Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Computational Investigation of the Photochemical Deoxygenation of Thiophene-*S*-oxide and Selenophene-*Se*-oxide

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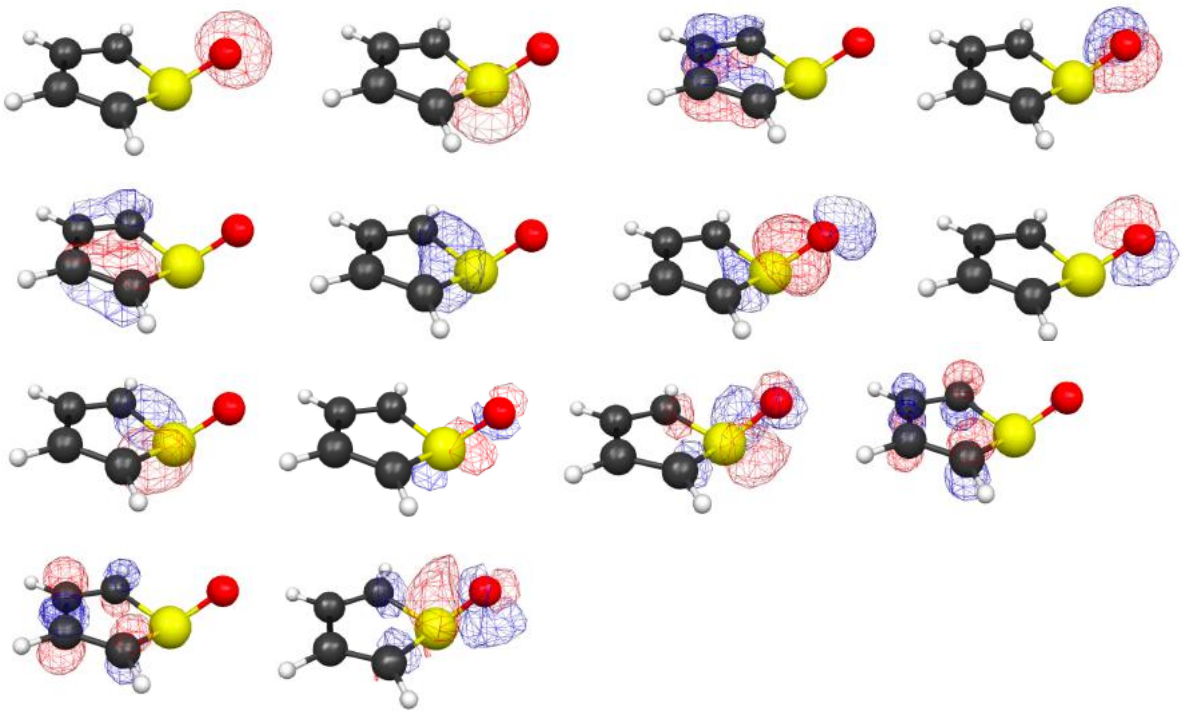
Table of Contents

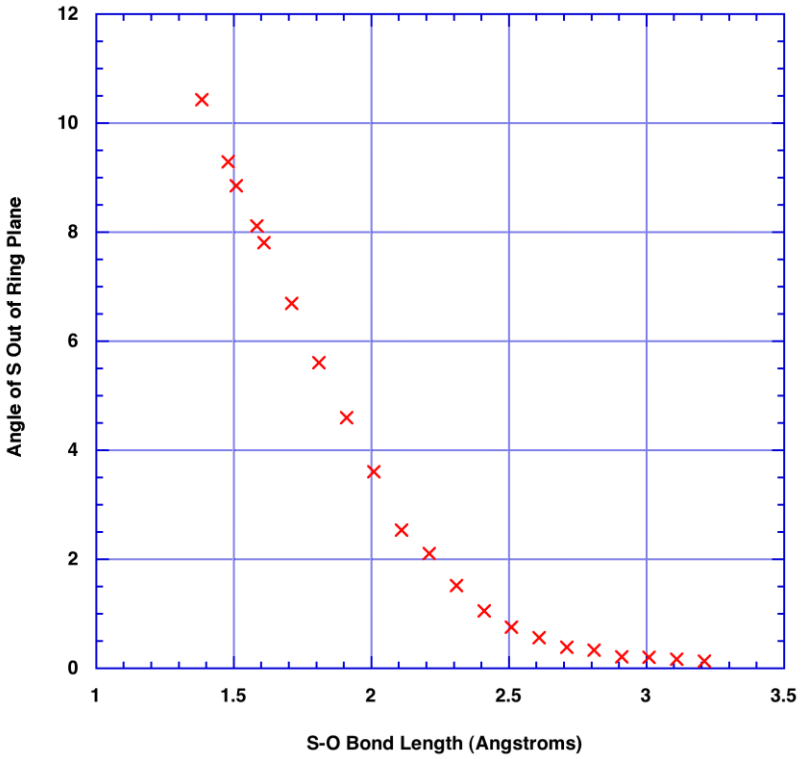
Illustrated Active Space orbitals for Thiophene-*S*-oxide (TO)

These represent the HF level orbitals used as starting points for the CASSCF calculations for thiophene-*S*-oxide. An analogous set was used for seleneophene-*Se*-oxide.



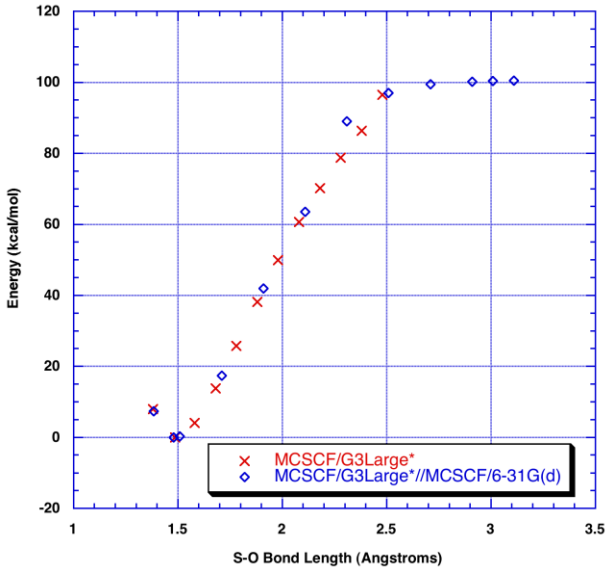
Thiophene-*S*-oxide: Angle of S out of plane of thiophene ring versus S-O distance. CASSCF/6-31G(d)

Note that the angle nears the asymptotic limit of zero (planar thiophene) as the S-O distance passes 3 Å.

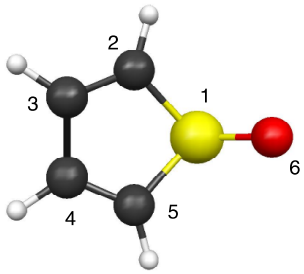


Control for basis sets in computational optimizations

The figure below illustrates the relative energies for TO in its ground electronic state with S–O at fixed distance. The red data were obtained with full CASSCG/G3Large* and the blue data were obtained using geometries from CASSCF/6-31G(d), i.e., CASSCF/G3Large* vs. CASSCF/G3Large*//CASSCF/6-31G(d). Due to the only minor difference, only the latter calculations were done in the rest of the study.



