Kato (ESI-Exp.) ESI-Exp: 1/1

Equations for the five correlation plots in Figs 6 and 7 as the following:

$y = 0.482x - 31.7$ ($R^2 = 0.996$) (A)

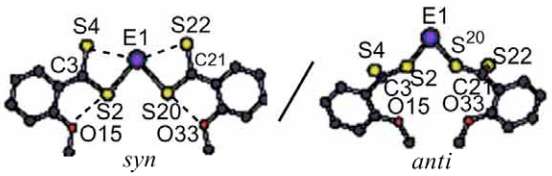
$y = 1.105x - 15.3$ ($R^2 = 0.9999$) (B)

$y = 0.965x - 36.2$ ($R^2 = 0.9998$) (C)

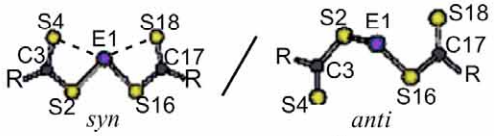
$y = 1.259x + 6.2$ ($R^2 = 0.999$) (D)

$y = 1.109x - 10.4$ ($R^2 = 0.999$) (E)

ESI-Table 1 Geometric parameters (bond distances and angles) of the optimized structures for $E(SSCC_6H_4OMe\text{-}2)_2$ **2e** – **4e** and $E(SSCMe)_2$ **2a** – **4a** (E = S, Se, Te)[a]



	E1 = S (**4e**)[b]	Se (**2e**)[c]	Te (**3e**)[c]
E1···S4	3.382	2.821	2.854
E1–S2	2.068	2.331	2.470
C3–S2	1.767	1.734	1.726
C3=S4	1.623	1.659	1.670
O15···S2	3.089	2.602	2.650
∠S2-E1-S20	106.9	87.6	80.9
∠S4-C3-S2	126.6	118.7	117.9
∠S4-E1-S20	133.1	155.2	146.7
∠S4-E1-S2	62.5	68.8	65.8
∠C3-S2-E1	105.3	94.0	93.9
∠C(3)-S4-E1	64.4	78.4	82.4
∠O15-S2-E1	125.7	173.9	172.9
ϕC3-S2-E1-S20	70.8	180.0	180.0
ϕS2-C3-C6-O15	25.7	0.0	0.0

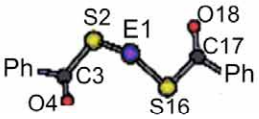


	E1 = S (**4a**)[b]	Se (**2a**)[c]	Te (**3a**)[c]
E1···S4	3.351	2.845	2.876
E1–S2	2.065	2.291	2.476
C3–S2	1.779	1.723	1.714
C3=S4	1.620	1.643	1.654
∠S2-E1-S9	106.1	88.1	82.3
∠S4-C3-S2	126.3	121.7	121.1
∠S4-E1-S9	127.4	157.0	148.3
∠S4-E1-S2	63.0	68.9	66.0
∠C3-S2-E1	105.3	92.9	92.4
ϕC3-S2-E1-S9	80.0	180.0	180.0
ϕS4-C3-S2-E1	-8.4	0.0	0.0

[a]Distances are in angstrom (Å), angles (∠) and torsion (ϕ) in degrees. [b]*anti*-Conformer (C2). [c]*syn*-Conformer (C2v).

ESI-Table 2 Geometric parameters (bond distances and angles) of the optimized structures for *anti*-E(SOCPh)$_2$ (E = S, Se, Te)[a]

	XRD values		
E =	S (**4d**)[b]	Se (**2d**)[d]	Te (**3d**)[e]
E···O(4)	3.007	3.11(2)	3.242(2)
E–S(2)	2.020	2.174(1)	2.379(2)
C(3)–S(2)	1.805	1.827(5)	1.832(6)
C(3)=O(4)	1.210	1.187(7)	1.199(9)
∠S(2)-E-S(16)	107.3[c]	105.0(1)	103.1(1)
∠O(4)-C(3)-S(2)	121.7	121.6(3)	121.0(4)
∠O(4)-E-O(18)	-	-	-
∠O(4)-E-S(2)	59.8	-	-
∠C(3)-S(2)-S(1)	101.6	102.1(2)	102.5(2)
ϕC(3)-S(2)-E-S(16)	80.7	-	-
ϕO(4)-C(3)-S(2)-E	-7.7	-	-



anti

	calculated values[f]		
E1 =	S (**4d**)	Se (**2d**)	Te (**3d**)
E1···O4	3.037	3.139	3.214
E1–S2	2.062	2.200	2.366
C3–S2	1.818	1.822	1.830
C3=O4	1.211	1.211	1.211
∠S2-E1-S16	106.6	102.1	99.6
∠O4-C3-S2	122.7	123.1	122.7
∠O4-E1-O18	123.4	117.4	115.2
∠O4-E1-S2	59.7	56.2	55.0
∠C3-S2-E1	100.5	101.1	100.7
ϕC3-S2-E1-S16	80.3	78.6	78.7
ϕO4-C3-S2-E1	11.5	11.6	10.2

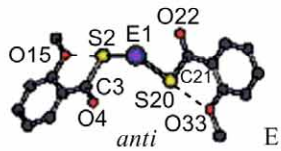
[a]Distances are in angstrom (Å), angles (∠) and torsion (ϕ) in degrees. [b]Values taken from compound $(PhCOS)_2$ (CCDC refcord: DBZOSS03). [c]Values taken from compound $F_3CSSSCF_3$ in ref 10. [d]Values taken from ref 8. [e]Values taken from ref 9. [f]*Anti*-conformer (C2 symmetry)

ESI-Table 3 Relative energies of the *syn*- and *anti*-conformers of $E(SE'CR)_2$ **2**–**13** (E = O, S, Se, Te; E' = O, S; R = Me, Ph, C_6H_4OMe-2)

compounds	energy (au) *syn*-	energy (au) *anti*-	ΔE^a kJ/mol
$O(SSCMe)_2$ (**12**)	-1821.1157772	-1821.1351023	-50.7
$S(SSCMe)_2$ (**4a**)	-2143.7575830	-2143.7727237	-39.8
$Se(SSCMe)_2$ (**2a**)	-4146.1850305	-4146.1874376	-6.3
$Te(SSCMe)_2$ (**3a**)	-8358.0438517	-8358.0278258	42.1
$O(SSCPh)_2$ (**10**)[b]	-	-	-
$S(SSCPh)_2$ (**4d**)	-2526.0211974	-2526.0438730	-59.5
$Se(SSCPh)_2$ (**2d**)	-4528.4496801	-4528.4580218	-21.9
$Te(SSCPh)_2$ (**3d**)	-8740.3097485	-8740.2979421	31.0
$O(SSCC_6H_4OMe\text{-}2)_2$ (**8**)[b]	-	-	-
$S(SSCC_6H_4OMe\text{-}2)_2$ (**4e**)	-2754.4739911	-2754.5023544	-74.5
$Se(SSCC_6H_4OMe\text{-}2)_2$ (**2e**)	-4756.9002324	-4756.9164138	-42.5
$Te(SSCC_6H_4OMe\text{-}2)_2$ (**3e**)	-8968.7560914	-8968.7543828	4.5
$O(SOCMe)_2$ (**13**)	-1175.9749332	-1175.9957708	-54.7
$S(SOCMe)_2$ (**7a**)	-1498.6180248	-1498.6380838	-52.7
$Se(SOCMe)_2$ (**5a**)	-3501.0401046	-3501.0532058	-34.4
$Te(SOCMe)_2$ (**6a**)	-7712.8862231	-7712.8905401	-11.3
$O(SOCPh)_2$ (**11**)[b]	-	-	-
$S(SOCPh)_2$ (**7d**)	-1880.8782175	-1880.9009239	-59.6
$Se(SOCPh)_2$ (**5d**)	-3883.3007571	-3883.3152784	-38.1
$Te(SOCPh)_2$ (**6d**)	-8095.1497105	-8095.1526333	-7.7
$O(SOCC_6H_4OMe\text{-}2)_2$ (**9**)[b]	-	-	-
$S(SOCC_6H_4OMe\text{-}2)_2$ (**7e**)	-2109.3331641	-2109.3515268	-48.2
$Se(SOCC_6H_4OMe\text{-}2)_2$ (**5e**)	-4111.7545049	-4111.7649057	-27.3
$Te(SOCC_6H_4OMe\text{-}2)_2$ (**6e**)	-8323.5999567	-8323.6008410	-2.3

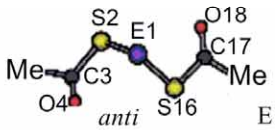
[a] E (*anti*-conformer) – E (*syn*-conformer). [b] For compounds **8**, **9**, **10** and **11**, the optimized structures of *syn*- and *trans*-conformers were not obtained.

