16865800	1233.6809	1244.6699	2732.7540
	S	-1.49346600	2.91967300	-0.17424700	2749.8962	3174.2749	3185.0590
	H	-2.62972800	2.51118300	0.42505200			
	H	-0.77518800	2.79014700	0.95895000			
	H	3.20079800	2.05284000	-0.73721300			
	H	2.33822400	2.22457200	1.00083100	18.0602	23.0500	31.2146
	S	2.22868200	2.82043600	-0.20409400	39.9740	46.9541	47.7596
	C	1.48831800	-0.81625800	-0.10138300	54.2189	62.6684	76.8463
	H	1.09910600	0.13471000	-0.47265100	81.7723	198.6171	213.7988
	Cl	1.56960400	-0.70645700	1.66600400	266.6526	266.6895	267.6457
CCS-5	Cl	3.10718600	-1.04662800	-0.79084100	268.7103	376.1773	376.7807
	Cl	0.39415800	-2.10561800	-0.60835700	681.2435	683.0954	774.8042
	C	-2.71561300	0.65005100	0.07316600	781.4750	788.2160	792.1746
	H	-3.53351500	1.34696600	0.26319400	1199.1409	1222.6756	1228.2452
	Cl	-2.50041100	-0.34637300	1.51785800	1229.7064	1242.8274	2729.8485
	Cl	-1.26008700	1.60782300	-0.25924000	2745.9320	3178.7163	3185.6521
	Cl	-3.15749400	-0.33738300	-1.32656300			
	C	1.69257400	0.43194300	0.25800000			
	H	2.68439200	0.41299400	0.71744200	12.4279	14.9792	18.0846
	Cl	1.87141100	1.05338500	-1.38767400	23.1837	27.1179	46.0620
	Cl	1.08529400	-1.23664700	0.24140600	53.8450	64.2155	68.8337
	Cl	0.63818500	1.47702300	1.22426500	82.2762	178.9857	223.5644
	C	-2.46306900	-0.20941800	0.07475800	265.8553	265.9142	266.3393
CCS-6	H	-1.51183200	-0.22405100	0.60882200	268.0144	375.7675	376.7626
	Cl	-3.57885000	0.82512800	0.97979100	680.1707	682.6982	775.5717
	Cl	-2.16233500	0.44091100	-1.54255700	783.5111	787.0959	790.0354
	Cl	-3.06340500	-1.87329200	-0.01003500	1200.5102	1227.8432	1236.9213
	S	5.15772300	-0.68477400	0.36206900	1238.7014	1255.3338	2731.3881
	H	4.52145500	-1.86625300	0.23183800	2748.1844	3162.5778	3194.4276
	H	4.97029400	-0.37211600	-0.93608000			
	C	1.62542700	0.61785100	-0.00042700			
	H	2.70076900	0.81507900	0.00271600	8.3522	13.2984	13.7093
	Cl	0.75468800	2.15880200	-0.01446300	21.0259	22.2024	38.2309
	Cl	1.25428700	-0.32811800	-1.45367700	40.8592	47.6691	52.1594
	Cl	1.24198900	-0.30880600	1.46182300	76.2302	181.5468	193.1499
	C	-2.28861700	-0.19705800	-0.00186700	265.9237	266.1535	266.7037
CCS-7	H	-1.24619000	0.12299500	-0.01020400	267.1458	376.8944	377.4752
	Cl	-3.06117500	0.44429700	-1.45910300	679.8897	690.2741	773.6861
	Cl	-2.31310500	-1.96668500	0.00573900	778.2866	789.1816	790.0629
	Cl	-3.04188700	0.45661800	1.45987600	1199.3966	1216.7887	1223.0521
	S	5.07812200	-0.53884900	0.00881800	1231.2118	1252.2856	2729.7536
	H	4.58989000	-1.24153500	-1.03309000	2745.9360	3163.2314	3209.3232
	H	4.49318700	-1.35353500	0.90992500			
	H	0.41725300	3.02118000	-0.18850300	19.0424	24.9488	33.3800
	H	-1.39892200	2.37213500	-0.42947700	36.3934	40.4631	42.2487
	S	-0.81429300	3.56834900	-0.21930000	52.7178	57.9173	67.4665
	C	-2.29622400	-1.12586800	0.46158300	111.7882	150.9225	183.6344
CCS-8	H	-3.19180400	-1.51002600	0.95269600	265.9121	266.5785	267.8046
