Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

ESI of

Formation of unexpected S-S covalent bond in H_2S dimer under confinement.

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Table S1: Optimized geometries in cartesian coordinates and all normal mode frequencies calculated at the LC-wHPBE/6-31++G** level of theory.

Species	Cartesian coordinates (Å)				Frequencies (cm^{-1})		
	S	-1.023256	-0.06782	0.054595	437.6006	567.4076	935.7246
H_2S_2	H	-1.287214	0.862608	-0.873514	941.4459	2786.0131	2787.5418
	S	1.023256	0.06782	0.054595			
	H	1.287214	-0.862605	-0.873517			
	H	2.322661	1.232566	-0.001317	32.475	62.1678	99.1775
	H	0.785926	0.036535	0.000883	101.2304	179.9824	299.9779
$(H_2S)_2$	S	2.120621	-0.08923	0.000109	1235.4364	1245.7379	2784.5608
	H	-2.32644	-0.759631	0.973958	2823.293	2831.1972	2842.5763
	H	-2.322726	-0.762656	-0.972735			
	S	-2.024335	0.105054	-0.000158			
C_{60}	C	-3.276636	0.476541	1.215409	271.3021	271.3088	271.3152
	C	-2.955239	1.792244	0.703505	271.3223	271.3343	346.6748
	C	-2.835062	1.99308	-0.656232	346.6967	346.7372	365.7942
	C	-3.030337	0.88809	-1.571266	365.8032	365.8186	365.8394
	C	-3.3366	-0.365657	-1.083457	415.2655	415.2767	415.294
	C	-3.462731	-0.576418	0.343474	415.3103	415.3276	447.8257
	C	-2.530975	0.278738	2.44069	447.8529	447.8667	447.8793
	C	-1.748754	1.472182	2.686061	447.8893	501.935	501.9377
	C	-2.010962	2.407577	1.61242	501.9583	501.9881	513.6365
	C	-0.990995	3.194762	1.118837	555.5115	555.5247	555.5372
	C	-1.764682	2.819155	-1.174212	555.5474	555.5671	556.5808
	C	-2.08064	1.031221	-2.654792	556.5951	556.6277	574.2833

	C	-1.481943	-0.086134	-3.19949	574.2954	574.3465	582.7744
	C	-1.803354	-1.401842	-2.687588	582.8546	582.8799	582.9033
	C	-2.708319	-1.538223	-1.655073	594.1402	594.1603	594.1923
	C	-2.446118	-2.473637	-0.581457	609.1584	609.1602	609.1683
	C	-2.912343	-1.87922	0.653735	688.7625	688.7707	688.7828
	C	-2.201783	-2.067718	1.821297	688.8034	688.843	739.4799
	C	-2.006508	-0.962711	2.736318	739.5008	739.5388	739.5532
	C	-0.478912	1.367996	3.215493	739.5616	745.9681	745.9789
	C	0.071442	0.065223	3.525734	746.0035	746.1695	746.1892
	C	-0.673941	-1.072044	3.291918	746.2056	746.2313	748.855
	C	-0.04565	-2.244613	2.720296	748.8954	748.9174	759.6994
	C	-0.989901	-2.859972	1.811361	759.7186	759.7459	759.7597
	C	-0.545629	-3.426423	0.634329	759.777	774.2506	774.2608
	C	-1.291288	-3.228593	-0.590922	774.2747	774.3219	776.5612
	C	-0.341599	-3.085448	-1.674453	776.5673	776.5915	776.599
	C	-0.591467	-2.194094	-2.697517	814.2094	814.2255	814.2329
	C	-1.298439	2.224689	-2.409408	814.2433	814.2921	814.2944
	C	2.530975	-0.278737	-2.440689	814.3206	814.3601	855.922
	C	2.006509	0.962711	-2.736317	855.9523	855.9794	980.7276
	C	2.201783	2.067717	-1.821297	995.158	995.1955	995.2322
	C	2.912344	1.879219	-0.653736	1015.0324	1015.0461	1015.0576
	C	3.462732	0.576419	-0.343475	1015.1254	1112.507	1112.5446
	C	2.955238	-1.792244	-0.703505	1112.5806	1112.5943	1167.2282
	C	2.010962	-2.407576	-1.612421	1167.2539	1167.2794	1167.3203
	C	1.748754	-1.472183	-2.68606	1167.341	1226.1031	1226.1371
	C	0.478912	-1.367997	-3.215493	1226.1424	1262.4121	1262.4525

	C	-0.071443	-0.065222	-3.525734	1262.4694	1300.0116	1300.0265
	C	0.67394	1.072045	-3.291918	1300.0743	1300.1374	1300.1623
	C	0.989901	2.859972	-1.811361	1346.0088	1346.0413	1346.07
	C	0.545629	3.426423	-0.634329	1346.1161	1346.1437	1352.0486
	C	1.291288	3.228592	0.590923	1352.0786	1352.162	1376.9641
	C	2.446118	2.473637	0.581458	1376.9946	1377.0316	1377.0474
	C	2.708319	1.538224	1.655073	1397.1926	1397.1979	1397.2764
	C	3.3366	0.365657	1.083457	1397.3056	1433.9053	1433.9197
	C	3.030336	-0.888089	1.571265	1433.9808	1433.9917	1434.013
	C	2.835062	-1.99308	0.656231	1452.556	1452.5779	1452.6067
	C	0.990995	-3.194763	-1.118838	1531.9941	1532.0238	1532.0372
	C	0.86488	-3.405513	0.308063	1532.0679	1532.119	1532.3347
	C	1.764681	-2.819155	1.174212	1532.3617	1532.3976	1551.902
	C	1.298438	-2.224689	2.409408	1551.9525	1551.9765	1552.0439
	C	2.08064	-1.03122	2.654792	1577.4343	1625.9597	1625.975
	C	1.481944	0.086134	3.19949	1625.9913	1626.0747	1648.0031
	C	1.803354	1.401842	2.687589	1648.0506	1648.0722	1709.6801
	C	0.591468	2.194094	2.697517	1709.6815	1709.725	1709.7491
	C	0.3416	3.085447	1.674453	1709.7719	1715.484	1715.4967
	C	0.04565	2.244612	-2.720296	1715.5181	1715.5549	1715.5806
	C	-0.86488	3.405512	-0.308062			
	C	3.276636	-0.476541	-1.215409			
$(H_2S)_2@C_{60}$	C	-2.9722	-0.44781	1.95109	77.2899	130.4295	164.7509
	C	-1.95614	-0.34868	2.93857	191.7402	210.2054	226.742
	C	-1.28436	0.87941	3.17124	272.3001	281.3167	301.5942

	C	-1.62521	2.02983	2.37851	303.2248	349.603	362.9112
	C	-2.62508	1.96443	1.40453	364.8172	372.9855	377.9108
	C	-3.2969	0.68559	1.16056	386.4041	392.8766	394.5103
	C	-2.83572	-1.74866	1.28101	400.1385	405.9382	409.5138
	C	-1.71898	-2.44214	1.89887	412.0663	418.7833	427.8902
	C	-1.1682	-1.56328	2.91255	429.8479	460.9962	466.9427
	C	0.20183	-1.54287	3.13304	477.0853	500.1931	511.9245
	C	0.12948	0.89666	3.3815	515.119	516.0082	525.9997
	C	-0.4027	2.78993	2.12615	532.0669	532.7929	538.3089
	C	-0.21197	3.4257	0.91142	546.6503	560.8489	562.8375
	C	-1.22684	3.35339	-0.11452	566.0425	568.1226	569.255
	C	-2.42783	2.63247	0.13165	570.6813	576.6899	579.1794
	C	-2.96303	1.76181	-0.89813	581.5881	582.8208	584.1882
	C	-3.495	0.5549	-0.25392	586.2897	590.8012	595.6301
	C	-3.41558	-0.71885	-0.90787	605.7498	609.3515	612.4627
	C	-3.04354	-1.87741	-0.08417	619.8714	637.4898	645.8807
	C	-0.86147	-3.22966	1.15053	666.1364	680.1876	681.936
	C	-1.07727	-3.36297	-0.27135	683.7792	687.2087	688.1299
	C	-2.13815	-2.70312	-0.86978	725.5616	732.7978	736.3545
	C	-1.94041	-2.03811	-2.14506	736.8918	739.7357	740.951
	C	-2.75753	-0.8269	-2.15809	748.6178	749.3763	757.8064
	C	-2.18007	0.34127	-2.76264	759.5848	762.3654	764.6977
	C	-2.30697	1.64487	-2.12398	769.506	769.8726	771.9673
	C	-1.08394	2.39254	-2.36788	773.4624	773.9584	779.379
	C	-0.55873	3.22552	-1.37568	782.5402	787.523	789.0455
	C	0.69081	2.07876	2.74285	790.1736	792.5461	794.0332