ESI-Table 4 Geometric parameters (bond distances and angles) of the optimized structures for compounds **5e – 7e** $E(SOCC_6H_4OMe\text{-}2)_2$ and **5a – 7a** $E(SOCMe)_2$ (E = S, Se, Te)[a]



anti

E1 =	S (**7e**)	Se (**5e**)	Te (**6e**)
E1···O4	2.980	3.091	3.195
E1–S2	2.068	2.206	2.371
C3–S2	1.817	1.818	1.826
C3=O4	1.214	1.213	1.246
O15---S2	2.689	2.735	2.796
∠S2-E-S16	106.5	102.2	100.1
∠O4-C3-S2	121.7	122.2	122.1
∠O4-E1-O22	122.2	116.9	117.9
∠O4-E1-S2	60.5	57.7	55.1
∠C3-S2-E1	99.9	100.6	100.2
∠O4-C3-O15	163.9	159.5	153.3
∠O15-S2-E1	164.5	162.2	165.2
ϕC3-S2-E1-S16	74.1	72.1	81.6
ϕC3-S2-O15-C6	22.1	27.7	32.9

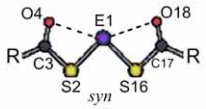
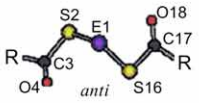


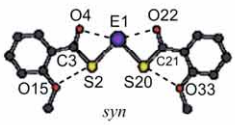
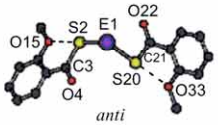
anti

E1 =	S (**7a**)[b]	Se (**5a**)[b]	Te (**6a**)[b]
E·1··O4	3.061	3.161	3.251
E1–S2	2.062	2.200	2.363
C3–S2	1.818	1.822	1.832
C3=O4	1.207	1.206	1.206
∠S2-E1-S9	105.5	102.5	101.6
∠O4-C3-S2	123.3	123.6	123.4
∠O4-E1-O11	127.3	122.3	121.4
∠O4-E1-S2	59.2	56.8	54.5
∠C3-S2-E1	101.3	101.8	101.6
ϕC3-S2-E-S9	81.4	80.3	81.3
ϕO4-C3-S2-E1	-7.1	7.0	5.3

[a]Distances are in angstrom (Å), angles (∠) and torsion (ϕ) in degrees.
[b]C2 symmetry.

ESI-Table 5 NBO analyses of E1(SOCR)$_2$ (E1 = O, S, Se, Te; R = Me, Ph, C_6H_4OMe-2) **5**, **6**, **7**, **9**, **11** and **13**

			E^b [kJ/mol]					
								
			syn			*anti*		
	E1(SOCR)$_2$		$n_{O4}\rightarrow\sigma^*_{E1\text{-}S16}$	$n_{O4}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{S2}\rightarrow\pi^*_{C3=O4}$	$n_{O4}\rightarrow\sigma^*_{E1\text{-}S16}$	$n_{O4}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{S2}\rightarrow\pi^*_{C3=O4}$
No.	R	E1	$n_{O18}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{O18}\rightarrow\sigma^*_{E1\text{-}S16}$	$n_{S9}\rightarrow\pi^*_{C10=O11}$	$n_{O18}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{O4}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{S9}\rightarrow\pi^*_{C10=O11}$
13	Me	O	-	-	86.2	-	-	92.2
7a		S	4.6	-	91.0	-	-	76.3
5a		Se	9.6	2.8	95,9	-	-	75.1
6a		Te	20.0	10.4	109.5	-	-	72.3
11[c]	Ph	O	-	-	-	-	-	-
7b		S	7.2	-	84.5	-	-	73.2
5d		Se	12.8	3.6	90.1	-	-	72.4
6d		Te	25.8	12.6	104.8	-	-	70.8

										
			syn				*anti*			
	E1(SOCR)$_2$		$n_{O4}\rightarrow\sigma^*_{E1\text{-}S20}$	$n_{O4}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{O15}\rightarrow\sigma^*_{S2\text{-}E1}$	$n_{S2}\rightarrow\pi^*_{C3=O4}$	$n_{O4}\rightarrow\sigma^*_{E1\text{-}S20}$	$n_{O4}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{O15}\rightarrow\sigma^*_{S2\text{-}E1}$	$n_{S2}\rightarrow\pi^*_{C3=O4}$
No.	R	E1	$n_{O22}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{O22}\rightarrow\sigma^*_{E1\text{-}S20}$	$n_{O33}\rightarrow\sigma^*_{S20\text{-}E1}$	$n_{O33}\rightarrow\pi^*_{C21=O22}$	$n_{O22}\rightarrow\sigma^*_{E1\text{-}S2}$	$n_{O22}\rightarrow\sigma^*_{E1\text{-}S20}$	$n_{O33}\rightarrow\sigma^*_{S20\text{-}E1}$	$n_{O33}\rightarrow{}^*\pi_{C21=O22}$
9[c]	2-$MeOC_6H_4$	O	-	-	-	-	-	-	-	-
7d		S	7.8	-	9.4	92.4	-	-	7.2	79.4
5e		Se	13.0	3.8	8.8	97.7	-	-	7.4	87.2
6e		Te	22.8	12.8	6.4	111.4	-	-	5.4	83.6

[a]Analyses for the calculation on compounds **5a**, **5d**, **5e**, **7a**, **7b**, **7d** and **13** were carried out at MP2/6-311G(2d, p) level of theory for O, S and Se and those of the compounds **6a**, **6d** and **6e** are at MP2/**7**433111/**7**43111/7411/2 +1s1p1d1f level for Te and 6.31G for C and H, respectively. [b]Stabilization energies associated with delocalization. [c]The optimized structures for the both *syn*- and *anti*-conformers of compounds **9** and **11** were not obtained.

Optimized Structures Given by Cartesian Coordinates for the compounds 2–7, 12, and 13

Quantum chemical calculations were performed on the chalcogen compounds using Gaussian 03 program.[35] The structures were optimized with the 6-311+G(d) basis sets for O, S, and Se and the reported ones of the (7433111/743111/7411/2 + 1s1p1d1f)[36] type for the Te atom with the 6-31G(d) basis sets for C and H at the Møller-Plesset second order energy correlation (MP2)[37] level.

ESI-Table 6 Optimized Structures Given by Cartesian Coordinates for the compounds **2**–**7**, **12**, and **13**

$O(SSCMe)_2$ (**12**)-*syn*
Total energy: -1821.1157772 hartrees

8	0	0.000000	0.000000	0.255524
16	0	0.000000	1.398020	1.236766
6	0	0.000000	2.581985	-0.038443
16	0	0.000000	2.226098	-1.621118
6	0	0.000000	3.976171	0.550963
1	0	0.000000	3.972877	1.647873
1	0	-0.886215	4.512615	0.202272
1	0	0.886215	4.512615	0.202272
16	0	0.000000	-1.398020	1.236766
6	0	0.000000	-2.581985	-0.038443
16	0	0.000000	-2.226098	-1.621118
6	0	0.000000	-3.976171	0.550963
1	0	0.000000	-3.972877	1.647873
1	0	-0.886215	-4.512615	0.202272
1	0	0.886215	-4.512615	0.202272

$O(SSCMe)_2$ (**12**)-*anti*
Total energy: -1821.1351023 hartrees

8	0	0.000000	0.000000	0.999657
16	0	0.774755	1.211701	0.131767
6	0	-0.537590	2.319984	-0.185733
16	0	-2.099910	2.039732	0.162146
6	0	0.000000	3.595919	-0.794675
1	0	0.153460	4.336325	-0.002852
1	0	0.955119	3.441052	-1.310782
1	0	-0.727990	3.992008	-1.505167
16	0	-0.774755	-1.211701	0.131767
6	0	0.537590	-2.319984	-0.185733
16	0	2.099910	-2.039732	0.162146
6	0	0.000000	-3.595919	-0.794675
1	0	-0.153460	-4.336325	-0.002852
1	0	-0.955119	-3.441052	-1.310782
1	0	0.727990	-3.992008	-1.505167

$S(SSCMe)_2$ (**4a**)-*syn*
Total energy: -2143.757583 hartrees

16	0	0.000000	0.000000	0.313768
16	0	0.000000	1.514825	-1.181787
6	0	0.000000	2.861173	-0.085667

16	0	0.000000	2.696026	1.538521
6	0	0.000000	4.192744	-0.801061
1	0	0.884672	4.762653	-0.503836
1	0	0.000000	4.079986	-1.889847
1	0	-0.884672	4.762653	-0.503836
16	0	0.000000	-1.514825	-1.181787
6	0	0.000000	-2.861173	-0.085667
16	0	0.000000	-2.696026	1.538521
6	0	0.000000	-4.192744	-0.801061
1	0	0.884672	-4.762653	-0.503836
1	0	0.000000	-4.079986	-1.889847
1	0	-0.884672	-4.762653	-0.503836

