O•••S *versus* N•••S Intramolecular Nonbonded Interactions in Neutral and Radical Cation Salts of TTF-Oxazoline Derivatives: Synthesis, Theoretical Investigations, Crystalline Structures, and Physical Properties

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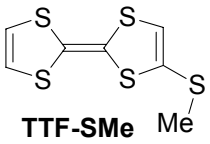
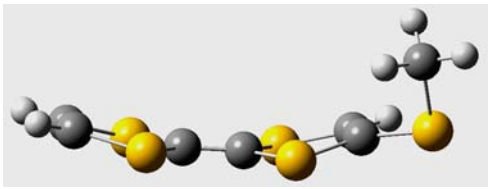
SUPPORTING INFORMATION

Geometry optimization for TTF-SMe



TTF-SMe



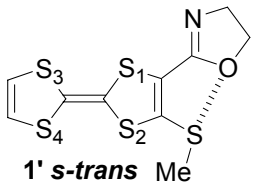
SCF Done: E(RB+HF-LYP) = -2261.25189838; E_{ZPC} = -2261.141022

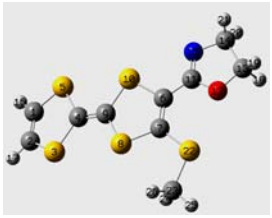
Cartesian coordinates for the optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.107312	-0.076931	0.556986
2	6	0	-3.780238	-1.350146	0.298390
3	16	0	-2.164601	-1.676786	-0.328641
4	6	0	-1.592748	0.003260	-0.129559
5	16	0	-2.895120	1.166116	0.248488
6	6	0	1.966873	1.592021	0.093163
7	6	0	2.324319	0.317985	-0.155854
8	16	0	1.009958	-0.784581	-0.659662
9	6	0	-0.296046	0.361315	-0.265267
10	16	0	0.275470	2.044877	-0.083790
11	1	0	-5.075263	0.252128	0.918116
12	1	0	-4.446446	-2.196777	0.420754
13	16	0	3.996222	-0.255284	-0.183799
14	6	0	4.014591	-1.413701	1.243779
15	1	0	5.023886	-1.834283	1.278775
16	1	0	3.809000	-0.882186	2.176130
17	1	0	3.294163	-2.223088	1.104274
18	1	0	2.667148	2.371903	0.370591

Low frequencies --- 32.4460 48.2703 72.9174; 80.4037 94.0438

Geometry optimization for TTF-(SMe)-OX 1' *s-trans*





SCF Done: E(RB+HF-LYP) = -2507.34735160; E_{ZPC} = -2507.1740376

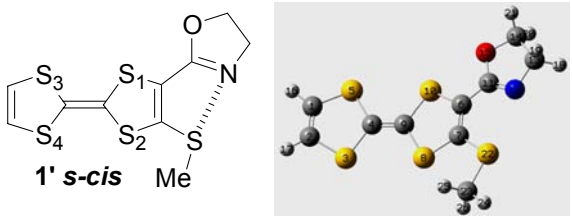
Cartesian coordinates for the optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.787843	-1.257987	0.554661
2	6	0	-4.990778	0.066297	0.538510
3	16	0	-3.672365	1.093541	-0.025986
4	6	0	-2.489396	-0.240366	-0.131191
5	16	0	-3.221736	-1.862282	0.014920
6	6	0	1.421598	-0.313797	-0.131286
7	6	0	1.218947	1.033709	-0.132045
8	16	0	-0.441920	1.568977	-0.466291
9	6	0	-1.163614	-0.048698	-0.317914
10	16	0	0.016574	-1.365401	-0.464331
11	6	0	2.673754	-1.032390	0.034538
12	8	0	3.817654	-0.287043	0.123742
13	6	0	4.889574	-1.236058	0.373803
14	6	0	4.210500	-2.612981	0.166159
15	7	0	2.776741	-2.309953	0.068245
16	1	0	-5.528373	-1.992627	0.850818
17	1	0	-5.917164	0.555040	0.818674
18	1	0	5.242631	-1.077042	1.398034
19	1	0	5.696862	-1.017984	-0.329010
20	1	0	4.396262	-3.301555	0.997330
21	1	0	4.540696	-3.110742	-0.754927
22	16	0	2.477297	2.265266	0.066694
23	6	0	1.515488	3.788169	0.399873
24	1	0	0.868449	3.674126	1.272616
25	1	0	2.273455	4.547369	0.614602
26	1	0	0.933784	4.112416	-0.466557