	C	2.85045	1.74843	-1.28	794.7914	797.5355	799.4955
	C	3.05983	1.87548	0.09171	802.8657	806.3266	806.9416
	C	3.41001	0.71068	0.89663	809.3946	813.9059	815.4198
	C	3.50756	-0.5496	0.25612	816.5852	830.9672	849.9709
	C	3.30798	-0.68175	-1.16525	852.9965	853.875	874.2916
	C	1.95206	0.35477	-2.93989	936.6178	951.4249	974.7962
	C	1.17704	1.56556	-2.91606	978.7632	987.2863	992.624
	C	1.7286	2.44634	-1.8986	1001.5719	1002.683	1010.3816
	C	0.87661	3.23897	-1.14662	1020.9535	1038.7434	1059.3648
	C	1.09798	3.37024	0.27862	1098.5077	1109.5184	1111.5011
	C	2.15198	2.70473	0.87866	1119.4451	1131.9067	1152.6534
	C	2.7391	0.8205	2.15988	1155.4103	1162.7391	1165.1733
	C	2.18449	-0.33541	2.76904	1190.157	1191.3368	1201.5078
	C	2.32091	-1.64001	2.12904	1208.5669	1230.2095	1231.6613
	C	2.97205	-1.75447	0.90284	1241.1099	1247.3264	1262.1422
	C	2.4344	-2.62235	-0.12971	1265.0366	1282.0021	1285.0102
	C	2.62926	-1.95985	-1.40503	1290.5217	1308.1878	1314.6966
	C	1.63164	-2.02775	-2.37254	1317.8242	1323.1324	1331.4672
	C	1.28197	-0.87108	-3.16957	1338.6904	1345.0679	1346.0766
	C	-0.19961	1.54969	-3.12682	1350.2368	1357.0042	1362.2296
	C	-0.87975	0.28734	-3.36909	1371.3037	1377.9407	1384.7394
	C	-0.12401	-0.89212	-3.38558	1385.7988	1390.0095	1390.3965
	C	-0.68579	-2.07596	-2.73728	1395.9129	1399.0783	1416.7951
	C	0.4117	-2.78184	-2.12181	1421.4041	1422.1194	1433.2258
	C	0.22608	-3.41297	-0.90545	1438.1978	1440.7629	1442.7684
	C	1.2462	-3.32668	0.11345	1466.0608	1472.1549	1495.5402

	C	0.57133	-3.20519	1.38013	1498.1843	1503.581	1509.1533
	C	1.09392	-2.38165	2.36958	1518.7777	1525.1753	1541.1762
	C	1.94742	2.0363	2.15347	1552.7238	1568.8953	1574.6902
	C	0.88285	-0.28041	3.37833	1578.524	1582.7673	1587.7359
	C	2.9761	0.44644	-1.94089	1599.8247	1610.9206	1614.1555
	S	-1.04313	0.02064	0.01644	1620.8826	1635.6271	1641.3812
	H	-1.04006	1.3754	0.17071	1650.4891	1659.5658	1668.7773
	S	0.94535	-0.23146	-0.02923	1671.6407	1675.7316	2031.6359
	H	1.30149	1.00998	-0.44205	2294.7338	2456.9551	2556.4674
	H	1.1314	-0.02061	1.3177			
	H	-1.20024	0.03009	-1.37162			
C_{70}	C	3.212338	-1.094467	-2.127622	-43.24	62.0428	126.9576
	C	2.434428	-2.290591	-1.923119	131.5882	199.8879	222.5101
	C	3.959623	-0.562571	-1.093913	237.1267	237.5635	238.633
	C	2.434127	-2.907347	-0.700254	265.2453	288.4505	291.0493
	C	1.195222	-3.438637	-0.159091	293.1067	311.1258	322.0334
	C	-0.000079	-3.42238	-0.905225	322.9516	334.6637	336.3755
	C	-1.195274	-3.438382	-0.159353	346.9488	359.2362	360.5147
	C	3.212316	1.685229	-1.698176	366.0944	384.971	389.3265
	C	2.434505	1.121197	-2.772522	402.7358	404.8382	431.0469
	C	3.959788	0.866504	-0.873235	433.8297	435.4501	436.6515
	C	2.434154	-0.232452	-2.981357	437.1475	450.6457	455.5319
	C	1.195236	-0.911276	-3.319336	465.3307	467.6869	469.7251
	C	-0.000137	-0.19671	-3.534298	486.4248	502.8398	508.3666
	C	-1.195323	-0.911102	-3.319361	508.7935	510.4007	530.4667

	C	-0.000064	-2.761261	-2.215699	531.2082	536.1091	537.7683
	C	1.19526	-2.170502	-2.671603	551.0444	553.3347	553.6616
	C	-1.195258	-2.17077	-2.671572	555.1793	557.0668	558.2514
	C	3.212277	2.135921	1.077965	561.2763	561.9116	564.2196
	C	2.434271	2.983367	0.209421	566.7065	571.8245	573.6227
	C	3.959657	1.098225	0.554342	575.0075	591.8524	593.5071
	C	2.434472	2.764158	-1.142505	599.5118	604.8116	608.0786
	C	1.195297	2.87535	-1.892404	609.6011	621.6593	630.6945
	C	-0.000027	3.300838	-1.27943	650.7549	650.894	658.7007
	C	-1.195266	2.875579	-1.892189	658.914	662.9931	688.5321
	C	-0.00003	1.253763	-3.310458	688.6117	698.2782	698.6089
	C	1.195319	1.870046	-2.889564	700.1695	701.4949	726.2258
	C	-1.195155	1.869857	-2.889649	728.6689	736.4522	740.6106
	C	3.212261	-0.365268	2.364708	742.7453	743.8586	749.0615
	C	2.434039	0.722638	2.90198	751.3378	752.8059	754.0394
	C	3.959554	-0.187753	1.215803	755.8455	759.9197	765.2843
	C	2.434401	1.940618	2.27553	766.4783	766.6567	768.2967
	C	1.195273	2.688163	2.149664	771.9428	773.5999	774.6834
	C	-0.000102	2.236638	2.743869	776.0358	777.2133	777.9343
	C	-1.195209	2.687991	2.149702	778.689	788.6228	789.1812
	C	-0.00007	3.535939	0.169458	789.5975	792.1321	792.6132
	C	1.195222	3.326292	0.885632	794.2463	795.5147	804.3886
	C	-1.195322	3.326447	0.885298	804.4485	805.5566	805.9535
	C	3.212531	-2.361887	0.383476	808.9378	809.1323	812.2968
	C	2.434117	-2.536451	1.58395	822.704	822.9252	858.6661
	C	3.959526	-1.214206	0.197215	858.9115	895.4422	919.5947

	C	2.434309	-1.564511	2.548973	940.3519	942.1837	947.4014
	C	1.195143	-1.213881	3.221065	948.8737	965.6976	994.8986
	C	-0.000134	-1.918555	2.975366	995.2435	1072.7392	1074.8107
	C	-1.195337	-1.214133	3.220997	1075.5056	1078.0243	1098.0611
	C	-0.00023	0.931444	3.415132	1117.432	1117.5906	1149.8668
	C	1.195115	0.18562	3.437265	1150.0954	1164.4735	1168.2291
	C	-1.195395	0.185757	3.437143	1191.3758	1208.7932	1209.3233
	C	-0.000093	-2.960197	1.941278	1230.2859	1230.8263	1234.8362
	C	1.195212	-3.211671	1.238609	1239.9791	1240.0741	1245.0888
	C	-1.195251	-3.211293	1.238716	1267.9779	1276.9811	1277.9235
	C	-3.212472	-0.36521	2.364883	1279.1116	1292.5983	1301.5488
	C	-2.434448	-1.564699	2.54927	1304.0637	1306.0874	1306.7811
	C	-2.434037	-2.536314	1.583938	1311.8593	1312.1221	1312.7361
	C	3.959526	-1.214206	0.197215	1313.4833	1337.4695	1338.0524
	C	2.434309	-1.564511	2.548973	1362.3285	1363.3633	1363.9658
	C	1.195143	-1.213881	3.221065	1364.7048	1375.7526	1381.5446
	C	-0.000134	-1.918555	2.975366	1384.9023	1386.4752	1387.1739
	C	-1.195337	-1.214133	3.220997	1399.116	1399.3308	1400.4244
	C	-0.00023	0.931444	3.415132	1408.8413	1410.2523	1415.9317
	C	1.195115	0.18562	3.437265	1416.3162	1427.8362	1430.841
	C	-1.195395	0.185757	3.437143	1431.2135	1456.1534	1456.9378
	C	-0.000093	-2.960197	1.941278	1477.6624	1478.9393	1483.1786
	C	1.195212	-3.211671	1.238609	1483.1943	1496.8085	1503.6912
	C	-1.195251	-3.211293	1.238716	1507.3018	1509.87	1511.3751
	C	-3.212472	-0.36521	2.364883	1511.9607	1529.4852	1557.4803
	C	-2.434448	-1.564699	2.54927	1557.8481	1592.7471	1594.9862