Comparison of computed (CASSCF/6-31G(d)) thiophene-*S*-oxide geometries with reported values for 2,5-diphenylthiophene-*S*-oxide and thiophene



Atoms	Bond Length (Å)	Atoms	Angle (°)
S_0 ^{1}A' (Ground State)			
S1-O6	1.510 (1.484)[a]	O6-S1-C2	113.9 (112.6)[a]
S1-C2	1.787 (1.781)[a]	S1-C2-C3	112.1 (108.9)[a]
C2-C3	1.345 (1.345)[a]	C2-C3-C4	112.8 (114.5)[a]
C3-C4	1.471 (1.433)[a]	C2-S1-C5	89.3 (91.3)[a]
T_1 ^{3}A"			
S1-O6	1.513	O6-S1-C2	110.9
S1-C2	1.782	S1-C2-C3	113.7
C2-C3	1.452	C2-C3-C4	112.2
C3-C4	1.363	C2-S1-C5	87.3
T_2 ^{3}A' (constrained S-O)			
S1-O6	1.500[c]	O6-S1-C2	120.6
S1-C2	1.736	S1-C2-C3	108.5
C2-C3	1.382	C2-C3-C4	113.5
C3-C4	1.426	C2-S1-C5	93.5
T_2 ^{3}A' (constrained S-O) Thiophene + O(^{3}P)			
S1-O6	4.000	O6-S1-C2	102.6
S1-C2	1.763 (1.714)[b]	S1-C2-C3	111.7 (111.5)[b]
C2-C3	1.362 (1.370)[b]	C2-C3-C4	113.1 (112.4)[b]
C3-C4	1.433 (1.432)[b]	C2-S1-C5	90.4 (92.2)[b]
S_1 ^{1}A' (Excited State) (constrained S-O)			
S1-O6	1.500[c]	O6-S1-C2	115.5
S1-C2	1.761	S1-C2-C3	108.2
C2-C3	1.383	C2-C3-C4	114.0
C3-C4	1.420	C2-S1-C5	92.4
S_2 ^{1}A" (constrained S-O)			
S1-O6	1.510[c]	O6-S1-C2	106.4
S1-C2	1.758	S1-C2-C3	111.3
C2-C3	1.395	C2-C3-C4	113.3
C3-C4	1.396	C2-S1-C5	90.6

[a] Values in parentheses are from the crystal structure of 2,5-diphenylthiophene-*S*-oxide.[1] [b] Values in parentheses are experimental parameters for thiophene.[2] [c]Constrained to this value.

Coordinates

Thiophene-*S*-oxide-Coordinates: S_0 A′ State

1.38Å S-O Bond Length

S	16.0	1.6100335373	-.5021242834	.0000000000
H	1.0	-1.7424797485	.1423629575	-1.3163189517
C	6.0	-.8450953250	.0384292144	-.7355988566
H	1.0	.6498815566	-.1694727270	-2.2937245745
C	6.0	.3859728527	-.1147481045	-1.2555271751
O	8.0	2.7246512577	.3172155488	.0000000000

TOTAL ENERGY = -626.2075682419

1.48Å S-O Bond Length

S	16.0	1.6727391380	-0.4086038296	0.0000000000
H	1.0	-1.7311402701	-0.3046121733	-1.3174730480
C	6.0	-0.8292828761	-0.2751506261	-0.7356040397
H	1.0	0.6869788356	-0.2455974950	-2.2915215191
C	6.0	0.4102634491	-0.2389025392	-1.2560002571
O	8.0	2.6774813331	0.6780852342	0.0000000000

TOTAL ENERGY = -626.2251080482

1.51Å S-O Bond Length:Optimized Ground State

S	16.0	1.5867450935	-.5305123333	.0000000000
H	1.0	-1.7385686200	.1924410918	-1.3177754645
C	6.0	-.8472477369	.0538425381	-.7355520953
H	1.0	.6501665394	-.1953546969	-2.2910690103
C	6.0	.3773759978	-.1400381860	-1.2561617749
O	8.0	2.7868025461	.3857308394	.0000000000

TOTAL ENERGY = -626.2259228775

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1.58Å S-O Bond Length

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S          16.0    1.5731680184  -0.5471732880   0.0000000000
H           1.0   -1.7361794202   0.2190985962  -1.3187065043
C           6.0   -0.8488027387   0.0624270806  -0.7353405342
H           1.0    0.6497044334  -0.2085852363  -2.2893644108
C           6.0    0.3722532812  -0.1530533349  -1.2561807426
O           8.0    2.8237185457   0.4239902420   0.0000000000
TOTAL ENERGY =    -626.2219823681
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1.61Å S-O Bond Length

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S          16.0    1.5684507073   -.5536988404    .0000000000
H           1.0   -1.7349877848    .2289320905  -1.3190279851
C           6.0    -.8490479016    .0660836885   -.7352720289
H           1.0     .6490624898   -.2143375696  -2.2888475037
C           6.0     .3704877073   -.1581051654  -1.2561367795
O           8.0    2.8360957267    .4386133046    .0000000000
TOTAL ENERGY =    -626.2190401201
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1.71Å S-O Bond Length