	Cl	-1.26076000	-2.50989900	0.06719200	268.6756	375.6794	376.4429
	Cl	-1.48401600	-0.02850000	1.58953500	681.2277	683.1521	775.9283
	Cl	-2.80046200	-0.27181000	-1.00311600	782.3675	787.7325	790.5658
	C	1.83069900	-0.34884400	0.02911800	1198.8838	1224.1786	1228.0726

	H	1.04389000	-0.90792100	0.53827100	1234.6207	1239.7086	2736.3930
	Cl	1.15886500	0.26562500	-1.48873400	2751.6397	3188.7821	3190.4527
	Cl	3.18024800	-1.45179600	-0.27251400			
	Cl	2.32091500	0.98339900	1.08949600			
	C	2.27624200	-1.08394300	0.03478000			
	H	3.33803600	-1.33401100	0.06495000	15.9974	22.8493	24.0561
	Cl	1.89109000	-0.12441500	1.47012900	26.4662	34.1805	36.6746
	Cl	1.97099000	-0.15421400	-1.44131000	40.8868	46.4586	58.9169
	Cl	1.35583300	-2.59913400	0.02360600	124.7563	151.5060	209.1413
	C	-1.68990500	-0.21474800	0.00375300	265.5731	266.9414	267.5549
CCS-9	H	-0.65100500	-0.54719100	0.04333900	268.6802	376.7855	377.6438
	Cl	-1.88508100	0.77635700	-1.45417100	682.4513	688.9051	774.1432
	Cl	-2.71656800	-1.65230100	-0.06746300	778.3315	787.8320	793.5524
	Cl	-2.01593100	0.73503700	1.45904000	1215.2981	1219.1745	1220.6600
	S	1.07822100	3.37823400	0.01051500	1227.1517	1228.0107	2732.7615
	H	0.11105000	2.51666800	-0.36386200	2749.5592	3189.8049	3193.7603
	H	0.22673000	4.42231600	0.02899900			
	C	2.39173700	0.30489000	-0.03179700			
	H	1.36018900	0.64628000	-0.13373800	12.2313	16.4399	17.9364
	Cl	3.33637500	1.01435800	-1.34593600	35.4979	41.2891	49.7666
	Cl	2.99076300	0.82842900	1.54636000	52.6042	55.1954	67.2137
	Cl	2.38472200	-1.46836200	-0.14715100	99.7712	131.7268	137.7245
	C	-1.26898100	-1.14588500	-0.03022800	265.4746	266.3475	266.4879
CCS-10	H	-0.54858100	-1.96420400	-0.08160500	269.1267	374.7278	376.3341
	Cl	-2.89744600	-1.83080700	-0.00332100	679.5079	685.0738	773.5609
	Cl	-0.93748000	-0.23429900	1.45529100	775.5301	788.7773	793.4133
	Cl	-1.03098800	-0.12535800	-1.45991800	1200.7774	1222.0052	1224.2065
	S	-4.10811800	2.15563300	-0.00710300	1231.6389	1235.9179	2732.8057
	H	-3.10990200	1.66323300	0.75330600	2748.9550	3187.7954	3192.1424
	H	-4.08943500	1.08321700	-0.82268900			
	C	-1.65270400	0.62565400	0.19383500			
	H	-2.66832300	0.56663000	0.59292900	13.1850	16.7038	18.6380
	Cl	-0.81655000	-0.87177500	0.63806800	26.6771	36.8933	49.3029
	Cl	-1.78503600	0.77365100	-1.56931600	50.0319	55.5557	69.8228
	Cl	-0.84941400	2.03718200	0.89119600	84.5745	185.6414	247.2162
	C	3.14366800	-0.19633700	-0.20516000	265.3226	265.6077	266.4041
CCS-11	H	4.19075000	-0.02332000	-0.45834300	267.0767	374.3662	374.7842
	Cl	2.14885500	0.64675300	-1.39963300	679.1163	682.0509	775.1114
	Cl	2.86011600	-1.94477900	-0.25940700	780.4154	787.3493	789.0911
	Cl	2.86790600	0.44172700	1.42240200	1200.4365	1227.9544	1228.3140
	S	-4.83279200	-1.15510500	0.32089700	1234.3922	1249.5321	2731.9946
	H	-3.83819600	-2.05008800	0.48934900	2747.9311	3169.2697	3188.3282
	H	-4.54522700	-0.99433100	-0.98660300			