$S(SSCMe)_2$ (**4a**)-*anti*
Total energy: -2143.7727237 hartrees

16	0	0.000000	0.000000	1.412030
16	0	1.114324	1.199729	0.162981
6	0	0.000000	2.487567	-0.354623
16	0	-1.593956	2.547430	-0.071716
6	0	0.780904	3.531365	-1.119235
1	0	1.404572	4.108892	-0.427667
1	0	1.441538	3.066446	-1.859566
1	0	0.090403	4.207111	-1.626098
16	0	-1.114324	-1.199729	0.162981
6	0	0.000000	-2.487567	-0.354623
16	0	1.593956	-2.547430	-0.071716
6	0	-0.780904	-3.531365	-1.119235
1	0	-1.404572	-4.108892	-0.427667
1	0	-1.441538	-3.066446	-1.859566
1	0	-0.090403	-4.207111	-1.626098

$Se(SSCMe)_2$ (**2a**)-*syn*
Total energy: -4146.1850305 hartrees

34	0	0.000000	0.000000	0.347072
16	0	0.000000	1.593619	-1.299238
6	0	0.000000	2.890510	-0.164675
16	0	0.000000	2.620939	1.455782
6	0	0.000000	4.271009	-0.777304
1	0	0.000000	4.231795	-1.870539
1	0	0.884644	4.819622	-0.441260
1	0	-0.884644	4.819622	-0.441260
16	0	0.000000	-1.593619	-1.299238
6	0	0.000000	-2.890510	-0.164675
16	0	0.000000	-2.620939	1.455782
6	0	0.000000	-4.271009	-0.777304
1	0	0.000000	-4.231795	-1.870539
1	0	0.884644	-4.819622	-0.441260
1	0	-0.884644	-4.819622	-0.441260

$Se(SSCMe)_2$ (**2a**)-*anti*
Total energy: -4146.1874376 hartrees

34	0	0.000000	0.000000	1.362255
16	0	0.000000	1.711467	-0.016370
6	0	-1.675447	1.840366	-0.611984
16	0	-2.879920	0.794154	-0.333913
6	0	-1.790711	3.079961	-1.471085
1	0	-1.557330	3.975207	-0.884401
1	0	-1.085134	3.033511	-2.308321
1	0	-2.805965	3.158645	-1.862680
16	0	0.000000	-1.711467	-0.016370
6	0	1.675447	-1.840366	-0.611984
16	0	2.879920	-0.794154	-0.333913
6	0	1.790711	-3.079961	-1.471085
1	0	1.557330	-3.975207	-0.884401
1	0	1.085134	-3.033511	-2.308321
1	0	2.805965	-3.158645	-1.862680

$Te(SSCMe)_2$ (**3a**)-*syn*
Total energy: -8358.0438517 hartrees

52	0	0.000000	0.000000	0.470705
16	0	0.000000	1.629611	-1.393969
6	0	0.000000	2.967381	-0.322626
16	0	0.000000	2.748532	1.316439
6	0	0.000000	4.338388	-0.958032
1	0	0.884601	4.893971	-0.632108
1	0	0.000000	4.275427	-2.049687
1	0	-0.884601	4.893971	-0.632108
16	0	0.000000	-1.629611	-1.393969
6	0	0.000000	-2.967381	-0.322626
16	0	0.000000	-2.748532	1.316439
6	0	0.000000	-4.338388	-0.958032
1	0	0.884601	-4.893971	-0.632108
1	0	0.000000	-4.275427	-2.049687
1	0	-0.884601	-4.893971	-0.632108

$Te(SSCMe)_2$ (**3a**)-*anti*
Total energy: -8358.0278258 hartrees

52	0	0.000000	0.000000	1.290812
16	0	0.000000	1.812256	-0.226366
6	0	-1.680063	1.905041	-0.841788
16	0	-2.851645	0.824313	-0.556971
6	0	-1.825236	3.138698	-1.704439
1	0	-1.673687	4.040364	-1.100541
1	0	-1.072473	3.139648	-2.500892
1	0	-2.821343	3.163302	-2.148940
16	0	0.000000	-1.812256	-0.226366
6	0	1.680063	-1.905041	-0.841788
16	0	2.851645	-0.824313	-0.556971
6	0	1.825236	-3.138698	-1.704439
1	0	1.673687	-4.040364	-1.100541
1	0	1.072473	-3.139648	-2.500892
1	0	2.821343	-3.163302	-2.148940

$S(SSCPh)_2$ (**4d**)-*syn*
Total energy: -2526.0211974 hartrees

16	0	0.000000	0.000000	0.876090
16	0	0.000000	1.502118	-0.643710
6	0	0.000000	2.853586	0.466108
16	0	0.000000	2.599084	2.088572
6	0	0.000000	4.190691	-0.183534
6	0	0.000000	4.335218	-1.584340
6	0	0.000000	5.349912	0.613293
6	0	0.000000	5.602893	-2.166022
6	0	0.000000	6.612887	0.025254
6	0	0.000000	6.748013	-1.366215
1	0	0.000000	3.464366	-2.235842
1	0	0.000000	5.250465	1.695051
1	0	0.000000	5.693289	-3.249648
1	0	0.000000	7.496635	0.658882
1	0	0.000000	7.735207	-1.822232
16	0	0.000000	-1.502118	-0.643710
6	0	0.000000	-2.853586	0.466108
16	0	0.000000	-2.599084	2.088572
6	0	0.000000	-4.190691	-0.183534
6	0	0.000000	-4.335218	-1.584340
6	0	0.000000	-5.349912	0.613293
6	0	0.000000	-5.602893	-2.166022
6	0	0.000000	-6.612887	0.025254
6	0	0.000000	-6.748013	-1.366215
1	0	0.000000	-3.464366	-2.235842
1	0	0.000000	-5.250465	1.695051
1	0	0.000000	-5.693289	-3.249648
1	0	0.000000	-7.496635	0.658882
1	0	0.000000	-7.735207	-1.822232

$S(SSCPh)_2$ (**4d**)-*anti*
Total energy: -2526.043873 hartrees

16	0	0.000000	0.000000	2.182973
16	0	0.481734	1.560171	0.924211
6	0	-1.090915	2.213544	0.408326
16	0	-2.540989	1.512285	0.628600
6	0	-0.874425	3.472491	-0.339140
6	0	0.000000	4.461519	0.149189
6	0	-1.544383	3.680082	-1.557558
6	0	0.179711	5.647522	-0.565586
6	0	-1.342892	4.859042	-2.273014
6	0	-0.480243	5.845042	-1.781145
1	0	0.495030	4.324285	1.107748
1	0	-2.213144	2.908886	-1.932292
1	0	0.839548	6.416675	-0.171309
1	0	-1.856421	5.007660	-3.219971
1	0	-0.330587	6.766161	-2.339356
16	0	-0.481734	-1.560171	0.924211

6	0	1.090915	-2.213544	0.408326
16	0	2.540989	-1.512285	0.628600
6	0	0.874425	-3.472491	-0.339140
6	0	0.000000	-4.461519	0.149189
6	0	1.544383	-3.680082	-1.557558
6	0	-0.179711	-5.647522	-0.565586
6	0	1.342892	-4.859042	-2.273014
6	0	0.480243	-5.845042	-1.781145
1	0	-0.495030	-4.324285	1.107748
1	0	2.213144	-2.908886	-1.932292
1	0	-0.839548	-6.416675	-0.171309
1	0	1.856421	-5.007660	-3.219971
1	0	0.330587	-6.766161	-2.339356

$Se(SSCPh)_2$ (**2d**)-*syn*
Total energy: -4528.4496801 hartrees

34	0	0.000000	0.000000	0.835743
16	0	0.000000	1.583095	-0.830491
6	0	0.000000	2.894471	0.304015
16	0	0.000000	2.566616	1.923769
6	0	0.000000	4.265367	-0.268334
6	0	0.000000	4.480467	-1.659876
6	0	0.000000	5.381691	0.588098
6	0	0.000000	5.776371	-2.175095
6	0	0.000000	6.673157	0.065208
6	0	0.000000	6.879232	-1.317546
1	0	0.000000	3.640751	-2.351029
1	0	0.000000	5.229763	1.664006
1	0	0.000000	5.922794	-3.252609
1	0	0.000000	7.523501	0.743050
1	0	0.000000	7.888528	-1.722323
16	0	0.000000	-1.583095	-0.830491
6	0	0.000000	-2.894471	0.304015
16	0	0.000000	-2.566616	1.923769
6	0	0.000000	-4.265367	-0.268334
6	0	0.000000	-4.480467	-1.659876
6	0	0.000000	-5.381691	0.588098
6	0	0.000000	-5.776371	-2.175095
6	0	0.000000	-6.673157	0.065208
6	0	0.000000	-6.879232	-1.317546
1	0	0.000000	-3.640751	-2.351029
1	0	0.000000	-5.229763	1.664006
1	0	0.000000	-5.922794	-3.252609
1	0	0.000000	-7.523501	0.743050
1	0	0.000000	-7.888528	-1.722323

$Se(SSCPh)_2$ (**2d**)-*anti*
Total energy: -4528.4580218 hartrees

34	0	0.000000	0.000000	2.162288
16	0	0.509109	1.631329	0.774577
6	0	-1.059492	2.242506	0.190665

