Supporting Information

Relativistic effect on ^{125}Te and ^{33}S NMR chemical shifts of various tellurium and sulfur species, together with ^{77}Se of selenium congeners, in the framework of zeroth-order regular approximation: applicability to tellurium compounds

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Table S1. List of symbols and definitions of σ(Z: Z = Te, Se, and S) with the relativistic effect at the nonreltivistic, scalar ZORA relativistic, and spin-orbit ZORA relativistic levels[a]

Term/Conditions	Non-relativistic	Scalar-ZORA relativistic (Rlt-sc)	Relativistic Effect at Rlt-sc
Diamagnetic ($\sigma^{d}(Z)$)	$\sigma^{d}(Z)_{Non}$	$\sigma^{d}(Z)_{Rlt\text{-}sc}$	$\sigma^{d}(Z)_{Rlt\text{-}sc} - \sigma^{d}(Z)_{Non} = \Delta\sigma^{d}(Z)_{Rlt\text{-}sc}$
Paramagnetic ($\sigma^{p}(Z)$)	$\sigma^{p}(Z)_{Non}$	$\sigma^{p}(Z)_{Rlt\text{-}sc}$	$\sigma^{p}(Z)_{Rlt\text{-}sc} - \sigma^{p}(Z)_{Non} = \Delta\sigma^{p}(Z)_{Rlt\text{-}sc}$
$\sigma^{d}(Z) + \sigma^{p}(Z)$	$\sigma^{d+p}(Z)_{Non}$	$\sigma^{d+p}(Z)_{Rlt\text{-}sc}$	$\sigma^{d+p}(Z)_{Rlt\text{-}sc} - \sigma^{d+p}(Z)_{Non} = \Delta\sigma^{d+p}(Z)_{Rlt\text{-}sc}$
Spin-orbit	---	---	---
Total[b]	$\sigma^{d+p}(Z)_{Non}$	$\sigma^{d+p}(Z)_{Rlt\text{-}sc}$	$\Delta\sigma^{d+p}(Z)_{Rlt\text{-}sc}$[c]

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Term/Conditions	Spin-orbit ZORA relativistic (Rlt-so)	Relativistic Effect at Rlt-so
Diamagnetic ($\sigma^{d}(Z)$)	$\sigma^{d}(Z)_{Rlt\text{-}so}$	$\Delta\sigma^{d}(Z)_{Rlt\text{-}so} = \sigma^{d}(Z)_{Rlt\text{-}so} - \sigma^{d}(Z)_{Non}$
Paramagnetic ($\sigma^{p}(Z)$)	$\sigma^{p}(Z)_{Rlt\text{-}so}$	$\Delta\sigma^{p}(Z)_{Rlt\text{-}so} = \sigma^{p}(Z)_{Rlt\text{-}so} - \sigma^{p}(Z)_{Non}$
$\sigma^{d}(Z) + \sigma^{p}(Z)$	$\sigma^{d+p}(Z)_{Rlt\text{-}so}$	$\Delta\sigma^{d+p}(Z)_{Rlt\text{-}so} = \sigma^{d+p}(Z)_{Rlt\text{-}so} - \sigma^{d+p}(Z)_{Non}$
Spin-orbit	$\sigma^{so}(Z)_{Rlt\text{-}so}$	$\sigma^{so}(Z)_{Rlt\text{-}so}$
Total ($\sigma^{t}(Z)$)	$\sigma^{d+p}(Z)_{Rlt\text{-}so} + \sigma^{so}(Z)_{Rlt\text{-}so}$	$\Delta\sigma^{d+p}(Z)_{Rlt\text{-}so} + \sigma^{so}(Z)_{Rlt\text{-}so} = \Delta\sigma^{t}(Z)_{Rlt\text{-}so}$

[a] Values of σ(Z) at Rlt-so are very close to those at Rlt-sc, except for $\sigma^{so}(Z)_{Rlt\text{-}so}$, where $\sigma^{so}(Z)_{Rlt\text{-}so}$, originates inherently as the spin-orbit effect. Therefore, the discussion is focused at the Rlt-so level. [b] The total turm could be used for $\sigma^{t}(Z)_{Rlt\text{-}sc}$ at the Rlt-sc level. However, the term is denoted by $\sigma^{d+p}(Z)_{Rlt\text{-}sc}$ in this paper, to clarify the absence of $\sigma^{so}(Z)_{Rlt\text{-}so}$ in the total term at the Non and Rlt-sc levels. [c] Similarly to the case of $\sigma^{d+p}(Z)_{Rlt\text{-}sc}$, $\Delta\sigma^{d+p}(Z)_{Rlt\text{-}sc}$ is employed to show the relativistic effect at the Rlt-sc level in this paper. It is appearent that $\Delta\sigma^{d+p}(Z)_{Rlt\text{-}sc}$ does not contain at the Rlt-sc level.