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S          16.0    1.5505550562  -0.5785319443   0.0000000000
H           1.0   -1.7292560127   0.2686204345  -1.3199364793
C           6.0   -0.8496329616   0.0799208951  -0.7347407529
H           1.0    0.6462285106  -0.2360701004  -2.2869379201
C           6.0    0.3637469446  -0.1770245423  -1.2559172530
O           8.0    2.8824942260   0.4936148763   0.0000000000
TOTAL ENERGY =    -626.2036363175
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1.81Å S-O Bond Length

```
S          16.0    1.5329814494  -0.6056694524   0.0000000000
H           1.0   -1.7213729384   0.3091587132  -1.3207991545
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C	6.0	-0.8487172817	0.0952428439	-0.7341306392
H	1.0	0.6423576734	-0.2591002735	-2.2851846298
C	6.0	0.3575719868	-0.1958936578	-1.2553896558
O	8.0	2.9250077501	0.5509758802	0.0000000000

TOTAL ENERGY = -626.1849411677

1.91Å S-O Bond Length

S	16.0	1.5156053589	-0.6361449207	0.0000000000
H	1.0	-1.7098934981	0.3531332042	-1.3216605194
C	6.0	-0.8453974482	0.1125672049	-0.7334819673
H	1.0	0.6383061170	-0.2828499702	-2.2836243153
C	6.0	0.3524746886	-0.2147481509	-1.2546816649
O	8.0	2.9614716452	0.6116402334	0.0000000000

TOTAL ENERGY = -626.1658436629

2.01Å S-O Bond Length

S	16.0	1.4987569804	-0.6726131854	0.0000000000
H	1.0	-1.6923136717	0.4042484405	-1.3223115621
C	6.0	-0.8376853549	0.1339753666	-0.7328322794
H	1.0	0.6349109046	-0.3083783865	-2.2824093303
C	6.0	0.3491614529	-0.2342462783	-1.2540422894
O	8.0	2.9867617992	0.6784459243	0.0000000000

TOTAL ENERGY = -626.1478826791

2.11Å S-O Bond Length

S	16.0	1.4828387955	-.7222748441	.0000000000
H	1.0	-1.6588109070	.4777038029	-1.3232799099
C	6.0	-.8197909963	.1651772405	-.7323567939
H	1.0	.6351047070	-.3347705527	-2.2816572131
C	6.0	.3499152432	-.2561522165	-1.2536004821
O	8.0	2.9863542806	.7578200110	.0000000000

TOTAL ENERGY = -626.1319830294

2.21Å S-O Bond Length

S	16.0	1.4830224414	-0.7537988454	0.0000000000
H	1.0	-1.6678225449	0.5021539123	-1.3150730466
C	6.0	-0.8309535332	0.1775430059	-0.7272713869
H	1.0	0.5994550867	-0.3527556957	-2.2943512788
C	6.0	0.3277915961	-0.2637305109	-1.2632454349
O	8.0	3.0415604894	0.8128348353	0.0000000000

TOTAL ENERGY = -626.1155598513

2.31Å S-O Bond Length

S	16.0	1.4672563703	-0.7909090412	0.0000000000
H	1.0	-1.6480815270	0.5464252346	-1.3144931477
C	6.0	-0.8223743103	0.1972414147	-0.7249435846
H	1.0	0.5914128542	-0.3772854262	-2.2927777639

C	6.0	0.3246182652	-0.2795354303	-1.2611679771
O	8.0	3.0634894571	0.8786841519	0.0000000000

TOTAL ENERGY = -626.1061524216

2.41Å S-O Bond Length

S	16.0	1.4506107819	-0.8195331326	0.0000000000
H	1.0	-1.6367350078	0.5768648581	-1.3136196813
C	6.0	-0.8196927314	0.2101375937	-0.7225152450
H	1.0	0.5815763357	-0.3981553250	-2.2905043284
C	6.0	0.3187470078	-0.2934265946	-1.2584459067
O	8.0	3.1013579144	0.9361875632	0.0000000000

TOTAL ENERGY = -626.1000496078

2.51Å S-O Bond Length

S	16.0	1.4340595230	-0.8410633973	0.0000000000
H	1.0	-1.6341165106	0.5936572799	-1.3131488297
C	6.0	-0.8226659751	0.2165045656	-0.7207615650
H	1.0	0.5685525627	-0.4166887997	-2.2887868773
C	6.0	0.3100174335	-0.3051434997	-1.2562291677
O	8.0	3.1533131323	0.9874710578	0.0000000000

TOTAL ENERGY = -626.096562771

2.61Å S-O Bond Length

S	16.0	1.4177708197	-0.8560969459	0.0000000000
H	1.0	-1.6389028176	0.5999923431	-1.3132069757
C	6.0	-0.8311299942	0.2166947882	-0.7196470386
H	1.0	0.5545585060	-0.4292923491	-2.2875781667
C	6.0	0.2985398800	-0.3153362863	-1.2545496949
O	8.0	3.2181610086	1.0333200359	0.0000000000

TOTAL ENERGY = -626.0946286349

2.71Å S-O Bond Length

S	16.0	1.4017907632	-0.8711348237	0.0000000000
H	1.0	-1.6443037085	0.6058066217	-1.3129844855
C	6.0	-0.8396635352	0.2167062046	-0.7188543089
H	1.0	0.5404738359	-0.4423340230	-2.2867109624
C	6.0	0.2865620505	-0.3251584822	-1.2534402018
O	8.0	3.2833357702	1.0790107392	0.0000000000

TOTAL ENERGY = -626.0935693455

2.81Å S-O Bond Length

S	16.0	1.3857739230	-0.8859613246	0.0000000000
H	1.0	-1.6506387121	0.6099604954	-1.3126662217
C	6.0	-0.8486669415	0.2157760775	-0.7182567475
H	1.0	0.5273472075	-0.4531199551	-2.2860838869
C	6.0	0.2746307090	-0.3339541490	-1.2526685791
O	8.0	3.3492163110	1.1240763811	0.0000000000

TOTAL ENERGY = -626.0929900427

2.91Å S-O Bond Length

S	16.0	1.3699577590	-0.9001647499	0.0000000000
H	1.0	-1.6571420417	0.6137755599	-1.3127332517
C	6.0	-0.8578564304	0.2146630728	-0.7179367016
H	1.0	0.5130112845	-0.4649539529	-2.2856765375
C	6.0	0.2621193466	-0.3431001799	-1.2520824021
O	8.0	3.4160188484	1.1688714520	0.0000000000

TOTAL ENERGY = -626.092665288

3.01Å S-O Bond Length

S	16.0	1.3542193622	-0.9145222076	0.0000000000
H	1.0	-1.6643198360	0.6167528767	-1.3125420153
C	6.0	-0.8673378992	0.2130479886	-0.7176742035
H	1.0	0.4997302634	-0.4748794388	-2.2853389193
C	6.0	0.2496925057	-0.3514073436	-1.2517109852
O	8.0	3.4829292824	1.2133341385	0.0000000000

TOTAL ENERGY = -626.0924696317

3.11Å S-O Bond Length

S	16.0	1.3388683371	-0.9287118737	0.0000000000
H	1.0	-1.6717288195	0.6194778649	-1.3124047053
C	6.0	-0.8770923357	0.2112569210	-0.7174791149
H	1.0	0.4853602113	-0.4845148743	-2.2856488037
C	6.0	0.2367478542	-0.3596699267	-1.2516300692
O	8.0	3.5504183194	1.2576538412	0.0000000000

TOTAL ENERGY = -626.0932559721

3.21Å S-O Bond Length

S	16.0	1.3231592038	-0.9424149549	0.0000000000
H	1.0	-1.6792074618	0.6215747343	-1.3124413467
C	6.0	-0.8868195188	0.2091593846	-0.7173503961
H	1.0	0.4716428065	-0.4944894645	-2.2854528574
C	6.0	0.2240281525	-0.3680086753	-1.2513951856
O	8.0	3.6181712831	1.3016969425	0.0000000000

TOTAL ENERGY = -626.0932148133

Thiophene-*S*-oxide-Coordinates: T_1 A″ State

1.38Å S-O Bond Length

S	16.0	1.7478470331	-0.4633150175	0.0000000000
H	1.0	-1.7387392753	0.0666345902	-1.2971793947
C	6.0	-0.8740735465	-0.0915577456	-0.6817814002
H	1.0	0.6916251199	-0.3483649662	-2.2726089754
C	6.0	0.4431659222	-0.3619487896	-1.2293745879
O	8.0	2.5455589597	0.6627647678	0.0000000000

TOTAL ENERGY = -626.1206762349

1.48Å S-O Bond Length

S	16.0	1.7312903933	-0.4903135819	0.0000000000
H	1.0	-1.7260131788	0.1051219487	-1.2982231751
C	6.0	-0.8673283820	-0.0773953997	-0.6816353886
H	1.0	0.6999792954	-0.3651426844	-2.2695638143
C	6.0	0.4411625120	-0.3866880402	-1.2296686730
O	8.0	2.5688824726	0.7298665315	0.0000000000

TOTAL ENERGY = -626.1397651783

1.52Å S-O Bond Length

S	16.0	1.7248035427	-0.5013891036	0.0000000000
H	1.0	-1.7213721674	0.1183294608	-1.2985171112
C	6.0	-0.8648218954	-0.0722307846	-0.6815452675
H	1.0	0.7026084500	-0.3720805067	-2.2685592940
C	6.0	0.4402738157	-0.3951914672	-1.2298320969
O	8.0	2.5785053442	0.7562250005	0.0000000000

TOTAL ENERGY = -626.1406751

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MODE 23	FREQUENCY=1350.52665	(CM**-1)
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MODE 30 FREQUENCY=3450.78202 (CM**-1)

1.60Å S-O Bond Length

S	16.0	1.7116322853	-0.5238832505	0.0000000000
H	1.0	-1.7120387263	0.1439757296	-1.2990518142
C	6.0	-0.8598399250	-0.0622575729	-0.6813985037
H	1.0	0.7075849679	-0.3868376533	-2.2663538831
C	6.0	0.4388012428	-0.4108333420	-1.2297121097
O	8.0	2.5977641554	0.8083218048	0.0000000000

TOTAL ENERGY = -626.1354612465

1.70Å S-O Bond Length

S	16.0	1.6952116952	-0.5536530144	0.0000000000
H	1.0	-1.6998858208	0.1718712742	-1.3002922880
C	6.0	-0.8528779384	-0.0499520854	-0.6812419240
H	1.0	0.7124930039	-0.4060719598	-2.2638490540
C	6.0	0.4378551501	-0.4274339147	-1.2291327522
O	8.0	2.6194104114	0.8731815006	0.0000000000

