SUPPLEMENTARY MATERIALS

Vibronic Emission Spectra of Dithiophene and Terthiophene and Their Complexes with H_2S and $(H_2S)_2$

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A. Coordinates, bond lengths and angles of T2···H_2S, T2···$(H_2S)_2$, T3···H_2S, T3···$(H_2S)_2$.

All coordinates in Tables A1 – A4 are given in bohrs.

A1. T2···H_2S complex

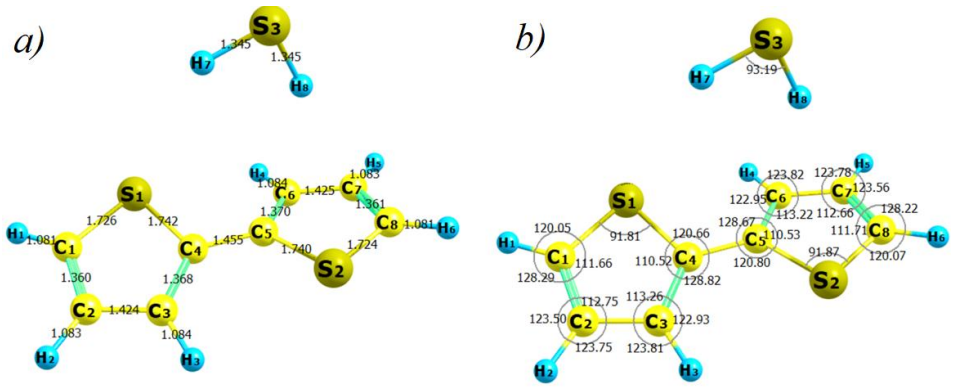

Fig. A1. T2···H_2S: *a)* the bond lengths (Å); *b)* the angles (in degrees)

Table A1. Cartesian coordinates of T2···H_2S

Atom	X	Y	Z
H1	2.608150000	-0.476940000	-6.926010000
C4	4.463190000	1.544890000	-4.683970000
S1	4.332240000	-0.106740000	-5.221690000
C1	3.062980000	0.293910000	-6.319890000
C2	2.768380000	1.621290000	-6.283930000

C3	3.568470000	2.337910000	-5.348670000
H3	3.470930000	3.401110000	-5.161440000
H2	2.000680000	2.080210000	-6.895260000
C5	5.440450000	1.921040000	-3.673530000
S2	6.107660000	3.527660000	-3.633880000
C8	7.095260000	3.144990000	-2.273170000
C7	6.931610000	1.852210000	-1.879830000
C6	5.983460000	1.150820000	-2.679660000
H5	7.457580000	1.409850000	-1.042360000
H6	7.738240000	3.899090000	-1.841420000
H4	5.699750000	0.118070000	-2.512470000
S3	8.755980000	0.358030000	-5.396790000
H7	7.578430000	0.142330000	-6.009010000
H8	8.176450000	0.886870000	-4.303800000

A2. T2···$(H_2S)_2$ complex

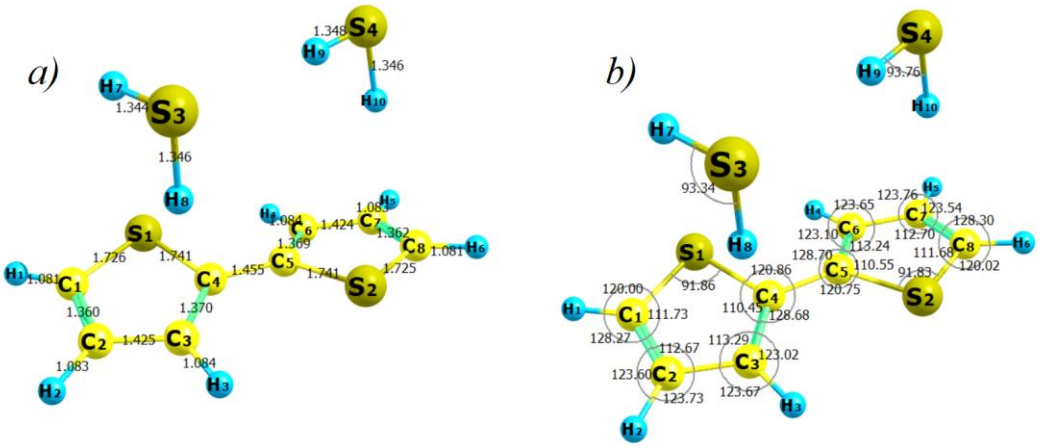

Fig. A2. T2···$(H_2S)_2$: *a)* the bond lengths (Å); *b)* the angles (in degrees)