Low frequencies --- 28.0782 28.5449 51.6501; 58.7714 66.0823

AIM ellipticity of O•••S interaction $\varepsilon = \lambda_1/\lambda_2 - 1 = 0.1316$

Geometry optimization for TTF-(SMe)-OX 1' *s-cis*



SCF Done: E(RB+HF-LYP) = -2507.34776122; E_{ZPC} = -2507.17442422

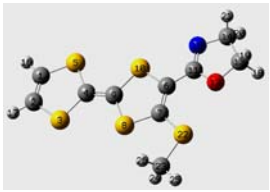
Cartesian coordinates for the optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.761360	-1.304053	0.518593
2	6	0	4.983656	0.017186	0.522526
3	16	0	3.675309	1.073710	-0.010078
4	6	0	2.471726	-0.240494	-0.126409
5	16	0	3.180640	-1.875500	-0.014793
6	6	0	-1.444538	-0.253017	-0.121001
7	6	0	-1.220405	1.092079	-0.103480
8	16	0	0.449556	1.607057	-0.415626
9	6	0	1.147343	-0.024702	-0.296999
10	16	0	-0.051993	-1.321942	-0.452024
11	6	0	-2.740144	-0.886482	0.040337
12	7	0	-3.870605	-0.292155	0.144943
13	6	0	-4.879403	-1.342448	0.345469
14	6	0	-4.114123	-2.670060	0.116226
15	8	0	-2.722960	-2.258599	0.079195
16	1	0	5.493784	-2.054575	0.794328
17	1	0	5.920140	0.487128	0.801296
18	1	0	-5.709298	-1.209546	-0.356643
19	1	0	-5.289599	-1.264457	1.360859
20	1	0	-4.348394	-3.143321	-0.843234
21	1	0	-4.224956	-3.400771	0.920593
22	16	0	-2.480139	2.307667	0.125680
23	6	0	-1.511717	3.858292	0.273564
24	1	0	-2.261326	4.629370	0.474376
25	1	0	-0.808654	3.822267	1.109330
26	1	0	-0.990267	4.114087	-0.652573

Low frequencies --- 27.6624 28.7883 51.1223; 63.8474 74.3044

AIM ellipticity of N•••S interaction $\varepsilon = \lambda_1/\lambda_2 - 1 = 0.1732$

Geometry optimization for TTF-(SMe)-OX 1'$^{+\bullet}$ *s-trans*



SCF Done: E(UB+HF-LYP) = -2507.12330602;

E_{ZPC} = -2506.94916902

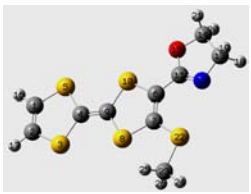
Cartesian coordinates for the optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.886737	-1.269889	-0.000559
2	6	0	-5.091229	0.060766	0.000406
3	16	0	-3.678777	1.085062	0.001170
4	6	0	-2.519110	-0.227579	-0.000007
5	16	0	-3.233874	-1.827299	-0.001128
6	6	0	1.433030	-0.300498	-0.000072
7	6	0	1.244633	1.063262	-0.000029
8	16	0	-0.438451	1.581547	-0.000120
9	6	0	-1.140345	-0.021115	0.000021
10	16	0	0.010617	-1.322613	0.000203
11	6	0	2.689706	-1.045544	0.000053
12	8	0	3.841123	-0.334987	-0.000868
13	6	0	4.917176	-1.333601	0.000024
14	6	0	4.158398	-2.688997	0.000711
15	7	0	2.732175	-2.322365	0.001077
16	1	0	-5.668540	-2.021570	-0.001058
17	1	0	-6.061698	0.544711	0.000798
18	1	0	5.519058	-1.158794	0.893904
19	1	0	5.519505	-1.159873	-0.893754
20	1	0	4.377605	-3.297004	0.884637
21	1	0	4.376966	-3.297574	-0.882993
22	16	0	2.533519	2.254414	-0.000284
23	6	0	1.620851	3.839768	-0.000314
24	1	0	1.016042	3.963446	0.902146
25	1	0	2.404207	4.602534	-0.000471
26	1	0	1.015847	3.963335	-0.902663

Low frequencies --- 36.9185 40.0380 46.1336; 60.4664 67.0617

AIM ellipticity of O•••S interaction $\varepsilon = \lambda_1/\lambda_2 - 1 = 0.1621$