TOTAL ENERGY = -626.1213302085

1.80Å S-O Bond Length

S	16.0	1.6781925801	-0.5910684389	0.0000000000
H	1.0	-1.6781705303	0.2087492612	-1.3017985711
C	6.0	-0.8372564348	-0.0318758682	-0.6817605260
H	1.0	0.7209728736	-0.4304106200	-2.2612594540
C	6.0	0.4417634442	-0.4430394430	-1.2280212148
O	8.0	2.6203205959	0.9426834324	0.0000000000

TOTAL ENERGY = -626.1041476714

1.90Å S-O Bond Length

S	16.0	1.6491480895	-0.7015412000	0.0000000000
H	1.0	-1.5804922918	0.2511361620	-1.3121753444
C	6.0	-0.7247660047	0.0049805565	-0.7137092101
H	1.0	0.7477101980	-0.4814698124	-2.2789079445
C	6.0	0.4751609934	-0.3863937867	-1.2484466601
O	8.0	2.4437971116	1.0243014729	0.0000000000

TOTAL ENERGY = -626.1102912111

2.00Å S-O Bond Length

S	16.0	1.6392211541	-0.7220346276	0.0000000000
H	1.0	-1.5890830317	0.2514155875	-1.3132118796
C	6.0	-0.7354484983	-0.0045058271	-0.7156085950
H	1.0	0.7334940447	-0.4760945933	-2.2803797910
C	6.0	0.4620239852	-0.3886518089	-1.2486462522
O	8.0	2.5022546725	1.0821752123	0.0000000000

TOTAL ENERGY = -626.1199712671

2.10Å S-O Bond Length

S	16.0	1.6270532638	-0.7302100086	0.0000000000
H	1.0	-1.6101246176	0.2329744435	-1.3128315515
C	6.0	-0.7555644235	-0.0224495211	-0.7160884520
H	1.0	0.7131759217	-0.4755078784	-2.2825754082
C	6.0	0.4432594087	-0.3941441392	-1.2496219430
O	8.0	2.5901283384	1.1359321084	0.0000000000

TOTAL ENERGY = -626.1307341192

2.30Å S-O Bond Length

S	16.0	1.6048048479	-0.7734623012	0.0000000000
H	1.0	-1.6210787726	0.2411766726	-1.3125034726
C	6.0	-0.7697270319	-0.0269297564	-0.7164786672
H	1.0	0.6905947673	-0.4929814621	-2.2837252037
C	6.0	0.4238116429	-0.4105044864	-1.2498992238
O	8.0	2.6892581452	1.2548278767	0.0000000000

TOTAL ENERGY = -626.1491282693

2.50Å S-O Bond Length

S	16.0	1.5850607934	-0.8331531908	0.0000000000
H	1.0	-1.6121515820	0.2806988533	-1.3135279355
C	6.0	-0.7700099054	-0.0130477815	-0.7163811958
H	1.0	0.6747618566	-0.5215679183	-2.2843887532
C	6.0	0.4119170652	-0.4291833058	-1.2502065130
O	8.0	2.7478665796	1.3799628711	0.0000000000

TOTAL ENERGY = -626.1627648632

Thiophene-*S*-oxide-Coordinates: T_2 A′ State

1.36Å S-O Bond Length

S	16.0	1.6423688302	-0.3141236056	0.0000000000
H	1.0	-1.6754300357	-0.0309144303	-1.3038026024
C	6.0	-0.7993819353	-0.2177351393	-0.7131725655
H	1.0	0.7555808953	-0.3959576619	-2.2933540795
C	6.0	0.4541295077	-0.4069415320	-1.2674683963
O	8.0	2.6118369217	0.6396749162	0.0000000000

TOTAL ENERGY = -626.0698374934

1.48Å S-O Bond Length

S	16.0	1.6293971968	-0.3432109857	0.0000000000
H	1.0	-1.6853652611	-0.0320847282	-1.3063722688
C	6.0	-0.8102461574	-0.2141565696	-0.7131808085
H	1.0	0.7461594211	-0.4092075744	-2.2895676029
C	6.0	0.4413786191	-0.4131516477	-1.2649728424
O	8.0	2.6756390288	0.7035831817	0.0000000000

TOTAL ENERGY = -626.0970885578

1.60Å S-O Bond Length

S	16.0	1.6144642928	-0.4220765755	0.0000000000
H	1.0	-1.6889937102	0.0559617962	-1.3097877205
C	6.0	-0.8192437276	-0.1379890322	-0.7126469917
H	1.0	0.7240568532	-0.4245752740	-2.2830961310
C	6.0	0.4219130090	-0.3904135499	-1.2582187267
O	8.0	2.7514391992	0.7036623221	0.0000000000

TOTAL ENERGY = -626.0995828952

1.70Å S-O Bond Length

S	16.0	1.6279480683	-0.5217828385	0.0000000000
H	1.0	-1.6751730782	0.0791687527	-1.3102169725
C	6.0	-0.8012878952	-0.0940440240	-0.7127863068
H	1.0	0.7208687059	-0.4503108834	-2.2815419195
C	6.0	0.4306969040	-0.3729822036	-1.2551096727
O	8.0	2.6830243698	0.8111890285	0.0000000000

TOTAL ENERGY = -626.1017079848

1.80Å S-O Bond Length

S	16.0	1.6238009200	-0.5659396882	0.0000000000
H	1.0	-1.6737167765	0.0980991327	-1.3123221822
C	6.0	-0.8013179688	-0.0832165649	-0.7149946955
H	1.0	0.7123155225	-0.4434778396	-2.2799916045
C	6.0	0.4257001064	-0.3710682025	-1.2518149801
O	8.0	2.6997511069	0.8770887928	0.0000000000

TOTAL ENERGY = -626.1078137554

1.90Å S-O Bond Length

S	16.0	1.6141523859	-0.5876851929	0.0000000000
H	1.0	-1.6849739052	0.0970977384	-1.3136066277
C	6.0	-0.8133840324	-0.0892301498	-0.7164068816
H	1.0	0.6962466072	-0.4333852118	-2.2803108882
C	6.0	0.4123936703	-0.3704422629	-1.2504393360
O	8.0	2.7605519079	0.9274940493	0.0000000000

TOTAL ENERGY = -626.1153446231

2.00Å S-O Bond Length

S	16.0	1.5976566825	-0.5670479680	0.0000000000
H	1.0	-1.7267383953	0.0374652495	-1.3132100833
C	6.0	-0.8501247948	-0.1286876846	-0.7169977999
H	1.0	0.6630306138	-0.4155409121	-2.2832601292
C	6.0	0.3813453100	-0.3678275416	-1.2515148090
O	8.0	2.9046899579	0.9467903812	0.0000000000

TOTAL ENERGY = -626.1245475289

2.10Å S-O Bond Length

S	16.0	1.4813182271	-0.0170721919	0.0000000000
H	1.0	-1.8407628066	-0.7334065578	-1.3140654548
C	6.0	-0.9679497950	-0.5447492050	-0.7181902595
H	1.0	0.5255911476	-0.2218213893	-2.2870814622
C	6.0	0.2541687215	-0.2810402444	-1.2525832591
O	8.0	3.5365461259	0.4142493635	0.0000000000

TOTAL ENERGY = -626.1354178426

2.20Å S-O Bond Length

S	16.0	1.4639048672	-0.0206739226	0.0000000000
H	1.0	-1.8550743774	-0.7362676842	-1.3137942756
C	6.0	-0.9823949560	-0.5477663519	-0.7177694002
H	1.0	0.5120589972	-0.2250210890	-2.2860426355
C	6.0	0.2405402983	-0.2840504703	-1.2515964078
O	8.0	3.6169861146	0.4312565387	0.0000000000

TOTAL ENERGY = -626.1459496792

2.30Å S-O Bond Length

S	16.0	1.4470374117	-0.0241878295	0.0000000000
H	1.0	-1.8696404512	-0.7392460172	-1.3138903944
C	6.0	-0.9972133865	-0.5508940749	-0.7174535150
H	1.0	0.4979345134	-0.2282017134	-2.2854552923
C	6.0	0.2262694310	-0.2871344669	-1.2510532153
O	8.0	3.6979656723	0.4483771383	0.0000000000

TOTAL ENERGY = -626.154235727

2.40Å S-O Bond Length

S	16.0	1.4304825153	-.0276430913	.0000000000
H	1.0	-1.8845725721	-.7423688583	-1.3137334670
C	6.0	-1.0122165265	-.5540843451	-.7172251877
H	1.0	.4835283580	-.2313476010	-2.2851084545
C	6.0	.2116028410	-.2902634704	-1.2507980200
O	8.0	3.7792730084	.4655557284	.0000000000

TOTAL ENERGY = -626.1605421607

2.50Å S-O Bond Length

S	16.0	1.4140904775	-0.0310724289	0.0000000000
H	1.0	-1.8995413695	-0.7455236644	-1.3137483220
C	6.0	-1.0273199957	-0.5572991465	-0.7170810757
H	1.0	0.4688659815	-0.2345130522	-2.2848999468
C	6.0	0.1967609831	-0.2934175060	-1.2506804291
O	8.0	3.8607052457	0.4827633611	0.0000000000

TOTAL ENERGY = -626.1652355464

2.60Å S-O Bond Length

S	16.0	1.3980409395	-0.0344256616	0.0000000000
H	1.0	-1.9149039445	-0.7487965005	-1.3136792878

C	6.0	-1.0426886539	-0.5605825074	-0.7169569932
H	1.0	0.4536212875	-0.2377716525	-2.2848407469
C	6.0	0.1815369114	-0.2966379987	-1.2505894374
O	8.0	3.9425472824	0.5000480703	0.0000000000

TOTAL ENERGY = -626.1686761919

2.70Å S-O Bond Length

S	16.0	1.3819877137	-0.0377836654	0.0000000000
H	1.0	-1.9301925684	-0.7520457116	-1.3136474918
C	6.0	-1.0579978380	-0.5638468745	-0.7168813347
H	1.0	0.4383955500	-0.2410253078	-2.2848157416
C	6.0	0.1662724088	-0.2998729186	-1.2505993063
O	8.0	4.0243564086	0.5173318639	0.0000000000

TOTAL ENERGY = -626.1711634019

2.80Å S-O Bond Length

S	16.0	1.3660685424	-0.0411147295	0.0000000000
H	1.0	-1.9455975756	-0.7553240742	-1.3135470002
C	6.0	-1.0734276693	-0.5671376402	-0.7168031828
H	1.0	0.4230993939	-0.2442877979	-2.2847730017
C	6.0	0.1509017378	-0.3031282436	-1.2505891352
O	8.0	4.1062614468	0.5346368229	0.0000000000

TOTAL ENERGY = -626.1729406221

2.90Å S-O Bond Length

S	16.0	1.3502254287	-0.0444294890	0.0000000000
H	1.0	-1.9610778946	-0.7586269855	-1.3135253649
C	6.0	-1.0889352058	-0.5704466974	-0.7167608446
H	1.0	0.4077224391	-0.2475598893	-2.2847622105
C	6.0	0.1354747462	-0.3063930361	-1.2506261485
O	8.0	4.1882352296	0.5519551460	0.0000000000