	C	-2.434037	-2.536314	1.583938	1597.0825	1601.2563	1603.4642
	C	-3.959495	-0.187675	1.215788	1609.1855	1611.5238	1624.9978
	C	-3.212481	2.136289	1.07817	1626.089	1636.1111	1636.4648
	C	-2.434152	1.940488	2.275415	1671.4603	1680.5316	1681.1594
	C	-2.434382	0.722658	2.902257	1684.0204	1685.235	1690.0543
	C	-3.959225	1.098076	0.554369	1696.3858	1696.6148	1699.7369
	C	-3.212457	1.685532	-1.698658	1700.9708	1706.904	2842.0831
	C	-2.434261	2.764251	-1.142569	2857.8012	2908.5926	3126.4357
	C	-2.434227	2.983571	0.209373			
	C	-3.959247	0.866334	-0.873354			
	C	-3.212452	-1.094542	-2.127967			
	C	-2.434224	-0.232517	-2.981606			
	C	-2.434218	1.121158	-2.772575			
	C	-3.959486	-0.562536	-1.094083			
	C	-3.212423	-2.361943	0.383389			
	C	-2.434117	-2.907345	-0.700404			
	C	-2.434351	-2.290839	-1.923371			
	C	-3.959085	-1.214066	0.197113			
$(H_2S)_2@C_{70}$	C	3.252642	-0.644424	-2.305927	-43.24	62.0428	126.9576
	C	2.453136	-1.848955	-2.351596	131.5882	199.8879	222.5101
	C	4.03832	-0.342135	-1.195719	237.1267	237.5635	238.633
	C	2.444229	-2.703519	-1.28279	265.2453	288.4505	291.0493
	C	1.191079	-3.321057	-0.864439	293.1067	311.1258	322.0334
	C	-0.010379	-3.148038	-1.586549	322.9516	334.6637	336.3755
	C	-1.215659	-3.310835	-0.8674	346.9488	359.2362	360.5147

	C	3.272559	1.993653	-1.314228	366.0944	384.971	389.3265
	C	2.472156	1.659233	-2.471973	402.7358	404.8382	431.0469
	C	4.056331	1.025843	-0.681071	433.8297	435.4501	436.6515
	C	2.462657	0.377209	-2.953298	437.1475	450.6457	455.5319
	C	1.210546	-0.208107	-3.418994	465.3307	467.6869	469.7251
	C	0.011207	0.53389	-3.478606	486.4248	502.8398	508.3666
	C	-1.196123	-0.197864	-3.424545	508.7935	510.4007	530.4667
	C	-0.002834	-2.23414	-2.731903	531.2082	536.1091	537.7683
	C	1.204237	-1.571024	-3.050892	551.0444	553.3347	553.6616
	C	-1.205508	-1.565105	-3.057225	555.1793	557.0668	558.2514
	C	3.267527	1.857558	1.502426	561.2763	561.9116	564.2196
	C	2.476909	2.861861	0.823989	566.7065	571.8245	573.6227
	C	4.05274	0.955822	0.782598	575.0075	591.8524	593.5071
	C	2.480362	2.929985	-0.545412	599.5118	604.8116	608.0786
	C	1.228305	3.193862	-1.251024	609.6011	621.6593	630.6945
	C	0.023691	3.484533	-0.56845	650.7549	650.894	658.7007
	C	-1.181443	3.201596	-1.24912	658.914	662.9931	688.5321
	C	0.018559	1.903092	-2.959282	688.6117	698.2782	698.6089
	C	1.224397	2.413085	-2.428695	700.1695	701.4949	726.2258
	C	-1.181945	2.421736	-2.427735	728.6689	736.4522	740.6106
	C	3.245072	-0.859226	2.240095	742.7453	743.8586	749.0615
	C	2.455641	0.095722	2.983064	751.3378	752.8059	754.0394
	C	4.031751	-0.453641	1.164291	755.8455	759.9197	765.2843
	C	2.465515	1.416099	2.622643	766.4783	766.6567	768.2967
	C	1.217689	2.169408	2.64676	771.9428	773.5999	774.6834
	C	0.011497	1.613036	3.126503	776.0358	777.2133	777.9343

	C	-1.187503	2.179175	2.642785	778.689	788.6228	789.1812
	C	0.021951	3.413379	0.895032	789.5975	792.1321	792.6132
	C	1.223801	3.05694	1.548348	794.2463	795.5147	804.3886
	C	-1.184205	3.066987	1.543175	804.4485	805.5566	805.9535
	C	3.233419	-2.397086	-0.111159	808.9378	809.1323	812.2968
	C	2.440671	-2.811331	1.023944	822.704	822.9252	858.6661
	C	4.020893	-1.25001	-0.055605	858.9115	895.4422	919.5947
	C	2.446188	-2.062152	2.169582	940.3519	942.1837	947.4014
	C	1.196521	-1.852315	2.891026	948.8737	965.6976	994.8986
	C	-0.009596	-2.480836	2.506369	995.2435	1072.7392	1074.8107
	C	-1.213361	-1.847191	2.892776	1075.5056	1078.0243	1098.0611
	C	0.0026	0.201677	3.516776	1117.432	1117.5906	1149.8668
	C	1.202636	-0.531023	3.388925	1150.0954	1164.4735	1168.2291
	C	-1.205682	-0.521774	3.391615	1191.3758	1208.7932	1209.3233
	C	-0.013748	-3.280715	1.279012	1230.2859	1230.8263	1234.8362
	C	1.189009	-3.386849	0.546244	1239.9791	1240.0741	1245.0888
	C	-1.216793	-3.375245	0.545512	1267.9779	1276.9811	1277.9235
	C	-3.25174	-0.835221	2.239726	1279.1116	1292.5983	1301.5488
	C	-2.467441	-2.049141	2.171368	1304.0637	1306.0874	1306.7811
	C	-2.46729	-2.794849	1.021175	1311.8593	1312.1221	1312.7361
	C	-4.020954	-0.421052	1.154938	1313.4833	1337.4695	1338.0524
	C	-3.234047	1.88481	1.493287	1362.3285	1363.3633	1363.9658
	C	-2.442022	1.436389	2.616618	1364.7048	1375.7526	1381.5446
	C	-2.452527	0.115274	2.982685	1384.9023	1386.4752	1387.1739
	C	-4.012323	0.983899	0.771072	1399.116	1399.3308	1400.4244
	C	-3.231692	2.0198	-1.315771	1408.8413	1410.2523	1415.9317

	C	-2.436502	2.954561	-0.548171	1416.3162	1427.8362	1430.841
	C	-2.43743	2.888233	0.819177	1431.2135	1456.1534	1456.9378
	C	-4.010753	1.05374	-0.683405	1477.6624	1478.9393	1483.1786
	C	-3.244025	-0.618645	-2.313481	1483.1943	1496.8085	1503.6912
	C	-2.442775	0.397855	-2.959513	1507.3018	1509.87	1511.3751
	C	-2.436025	1.67951	-2.473556	1511.9607	1529.4852	1557.4803
	C	-4.016681	-0.308674	-1.197176	1557.8481	1592.7471	1594.9862
	C	-3.258605	-2.379664	-0.116779	1597.0825	1601.2563	1603.4642
	C	-2.465993	-2.688078	-1.288263	1609.1855	1611.5238	1624.9978
	C	-2.461864	-1.835142	-2.361462	1626.089	1636.1111	1636.4648
	C	-4.026215	-1.220551	-0.061816	1671.4603	1680.5316	1681.1594
	S	-1.467508	0.067912	-0.001445	1684.0204	1685.235	1690.0543
	H	-0.824648	-0.532257	0.997648	1696.3858	1696.6148	1699.7369
	S	1.220437	-0.116498	0.009519	1700.9708	1706.904	2842.0831
	H	2.446236	0.319941	-0.036362	2857.8012	2908.5926	3126.4357
	H	0.731106	1.110611	-0.092104			
	H	-0.828122	-0.623935	-0.941414			
C_{84}	C	2.555232	-1.833413	2.772631	215.9142	216.3442	221.5773
	C	3.207492	-2.202534	1.574766	226.655	226.8816	275.7223
	C	2.602372	-3.244344	0.85788	280.6094	282.8491	286.2507
	C	1.284003	-2.326374	3.117419	289.0624	294.0262	295.3489
	C	0.609399	-3.268825	2.324258	336.1633	339.4951	349.1083
	C	1.347625	-3.77973	1.23379	353.0798	356.9374	359.5874
	C	3.971566	-1.181849	0.845636	366.6584	369.393	372.0628
	C	4.054812	-1.267356	-0.558417	373.6112	377.4828	384.9805