16	0	-2.505436	1.525187	0.379802
6	0	-0.836637	3.481644	-0.589923
6	0	0.000000	4.503165	-0.102472
6	0	-1.463864	3.636002	-1.838850
6	0	0.183781	5.668911	-0.848537
6	0	-1.257377	4.794952	-2.584924
6	0	-0.433025	5.813631	-2.093840
1	0	0.461759	4.405741	0.877319
1	0	-2.104780	2.840657	-2.211836
1	0	0.814163	6.463282	-0.456053
1	0	-1.737224	4.902608	-3.554830
1	0	-0.279628	6.719012	-2.676282
16	0	-0.509109	-1.631329	0.774577
6	0	1.059492	-2.242506	0.190665
16	0	2.505436	-1.525187	0.379802
6	0	0.836637	-3.481644	-0.589923
6	0	0.000000	-4.503165	-0.102472
6	0	1.463864	-3.636002	-1.838850
6	0	-0.183781	-5.668911	-0.848537
6	0	1.257377	-4.794952	-2.584924
6	0	0.433025	-5.813631	-2.093840
1	0	-0.461759	-4.405741	0.877319
1	0	2.104780	-2.840657	-2.211836
1	0	-0.814163	-6.463282	-0.456053
1	0	1.737224	-4.902608	-3.554830
1	0	0.279628	-6.719012	-2.676282

$Te(SSCPh)_2$ (**3d**)-*syn*
Total energy: -8740.3097485 hartrees

52	0	0.000000	0.000000	1.006658
16	0	0.000000	1.613121	-0.868498
6	0	0.000000	2.977514	0.187237
16	0	0.000000	2.727558	1.830092
6	0	0.000000	4.326217	-0.436682
6	0	0.000000	4.484112	-1.836337
6	0	0.000000	5.476746	0.374409
6	0	0.000000	5.758091	-2.403290
6	0	0.000000	6.745798	-0.201278
6	0	0.000000	6.895193	-1.591290
1	0	0.000000	3.614881	-2.489615
1	0	0.000000	5.371634	1.456075
1	0	0.000000	5.860653	-3.485895
1	0	0.000000	7.623341	0.441014
1	0	0.000000	7.887189	-2.036805
16	0	0.000000	-1.613121	-0.868498
6	0	0.000000	-2.977514	0.187237
16	0	0.000000	-2.727558	1.830092
6	0	0.000000	-4.326217	-0.436682
6	0	0.000000	-4.484112	-1.836337
6	0	0.000000	-5.476746	0.374409
6	0	0.000000	-5.758091	-2.403290

6	0	0.000000	-6.745798	-0.201278
6	0	0.000000	-6.895193	-1.591290
1	0	0.000000	-3.614881	-2.489615
1	0	0.000000	-5.371634	1.456075
1	0	0.000000	-5.860653	-3.485895
1	0	0.000000	-7.623341	0.441014
1	0	0.000000	-7.887189	-2.036805

$Te(SSCPh)_2$ (**3d**)-*anti*
Total energy: -8740.2979421 hartrees

52	0	0.000000	0.000000	2.113893
16	0	0.699496	1.668463	0.589256
6	0	-0.824808	2.386428	-0.019696
16	0	-2.310642	1.763253	0.194014
6	0	-0.526481	3.588977	-0.831758
6	0	0.386289	4.560530	-0.379572
6	0	-1.171683	3.765526	-2.068961
6	0	0.633860	5.696577	-1.152292
6	0	-0.901265	4.893363	-2.842075
6	0	0.000000	5.862140	-2.386719
1	0	0.866692	4.445850	0.589499
1	0	-1.871400	3.008382	-2.414930
1	0	1.324955	6.453029	-0.788055
1	0	-1.393693	5.016566	-3.803798
1	0	0.203251	6.743869	-2.989837
16	0	-0.699496	-1.668463	0.589256
6	0	0.824808	-2.386428	-0.019696
16	0	2.310642	-1.763253	0.194014
6	0	0.526481	-3.588977	-0.831758
6	0	-0.386289	-4.560530	-0.379572
6	0	1.171683	-3.765526	-2.068961
6	0	-0.633860	-5.696577	-1.152292
6	0	0.901265	-4.893363	-2.842075
6	0	0.000000	-5.862140	-2.386719
1	0	-0.866692	-4.445850	0.589499
1	0	1.871400	-3.008382	-2.414930
1	0	-1.324955	-6.453029	-0.788055
1	0	1.393693	-5.016566	-3.803798
1	0	-0.203251	-6.743869	-2.989837

$S(SSCC_6H_4OMe\text{-}2)_2$ (**4e**)-*syn*
Total energy: -2754.4739911 hartrees

16	0	0.000000	0.000000	1.335593
16	0	0.000000	1.498638	-0.195671
6	0	0.000000	2.860966	0.897852
16	0	0.000000	2.596679	2.527056
6	0	0.000000	4.228580	0.302901
6	0	0.000000	4.495091	-1.089173
6	0	0.000000	5.339518	1.167210
6	0	0.000000	5.809729	-1.573011
6	0	0.000000	6.645809	0.690743

6	0	0.000000	6.883251	-0.684689
1	0	0.000000	5.154064	2.236720
1	0	0.000000	6.002360	-2.640424
1	0	0.000000	7.474978	1.393286
1	0	0.000000	7.899538	-1.072076
8	0	0.000000	3.409909	-1.908598
6	0	0.000000	3.605264	-3.315204
1	0	0.000000	2.602074	-3.740749
1	0	0.897234	4.143933	-3.637323
1	0	-0.897234	4.143933	-3.637323
16	0	0.000000	-1.498638	-0.195671
6	0	0.000000	-2.860966	0.897852
16	0	0.000000	-2.596679	2.527056
6	0	0.000000	-4.228580	0.302901
6	0	0.000000	-4.495091	-1.089173
6	0	0.000000	-5.339518	1.167210
6	0	0.000000	-5.809729	-1.573011
6	0	0.000000	-6.645809	0.690743
6	0	0.000000	-6.883251	-0.684689
1	0	0.000000	-5.154064	2.236720
1	0	0.000000	-6.002360	-2.640424
1	0	0.000000	-7.474978	1.393286
1	0	0.000000	-7.899538	-1.072076
8	0	0.000000	-3.409909	-1.908598
6	0	0.000000	-3.605264	-3.315204
1	0	0.000000	-2.602074	-3.740749
1	0	0.897234	-4.143933	-3.637323
1	0	-0.897234	-4.143933	-3.637323

$S(SSCC_6H_4OMe\text{-}2)_2$ (**4e**)-*anti*
Total energy: -2754.5023544 hartrees

16	0	0.000000	0.000000	2.862998
16	0	0.695766	1.473630	1.590361
6	0	-0.749001	2.182101	0.861375
16	0	-2.298482	1.799112	1.154442
6	0	-0.295885	3.208172	-0.108105
6	0	0.395177	2.803195	-1.267424
6	0	-0.503178	4.572496	0.136817
6	0	0.900917	3.762298	-2.151506
6	0	0.000000	5.527769	-0.747303
6	0	0.708830	5.119879	-1.881495
1	0	-1.041808	4.870419	1.034216
1	0	1.424342	3.454463	-3.052391
1	0	-0.153046	6.585197	-0.548103
1	0	1.103494	5.861324	-2.572305
8	0	0.449430	1.458681	-1.488430
6	0	1.658045	0.946790	-2.048073
1	0	1.743834	1.191439	-3.112490
1	0	2.523087	1.342449	-1.504037
1	0	1.591701	-0.133049	-1.923996
16	0	-0.695766	-1.473630	1.590361

6	0	0.749001	-2.182101	0.861375
16	0	2.298482	-1.799112	1.154442
6	0	0.295885	-3.208172	-0.108105
6	0	-0.395177	-2.803195	-1.267424
6	0	0.503178	-4.572496	0.136817
6	0	-0.900917	-3.762298	-2.151506
6	0	0.000000	-5.527769	-0.747303
6	0	-0.708830	-5.119879	-1.881495
1	0	1.041808	-4.870419	1.034216
1	0	-1.424342	-3.454463	-3.052391
1	0	0.153046	-6.585197	-0.548103
1	0	-1.103494	-5.861324	-2.572305
8	0	-0.449430	-1.458681	-1.488430
6	0	-1.658045	-0.946790	-2.048073
1	0	-1.743834	-1.191439	-3.112490
1	0	-2.523087	-1.342449	-1.504037
1	0	-1.591701	0.133049	-1.923996

$Se(SSCC_6H_4OMe\text{-}2)_2$ (**2e**)-*syn*
Total energy: -4756.9002324 hartrees