TOTAL ENERGY = -626.1741968609

3.00Å S-O Bond Length

S	16.0	1.3344710810	-0.0477269369	0.0000000000
H	1.0	-1.9766192378	-0.7619592474	-1.3135234868
C	6.0	-1.1044728003	-0.5737626962	-0.7167473709
H	1.0	0.3921606372	-0.2508515697	-2.2848097977
C	6.0	0.1198983042	-0.3096869386	-1.2506550071
O	8.0	4.2703319115	0.5692991271	0.0000000000

TOTAL ENERGY = -626.1750752019

3.10Å S-O Bond Length

S	16.0	1.3187067512	-0.0510292131	0.0000000000
H	1.0	-1.9921824759	-0.7652896734	-1.3134868872
C	6.0	-1.1200408487	-0.5770820677	-0.7167265014
H	1.0	0.3766588406	-0.2541336041	-2.2848092213

C	6.0	0.1043491506	-0.3129770582	-1.2506866120
O	8.0	4.3524484937	0.5866506969	0.0000000000

TOTAL ENERGY = -626.1756819644

3.20Å S-O Bond Length

S	16.0	1.2874032150	-0.0580835272	0.0000000000
H	1.0	-2.0240751755	-0.7689375241	-1.3135180730
C	6.0	-1.1517197137	-0.5816175836	-0.7167017489
H	1.0	0.3453537847	-0.2601904841	-2.2848398654
C	6.0	0.0730218765	-0.3187419450	-1.2506651063
O	8.0	4.5175241800	0.6174299906	0.0000000000

TOTAL ENERGY = -626.1760950952

Thiophene-*S*-oxide-Coordinates: ^{1}A″ State

1.48Å S-O Bond Length

S	16.0	1.6561888376	-0.3002565885	0.0000000000
H	1.0	-1.7590303280	-0.1013836034	-1.3169268787
C	6.0	-0.9108655883	-0.2263771388	-0.6736077920
H	1.0	0.7232520004	-0.5039927567	-2.2337957855
C	6.0	0.4511168243	-0.4244059937	-1.2008154844
O	8.0	2.7706205906	0.6736232134	0.0000000000

TOTAL ENERGY = -626.0445753954

1.51Å S-O Bond Length

S	16.0	1.6054651894	-0.6124315050	0.0000000000
H	1.0	-1.6445937184	0.3871195458	-1.3037482705
C	6.0	-0.7841015998	0.1775523657	-0.6981030920
H	1.0	0.7349191595	-0.3045946775	-2.2695889510
C	6.0	0.4170577321	-0.2694237338	-1.2496166892
O	8.0	2.5725693145	0.5472277603	0.0000000000

TOTAL ENERGY = -626.0471348673

1.60Å S-O Bond Length

S	16.0	1.5858540739	-0.6474666122	0.0000000000
H	1.0	-1.6030206711	0.4589079431	-1.3063113270
C	6.0	-0.7541326299	0.1989836208	-0.7040974679
H	1.0	0.7067000512	-0.4129234483	-2.2732643706
C	6.0	0.4219843594	-0.2919734896	-1.2503522934
O	8.0	2.5577268901	0.6235421328	0.0000000000

TOTAL ENERGY = -626.0604208931

1.70Å S-O Bond Length

S	16.0	1.5734114251	-0.6886564780	0.0000000000
H	1.0	-1.5781666098	0.5068304209	-1.3060210227
C	6.0	-0.7353074816	0.2157121005	-0.7096682696
H	1.0	0.6798861067	-0.4637733865	-2.2815196909

C	6.0	0.4204779340	-0.3032105292	-1.2570293873
O	8.0	2.5568590095	0.6980052867	0.0000000000

TOTAL ENERGY = -626.0683820406

1.80Å S-O Bond Length

S	16.0	1.5576391061	-0.7148427145	0.0000000000
H	1.0	-1.5714777179	0.5259638216	-1.3092734209
C	6.0	-0.7348444100	0.2174596390	-0.7130159463
H	1.0	0.6719238511	-0.4645812587	-2.2812834431
C	6.0	0.4142118481	-0.3093166516	-1.2552365090
O	8.0	2.5972539028	0.7545793061	0.0000000000

TOTAL ENERGY = -626.0717823754

1.90Å S-O Bond Length

S	16.0	1.5432143074	-0.7414753624	0.0000000000
H	1.0	-1.5679226707	0.5416135019	-1.3120360857
C	6.0	-0.7373033622	0.2171400967	-0.7158857324
H	1.0	0.6656193213	-0.4565795533	-2.2813941068
C	6.0	0.4070756969	-0.3120446658	-1.2536758732
O	8.0	2.6408312128	0.8094073311	0.0000000000

TOTAL ENERGY = -626.0729876633

2.00Å S-O Bond Length

S	16.0	1.5298925140	-0.7699016339	0.0000000000
H	1.0	-1.5644013706	0.5575598998	-1.3138380115
C	6.0	-0.7398104129	0.2174995015	-0.7179454187
H	1.0	0.6596483290	-0.4474724528	-2.2821214130
C	6.0	0.4000611655	-0.3136114624	-1.2529456678
O	8.0	2.6820556400	0.8648827957	0.0000000000

TOTAL ENERGY = -626.073479808

2.20Å S-O Bond Length

S	16.0	1.5055560665	-0.8159704407	0.0000000000
H	1.0	-1.5720742055	0.5757917642	-1.3135646600
C	6.0	-0.7566227239	0.2118831494	-0.7187627629
H	1.0	0.6373579253	-0.4369686087	-2.2853080989
C	6.0	0.3783786943	-0.3181146390	-1.2535715954
O	8.0	2.7922379905	0.9685321864	0.0000000000

TOTAL ENERGY = -626.0754986414

Thiophene-*S*-oxide-Coordinates: ^{1}A′ State

1.40Å S-O Bond Length

S	16.0	1.5931842910	-0.4094607967	0.0000000000
H	1.0	-1.6324440311	0.4492484982	-1.2995772644
C	6.0	-0.8052011858	0.1007608143	-0.7106871465
H	1.0	0.6723757020	-0.3796796970	-2.3007589082
C	6.0	0.3616665509	-0.3795655847	-1.2773705055

O	8.0	2.5441634166	0.6179820014	0.0000000000

TOTAL ENERGY = -626.0632473765

1.50Å S-O Bond Length

S	16.0	1.5786104562	-0.4416816916	0.0000000000
H	1.0	-1.6575861754	0.4043912612	-1.3031005411
C	6.0	-0.8190864113	0.0927797804	-0.7101833719
H	1.0	0.6697198186	-0.3886821947	-2.2949403671
C	6.0	0.3632411027	-0.3529570652	-1.2716186342
O	8.0	2.5952698580	0.6612252224	0.0000000000

TOTAL ENERGY = -626.0801421652

1.60Å S-O Bond Length

S	16.0	1.5651513689	-0.4827903554	0.0000000000
H	1.0	-1.6776602569	0.3576858448	-1.3068109629
C	6.0	-0.8277074826	0.0881932966	-0.7102898594
H	1.0	0.6673815643	-0.3996301902	-2.2870645972
C	6.0	0.3700588020	-0.3216024161	-1.2636386019
O	8.0	2.6277033781	0.7104972852	0.0000000000

TOTAL ENERGY = -626.0831550864

1.70Å S-O Bond Length

S	16.0	1.5589964510	-0.5359214592	0.0000000000
H	1.0	-1.6854191910	0.3426649447	-1.3084472384
C	6.0	-0.8283884168	0.0967115108	-0.7122426584
H	1.0	0.6576176541	-0.4102344519	-2.2854436035
C	6.0	0.3723933839	-0.3010643618	-1.2611643667
O	8.0	2.6397333202	0.7763314965	0.0000000000

TOTAL ENERGY = -626.0824331116

1.80Å S-O Bond Length

S	16.0	1.5485730095	-0.5728603456	0.0000000000
H	1.0	-1.6857538452	0.3509263682	-1.3108922239
C	6.0	-0.8290659763	0.1036949509	-0.7148332731
H	1.0	0.6495332169	-0.4091359402	-2.2831877433
C	6.0	0.3683637649	-0.2994965410	-1.2575357079
O	8.0	2.6686926096	0.8361577816	0.0000000000

TOTAL ENERGY = -626.081331782

1.90Å S-O Bond Length

S	16.0	1.5369080731	-0.6017803970	0.0000000000
H	1.0	-1.6889226819	0.3588567682	-1.3130229884
C	6.0	-0.8340092752	0.1048948918	-0.7172217487
H	1.0	0.6403968853	-0.4020262211	-2.2822498438
C	6.0	0.3602848251	-0.2995766551	-1.2552846785
O	8.0	2.7130997868	0.8903901873	0.0000000000

TOTAL ENERGY = -626.0797112881

2.00Å S-O Bond Length

S	16.0	1.5260313973	-0.6265555117	0.0000000000
H	1.0	-1.6968107899	0.3612067018	-1.3139997874
C	6.0	-0.8426834380	0.1021689101	-0.7190975160
H	1.0	0.6274713755	-0.3933569886	-2.2838764964
C	6.0	0.3486715740	-0.2986111974	-1.2553559132
O	8.0	2.7679047680	0.9411659339	0.0000000000

TOTAL ENERGY = -626.0787569968

Selenophene-*Se*-oxide-Coordinates: S_0 A′ State

1.65Å S-O Bond Length

C	6.0	-.8434234720	.0604081850	-.7375828784
SE	34.0	1.7071384915	-.6184554663	.0000000000
C	6.0	.3470106986	-.1879992344	-1.3095936583
H	1.0	.5603507407	-.2417836683	-2.3588677665
O	8.0	2.9041269549	.5285611667	.0000000000
H	1.0	-1.7410706905	.2528218675	-1.2968645279

TOTAL ENERGY = -2628.2376050816

MODE	1	FREQUENCY= 0.00003	(CM**-1)
MODE	2	FREQUENCY= 0.00002	(CM**-1)
MODE	3	FREQUENCY= 0.00001	(CM**-1)
MODE	4	FREQUENCY= 0.00000	(CM**-1)
MODE	5	FREQUENCY= 0.00000	(CM**-1)
MODE	6	FREQUENCY= 0.00001	(CM**-1)
MODE	7	FREQUENCY= 166.80894	(CM**-1)
MODE	8	FREQUENCY= 217.42142	(CM**-1)
MODE	9	FREQUENCY= 401.64689	(CM**-1)
MODE	10	FREQUENCY= 449.18379	(CM**-1)
MODE	11	FREQUENCY= 481.51128	(CM**-1)
MODE	12	FREQUENCY= 570.38526	(CM**-1)
MODE	13	FREQUENCY= 702.70848	(CM**-1)
MODE	14	FREQUENCY= 706.24163	(CM**-1)
MODE	15	FREQUENCY= 746.16736	(CM**-1)
MODE	16	FREQUENCY= 873.32240	(CM**-1)
MODE	17	FREQUENCY= 882.86263	(CM**-1)
MODE	18	FREQUENCY= 938.95257	(CM**-1)
MODE	19	FREQUENCY= 941.07312	(CM**-1)
MODE	20	FREQUENCY=1035.89102	(CM**-1)
MODE	21	FREQUENCY=1193.57354	(CM**-1)
MODE	22	FREQUENCY=1194.83270	(CM**-1)
MODE	23	FREQUENCY=1391.51387	(CM**-1)
MODE	24	FREQUENCY=1476.53265	(CM**-1)
MODE	25	FREQUENCY=1638.02456	(CM**-1)