	C	2.629083	-0.474787	3.266497	386.5357	387.3184	431.7355
	C	3.338756	0.46517	2.602714	444.9527	447.9529	449.5174
	C	4.046721	0.121248	1.378929	458.4898	463.1484	463.891
	C	1.369841	-0.122442	3.868875	467.2131	472.1021	481.1655
	C	0.840697	1.182213	3.736357	491.4756	493.764	494.3805
	C	-0.551728	1.27126	3.812558	497.7808	505.4366	507.6262
	C	-0.840684	-1.182183	3.736369	514.846	515.8623	516.8202
	C	0.551742	-1.27123	3.812566	517.4503	518.0916	520.4639
	C	-1.369827	0.122473	3.868879	529.5157	530.0199	534.0049
	C	-1.582046	-2.191977	2.975909	535.1369	537.5195	541.443
	C	-1.455003	-3.782533	1.122212	544.7296	549.7484	561.3055
	C	-0.854316	-3.227425	2.258845	589.3903	595.3881	601.4759
	C	-2.845545	-1.823432	2.498584	602.7113	617.0179	623.9972
	C	3.369452	2.332456	1.277796	624.328	625.859	643.2671
	C	4.054816	1.26735	0.558403	645.7429	648.1837	650.3694
	C	3.971565	1.181843	-0.84565	653.5826	662.841	662.9381
	C	4.046716	-0.121254	-1.378944	665.6778	665.9357	673.5262
	C	2.680791	3.289789	0.596022	675.8797	675.9168	677.1059
	C	1.582057	2.192	2.975886	678.4477	679.9646	685.9975
	C	2.845554	1.823453	2.49856	691.4362	700.2536	700.7639
	C	1.455007	3.782542	1.122176	701.1818	703.6997	704.0228
	C	0.854325	3.227443	2.258817	705.1492	710.8191	711.3514
	C	2.602373	3.24434	-0.857889	719.8697	722.0236	725.4373
	C	3.20749	2.202529	-1.574778	726.1616	729.6415	734.534
	C	2.555225	1.833409	-2.772641	735.2215	737.5679	737.9414
	C	2.629073	0.474783	-3.266508	740.1822	740.6512	744.7344

	C	3.338746	-0.465174	-2.602725	747.0629	747.8247	747.8998
	C	-0.674624	4.193718	0.023593	751.1151	752.0606	752.2499
	C	0.67463	4.193718	-0.023627	752.7527	755.4039	758.7223
	C	1.347626	3.779728	-1.233794	761.6962	764.9427	766.1969
	C	0.609396	3.268824	-2.324261	768.1972	771.799	772.5624
	C	1.283995	2.326372	-3.117423	778.7373	784.0249	797.2661
	C	-1.283991	2.326399	3.117405	800.355	820.8716	838.2333
	C	-0.609391	3.268843	2.324234	847.4089	853.1994	853.8782
	C	-1.347621	3.77974	1.233764	869.8824	887.4176	887.9697
	C	2.680785	-3.289794	-0.596032	893.4937	899.4523	910.9782
	C	3.369444	-2.332461	-1.277808	933.6069	933.6166	939.9528
	C	2.845542	-1.823457	-2.49857	967.9573	1046.2089	1049.6953
	C	1.369827	0.12244	-3.86888	1051.4368	1059.3172	1060.1209
	C	-0.551744	-1.27126	-3.812555	1064.0661	1066.8994	1078.9645
	C	0.840682	-1.182214	-3.73636	1085.9905	1159.1097	1161.8588
	C	1.582042	-2.192002	-2.975891	1164.3133	1172.1713	1175.1371
	C	0.854312	-3.227445	-2.25882	1182.625	1200.3938	1202.4594
	C	1.454997	-3.782544	-1.122182	1216.8339	1218.5047	1223.4234
	C	-1.455001	3.782535	-1.122207	1228.3113	1237.5824	1258.2615
	C	-0.854319	3.227426	-2.258842	1269.3021	1270.6721	1272.809
	C	-1.582053	2.191978	-2.975903	1281.6382	1284.908	1303.5093
	C	-0.840695	1.182184	-3.736366	1304.9529	1306.7001	1308.8186
	C	0.55173	1.271229	-3.812567	1313.5299	1317.9484	1322.9866
	C	-1.369841	-0.122471	-3.868874	1326.7816	1328.0051	1332.4293
	C	-1.284006	-2.326397	-3.1174	1344.9996	1346.334	1352.6269
	C	-0.609404	-3.268842	-2.324232	1355.2985	1366.3824	1383.9265

	C	-1.347631	-3.779738	-1.23376	1384.8309	1386.6545	1393.4094
	C	-0.67463	-4.193717	-0.023591	1393.8971	1399.1876	1403.1704
	C	0.674624	-4.193719	0.023624	1405.9929	1409.4079	1411.7522
	C	-3.338755	0.465154	-2.602717	1416.4718	1420.259	1426.1767
	C	-2.629084	-0.474809	-3.266494	1429.6307	1430.1821	1435.0743
	C	-2.555234	-1.833431	-2.772617	1438.0281	1438.1428	1441.4768
	C	-3.207496	-2.202542	-1.574749	1444.4792	1450.7035	1455.9402
	C	-2.602376	-3.244346	-0.857854	1459.8309	1463.4239	1469.9804
	C	-2.680787	3.289789	-0.596048	1475.5753	1477.5069	1484.8356
	C	-3.369449	2.332451	-1.277815	1491.2405	1500.3778	1511.8526
	C	-2.845551	1.823436	-2.498574	1515.6177	1526.9464	1527.35
	C	-2.555221	1.833435	2.772626	1530.0115	1533.623	1551.0812
	C	-3.207487	2.202546	1.57476	1573.6305	1587.0478	1589.1534
	C	-2.602369	3.24435	0.857863	1594.8921	1599.6413	1612.708
	C	-4.046717	-0.121238	1.378945	1613.6413	1615.5844	1632.5913
	C	-3.338747	-0.465149	2.60273	1639.8703	1643.9774	1647.2126
	C	-2.629071	0.474813	3.266503	1647.8765	1654.395	1659.1308
	C	-4.054814	1.267352	-0.558413	1660.0323	1670.9144	1671.2863
	C	-3.971564	1.181856	0.845641	1678.3459	1688.517	1710.0811
	C	-2.680789	-3.289784	0.596057	1719.2714	1719.4997	1719.6048
	C	-4.046721	0.121243	-1.37893	1748.9838	1750.1662	1756.9378
	C	-3.971569	-1.18185	-0.845627	1759.806	1765.4457	1768.4121
	C	-4.054814	-1.267346	0.558428			
	C	-3.369448	-2.332447	1.277827			
$(H_2S)_2@C_{84}$	C	-2.626321	1.885699	2.685318	41.0582	52.3885	75.8602
	C	-3.247701	2.266724	1.47273	100.5679	125.4373	134.2129

	C	-2.577268	3.286956	0.7769	207.2231	214.4304	215.0242
	C	-1.34756	2.347628	3.063116	237.3754	239.4936	241.5371
	C	-0.618747	3.269475	2.295956	273.6738	277.0282	283.4756
	C	-1.31635	3.791253	1.187397	288.0573	301.4092	309.5115
	C	-4.04528	1.268317	0.727262	311.2417	327.6547	330.2791
	C	-4.069349	1.355359	-0.684668	335.4692	340.2372	349.5296
	C	-2.743713	0.528462	3.172694	352.7047	360.508	367.4526
	C	-3.472341	-0.392754	2.495325	370.287	371.6769	374.7782
	C	-4.177211	-0.039144	1.262242	380.6552	386.6908	392.9957
	C	-1.500492	0.152367	3.803597	400.5514	401.6949	411.2888
	C	-0.987938	-1.157809	3.688701	433.2662	449.8702	454.0558
	C	0.403593	-1.272253	3.806052	456.2012	467.1815	467.8665
	C	0.743231	1.166191	3.739781	469.1849	471.9969	488.8054
	C	-0.653068	1.280862	3.77303	489.7186	492.2549	502.5437
	C	1.24557	-0.143769	3.887282	505.7849	506.425	508.9357
	C	1.539571	2.153866	3.009506	509.7194	512.9076	515.3264
	C	1.501689	3.737447	1.163384	515.6459	518.0826	522.7332
	C	0.849561	3.198849	2.276443	522.9695	526.0745	532.1433
	C	2.817536	1.763764	2.575589	532.9186	533.5972	536.2541
	C	-3.495592	-2.261163	1.168941	540.4339	546.4306	552.4341
	C	-4.179526	-1.192179	0.437303	555.3168	563.3039	572.2789
	C	-4.03176	-1.106365	-0.969918	590.881	600.7406	601.3267
	C	-4.052397	0.203815	-1.506412	606.2861	617.0376	624.4037
	C	-2.783029	-3.222499	0.509936	625.1217	638.2928	643.7163
	C	-1.735098	-2.146429	2.910283	645.9325	648.8072	654.1444
	C	-2.986214	-1.756927	2.399859	663.9254	670.4853	673.9007