34	0	0.000000	0.000000	1.310629
16	0	0.000000	1.570670	-0.358627
6	0	0.000000	2.916122	0.738448
16	0	0.000000	2.615064	2.369406
6	0	0.000000	4.299305	0.183801
6	0	0.000000	4.603724	-1.201435
6	0	0.000000	5.385843	1.079425
6	0	0.000000	5.932634	-1.645816
6	0	0.000000	6.705037	0.640284
6	0	0.000000	6.980891	-0.727940
1	0	0.000000	5.172823	2.143979
1	0	0.000000	6.156201	-2.707149
1	0	0.000000	7.514072	1.365943
1	0	0.000000	8.007597	-1.086837
8	0	0.000000	3.544627	-2.053191
6	0	0.000000	3.785050	-3.452927
1	0	0.000000	2.795899	-3.909968
1	0	0.897162	4.333617	-3.758318
1	0	-0.897162	4.333617	-3.758318
16	0	0.000000	-1.570670	-0.358627
6	0	0.000000	-2.916122	0.738448
16	0	0.000000	-2.615064	2.369406
6	0	0.000000	-4.299305	0.183801
6	0	0.000000	-4.603724	-1.201435
6	0	0.000000	-5.385843	1.079425
6	0	0.000000	-5.932634	-1.645816
6	0	0.000000	-6.705037	0.640284
6	0	0.000000	-6.980891	-0.727940
1	0	0.000000	-5.172823	2.143979
1	0	0.000000	-6.156201	-2.707149
1	0	0.000000	-7.514072	1.365943

1	0	0.000000	-8.007597	-1.086837
8	0	0.000000	-3.544627	-2.053191
6	0	0.000000	-3.785050	-3.452927
1	0	0.000000	-2.795899	-3.909968
1	0	0.897162	-4.333617	-3.758318
1	0	-0.897162	-4.333617	-3.758318

$Se(SSCC_6H_4OMe\text{-}2)_2$ (**2e**)-*anti*
Total energy: -4756.9164138 hartrees

34	0	0.000000	0.000000	3.034434
16	0	0.477363	1.638693	1.623173
6	0	-0.959822	1.880812	0.637805
16	0	-2.416785	1.181147	0.806103
6	0	-0.618674	2.841293	-0.444189
6	0	0.285146	2.470655	-1.467231
6	0	-1.203441	4.113111	-0.462835
6	0	0.586581	3.381131	-2.487586
6	0	-0.894235	5.021771	-1.477117
6	0	0.000000	4.651335	-2.482583
1	0	-1.899893	4.378228	0.330238
1	0	1.274542	3.113652	-3.283351
1	0	-1.348027	6.009226	-1.480186
1	0	0.246700	5.350693	-3.278187
8	0	0.769032	1.205729	-1.386672
6	0	1.623341	0.746802	-2.421357
1	0	1.119113	0.780573	-3.394919
1	0	2.548852	1.332710	-2.463738
1	0	1.855887	-0.285234	-2.159716
16	0	-0.477363	-1.638693	1.623173
6	0	0.959822	-1.880812	0.637805
16	0	2.416785	-1.181147	0.806103
6	0	0.618674	-2.841293	-0.444189
6	0	-0.285146	-2.470655	-1.467231
6	0	1.203441	-4.113111	-0.462835
6	0	-0.586581	-3.381131	-2.487586
6	0	0.894235	-5.021771	-1.477117
6	0	0.000000	-4.651335	-2.482583
1	0	1.899893	-4.378228	0.330238
1	0	-1.274542	-3.113652	-3.283351
1	0	1.348027	-6.009226	-1.480186
1	0	-0.246700	-5.350693	-3.278187
8	0	-0.769032	-1.205729	-1.386672
6	0	-1.623341	-0.746802	-2.421357
1	0	-1.119113	-0.780573	-3.394919
1	0	-2.548852	-1.332710	-2.463738
1	0	-1.855887	0.285234	-2.159716

$Te(SSCC_6H_4OMe\text{-}2)_2$ (**3e**)-*syn*
Total energy: -8968.7560914 hartrees

52	0	0.000000	0.000000	1.446993
16	0	0.000000	1.602017	-0.433335

6	0	0.000000	2.989310	0.593320
16	0	0.000000	2.740265	2.244331
6	0	0.000000	4.357958	0.005906
6	0	0.000000	4.630848	-1.387972
6	0	0.000000	5.465369	0.877461
6	0	0.000000	5.951624	-1.857537
6	0	0.000000	6.774780	0.410314
6	0	0.000000	7.020219	-0.963484
1	0	0.000000	5.279392	1.947258
1	0	0.000000	6.153347	-2.923180
1	0	0.000000	7.599317	1.118320
1	0	0.000000	8.038616	-1.345380
8	0	0.000000	3.558560	-2.221290
6	0	0.000000	3.777928	-3.624645
1	0	0.000000	2.781510	-4.065685
1	0	0.897086	4.321455	-3.939474
1	0	-0.897086	4.321455	-3.939474
16	0	0.000000	-1.602017	-0.433335
6	0	0.000000	-2.989310	0.593320
16	0	0.000000	-2.740265	2.244331
6	0	0.000000	-4.357958	0.005906
6	0	0.000000	-4.630848	-1.387972
6	0	0.000000	-5.465369	0.877461
6	0	0.000000	-5.951624	-1.857537
6	0	0.000000	-6.774780	0.410314
6	0	0.000000	-7.020219	-0.963484
1	0	0.000000	-5.279392	1.947258
1	0	0.000000	-6.153347	-2.923180
1	0	0.000000	-7.599317	1.118320
1	0	0.000000	-8.038616	-1.345380
8	0	0.000000	-3.558560	-2.221290
6	0	0.000000	-3.777928	-3.624645
1	0	0.000000	-2.781510	-4.065685
1	0	0.897086	-4.321455	-3.939474
1	0	-0.897086	-4.321455	-3.939474

$Te(SSCC_6H_4OMe\text{-}2)_2$ (**3e**)-*anti*
Total energy: -8968.7543828 hartrees

52	0	0.000000	0.000000	2.849387
16	0	0.538955	1.722641	1.306892
6	0	-0.947404	2.023998	0.388945
16	0	-2.393869	1.320776	0.605955
6	0	-0.644489	3.026481	-0.664738
6	0	0.162343	2.655942	-1.762790
6	0	-1.134538	4.333829	-0.568559
6	0	0.484440	3.605465	-2.739264
6	0	-0.811238	5.279985	-1.544148
6	0	0.000000	4.912869	-2.619513
1	0	-1.758105	4.599298	0.283038
1	0	1.099640	3.336772	-3.592537
1	0	-1.187218	6.296307	-1.461443

1	0	0.257109	5.644244	-3.382298
8	0	0.523678	1.347060	-1.795564
6	0	1.531670	0.954991	-2.716076
1	0	1.175956	1.025791	-3.751145
1	0	2.433321	1.565637	-2.591434
1	0	1.747277	-0.084630	-2.472410
16	0	-0.538955	-1.722641	1.306892
6	0	0.947404	-2.023998	0.388945
16	0	2.393869	-1.320776	0.605955
6	0	0.644489	-3.026481	-0.664738
6	0	-0.162343	-2.655942	-1.762790
6	0	1.134538	-4.333829	-0.568559
6	0	-0.484440	-3.605465	-2.739264
6	0	0.811238	-5.279985	-1.544148
6	0	0.000000	-4.912869	-2.619513
1	0	1.758105	-4.599298	0.283038
1	0	-1.099640	-3.336772	-3.592537
1	0	1.187218	-6.296307	-1.461443
1	0	-0.257109	-5.644244	-3.382298
8	0	-0.523678	-1.347060	-1.795564
6	0	-1.531670	-0.954991	-2.716076
1	0	-1.175956	-1.025791	-3.751145
1	0	-2.433321	-1.565637	-2.591434
1	0	-1.747277	0.084630	-2.472410

$O(SOCMe)_2$ (**13**)-*syn*
Total energy: -1175.9749332 hartrees

8	0	0.000000	0.000000	0.060603
16	0	0.000000	1.399954	-0.918246
6	0	0.000000	2.573058	0.433346
8	0	0.000000	2.238531	1.592271
6	0	0.000000	3.999670	-0.064573
1	0	0.000000	4.062374	-1.156860
1	0	0.887501	4.502959	0.327789
1	0	-0.887501	4.502959	0.327789
16	0	0.000000	-1.399954	-0.918246
6	0	0.000000	-2.573058	0.433346
8	0	0.000000	-2.238531	1.592271
6	0	0.000000	-3.999670	-0.064573
1	0	0.000000	-4.062374	-1.156860
1	0	0.887501	-4.502959	0.327789
1	0	-0.887501	-4.502959	0.327789

$O(SOCMe)_2$ (**13**)-*anti*
Total energy: -1175.9957708 hartrees

8	0	0.000000	0.000000	1.116059
16	0	0.866744	1.150304	0.246710
6	0	-0.470781	2.263506	-0.162534
8	0	-1.625464	2.012551	0.102817
6	0	0.000000	3.516394	-0.861642
1	0	-0.178938	4.369282	-0.200732