```
MODE    26    FREQUENCY=1709.64646 (CM**-1)
MODE    27    FREQUENCY=3385.71367 (CM**-1)
MODE    28    FREQUENCY=3399.21962 (CM**-1)
MODE    29    FREQUENCY=3441.30481 (CM**-1)
MODE    30    FREQUENCY=3442.92396 (CM**-1)
```

Selenophene-*Se*-oxide-Coordinates: S_1 A′ State

1.65Å S-O Bond Length

```
C            6.0  -0.7874425669   0.1224620607  -0.7096041026
SE          34.0   1.6899101783  -0.5949009850   0.0000000000
C            6.0   0.3550200202  -0.3521004616  -1.3266614167
H            1.0   0.6189147228  -0.3594383524  -2.3625090790
O            8.0   2.8751933754   0.5529682342   0.0000000000
H            1.0  -1.6316840177   0.4591410501  -1.2820545552
TOTAL ENERGY =   -2628.0946614705
```

Selenophene-*Se*-oxide-Coordinates: S_2 A″ State

1.65Å S-O Bond Length

```
C            6.0  -0.7605215373   0.1894422587  -0.7058506210
SE          34.0   1.7185915034  -0.6708622910   0.0000000000
C            6.0   0.3971077120  -0.2665149702  -1.3114675173
H            1.0   0.6366200072  -0.3712137707  -2.3477074431
O            8.0   2.6258476435   0.7073199525   0.0000000000
H            1.0  -1.6295733067   0.4412204998  -1.2846640426
TOTAL ENERGY =   -2628.0726859380
```

Selenophene-*Se*-oxide-Coordinates: T_1 A″ State

1.65Å S-O Bond Length