	C	-1.57608	-3.731815	1.070037	677.2746	680.4963	682.7491
	C	-0.997977	-3.192023	2.221629	683.4747	689.5267	692.1347
	C	-2.654812	-3.182067	-0.939286	697.9387	699.4717	699.6704
	C	-3.231207	-2.133781	-1.67148	706.8384	711.5968	712.1131
	C	-2.514374	-1.777312	-2.839728	715.3839	728.9645	731.4062
	C	-2.541123	-0.41902	-3.331932	733.4701	734.8587	736.5021
	C	-3.267949	0.529262	-2.696168	740.4315	741.1478	751.2053
	C	0.588798	-4.184477	0.042209	751.868	758.6288	762.8611
	C	-0.760782	-4.155808	-0.045524	765.3029	765.7741	768.1644
	C	-1.390957	-3.734226	-1.272395	769.4081	773.4047	778.4166
	C	-0.601046	-3.241649	-2.33259	778.8844	783.5704	784.0152
	C	-1.237483	-2.2912	-3.142038	785.7944	787.1376	791.9345
	C	1.141611	-2.338163	3.139432	794.9455	796.8473	798.1352
	C	0.466547	-3.263032	2.330484	798.4358	800.8909	803.3515
	C	1.23555	-3.786828	1.269251	804.5793	805.26	805.9054
	C	-2.604555	3.332269	-0.676852	807.3762	807.5227	809.4186
	C	-3.305871	2.395058	-1.376382	811.0983	822.3152	838.1964
	C	-2.742337	1.873642	-2.575223	845.4194	847.1787	854.872
	C	-1.250731	-0.09373	-3.889972	863.032	884.121	888.6604
	C	0.705575	1.25465	-3.775529	891.0291	897.4661	908.6917
	C	-0.694732	1.195044	-3.74344	931.2633	932.3846	932.704
	C	-1.449345	2.214635	-3.011547	967.1117	1039.3619	1042.1194
	C	-0.717432	3.231765	-2.277354	1046.6452	1048.5049	1055.6205
	C	-1.346924	3.794578	-1.162053	1063.1286	1066.7393	1076.0554
	C	1.420252	-3.791907	-1.073186	1079.0835	1150.3906	1158.6405
	C	0.864844	-3.228695	-2.224776	1160.491	1162.3906	1163.7353

	C	1.645262	-2.214151	-2.913059	1181.6608	1191.4296	1200.3515
	C	0.939402	-1.196522	-3.692437	1206.7115	1208.4607	1212.9974
	C	-0.455575	-1.255758	-3.808113	1214.2967	1217.5799	1221.1629
	C	1.506048	0.092386	-3.807205	1223.4801	1253.2202	1254.8786
	C	1.442209	2.292123	-3.064464	1256.7201	1268.361	1268.7383
	C	0.752634	3.242754	-2.295955	1280.9474	1291.1443	1298.4851
	C	1.469678	3.735729	-1.186696	1299.774	1304.2261	1311.0097
	C	0.761163	4.159424	-0.002054	1312.5217	1315.9088	1320.8234
	C	-0.590989	4.18814	0.003566	1321.4945	1328.1653	1333.5126
	C	3.45236	-0.531082	-2.497391	1336.5243	1337.4797	1345.9089
	C	2.764219	0.418474	-3.17689	1358.418	1371.2078	1375.3387
	C	2.700464	1.778344	-2.685624	1377.5739	1378.8098	1384.9766
	C	3.338768	2.13605	-1.472775	1386.6571	1394.0063	1394.5956
	C	2.709207	3.181198	-0.775182	1401.8825	1407.7931	1407.9337
	C	2.645823	-3.329177	-0.513007	1412.5833	1414.7825	1420.5011
	C	3.393748	-2.394964	-1.170267	1425.6809	1431.1767	1431.8738
	C	2.910025	-1.873891	-2.402629	1433.068	1437.0296	1439.6273
	C	2.438505	-1.874694	2.837014	1443.8063	1446.8331	1451.7864
	C	3.138157	-2.258115	1.668059	1456.3559	1465.5472	1466.4557
	C	2.520175	-3.283289	0.935941	1472.6587	1474.6255	1486.5667
	C	4.061895	0.044198	1.507722	1496.2636	1506.4976	1507.0141
	C	3.287343	0.399628	2.696018	1520.1828	1523.566	1526.8986
	C	2.522093	-0.519255	3.330415	1533.1637	1544.9813	1561.2573
	C	4.117835	-1.354478	-0.438365	1574.1862	1584.9756	1588.8322
	C	3.977884	-1.262354	0.967897	1592.6643	1593.4919	1597.1892
	C	2.740526	3.227143	0.679117	1606.4233	1614.3191	1624.8018

	C	4.169168	-0.204829	-1.263577	1635.7654	1638.8281	1641.6599
	C	4.098142	1.10733	-0.726566	1644.7495	1649.2941	1659.1899
	C	4.130132	1.195024	0.687273	1662.5721	1666.2523	1671.8478
	C	3.40444	2.263399	1.378659	1680.1332	1697.8968	1708.259
	S	-1.482059	-0.13234	0.097758	1710.4446	1713.4142	1736.0891
	H	-0.787591	0.486134	1.055313	1737.4039	1747.7395	1749.5337
	S	1.499235	0.055259	-0.031229	1756.3282	1759.5408	2806.9427
	H	0.888623	0.158088	-1.213516	2822.2182	2829.7695	2838.9906
	H	0.900702	-1.103821	0.250702			
	H	-1.168496	0.794694	-0.81279			