Table A2. Cartesian coordinates of T2···$(H_2S)_2$

Atom	X	Y	Z
H1	2.056300000	-0.413910000	-6.545160000
C4	4.305090000	1.487780000	-4.574690000
S1	3.795640000	-0.156230000	-4.836150000
C1	2.670470000	0.326600000	-6.052280000
C2	2.694600000	1.671290000	-6.255290000
C3	3.628610000	2.337570000	-5.410200000
H3	3.775740000	3.411660000	-5.405350000
H2	2.065690000	2.179920000	-6.975820000
C5	5.327060000	1.803820000	-3.588610000
S2	6.232230000	3.288160000	-3.688450000
C8	7.144670000	2.890910000	-2.279940000
C7	6.780800000	1.682490000	-1.768750000
C6	5.740210000	1.060360000	-2.516400000
H5	7.228490000	1.248020000	-0.883050000
H6	7.894200000	3.576330000	-1.909910000

H4	5.305580000	0.101430000	-2.258850000
S3	9.341700000	0.369030000	-4.699920000
H9	8.499970000	0.676270000	-5.707000000
H10	8.568070000	0.943090000	-3.760040000
H7	6.174670000	-0.182130000	-7.732470000
S4	6.665940000	1.068220000	-7.772160000
H8	5.681070000	1.563750000	-6.999240000

A3. T3···H_2S complex

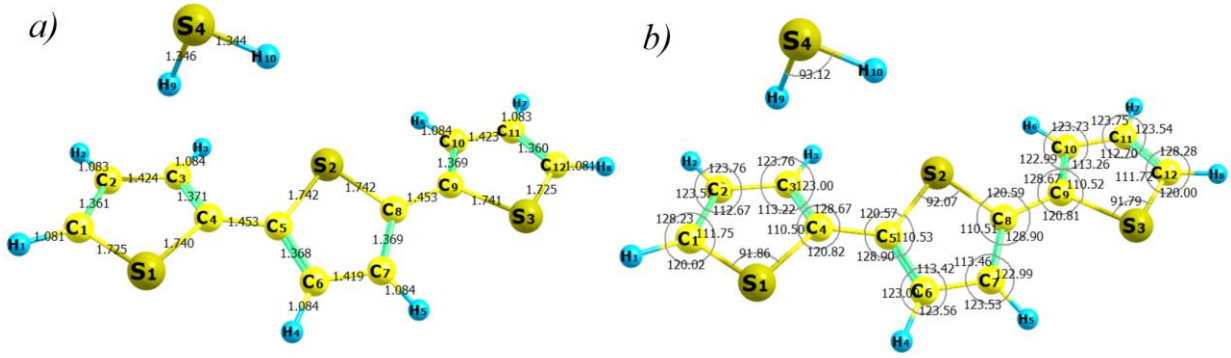

Fig. A3. T3···H_2S: *a)* the bond lengths (Å); *b)* the angles (in degrees)

Table A3. Cartesian coordinates of T3···H_2S

Atom	X	Y	Z
C4	2.665530000	-0.774600000	-6.624720000
S1	2.642560000	-0.640090000	-8.359800000
C1	1.756310000	-2.110940000	-8.518110000
C2	1.504520000	-2.680620000	-7.308130000
C3	2.022980000	-1.916920000	-6.223170000
H1	1.473620000	-2.469260000	-9.497980000
H2	0.960010000	-3.608980000	-7.184840000
H3	1.903690000	-2.192150000	-5.181450000
C8	4.488220000	1.461440000	-3.960380000
S2	3.926960000	-0.165940000	-4.224890000
C5	3.320290000	0.233310000	-5.808520000
C6	3.576400000	1.544540000	-6.103880000
C7	4.236440000	2.239720000	-5.057630000
H5	4.492000000	3.291910000	-5.106080000
H4	3.275820000	2.009410000	-7.035750000
C9	5.129320000	1.828290000	-2.709430000
S4	6.200660000	3.198350000	-2.624380000
C12	6.480490000	2.943720000	-0.941350000
C11	5.801450000	1.860480000	-0.476270000
C10	5.027600000	1.222030000	-1.486050000
H7	5.840200000	1.526650000	0.553630000
H8	7.132940000	3.610250000	-0.395010000
H6	4.401490000	0.355430000	-1.306920000