```
C            6.0  -0.8825568173   0.1717108447  -0.6817666193
SE          34.0   1.7416653623  -0.6426607443   0.0000000000
C            6.0   0.3454210229  -0.3159203077  -1.2867772778
H            1.0   0.5724977491  -0.2595512578  -2.3331801982
O            8.0   2.7821301692   0.6516037244   0.0000000000
H            1.0  -1.7184869543   0.4867383113  -1.2774160924
TOTAL ENERGY =   -2628.1529534262
```

```
MODE     1    FREQUENCY=    0.00004 (CM**-1)
MODE     2    FREQUENCY=    0.00001 (CM**-1)
MODE     3    FREQUENCY=    0.00001 (CM**-1)
MODE     4    FREQUENCY=    0.00000 (CM**-1)
MODE     5    FREQUENCY=    0.00001 (CM**-1)
MODE     6    FREQUENCY=    0.00001 (CM**-1)
MODE     7    FREQUENCY=  133.83622 (CM**-1)
MODE     8    FREQUENCY=  225.15098 (CM**-1)
MODE     9    FREQUENCY=  282.11014 (CM**-1)
MODE    10    FREQUENCY=  440.89438 (CM**-1)
MODE    11    FREQUENCY=  444.47409 (CM**-1)
```

MODE 12 FREQUENCY= 452.27096 (CM**-1)
MODE 13 FREQUENCY= 507.43525 (CM**-1)
MODE 14 FREQUENCY= 588.89532 (CM**-1)
MODE 15 FREQUENCY= 725.46632 (CM**-1)
MODE 16 FREQUENCY= 736.08216 (CM**-1)
MODE 17 FREQUENCY= 855.11303 (CM**-1)
MODE 18 FREQUENCY= 873.41969 (CM**-1)
MODE 19 FREQUENCY= 905.75649 (CM**-1)
MODE 20 FREQUENCY= 959.21042 (CM**-1)
MODE 21 FREQUENCY=1085.87215 (CM**-1)
MODE 22 FREQUENCY=1210.67073 (CM**-1)
MODE 23 FREQUENCY=1321.32944 (CM**-1)
MODE 24 FREQUENCY=1393.38761 (CM**-1)
MODE 25 FREQUENCY=1460.29510 (CM**-1)
MODE 26 FREQUENCY=1646.89747 (CM**-1)
MODE 27 FREQUENCY=3396.70645 (CM**-1)
MODE 28 FREQUENCY=3413.85901 (CM**-1)
MODE 29 FREQUENCY=3435.90279 (CM**-1)
MODE 30 FREQUENCY=3439.09351 (CM**-1)

Selenophene-*Se*-oxide-Coordinates: T_2 A′ State

1.65Å S-O Bond Length

C	6.0	-0.8262212761	0.0590556316	-0.7137100424
SE	34.0	1.6797144018	-0.5480288509	0.0000000000
C	6.0	0.3390500976	-0.3531029260	-1.3219753251
H	1.0	0.5937268646	-0.3503333078	-2.3607109264
O	8.0	3.0143421125	0.4221612723	0.0000000000
H	1.0	-1.6717734156	0.3953846855	-1.2843397347 -

TOTAL ENERGY = 2628.1091017991

Dibenzothiophene-*S*-oxide-Coordinates: S_0 A′ State

S	16.0	1.6213256014	-.4184904228	.0000000000
C	6.0	-2.0024416587	.1148183371	1.6029682735
C	6.0	-.9467240768	-.0257524420	.7367079883
C	6.0	.5970059706	-.1462881257	2.6108556731
C	6.0	.3543561662	-.1727227364	1.2565125096
O	8.0	2.6480785308	.6869948846	.0000000000
C	6.0	-1.7634090579	.1355060410	2.9824039317
C	6.0	-.4872979773	.0155819059	3.4818117291
H	1.0	1.5966982025	-.2425519677	2.9939922912
H	1.0	-.3182926580	.0449790147	4.5427968650
H	1.0	-2.5919001382	.2536715453	3.6572896537
H	1.0	-3.0073767437	.2200270728	1.2357728641

TOTAL ENERGY = -931.5392139852

MODE 1 FREQUENCY= 0.00003 (CM**-1)