Table S2: Natural population analysis of $(H_2S)_2@C_{60}$

Atom	charge	core	valence	rydberg	total
C	-0.0424	1.9987	4.0170	0.0267	6.0424
C	-0.0587	1.9987	4.0319	0.0280	6.0587
C	-0.0620	1.9988	4.0444	0.0188	6.0620
C	0.0415	1.9988	3.9413	0.0185	5.9585
C	-0.0437	1.9987	4.0156	0.0294	6.0437
C	-0.0223	1.9987	4.0031	0.0204	6.0223
C	-0.0080	1.9987	3.9836	0.0257	6.0080
C	-0.0307	1.9987	4.0095	0.0225	6.0307
C	0.0431	1.9988	3.9422	0.0160	5.9569
C	-0.0241	1.9987	4.0030	0.0224	6.0241
C	0.0145	1.9987	3.9713	0.0155	5.9855
C	-0.0597	1.9988	4.0330	0.0280	6.0597
C	0.0297	1.9987	3.9545	0.0171	5.9703
C	-0.0538	1.9988	4.0288	0.0263	6.0538
C	-0.0850	1.9987	4.0619	0.0244	6.0850
C	-0.0192	1.9987	3.9954	0.0251	6.0192
C	-0.0625	1.9988	4.0402	0.0235	6.0625
C	-0.0668	1.9987	4.0370	0.0311	6.0668
C	0.0271	1.9987	3.9556	0.0186	5.9729
C	0.0009	1.9987	3.9802	0.0202	5.9991
C	-0.0159	1.9988	3.9925	0.0247	6.0159
C	0.0002	1.9987	3.9843	0.0168	5.9998
C	-0.0104	1.9988	3.9878	0.0239	6.0104
C	-0.0545	1.9987	4.0315	0.0243	6.0545
C	-0.1282	1.9988	4.1037	0.0257	6.1282
C	0.0059	1.9987	3.9727	0.0227	5.9941
C	-0.0273	1.9987	4.0122	0.0164	6.0273
C	-0.0282	1.9987	4.0033	0.0261	6.0282
C	-0.0154	1.9987	3.9934	0.0233	6.0154
C	-0.0368	1.9987	4.0125	0.0256	6.0368
C	-0.0152	1.9987	3.9925	0.0240	6.0152
C	-0.0046	1.9986	3.9896	0.0164	6.0046
C	-0.0729	1.9988	4.0451	0.0290	6.0729
C	-0.0473	1.9987	4.0232	0.0254	6.0473
C	-0.0689	1.9987	4.0444	0.0258	6.0689
C	0.0344	1.9987	3.9521	0.0148	5.9656
C	-0.0530	1.9987	4.0266	0.0277	6.0530
C	0.0361	1.9987	3.9504	0.0148	5.9639
C	-0.0151	1.9987	3.9923	0.0240	6.0151
C	-0.0186	1.9987	4.0001	0.0198	6.0186
C	-0.0528	1.9987	4.0290	0.0252	6.0528
C	-0.0976	1.9987	4.0718	0.0271	6.0976
C	0.0430	1.9987	3.9430	0.0153	5.9570
C	-0.0268	1.9987	4.0010	0.0272	6.0268
C	-0.0136	1.9987	3.9981	0.0168	6.0136
C	-0.0228	1.9987	4.0007	0.0233	6.0228
C	0.0218	1.9988	3.9591	0.0203	5.9782
C	-0.0673	1.9987	4.0458	0.0227	6.0673
C	-0.0330	1.9988	4.0092	0.0251	6.0330
C	-0.0405	1.9988	4.0170	0.0248	6.0405
C	0.0046	1.9987	3.9810	0.0157	5.9954
C	-0.0153	1.9988	3.9953	0.0212	6.0153
C	-0.0440	1.9987	4.0226	0.0227	6.0440
C	0.0336	1.9987	3.9522	0.0155	5.9664
C	-0.0251	1.9988	4.0013	0.0251	6.0251
C	-0.0053	1.9987	3.9859	0.0207	6.0053
C	-0.0517	1.9987	4.0305	0.0226	6.0517
C	-0.0069	1.9987	3.9881	0.0201	6.0069
C	-0.0476	1.9987	4.0235	0.0254	6.0476
C	0.0148	1.9987	3.9709	0.0156	5.9852
S	0.3128	9.9986	5.5968	0.0918	15.6873
H	0.1967	0.0000	0.7969	0.0065	0.8033
S	0.3220	9.9986	5.5783	0.1011	15.6780
H	0.1937	0.0000	0.8009	0.0054	0.8063
H	0.2072	0.0000	0.7876	0.0052	0.7928
H	0.2184	0.0000	0.7753	0.0064	0.7817

Table S3: Natural population analysis of $(H_2S)_2@C_{70}$

Atom	charge	core	valence	rydberg	total
C	0.0307	1.9987	3.9557	0.0149	5.9693
C	0.0034	1.9987	3.9765	0.0214	5.9966
C	-0.0249	1.9987	3.9989	0.0272	6.0249
C	0.0020	1.9987	3.9774	0.0219	5.9980
C	-0.0174	1.9988	3.9953	0.0232	6.0174
C	0.0247	1.9988	3.9621	0.0145	5.9753
C	-0.0227	1.9988	4.0004	0.0235	6.0227
C	-0.0277	1.9988	4.0032	0.0258	6.0277
C	0.0047	1.9987	3.9768	0.0197	5.9953
C	0.0180	1.9987	3.9673	0.0161	5.9820
C	0.0089	1.9987	3.9711	0.0213	5.9911
C	-0.0070	1.9988	3.9878	0.0204	6.0070
C	0.0278	1.9988	3.9591	0.0143	5.9723
C	-0.0330	1.9989	4.0091	0.0251	6.0330
C	-0.0249	1.9989	4.0027	0.0233	6.0249
C	0.0042	1.9988	3.9783	0.0187	5.9958
C	0.0189	1.9988	3.9676	0.0147	5.9811
C	-0.0096	1.9987	3.9897	0.0212	6.0096
C	-0.0098	1.9988	3.9867	0.0243	6.0098
C	-0.0283	1.9987	4.0022	0.0275	6.0283
C	0.0361	1.9987	3.9496	0.0156	5.9639
C	-0.0297	1.9988	4.0073	0.0236	6.0297
C	0.0232	1.9988	3.9636	0.0144	5.9768
C	-0.0142	1.9988	3.9940	0.0215	6.0142
C	-0.0190	1.9989	3.9969	0.0233	6.0190
C	-0.0021	1.9988	3.9848	0.0186	6.0021
C	0.0316	1.9988	3.9554	0.0142	5.9684
C	0.0214	1.9987	3.9631	0.0168	5.9786
C	0.0080	1.9987	3.9709	0.0224	5.9920
C	0.0206	1.9987	3.9609	0.0198	5.9794
C	0.0075	1.9987	3.9739	0.0198	5.9925
C	-0.0137	1.9988	3.9934	0.0214	6.0137
C	0.0265	1.9988	3.9604	0.0143	5.9735
C	-0.0101	1.9988	3.9899	0.0214	6.0101
C	-0.0216	1.9989	3.9992	0.0236	6.0216
C	0.0220	1.9988	3.9651	0.0141	5.9780
C	-0.0010	1.9988	3.9834	0.0187	6.0010
C	0.0197	1.9987	3.9658	0.0158	5.9804
C	-0.0089	1.9988	3.9853	0.0248	6.0089
C	-0.0232	1.9987	3.9968	0.0276	6.0232
C	0.0004	1.9987	3.9779	0.0230	5.9996
C	-0.0051	1.9988	3.9851	0.0212	6.0051
C	0.0225	1.9988	3.9642	0.0145	5.9775
C	-0.0296	1.9989	4.0065	0.0243	6.0296
C	-0.0201	1.9989	3.9969	0.0244	6.0201
C	0.0013	1.9988	3.9813	0.0186	5.9987
C	0.0141	1.9988	3.9718	0.0152	5.9859
C	-0.0308	1.9989	4.0058	0.0261	6.0308
C	0.0303	1.9988	3.9562	0.0147	5.9697
C	0.0260	1.9988	3.9608	0.0144	5.9740
C	-0.0201	1.9987	3.9986	0.0228	6.0201
C	0.0025	1.9987	3.9788	0.0200	5.9975
C	-0.0033	1.9988	3.9814	0.0232	6.0033
C	0.0124	1.9987	3.9684	0.0205	5.9876
C	0.0214	1.9987	3.9649	0.0149	5.9786
C	-0.0155	1.9988	3.9918	0.0249	6.0155
C	0.0279	1.9987	3.9574	0.0159	5.9721
C	-0.0096	1.9987	3.9844	0.0265	6.0096
C	-0.0232	1.9987	4.0000	0.0244	6.0232
C	0.0111	1.9987	3.9708	0.0194	5.9889
C	0.0028	1.9987	3.9769	0.0216	5.9972
C	0.0384	1.9987	3.9461	0.0168	5.9616
C	-0.0331	1.9987	4.0078	0.0265	6.0331
C	0.0332	1.9987	3.9523	0.0159	5.9668
C	-0.0139	1.9988	3.9901	0.0251	6.0139
C	0.0414	1.9987	3.9432	0.0167	5.9586
C	0.0276	1.9987	3.9591	0.0146	5.9724
C	0.0026	1.9987	3.9765	0.0221	5.9974
C	-0.0066	1.9987	3.9856	0.0224	6.0066
C	0.0001	1.9987	3.9757	0.0256	6.0000
S	-0.3034	9.9992	6.2382	0.0660	16.3034
H	0.1347	0.0000	0.8560	0.0093	0.8653
S	-0.3002	9.9990	6.2435	0.0576	16.3002
H	0.0948	0.0000	0.8991	0.0062	0.9052
H	0.1237	0.0000	0.8659	0.0105	0.8764
H	0.1350	0.0000	0.8558	0.0092	0.8650