S3	5.681500000	-3.472710000	-6.420940000
H9	4.407390000	-3.109000000	-6.656120000
H10	5.949090000	-2.354820000	-5.723620000

A4. T3···$(H_2S)_2$ complex

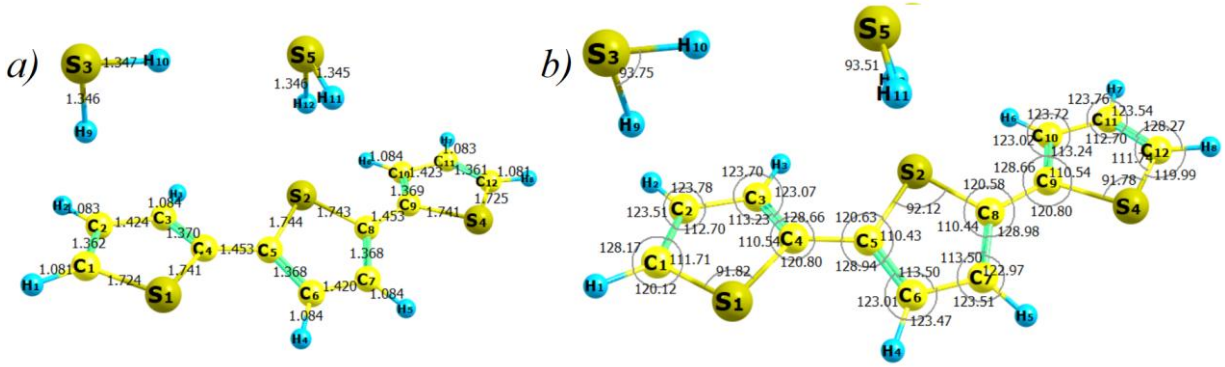

Fig. A4. T3···$(H_2S)_2$: *a)* the bond lengths (Å); *b)* the angles (in degrees)

Table A4. Cartesian coordinates of T3···$(H_2S)_2$

Atom	X	Y	Z
C4	2.386980000	-0.830830000	-6.631900000
S1	2.355570000	-0.764010000	-8.371710000
C1	1.289270000	-2.116080000	-8.459300000
C2	0.985470000	-2.599090000	-7.222490000
C3	1.612550000	-1.864560000	-6.176660000
H1	0.944580000	-2.473850000	-9.419430000
H2	0.327930000	-3.443660000	-7.055070000
H3	1.477620000	-2.083260000	-5.123610000
C8	4.466200000	1.298060000	-4.064960000
S2	3.688600000	-0.251920000	-4.244220000
C5	3.167170000	0.124560000	-5.864870000
C6	3.605130000	1.367750000	-6.230700000
C7	4.338440000	2.032080000	-5.212200000
H5	4.736460000	3.034580000	-5.318430000
H4	3.384360000	1.811560000	-7.194640000
C9	5.133990000	1.650760000	-2.824200000
S4	6.381760000	2.864870000	-2.797240000
C12	6.600860000	2.678580000	-1.096490000
C11	5.771510000	1.730490000	-0.582370000
C10	4.931590000	1.141920000	-1.569270000
H7	5.749370000	1.459580000	0.466290000
H8	7.332010000	3.281610000	-0.576650000
H6	4.189160000	0.382380000	-1.352440000
S5	6.674700000	-2.772590000	-5.706930000
H11	7.018940000	-1.846370000	-6.618690000
H12	5.747250000	-1.983040000	-5.133590000

S3	4.132790000	-5.029890000	-8.037230000
H9	3.137650000	-4.125570000	-7.983710000
H10	4.963770000	-4.291830000	-7.275370000