1	0	1.063205	3.477585	-1.116857
1	0	-0.589953	3.651850	-1.771482
16	0	-0.866744	-1.150304	0.246710
6	0	0.470781	-2.263506	-0.162534
8	0	1.625464	-2.012551	0.102817
6	0	0.000000	-3.516394	-0.861642
1	0	0.178938	-4.369282	-0.200732
1	0	-1.063205	-3.477585	-1.116857
1	0	0.589953	-3.651850	-1.771482

$S(SOCMe)_2$ (**7a**)-*syn*
Total energy: -1498.6180248 hartrees

16	0	0.000000	0.000000	0.567405
16	0	0.000000	1.527776	-0.902399
6	0	0.000000	2.864929	0.278642
8	0	0.000000	2.665952	1.475710
6	0	0.000000	4.235178	-0.353174
1	0	0.886210	4.774292	-0.007425
1	0	0.000000	4.191731	-1.444498
1	0	-0.886210	4.774292	-0.007425
16	0	0.000000	-1.527776	-0.902399
6	0	0.000000	-2.864929	0.278642
8	0	0.000000	-2.665952	1.475710
6	0	0.000000	-4.235178	-0.353174
1	0	0.886210	-4.774292	-0.007425
1	0	0.000000	-4.191731	-1.444498
1	0	-0.886210	-4.774292	-0.007425

$S(SOCMe)_2$ (**7a**)-*anti*
Total energy: -1498.6380838 hartrees

16	0	0.000000	0.000000	1.349654
16	0	0.925683	1.355864	0.102327
6	0	-0.460343	2.451484	-0.324697
8	0	-1.603036	2.227408	-0.007514
6	0	0.000000	3.662089	-1.099213
1	0	0.330049	4.429360	-0.391371
1	0	0.835956	3.421097	-1.761125
1	0	-0.840943	4.048183	-1.678391
16	0	-0.925683	-1.355864	0.102327
6	0	0.460343	-2.451484	-0.324697
8	0	1.603036	-2.227408	-0.007514
6	0	0.000000	-3.662089	-1.099213
1	0	-0.330049	-4.429360	-0.391371
1	0	-0.835956	-3.421097	-1.761125
1	0	0.840943	-4.048183	-1.678391

$Se(SOCMe)_2$ (**5a**)-*syn*
Total energy: -3501.0401046 hartrees

34	0	0.000000	0.000000	0.544509
16	0	0.000000	1.602919	-1.045602
6	0	0.000000	2.914813	0.154155

8	0	0.000000	2.684768	1.349596
6	0	0.000000	4.305459	-0.431638
1	0	0.000000	4.298332	-1.523462
1	0	0.885998	4.832995	-0.067707
1	0	-0.885998	4.832995	-0.067707
16	0	0.000000	-1.602919	-1.045602
6	0	0.000000	-2.914813	0.154155
8	0	0.000000	-2.684768	1.349596
6	0	0.000000	-4.305459	-0.431638
1	0	0.000000	-4.298332	-1.523462
1	0	0.885998	-4.832995	-0.067707
1	0	-0.885998	-4.832995	-0.067707

$Se(SOCMe)_2$ (**5a**)-*anti*
Total energy: -3501.0532058 hartrees

34	0	0.000000	0.000000	1.247373
16	0	0.000000	1.715227	-0.129703
6	0	-1.757691	1.817338	-0.597166
8	0	-2.582643	0.996857	-0.278965
6	0	-2.039541	3.054712	-1.416327
1	0	-2.125730	3.914615	-0.744364
1	0	-1.232752	3.253717	-2.126672
1	0	-2.983447	2.914657	-1.946376
16	0	0.000000	-1.715227	-0.129703
6	0	1.757691	-1.817338	-0.597166
8	0	2.582643	-0.996857	-0.278965
6	0	2.039541	-3.054712	-1.416327
1	0	2.125730	-3.914615	-0.744364
1	0	1.232752	-3.253717	-2.126672
1	0	2.983447	-2.914657	-1.946376

$Te(SOCMe)_2$ (**6a**)-*syn*
Total energy: -7712.8862231 hartrees

52	0	0.000000	0.000000	0.556116
16	0	0.000000	1.673699	-1.220577
6	0	0.000000	2.937381	0.007752
8	0	0.000000	2.640269	1.199731
6	0	0.000000	4.365312	-0.476411
1	0	0.885496	4.866616	-0.075077
1	0	0.000000	4.433813	-1.565546
1	0	-0.885496	4.866616	-0.075077
16	0	0.000000	-1.673699	-1.220577
6	0	0.000000	-2.937381	0.007752
8	0	0.000000	-2.640269	1.199731
6	0	0.000000	-4.365312	-0.476411
1	0	0.885496	-4.866616	-0.075077
1	0	0.000000	-4.433813	-1.565546
1	0	-0.885496	-4.866616	-0.075077

$Te(SOCMe)_2$ (**6a**)-*anti*
Total energy: -7712.8905401 hartrees

52	0	0.000000	0.000000	1.155466
16	0	0.000000	1.814487	-0.362598
6	0	-1.773142	1.922115	-0.809199
8	0	-2.601051	1.129061	-0.435385
6	0	-2.046462	3.113417	-1.696608
1	0	-1.887882	4.036359	-1.130265
1	0	-1.363336	3.118229	-2.550798
1	0	-3.080761	3.063526	-2.041554
16	0	0.000000	-1.814487	-0.362598
6	0	1.773142	-1.922115	-0.809199
8	0	2.601051	-1.129061	-0.435385
6	0	2.046462	-3.113417	-1.696608
1	0	1.887882	-4.036359	-1.130265
1	0	1.363336	-3.118229	-2.550798
1	0	3.080761	-3.063526	-2.041554

$S(SOCPh)_2$ (**7d**)-*syn*
Total energy: -1880.8782175 hartrees

16	0	0.000000	0.000000	0.909247
16	0	0.000000	1.515413	-0.576746
6	0	0.000000	2.841148	0.629921
8	0	0.000000	2.586795	1.821442
6	0	0.000000	4.221752	0.077332
6	0	0.000000	4.486893	-1.300624
6	0	0.000000	5.282219	0.996767
6	0	0.000000	5.807099	-1.751546
6	0	0.000000	6.597825	0.536547
6	0	0.000000	6.863911	-0.836498
1	0	0.000000	3.676698	-2.026841
1	0	0.000000	5.058396	2.060061
1	0	0.000000	6.010423	-2.819505
1	0	0.000000	7.418169	1.250100
1	0	0.000000	7.891318	-1.192778
16	0	0.000000	-1.515413	-0.576746
6	0	0.000000	-2.841148	0.629921
8	0	0.000000	-2.586795	1.821442
6	0	0.000000	-4.221752	0.077332
6	0	0.000000	-4.486893	-1.300624
6	0	0.000000	-5.282219	0.996767
6	0	0.000000	-5.807099	-1.751546
6	0	0.000000	-6.597825	0.536547
6	0	0.000000	-6.863911	-0.836498
1	0	0.000000	-3.676698	-2.026841
1	0	0.000000	-5.058396	2.060061
1	0	0.000000	-6.010423	-2.819505
1	0	0.000000	-7.418169	1.250100
1	0	0.000000	-7.891318	-1.192778

$S(SOCPh)_2$ (**7d**)-*anti*
Total energy: -1880.9009239 hartrees

16	0	0.000000	0.000000	2.213812

16	0	0.536802	1.547709	0.961723
6	0	-1.101562	2.203122	0.521227
8	0	-2.130818	1.616972	0.774805
6	0	-1.028469	3.469708	-0.251329
6	0	0.000000	4.404260	-0.052637
6	0	-2.033732	3.714273	-1.200005
6	0	0.015741	5.580800	-0.804326
6	0	-2.002182	4.887038	-1.952536
6	0	-0.977130	5.819779	-1.758626
1	0	0.758670	4.234490	0.707734
1	0	-2.824509	2.980337	-1.333727
1	0	0.803634	6.312214	-0.642282
1	0	-2.775433	5.074491	-2.693600
1	0	-0.957184	6.735213	-2.345227
16	0	-0.536802	-1.547709	0.961723
6	0	1.101562	-2.203122	0.521227
8	0	2.130818	-1.616972	0.774805
6	0	1.028469	-3.469708	-0.251329
6	0	0.000000	-4.404260	-0.052637
6	0	2.033732	-3.714273	-1.200005
6	0	-0.015741	-5.580800	-0.804326
6	0	2.002182	-4.887038	-1.952536
6	0	0.977130	-5.819779	-1.758626
1	0	-0.758670	-4.234490	0.707734
1	0	2.824509	-2.980337	-1.333727
1	0	-0.803634	-6.312214	-0.642282
1	0	2.775433	-5.074491	-2.693600
1	0	0.957184	-6.735213	-2.345227