Table S2. The σ^{d}(Se), σ^{p}(Se), σ^{d+p}(Se), σ^{so}(Se), and σ^{t}(Se) Values Calculated with the QZ4Pae Basis Sets at the Nonrelativistic (Non) and Spin-orbit ZORA Relativistic (Rlt-so) Levels for Various Selenium Species[a-d]

Species	σ^{d}_{Non}	σ^{p}_{Non}	σ^{d+p}_{Non}	σ^{d}_{Rlt-so}	$\Delta\sigma^{d}_{Rlt-so}$	σ^{p}_{Rlt-so}	$\Delta\sigma^{p}_{Rlt-so}$
H_2Se (C_{2v})	2994.3	-937.2	2057.1	2973.2	-21.0	-968.2	-31.0
HSe^- ($C_{\infty v}$)	3004.6	-501.3	2503.3	2982.8	-21.8	-524.2	-22.9
H_3Se^+ (C_{3v})	2983.0	-1112.2	1870.8	2962.8	-20.2	-1137.2	-25.0
H_4Se (C_{2v})	2982.7	-910.7	2072.1	2961.8	-20.9	-936.4	-25.8
H_5Se^- (C_{4v})	2977.1	-992.9	1984.3	2955.7	-21.5	-1001.4	-8.5
H_5Se^+ (C_{4v})	2970.3	-1253.4	1717.0	2949.5	-20.9	-1267.7	-14.3
H_6Se (O_h)	2957.8	-1068.4	1889.4	2934.1	-23.7	-1070.3	-1.9
$MeSe^-$ (C_s)	3004.1	-1215.6	1788.5	2981.9	-22.2	-1261.4	-45.8
MeSeH (C_s)	2992.5	-1187.1	1805.4	2971.1	-21.4	-1222.6	-35.5
Me_2Se (C_{2v})	2992.0	-1388.4	1603.6	2969.6	-22.5	-1425.5	-37.0
EtSeH (C_s)	2992.4	-1261.5	1731.0	2971.1	-21.4	-1298.0	-36.5
Et_2Se (C_{2v})	2992.9	-1553.0	1439.9	2970.4	-22.5	-1594.7	-41.6
MeSeSeMe (C_2)	2994.9	-1716.9	1278.0	2972.6	-22.3	-1810.6	-93.7
Me_3Se^+ (C_3)	2975.5	-1607.3	1368.2	2952.6	-22.9	-1639.2	-31.9
Me_4Se (C_{2v})	2972.2	-1352.6	1619.5	2948.8	-23.4	-1381.0	-28.4
Me_5Se^- (C_s)	2967.1	-1261.5	1705.5	2942.9	-24.1	-1277.0	-15.5
Me_5Se^+ (C_s)	2965.2	-1563.1	1402.1	2941.0	-24.2	-1582.7	-19.6
Me_6Se (C_i)	2961.6	-1210.4	1751.2	2937.5	-24.1	-1221.9	-11.6
H_2SeF_2 (C_{2v})	2980.2	-1775.6	1204.6	2959.6	-20.7	-1815.7	-40.1
H_2SeO (C_s)	2984.5	-1966.4	1018.1	2963.3	-21.1	-2012.5	-46.2
H_2SeO_2 (C_{2v})	2981.5	-2090.9	890.6	2960.4	-21.1	-2136.6	-45.7
H_4SeO (C_{2v})	2971.8	-1487.3	1484.5	2950.9	-20.8	-1510.1	-22.8
H_2SeF_2O (C_{2v})	2973.9	-1974.5	999.4	2953.6	-20.4	-2016.4	-41.8
Me_2SeF_2 (C_{2v})	2973.4	-2043.1	930.3	2950.7	-22.7	-2090.8	-47.7
$(CF_3)_2SeF_2$ (C_{2v})	2976.3	-2147.1	829.2	2954.7	-21.6	-2202.9	-55.8
Me_2SeCl_2 (C_{2v})	2975.5	-1719.3	1256.2	2953.1	-22.4	-1761.0	-41.7
Me_2SeBr_2 (C_{2v})	2981.1	-1649.1	1332.0	2958.6	-22.5	-1699.8	-50.7
Me_2SeO (C_s)	2981.8	-2144.7	837.1	2959.5	-22.2	-2193.7	-49.1
Me_2SeO_2 (C_{2v})	2976.2	-2223.5	752.7	2953.6	-22.6	-2272.5	-49.0
Me_2SeF_2O (C_{2v})	2968.6	-2116.8	851.8	2945.8	-22.8	-2162.0	-45.1
F_2SeO (C_s)	2985.7	-2707.1	278.6	2964.9	-20.8	-2788.7	-81.6
Cl_2SeO (C_s)	2985.7	-2833.9	151.8	2964.7	-21.1	-2925.5	-91.7
F_2SeO_2 (C_{2v})	2985.3	-2239.9	745.4	2964.0	-21.3	-2295.5	-55.6
SeF_4 (C_{2v})	2980.4	-2512.6	467.9	2958.8	-21.7	-2583.5	-71.0
$SeCl_4$ (C_s^e)	2984.2	-2712.4	271.8	2963.0	-21.2	-2818.5	-106.1
SeF_5^- (C_s^f)	2978.8	-2360.0	618.8	2957.2	-21.6	-2431.5	-71.5
SeF_5^+ (C_{4v})	2983.3	-2214.0	769.3	2961.7	-21.5	-2274.0	-60.0
$HSeF_5$ (C_{4v})	2966.8	-1984.2	982.6	2944.0	-22.8	-2037.3	-53.1
$MeSeF_5$ (C_s)	2959.4	-2054.8	904.6	2937.4	-22.1	-2109.3	-54.5
SeF_6 (O_h)	2970.1	-2015.6	954.5	2946.6	-23.5	-2068.3	-52.7