Table S4: Natural population analysis of $(H_2S)_2@C_{84}$

Atom	charge	core	valence	rydberg	total
C	0.0176	1.9988	3.9701	0.0135	5.9824
C	-0.0099	1.9989	3.9902	0.0208	6.0099
C	-0.0016	1.9986	3.9818	0.0212	6.0016
C	-0.0262	1.9989	4.0041	0.0231	6.0262
C	0.0407	1.9986	3.9461	0.0146	5.9594
C	-0.0389	1.9989	4.0180	0.0220	6.0389
C	-0.0007	1.9988	3.9799	0.0220	6.0007
C	-0.0029	1.9988	3.9821	0.0220	6.0029
C	-0.0110	1.9988	3.9891	0.0231	6.0110
C	0.0160	1.9988	3.9641	0.0212	5.9840
C	0.0375	1.9988	3.9499	0.0139	5.9625
C	0.0118	1.9988	3.9759	0.0135	5.9882
C	-0.0311	1.9989	4.0090	0.0232	6.0311
C	0.0467	1.9986	3.9403	0.0145	5.9533
C	-0.0018	1.9986	3.9818	0.0214	6.0018
C	-0.0180	1.9989	3.9979	0.0212	6.0180
C	-0.0477	1.9989	4.0273	0.0215	6.0477
C	0.0463	1.9987	3.9416	0.0134	5.9537
C	-0.0176	1.9989	3.9991	0.0196	6.0176
C	-0.0222	1.9990	4.0015	0.0217	6.0222
C	-0.0114	1.9986	3.9918	0.0209	6.0114
C	-0.0142	1.9988	3.9940	0.0214	6.0142
C	0.0013	1.9988	3.9789	0.0210	5.9987
C	-0.0132	1.9988	3.9899	0.0245	6.0132
C	0.0213	1.9988	3.9648	0.0152	5.9787
C	0.0455	1.9986	3.9422	0.0138	5.9545
C	-0.0040	1.9989	3.9868	0.0183	6.0040
C	-0.0147	1.9988	3.9979	0.0181	6.0147
C	-0.0092	1.9986	3.9901	0.0206	6.0092
C	-0.0032	1.9987	3.9835	0.0210	6.0032
C	-0.0041	1.9986	3.9826	0.0228	6.0041
C	-0.0105	1.9989	3.9920	0.0197	6.0105
C	-0.0196	1.9986	3.9969	0.0241	6.0196
C	0.0309	1.9988	3.9551	0.0152	5.9692
C	0.0357	1.9988	3.9479	0.0175	5.9643
C	0.0524	1.9985	3.9338	0.0152	5.9476
C	-0.0207	1.9989	3.9979	0.0240	6.0207
C	0.0244	1.9988	3.9640	0.0127	5.9756
C	-0.0299	1.9989	4.0088	0.0222	6.0299
C	-0.0027	1.9987	3.9835	0.0206	6.0027
C	-0.0280	1.9989	4.0075	0.0216	6.0280
C	0.0364	1.9986	3.9511	0.0138	5.9636
C	-0.0368	1.9989	4.0157	0.0222	6.0368
C	0.0424	1.9986	3.9451	0.0140	5.9576
C	-0.0167	1.9988	3.9957	0.0221	6.0167
C	-0.0279	1.9988	4.0063	0.0228	6.0279
C	-0.0442	1.9989	4.0217	0.0236	6.0442
C	0.0295	1.9988	3.9577	0.0140	5.9705
C	-0.0189	1.9989	3.9979	0.0221	6.0189
C	-0.0126	1.9989	3.9936	0.0201	6.0126
C	-0.0099	1.9987	3.9884	0.0229	6.0099
C	-0.0234	1.9987	4.0014	0.0233	6.0234
C	-0.0411	1.9989	4.0178	0.0244	6.0411
C	0.0422	1.9987	3.9451	0.0140	5.9578
C	0.0043	1.9987	3.9758	0.0213	5.9958
C	-0.0262	1.9989	4.0071	0.0201	6.0262
C	0.0457	1.9986	3.9419	0.0139	5.9544
C	-0.0395	1.9989	4.0175	0.0232	6.0395
C	-0.0311	1.9989	4.0071	0.0251	6.0311
C	0.0282	1.9986	3.9581	0.0151	5.9718
C	0.0140	1.9989	3.9737	0.0135	5.9860
C	-0.0176	1.9989	3.9931	0.0256	6.0176
C	0.0502	1.9985	3.9364	0.0148	5.9498
C	0.0195	1.9988	3.9597	0.0221	5.9805
C	0.0368	1.9988	3.9498	0.0147	5.9632
C	-0.0354	1.9988	4.0119	0.0247	6.0354
C	0.0304	1.9988	3.9563	0.0145	5.9696
C	-0.0289	1.9989	4.0043	0.0257	6.0289
C	0.0332	1.9988	3.9542	0.0138	5.9668
C	-0.0142	1.9988	3.9913	0.0241	6.0142
C	-0.0160	1.9988	3.9999	0.0173	6.0160
C	-0.0303	1.9988	4.0108	0.0207	6.0303
C	-0.0026	1.9988	3.9846	0.0192	6.0026
C	-0.0119	1.9988	3.9919	0.0212	6.0119
C	0.0322	1.9988	3.9549	0.0142	5.9679
C	-0.0067	1.9989	3.9848	0.0230	6.0067
C	0.0533	1.9985	3.9331	0.0152	5.9468
C	0.0515	1.9988	3.9358	0.0140	5.9485
C	-0.0217	1.9988	3.9971	0.0258	6.0217
C	0.0486	1.9985	3.9379	0.0151	5.9515
C	-0.0097	1.9988	3.9894	0.0215	6.0097
C	-0.0056	1.9988	3.9844	0.0224	6.0056
C	-0.0033	1.9988	3.9831	0.0214	6.0033
C	-0.0162	1.9988	3.9959	0.0214	6.0162
S	-0.3179	9.9992	6.2587	0.0600	16.3179
H	0.1539	0.0000	0.8391	0.0070	0.8461
S	-0.3187	9.9992	6.2596	0.0600	16.3187
H	0.1368	0.0000	0.8566	0.0067	0.8632
H	0.1513	0.0000	0.8417	0.0070	0.8487
H	0.1322	0.0000	0.8609	0.0069	0.8678

Table S5: Electron density and Laplacian showing the weak interaction between $(H_2S)_2$ and cage in $(H_2S)_2@C_{60}$, $(H_2S)_2@C_{70}$, and $(H_2S)_2@C_{84}$.

Species	Atoms	CP	ρ_{BCP}	$\Delta^2\rho_{BCP}$
$(H_2S)_2@C_{60}$	C15-H62	(3,-1)	0.04413	0.09303
	C26-H66	(3,-1)	0.05922	0.08059
	C42-H65	(3,-1)	0.04803	0.08683
	C60-H64	(3,-1)	0.04042	0.09402
$(H_2S)_2@C_{70}$	C17-H76	(3,-1)	0.01600	0.05136
	C44-H72	(3,-1)	0.01646	0.05240
	C10-H74	(3,-1)	0.04134	0.11470
	C22-H75	(3,-1)	0.01379	0.04492
$(H_2S)_2@C_{84}$	C46-H90	(3,-1)	0.01059	0.03509
	C56-H88	(3,-1)	0.00895	0.03074

Table S6: The stabilization energy in kcal mol^{-1} of $(H_2S)_2$ encapsulated in C_{60} fullerene, at different method of DFT functionals.

Method	Species
	$(H_2S)_2@C_{60}$
LC-wHPBE/6-31++G**	186.38
LC-BLYP/6-31++G**	206.07
LC-wB97X/6-31++G**	206.44
wB97XD/6-31++G**	186.64
M06-2X/6-31++G**	165.70

Table S7: Comparison of UHF and RHF results of $(H_2S)_2@C_{60}$ at LC-wHPBE/6-31++G** level of theory.

Method	S-S (Å)	S-H (Å)	H-S-H (deg.)	$\Delta E_{stabilization}$
RLC-wHPBE/6-31++G**	2.00	1.36	97.02	186.38
ULC-wHPBE/6-31++G**	1.99	1.37	97.34	185.74

Table S8: Natural electronic configuration, valence electron and natural charge on bare $(H_2S)_2$

Atom	electronic configuration	valence electron	natural charge
S	[core]3S(1.72)3p(4.47)4S(0.01)3d(0.05)4p(0.09)	6.34	-0.33
H	1S(0.83)2S(0.01)	0.84	0.16
S	[core]3S(1.71)3p(4.47)4S(0.01)3d(0.05)4p(0.09)	6.33	-0.33
H	1S(0.83)2S(0.01)	0.84	0.16
H	1S(0.83)	0.83	0.17
H	1S(0.83)	0.83	0.17
$(H_2S)_2$	Total valence electrons and charge in $(H_2S)_2$	16.01	0.00

Table S9: Natural electronic configuration, valence electron and natural charge on $(H_2S)_2$ unit obtained from NBO analysis of $(H_2S)_2@C_{70}$

Atom	electronic configuration	valence electron	natural charge
S	[core]3S(1.73)3p(4.51)3d(0.02)4p(0.03)5p(0.02)	6.31	-0.30
H	1S(0.86)	0.86	0.13
S	[core]3S(1.71)3p(4.53)3d(0.02)4p(0.02)5p(0.01)	6.29	-0.30
H	1S(0.90)	0.90	0.09
H	1S(0.87)2S(0.01)	0.88	0.12
H	1S(0.86)	0.86	0.14
$(H_2S)_2$	Total valence electrons and charge in $(H_2S)_2$	16.10	-0.11