```
MODE     2    FREQUENCY=    0.00001 (CM**-1)
MODE     3    FREQUENCY=    0.00000 (CM**-1)
MODE     4    FREQUENCY=    0.00000 (CM**-1)
MODE     5    FREQUENCY=    0.00001 (CM**-1)
MODE     6    FREQUENCY=    0.00001 (CM**-1)
MODE     7    FREQUENCY=   84.42347 (CM**-1)
MODE     8    FREQUENCY=  112.24822 (CM**-1)
MODE     9    FREQUENCY=  117.95918 (CM**-1)
MODE    10    FREQUENCY=  188.62551 (CM**-1)
MODE    11    FREQUENCY=  218.07551 (CM**-1)
MODE    12    FREQUENCY=  292.18302 (CM**-1)
MODE    13    FREQUENCY=  370.33019 (CM**-1)
MODE    14    FREQUENCY=  419.88229 (CM**-1)
MODE    15    FREQUENCY=  423.28944 (CM**-1)
MODE    16    FREQUENCY=  449.50397 (CM**-1)
MODE    17    FREQUENCY=  478.69357 (CM**-1)
MODE    18    FREQUENCY=  505.83165 (CM**-1)
MODE    19    FREQUENCY=  526.76065 (CM**-1)
MODE    20    FREQUENCY=  569.13355 (CM**-1)
MODE    21    FREQUENCY=  613.08384 (CM**-1)
MODE    22    FREQUENCY=  671.17462 (CM**-1)
MODE    23    FREQUENCY=  740.11754 (CM**-1)
MODE    24    FREQUENCY=  753.60889 (CM**-1)
MODE    25    FREQUENCY=  755.74085 (CM**-1)
MODE    26    FREQUENCY=  772.30827 (CM**-1)
MODE    27    FREQUENCY=  830.41832 (CM**-1)
MODE    28    FREQUENCY=  845.87552 (CM**-1)
MODE    29    FREQUENCY=  861.18093 (CM**-1)
MODE    30    FREQUENCY=  865.08608 (CM**-1)
MODE    31    FREQUENCY=  908.61929 (CM**-1)
MODE    32    FREQUENCY=  982.89547 (CM**-1)
MODE    33    FREQUENCY=  983.43409 (CM**-1)
MODE    34    FREQUENCY=1053.05336 (CM**-1)
MODE    35    FREQUENCY=1056.94397 (CM**-1)
MODE    36    FREQUENCY=1100.14521 (CM**-1)
MODE    37    FREQUENCY=1107.06196 (CM**-1)
MODE    38    FREQUENCY=1118.08651 (CM**-1)
MODE    39    FREQUENCY=1119.54713 (CM**-1)
MODE    40    FREQUENCY=1141.82459 (CM**-1)
MODE    41    FREQUENCY=1142.91740 (CM**-1)
MODE    42    FREQUENCY=1176.83242 (CM**-1)
MODE    43    FREQUENCY=1178.03530 (CM**-1)
MODE    44    FREQUENCY=1229.04273 (CM**-1)
MODE    45    FREQUENCY=1234.34962 (CM**-1)
MODE    46    FREQUENCY=1307.46732 (CM**-1)
MODE    47    FREQUENCY=1321.31263 (CM**-1)
MODE    48    FREQUENCY=1384.63098 (CM**-1)
```

```
MODE    49    FREQUENCY=1414.81177 (CM**-1)
MODE    50    FREQUENCY=1438.73731 (CM**-1)
MODE    51    FREQUENCY=1584.33234 (CM**-1)
MODE    52    FREQUENCY=1597.70844 (CM**-1)
MODE    53    FREQUENCY=1626.43717 (CM**-1)
MODE    54    FREQUENCY=1627.13222 (CM**-1)
MODE    55    FREQUENCY=1773.10265 (CM**-1)
MODE    56    FREQUENCY=1774.67038 (CM**-1)
MODE    57    FREQUENCY=1787.22994 (CM**-1)
MODE    58    FREQUENCY=1788.07865 (CM**-1)
MODE    59    FREQUENCY=3351.93548 (CM**-1)
MODE    60    FREQUENCY=3352.05913 (CM**-1)
MODE    61    FREQUENCY=3368.41493 (CM**-1)
MODE    62    FREQUENCY=3368.91712 (CM**-1)
MODE    63    FREQUENCY=3379.87298 (CM**-1)
MODE    64    FREQUENCY=3382.50052 (CM**-1)
MODE    65    FREQUENCY=3396.45308 (CM**-1)
MODE    66    FREQUENCY=3401.51924 (CM**-1)
```

Dibenzothiophene-*S*-oxide-Coordinates: T_1 A″ State

```
S          16.0    1.6662437036  -0.3889254683   0.0000000000
C           6.0   -2.0357347178   0.1956695537   1.6220945824
C           6.0   -0.9392164449   0.0116305201   0.6895817346
C           6.0    0.6085812150  -0.2545590941   2.5742771252
C           6.0    0.3867978894  -0.2151971525   1.2502918697
O           8.0    2.5920672943   0.8023629892   0.0000000000
C           6.0   -1.8020144328   0.1525380503   2.9453416371
C           6.0   -0.4853602502  -0.0740022071   3.4701481845
H           1.0    1.5974940372  -0.4118833497   2.9666691866
H           1.0   -0.3263841784  -0.1061104733   4.5304191206
H           1.0   -2.6127441245   0.2905528845   3.6379601334
H           1.0   -3.0277392625   0.3700931247   1.2477906924
TOTAL ENERGY =   -931.4166929194
```

Dibenzothiophene-*S*-oxide-Coordinates: T_2 A′ State

```
S          16.0    1.5899328245  -0.3946139150   0.0000000000
C           6.0   -2.0147001611   0.1132171356   1.6003613503
C           6.0   -0.9843867546  -0.0187108718   0.7374799902
C           6.0    0.6088886506  -0.1393680905   2.6525374151
C           6.0    0.3554869626  -0.1485349618   1.2469365684
O           8.0    2.6842448273   0.6440384575   0.0000000000
C           6.0   -1.7684286297   0.1191908395   3.0102024604
C           6.0   -0.4327278514  -0.0042355105   3.5024996327
H           1.0    1.6167984954  -0.2271075517   3.0143907344
H           1.0   -0.2658354664   0.0128227180   4.5641871875
H           1.0   -2.5874155127   0.2240204284   3.6950327294
H           1.0   -3.0239981474   0.2235896609   1.2464811383
```

TOTAL ENERGY = -931.3778197803

Dibenzothiophene-*S*-oxide-Coordinates: S_1 A′ State

S	16.0	1.5829020845	-0.2633677408	0.0000000000
C	6.0	-1.9596794401	0.2692275864	1.6259751066
C	6.0	-0.9192122873	-0.0032415458	0.7143868070
C	6.0	0.5890854975	-0.3773201843	2.6430980570
C	6.0	0.3467616051	-0.3455488068	1.2560894244
O	8.0	2.5340148372	0.8965393819	0.0000000000
C	6.0	-1.7331832738	0.1884672564	2.9700782677
C	6.0	-0.4542479099	-0.1440539342	3.4875413193
H	1.0	1.5698925008	-0.6014628613	3.0230933807
H	1.0	-0.3111858114	-0.2032489182	4.5510169558
H	1.0	-2.5360532496	0.3910519676	3.6559612804
H	1.0	-2.9343381237	0.5386997095	1.2600358786

TOTAL ENERGY = -931.3780312157

Dibenzothiophene-*S*-oxide-Coordinates: S_2 A″ State

S	16.0	1.6745640182	-0.3407847971	0.0000000000
C	6.0	-1.9919635521	0.2973448789	1.6153606780
C	6.0	-0.9292543336	0.0777018294	0.6933532518
C	6.0	0.5833069723	-0.3927371214	2.5978813882
C	6.0	0.3747540696	-0.2900096779	1.2097493827
O	8.0	2.4375048193	0.9608445069	0.0000000000
C	6.0	-1.7568830174	0.1628468392	2.9422995719
C	6.0	-0.4616791902	-0.1933116248	3.4448589823
H	1.0	1.5588567214	-0.6394889361	2.9756777833
H	1.0	-0.3268728870	-0.2967315672	4.5056811436
H	1.0	-2.5537244054	0.3263902461	3.6450459364
H	1.0	-2.9678916158	0.5678346167	1.2564888044

TOTAL ENERGY = -931.3472646063

References

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2. B. Bak, D. Christensen, L. Hansen-Nygaard and J. Rastrup-Andersen, *J. Mol. Spectrosc.*, 1961, **7**, 58-63.