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Species	$\sigma^{d+p}_{Rlt\text{-}so}$	$\Delta\sigma^{d+p}_{Rlt\text{-}so}$	$\sigma^{so}_{Rlt\text{-}so}$	$\sigma^{t}_{Rlt\text{-}so}$	$\Delta\sigma^{t}_{Rlt\text{-}so}$
H_2Se (C_{2v})	2005.0	-52.0	182.7	2187.8	130.7
HSe^- ($C_{\infty v}$)	2458.6	-44.7	197.3	2655.9	152.6
H_3Se^+ (C_{3v})	1825.6	-45.2	163.7	1989.3	118.5
H_4Se (C_{2v})	2025.4	-46.7	183.6	2209.0	136.9
H_5Se^- (C_{4v})	1954.3	-30.0	154.5	2108.8	124.5
H_5Se^+ (C_{4v})	1681.7	-35.2	157.5	1839.2	122.3
H_6Se (O_h)	1863.8	-25.6	161.3	2025.2	135.8
$MeSe^-$ (C_s)	1720.6	-67.9	213.5	1934.1	145.6
MeSeH (C_s)	1748.5	-56.9	183.3	1931.8	126.4
Me_2Se (C_{2v})	1544.1	-59.5	180.7	1724.8	121.2
EtSeH (C_s)	1673.1	-57.9	176.9	1849.9	119.0
Et_2Se (C_{2v})	1375.7	-64.2	169.9	1545.6	105.7
MeSeSeMe (C_2)	1162.0	-116.0	220.7	1382.6	104.7
Me_3Se^+ (C_3)	1313.4	-54.8	163.9	1477.3	109.1
Me_4Se (C_{2v})	1567.7	-51.8	171.1	1738.9	119.4
Me_5Se^- (C_s)	1665.9	-39.6	150.7	1816.6	111.0
Me_5Se^+ (C_s)	1358.3	-43.8	157.8	1516.1	114.0
Me_6Se (C_i)	1715.5	-35.7	163.6	1879.1	127.9
H_2SeF_2 (C_{2v})	1143.9	-60.7	139.1	1283.0	78.4
H_2SeO (C_s)	950.8	-67.3	148.4	1099.2	81.1
H_2SeO_2 (C_{2v})	823.9	-66.7	143.9	967.8	77.1
H_4SeO (C_{2v})	1440.9	-43.6	157.7	1598.6	114.1
H_2SeF_2O (C_{2v})	937.2	-62.2	145.7	1082.9	83.5
Me_2SeF_2 (C_{2v})	859.9	-70.4	136.6	996.5	66.2
$(CF_3)_2SeF_2$ (C_{2v})	751.8	-77.4	117.3	869.1	39.9
Me_2SeCl_2 (C_{2v})	1192.1	-64.1	147.4	1339.5	83.4
Me_2SeBr_2 (C_{2v})	1258.8	-73.2	97.2	1356.0	24.0
Me_2SeO (C_s)	765.8	-71.3	149.0	914.8	77.7
Me_2SeO_2 (C_{2v})	681.1	-71.6	145.7	826.9	74.1
Me_2SeF_2O (C_{2v})	783.8	-68.0	145.5	929.3	77.6
F_2SeO (C_s)	176.1	-102.5	104.7	280.9	2.3
Cl_2SeO (C_s)	39.1	-112.7	124.7	163.9	12.0
F_2SeO_2 (C_{2v})	668.5	-76.9	147.1	815.6	70.2
SeF_4 (C_{2v})	375.2	-92.6	95.2	470.4	2.6
$SeCl_4$ (C_s[e])	144.5	-127.3	143.9	288.4	16.6
SeF_5^- (C_s[f])	525.7	-93.1	98.5	624.2	5.4
SeF_5^+ (C_{4v})	687.8	-81.5	203.8	891.6	122.3
$HSeF_5$ (C_{4v})	906.7	-75.9	189.9	1096.6	114.0
$MeSeF_5$ (C_s)	828.1	-76.5	183.9	1012.0	107.4
SeF_6 (O_h)	878.2	-76.2	212.4	1090.7	136.2