Table S10: Natural electronic configuration, valence electron and natural charge on $(H_2S)_2$ unit obtained from NBO analysis of $(H_2S)_2@C_{84}$

Atom	electronic configuration	valence electron	natural charge
S	[core]3S(1.75)3p(4.51)3d(0.02)4p(0.03)5p(0.01)	6.32	-0.32
H	1S(0.84)	0.84	0.15
S	[core]3S(1.75)3p(4.51)3d(0.02)4p(0.03)5p(0.01)	6.32	-0.32
H	1S(0.86)	0.86	0.14
H	1S(0.84)	0.84	0.15
H	1S(0.86)	0.86	0.13
$(H_2S)_2$	Total valence electrons and charge in $(H_2S)_2$	16.04	-0.06

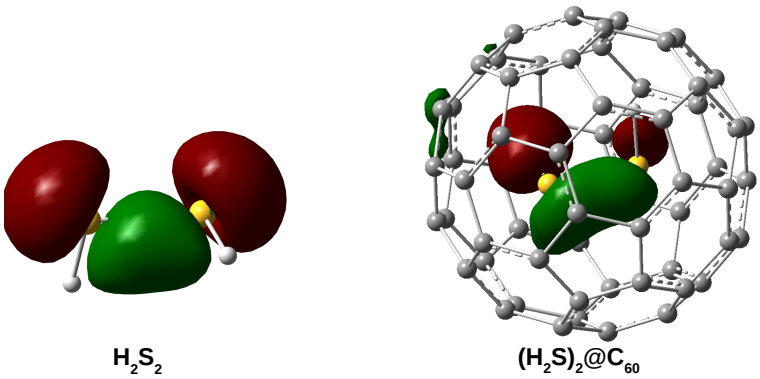

Figure S1: Spatial representation of the S-S bond MO in H_2S_2 and $(H_2S)_2@C_{60}$ obtained at LC-wHPBE/6-31++G** level of theory

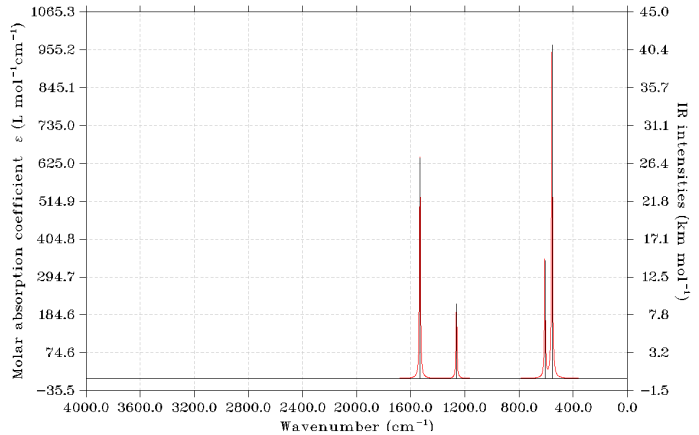

Figure S2: IR plot for the C_{60} molecule obtained at LC-wHPBE/6-31++G** level of theory.

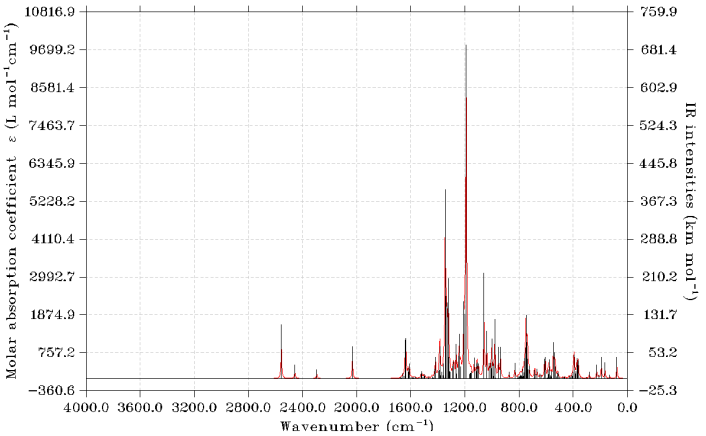

Figure S3: IR plot for the $(H_2S)_2@C_{60}$ molecule obtained at LC-wHPBE/6-31++G** level of theory

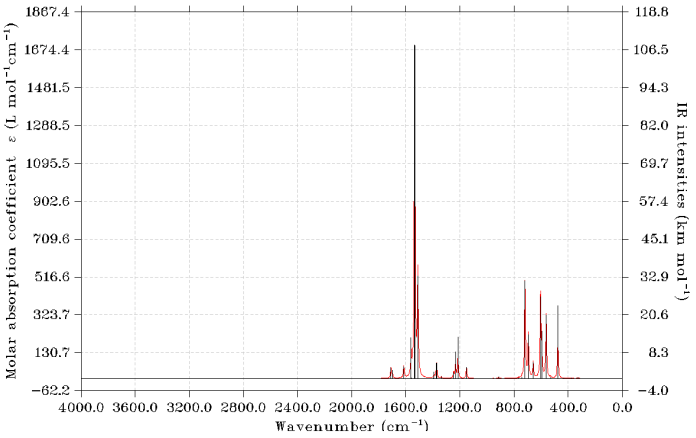

Figure S4: IR plot for the C_{70} molecule obtained at LC-wHPBE/6-31++G** level of theory.

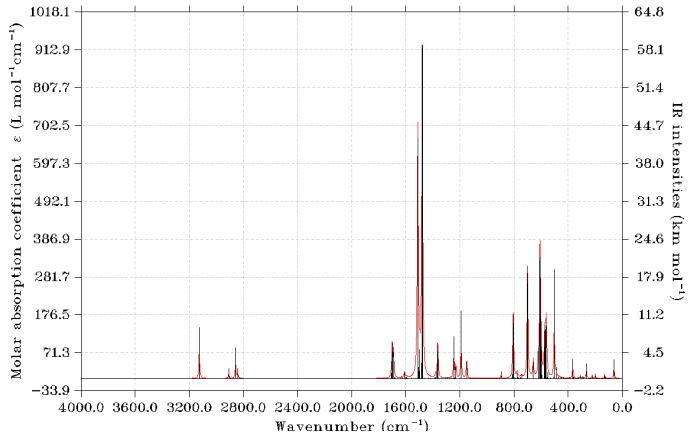

Figure S5: IR plot for the $(H_2S)_2@C_{70}$ molecule obtained at LC-wHPBE/6-31++G** level of theory

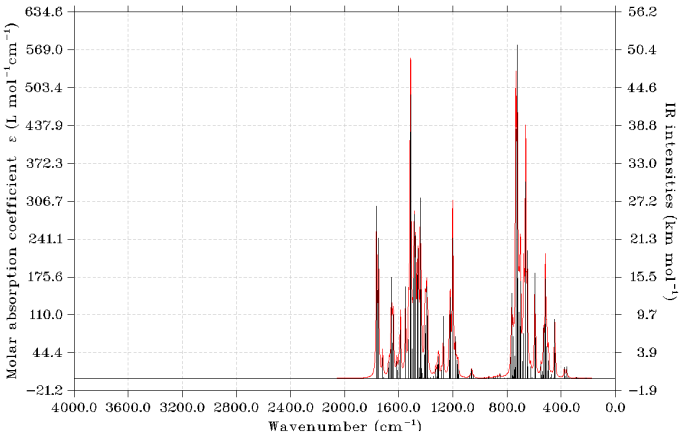

Figure S6: IR plot for the C_{84} molecule obtained at LC-wHPBE/6-31++G** level of theory.

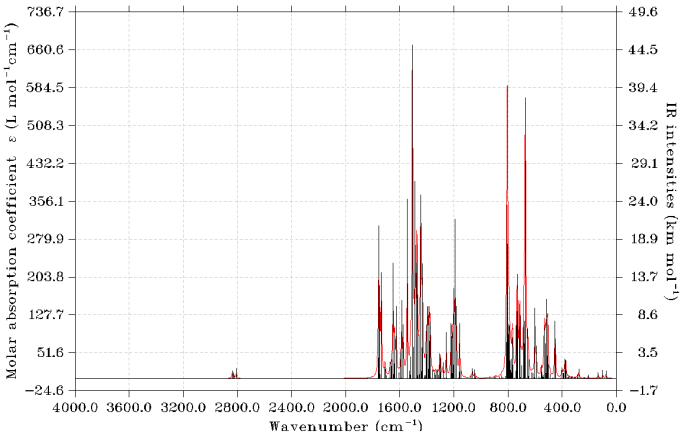

Figure S7: IR plot for the $(H_2S)_2@C_{84}$ molecule obtained at LC-wHPBE/6-31++G** level of theory