$Se(SOCPh)_2$ (**5d**)-*syn*
Total energy: -3883.3007571 hartrees

34	0	0.000000	0.000000	0.864097
16	0	0.000000	1.591163	-0.740838
6	0	0.000000	2.890923	0.482604
8	0	0.000000	2.607981	1.672231
6	0	0.000000	4.287214	-0.027934
6	0	0.000000	4.590935	-1.398005
6	0	0.000000	5.321366	0.921357
6	0	0.000000	5.923288	-1.811407
6	0	0.000000	6.649321	0.498058
6	0	0.000000	6.954017	-0.866971
1	0	0.000000	3.800185	-2.145343
1	0	0.000000	5.068247	1.978074
1	0	0.000000	6.156804	-2.873196
1	0	0.000000	7.449373	1.234322
1	0	0.000000	7.991071	-1.194145
16	0	0.000000	-1.591163	-0.740838
6	0	0.000000	-2.890923	0.482604
8	0	0.000000	-2.607981	1.672231
6	0	0.000000	-4.287214	-0.027934
6	0	0.000000	-4.590935	-1.398005

6	0	0.000000	-5.321366	0.921357
6	0	0.000000	-5.923288	-1.811407
6	0	0.000000	-6.649321	0.498058
6	0	0.000000	-6.954017	-0.866971
1	0	0.000000	-3.800185	-2.145343
1	0	0.000000	-5.068247	1.978074
1	0	0.000000	-6.156804	-2.873196
1	0	0.000000	-7.449373	1.234322
1	0	0.000000	-7.991071	-1.194145

$Se(SOCPh)_2$ (**5d**)-*anti*
Total energy: -3883.3152784 hartrees

34	0	0.000000	0.000000	2.170523
16	0	0.810716	1.507769	0.787734
6	0	-0.708123	2.382934	0.290945
8	0	-1.819393	1.970834	0.538282
6	0	-0.429067	3.593300	-0.526751
6	0	0.722275	4.373384	-0.336618
6	0	-1.367797	3.943652	-1.510130
6	0	0.926855	5.503071	-1.131090
6	0	-1.147406	5.066958	-2.305325
6	0	0.000000	5.846238	-2.119408
1	0	1.432812	4.123239	0.447553
1	0	-2.256072	3.329740	-1.636695
1	0	1.811315	6.116229	-0.976844
1	0	-1.868881	5.335303	-3.073266
1	0	0.167299	6.723849	-2.739371
16	0	-0.810716	-1.507769	0.787734
6	0	0.708123	-2.382934	0.290945
8	0	1.819393	-1.970834	0.538282
6	0	0.429067	-3.593300	-0.526751
6	0	-0.722275	-4.373384	-0.336618
6	0	1.367797	-3.943652	-1.510130
6	0	-0.926855	-5.503071	-1.131090
6	0	1.147406	-5.066958	-2.305325
6	0	0.000000	-5.846238	-2.119408
1	0	-1.432812	-4.123239	0.447553
1	0	2.256072	-3.329740	-1.636695
1	0	-1.811315	-6.116229	-0.976844
1	0	1.868881	-5.335303	-3.073266
1	0	-0.167299	-6.723849	-2.739371

$Te(SOCPh)_2$ (**6d**)-*syn*
Total energy: -8095.1497105 hartrees

52	0	0.000000	0.000000	0.845125
16	0	0.000000	1.660247	-0.946566
6	0	0.000000	2.917070	0.294664
8	0	0.000000	2.581745	1.482918
6	0	0.000000	4.337788	-0.134511
6	0	0.000000	4.712560	-1.487451
6	0	0.000000	5.320870	0.868608

6	0	0.000000	6.064674	-1.830081
6	0	0.000000	6.669052	0.514794
6	0	0.000000	7.044538	-0.832643
1	0	0.000000	3.957967	-2.271148
1	0	0.000000	5.012986	1.910840
1	0	0.000000	6.353836	-2.878119
1	0	0.000000	7.429855	1.291590
1	0	0.000000	8.097353	-1.104975
16	0	0.000000	-1.660247	-0.946566
6	0	0.000000	-2.917070	0.294664
8	0	0.000000	-2.581745	1.482918
6	0	0.000000	-4.337788	-0.134511
6	0	0.000000	-4.712560	-1.487451
6	0	0.000000	-5.320870	0.868608
6	0	0.000000	-6.064674	-1.830081
6	0	0.000000	-6.669052	0.514794
6	0	0.000000	-7.044538	-0.832643
1	0	0.000000	-3.957967	-2.271148
1	0	0.000000	-5.012986	1.910840
1	0	0.000000	-6.353836	-2.878119
1	0	0.000000	-7.429855	1.291590
1	0	0.000000	-8.097353	-1.104975

$Te(SOCPh)_2$ (**6d**)-*anti*
Total energy: -8095.1526333 hartrees

52	0	0.000000	0.000000	2.103752
16	0	0.000000	1.807794	0.576963
6	0	-1.763029	1.841206	0.087724
8	0	-2.540329	0.961694	0.385139
6	0	-2.108061	3.000152	-0.778792
6	0	-1.450428	4.236158	-0.675650
6	0	-3.142444	2.823649	-1.712202
6	0	-1.831201	5.289435	-1.509186
6	0	-3.505474	3.878690	-2.547558
6	0	-2.851187	5.111689	-2.448290
1	0	-0.669121	4.384351	0.065969
1	0	-3.642820	1.860333	-1.772341
1	0	-1.331457	6.251147	-1.423053
1	0	-4.299260	3.741004	-3.277779
1	0	-3.139227	5.933882	-3.099134
16	0	0.000000	-1.807794	0.576963
6	0	1.763029	-1.841206	0.087724
8	0	2.540329	-0.961694	0.385139
6	0	2.108061	-3.000152	-0.778792
6	0	1.450428	-4.236158	-0.675650
6	0	3.142444	-2.823649	-1.712202
6	0	1.831201	-5.289435	-1.509186
6	0	3.505474	-3.878690	-2.547558
6	0	2.851187	-5.111689	-2.448290
1	0	0.669121	-4.384351	0.065969
1	0	3.642820	-1.860333	-1.772341

1	0	1.331457	-6.251147	-1.423053
1	0	4.299260	-3.741004	-3.277779
1	0	3.139227	-5.933882	-3.099134

$S(SOCC_6H_4OMe\text{-}2)_2$ (**7e**)-*syn*
Total energy: -2109.3331641 hartrees

16	0	0.000000	0.000000	1.352658
16	0	0.000000	1.511725	-0.151307
6	0	0.000000	2.831018	1.047238
8	0	0.000000	2.562785	2.240361
6	0	0.000000	4.243434	0.565000
6	0	0.000000	4.637212	-0.789954
6	0	0.000000	5.235460	1.557185
6	0	0.000000	5.995904	-1.128544
6	0	0.000000	6.586639	1.222521
6	0	0.000000	6.963102	-0.122071
1	0	0.000000	4.915359	2.595210
1	0	0.000000	6.308152	-2.167378
1	0	0.000000	7.340885	2.004694
1	0	0.000000	8.015249	-0.397712
8	0	0.000000	3.631766	-1.704721
6	0	0.000000	3.964626	-3.085800
1	0	0.000000	3.008885	-3.608707
1	0	0.897159	4.532844	-3.352515
1	0	-0.897159	4.532844	-3.352515
16	0	0.000000	-1.511725	-0.151307
6	0	0.000000	-2.831018	1.047238
8	0	0.000000	-2.562785	2.240361
6	0	0.000000	-4.243434	0.565000
6	0	0.000000	-4.637212	-0.789954
6	0	0.000000	-5.235460	1.557185
6	0	0.000000	-5.995904	-1.128544
6	0	0.000000	-6.586639	1.222521
6	0	0.000000	-6.963102	-0.122071
1	0	0.000000	-4.915359	2.595210
1	0	0.000000	-6.308152	-2.167378
1	0	0.000000	-7.340885	2.004694
1	0	0.000000	-8.015249	-0.397712
8	0	0.000000	-3.631766	-1.704721
6	0	0.000000	-3.964626	-3.085800
1	0	0.000000	-3.008885	-3.608707
1	0	0.897159	-4.532844	-3.352515
1	0	-0.897159	-4.532844	-3.352515

$S(SOCC_6H_4OMe\text{-}2)_2$ (**7e**)-*anti*
Total energy: -2109.3515267 hartrees

16	0	0.000000	0.000000	2.588728
16	0	0.000000	1.645998	1.337289
6	0	-1.721488	1.597610	0.758975
8	0	-2.498403	0.749092	1.147746
6	0	-2.103257	2.578706	-0.301513