Geometry optimization for TTF-(SMe)-OX 1'$^{+\bullet}$ *s-cis*



SCF Done: E(UB+HF-LYP) = -2507.12431372;

E_{ZPC} = -2506.95020872

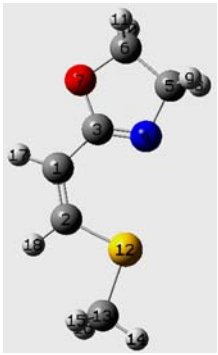
Cartesian coordinates for the optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.859956	-1.299063	-0.000169
2	6	0	5.078620	0.028694	0.000160
3	16	0	3.677094	1.069560	0.000406
4	6	0	2.502257	-0.230720	0.000016
5	16	0	3.200007	-1.838782	-0.000391
6	6	0	-1.451004	-0.256863	-0.000023
7	6	0	-1.244540	1.108778	-0.000046
8	16	0	0.442013	1.604173	-0.000059
9	6	0	1.127630	-0.007049	0.000022
10	16	0	-0.041834	-1.292515	0.000081
11	6	0	-2.748132	-0.918773	0.000019
12	7	0	-3.876401	-0.322294	0.000032
13	6	0	-4.902638	-1.379712	-0.000032
14	6	0	-4.107079	-2.713875	0.000302
15	8	0	-2.707961	-2.278764	0.000017
16	1	0	5.633191	-2.059501	-0.000330
17	1	0	6.054217	0.502197	0.000299
18	1	0	-5.538742	-1.264792	-0.883865
19	1	0	-5.539144	-1.264582	0.883479
20	1	0	-4.259092	-3.322536	-0.893252
21	1	0	-4.258900	-3.321930	0.894308
22	16	0	-2.528984	2.293219	-0.000098
23	6	0	-1.599391	3.872283	-0.000167
24	1	0	-2.374548	4.643298	-0.000190
25	1	0	-0.992633	3.990716	0.901957
26	1	0	-0.992651	3.990635	-0.902313

Low frequencies --- 37.7368 41.6301 46.4970; 60.9422 66.6638

AIM ellipticity of O•••S interaction $\varepsilon = \lambda_1/\lambda_2 - 1 = 0.1643$

Geometry optimization for MeS-Oxazoline 1"



SCF Done: E(RB+HF-LYP) = -762.204029466;

E_{ZPC} = -762.059758

Cartesian coordinates for the optimized geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.061717	1.374572	-0.000745
2	6	0	1.365820	1.017432	0.001134
3	6	0	-1.052654	0.444959	-0.001591
4	7	0	-0.985259	-0.835283	0.006110
5	6	0	-2.364909	-1.337770	-0.014029
6	6	0	-3.253183	-0.064678	0.018775
7	8	0	-2.299059	1.025687	-0.014712
8	1	0	-2.537582	-1.992173	0.848436
9	1	0	-2.525905	-1.938769	-0.917587
10	1	0	-3.843713	0.033316	0.935129
11	1	0	-3.912446	0.038065	-0.847885
12	16	0	2.017873	-0.607294	0.003808
13	6	0	3.806633	-0.198746	-0.002422
14	1	0	4.339609	-1.153541	-0.000370
15	1	0	4.087647	0.356998	-0.901790
16	1	0	4.092402	0.363429	0.891453
17	1	0	-0.192411	2.429877	-0.001932
18	1	0	2.115164	1.806371	0.001819

Low frequencies --- 26.1863 44.8658 97.4493; 99.9181 144.2476

AIM analysis of the N•••S interaction:

electron density $10^2\rho_B$ = 1.23

Laplacian $10^2\nabla^2\rho_B$ = 4.11

ellipticity $\varepsilon = \lambda_1/\lambda_2 - 1$ = 0.1303

Summary of Optimized Potential Surface Scan

	1	2	3	4	5
EIGENVALUES --	-762.20403	-762.20351	-762.20188	-762.19938	-762.19657
D1	0.00000	15.00000	30.00000	45.00000	60.00000

	6	7	8	9	10
EIGENVALUES --	-762.19414	-762.19275	-762.19283	-762.19574	-762.19870
D1	75.00000	90.00000	105.00000	120.00000	135.00000

	11	12	13
EIGENVALUES --	-762.20128	-762.20291	-762.20346
D1	150.00000	165.00000	180.00000