6	0	-1.424666	3.787297	-0.565097
6	0	-3.212699	2.237029	-1.089051
6	0	-1.854646	4.620885	-1.604656
6	0	-3.640467	3.064118	-2.124802
6	0	-2.956242	4.253739	-2.380770
1	0	-3.725843	1.305167	-0.867874
1	0	-1.346368	5.557226	-1.809324
1	0	-4.496618	2.780496	-2.730868
1	0	-3.278466	4.909157	-3.186773
8	0	-0.380097	4.077951	0.254297
6	0	0.455853	5.178547	-0.076883
1	0	0.850137	5.077184	-1.093455
1	0	-0.082345	6.126935	0.024531
1	0	1.272025	5.143224	0.643744
16	0	0.000000	-1.645998	1.337289
6	0	1.721488	-1.597610	0.758975
8	0	2.498403	-0.749092	1.147746
6	0	2.103257	-2.578706	-0.301513
6	0	1.424666	-3.787297	-0.565097
6	0	3.212699	-2.237029	-1.089051
6	0	1.854646	-4.620885	-1.604656
6	0	3.640467	-3.064118	-2.124802
6	0	2.956242	-4.253739	-2.380770
1	0	3.725843	-1.305167	-0.867874
1	0	1.346368	-5.557226	-1.809324
1	0	4.496618	-2.780496	-2.730868
1	0	3.278466	-4.909157	-3.186773
8	0	0.380097	-4.077951	0.254297
6	0	-0.455853	-5.178547	-0.076883
1	0	-0.850137	-5.077184	-1.093455
1	0	0.082345	-6.126935	0.024531
1	0	-1.272025	-5.143224	0.643744

$Se(SOCC_6H_4OMe\text{-}2)_2$ (**5e**)-*syn*
Total energy: -4111.7545049 hartrees

34	0	0.000000	0.000000	1.300651
16	0	0.000000	1.585933	-0.322088
6	0	0.000000	2.887457	0.886766
8	0	0.000000	2.599072	2.079323
6	0	0.000000	4.309646	0.435335
6	0	0.000000	4.731989	-0.911667
6	0	0.000000	5.280736	1.448555
6	0	0.000000	6.098094	-1.219881
6	0	0.000000	6.638667	1.142906
6	0	0.000000	7.043790	-0.193292
1	0	0.000000	4.939261	2.479753
1	0	0.000000	6.432887	-2.251645
1	0	0.000000	7.375993	1.941067
1	0	0.000000	8.101546	-0.446602
8	0	0.000000	3.748395	-1.849391
6	0	0.000000	4.114209	-3.222208

1	0	0.000000	3.171188	-3.767583
1	0	0.897166	4.688529	-3.475606
1	0	-0.897166	4.688529	-3.475606
16	0	0.000000	-1.585933	-0.322088
6	0	0.000000	-2.887457	0.886766
8	0	0.000000	-2.599072	2.079323
6	0	0.000000	-4.309646	0.435335
6	0	0.000000	-4.731989	-0.911667
6	0	0.000000	-5.280736	1.448555
6	0	0.000000	-6.098094	-1.219881
6	0	0.000000	-6.638667	1.142906
6	0	0.000000	-7.043790	-0.193292
1	0	0.000000	-4.939261	2.479753
1	0	0.000000	-6.432887	-2.251645
1	0	0.000000	-7.375993	1.941067
1	0	0.000000	-8.101546	-0.446602
8	0	0.000000	-3.748395	-1.849391
6	0	0.000000	-4.114209	-3.222208
1	0	0.000000	-3.171188	-3.767583
1	0	0.897166	-4.688529	-3.475606
1	0	-0.897166	-4.688529	-3.475606

$Se(SOCC_6H_4OMe\text{-}2)_2$ (**5e**)-*anti*
Total energy: -4111.7649057 hartrees

34	0	0.000000	0.000000	2.579597
16	0	0.190508	1.707159	1.194215
6	0	-1.509471	1.811772	0.557309
8	0	-2.397662	1.091401	0.962708
6	0	-1.718838	2.741241	-0.594903
6	0	-0.953924	3.900465	-0.842768
6	0	-2.748785	2.399039	-1.483239
6	0	-1.220529	4.684905	-1.971407
6	0	-3.011439	3.177019	-2.608788
6	0	-2.243040	4.317193	-2.849596
1	0	-3.330726	1.506174	-1.270607
1	0	-0.647690	5.585085	-2.167816
1	0	-3.805552	2.893799	-3.294305
1	0	-2.436957	4.934005	-3.724210
8	0	0.000000	4.197205	0.078976
6	0	0.919943	5.240369	-0.213006
1	0	1.425382	5.059929	-1.167584
1	0	0.419644	6.214498	-0.231599
1	0	1.644064	5.217591	0.600435
16	0	-0.190508	-1.707159	1.194215
6	0	1.509471	-1.811772	0.557309
8	0	2.397662	-1.091401	0.962708
6	0	1.718838	-2.741241	-0.594903
6	0	0.953924	-3.900465	-0.842768
6	0	2.748785	-2.399039	-1.483239
6	0	1.220529	-4.684905	-1.971407
6	0	3.011439	-3.177019	-2.608788

6	0	2.243040	-4.317193	-2.849596
1	0	3.330726	-1.506174	-1.270607
1	0	0.647690	-5.585085	-2.167816
1	0	3.805552	-2.893799	-3.294305
1	0	2.436957	-4.934005	-3.724210
8	0	0.000000	-4.197205	0.078976
6	0	-0.919943	-5.240369	-0.213006
1	0	-1.425382	-5.059929	-1.167584
1	0	-0.419644	-6.214498	-0.231599
1	0	-1.644064	-5.217591	0.600435

$Te(SOCC_6H_4OMe\text{-}2)_2$ (**6e**)-*syn*
Total energy: -8323.5999567 hartrees

52	0	0.000000	0.000000	1.269788
16	0	0.000000	1.654027	-0.532928
6	0	0.000000	2.922673	0.688001
8	0	0.000000	2.588083	1.880071
6	0	0.000000	4.362081	0.306345
6	0	0.000000	4.849167	-1.020730
6	0	0.000000	5.283741	1.366311
6	0	0.000000	6.230000	-1.257610
6	0	0.000000	6.654866	1.128392
6	0	0.000000	7.124639	-0.186385
1	0	0.000000	4.892335	2.379734
1	0	0.000000	6.616366	-2.271131
1	0	0.000000	7.351929	1.961960
1	0	0.000000	8.193464	-0.388145
8	0	0.000000	3.918744	-2.009550
6	0	0.000000	4.360558	-3.359946
1	0	0.000000	3.448865	-3.956239
1	0	0.897124	4.947914	-3.582128
1	0	-0.897124	4.947914	-3.582128
16	0	0.000000	-1.654027	-0.532928
6	0	0.000000	-2.922673	0.688001
8	0	0.000000	-2.588083	1.880071
6	0	0.000000	-4.362081	0.306345
6	0	0.000000	-4.849167	-1.020730
6	0	0.000000	-5.283741	1.366311
6	0	0.000000	-6.230000	-1.257610
6	0	0.000000	-6.654866	1.128392
6	0	0.000000	-7.124639	-0.186385
1	0	0.000000	-4.892335	2.379734
1	0	0.000000	-6.616366	-2.271131
1	0	0.000000	-7.351929	1.961960
1	0	0.000000	-8.193464	-0.388145
8	0	0.000000	-3.918744	-2.009550
6	0	0.000000	-4.360558	-3.359946
1	0	0.000000	-3.448865	-3.956239
1	0	0.897124	-4.947914	-3.582128
1	0	-0.897124	-4.947914	-3.582128

$Te(SOCC_6H_4OMe\text{-}2)_2$ (**6e**)-*anti*
Total energy: -8323.600841

52	0	0.000000	0.000000	2.143429
16	0	0.649506	1.697722	0.620883
6	0	-0.981569	2.408030	0.209210
8	0	-2.018975	1.847936	0.494785
6	0	-0.959039	3.768488	-0.406025
6	0	0.047579	4.229428	-1.279982
6	0	-2.014767	4.623609	-0.058540
6	0	0.000000	5.542069	-1.764228
6	0	-2.058831	5.931593	-0.538052
6	0	-1.048402	6.385991	-1.387206
1	0	-2.786361	4.243686	0.606373
1	0	0.761082	5.908658	-2.445197
1	0	-2.873442	6.590669	-0.250358
1	0	-1.070871	7.404446	-1.768251
8	0	0.998149	3.322738	-1.627641
6	0	2.149919	3.786375	-2.319810
1	0	1.897147	4.115418	-3.333535
1	0	2.632977	4.601645	-1.770734
1	0	2.816921	2.926697	-2.370929
16	0	-0.649506	-1.697722	0.620883
6	0	0.981569	-2.408030	0.209210
8	0	2.018975	-1.847936	0.494785
6	0	0.959039	-3.768488	-0.406025
6	0	-0.047579	-4.229428	-1.279982
6	0	2.014767	-4.623609	-0.058540
6	0	0.000000	-5.542069	-1.764228
6	0	2.058831	-5.931593	-0.538052
6	0	1.048402	-6.385991	-1.387206
1	0	2.786361	-4.243686	0.606373
1	0	-0.761082	-5.908658	-2.445197
1	0	2.873442	-6.590669	-0.250358
1	0	1.070871	-7.404446	-1.768251
8	0	-0.998149	-3.322738	-1.627641
6	0	-2.149919	-3.786375	-2.319810
1	0	-1.897147	-4.115418	-3.333535
1	0	-2.632977	-4.601645	-1.770734
1	0	-2.816921	-2.926697	-2.370929