[a] Structures optimized at the MP2 level of Gaussian 03 being employed. [b] σ(Se) are denoted by σ in Table. [c] $\Delta\sigma_{Rlt\text{-}so} = \sigma_{Rlt\text{-}so} - \sigma_{Non}$. [d] $\Delta\sigma^{t}_{Rlt\text{-}so} = \sigma^{t}_{Rlt\text{-}so} - \sigma^{d+p}_{Non} = \Delta\sigma^{d+p}_{Rlt\text{-}so} + \sigma^{so}_{Rlt\text{-}so}$. [e] Very close to C_{2v}. [f] Very close to C_{4v}.

Table S3. The σ^{d}(S), σ^{p}(S), σ^{d+p}(S), σ^{so}(S), and σ^{t}(S) Values Calculated with the QZ4Pae Basis Sets at the Nonrelativistic (Non) and Spin-orbit ZORA Relativistic (Rlt-so) Levels for Various Sulfur Species[a-d]

Species	σ^{d}_{Non}	σ^{p}_{Non}	σ^{d+p}_{Non}	σ^{d}_{Rlt-so}	$\Delta\sigma^{d}_{Rlt-so}$	σ^{p}_{Rlt-so}	$\Delta\sigma^{p}_{Rlt-so}$
H_2S (C_{2v})	1053.2	-356.6	696.6	1049.7	-3.6	-357.6	-1.0
HS^- ($C_{\infty v}$)	1058.6	-163.0	895.6	1056.1	-2.4	-165.4	-2.4
H_3S^+ (C_{3v})	1047.2	-447.5	599.7	1042.3	-4.9	-447.0	0.5
H_4S (C_{2v})	1045.3	-262.9	782.4	1037.1	-8.2	-256.6	6.3
H_5S^- (C_{4v})	1046.2	-345.3	700.9	1036.0	-10.2	-338.7	6.7
H_5S^+ (C_{4v})	1042.1	-477.3	564.8	1033.0	-9.1	-469.2	8.1
H_6S (O_h)	1036.8	-341.3	695.6	1032.5	-4.4	-336.3	5.0
MeS^- (C_s)	1059.2	-456.2	603.0	1056.0	-3.2	-459.0	-2.8
MeSH (C_s)	1054.5	-462.1	592.3	1051.0	-3.5	-464.3	-2.2
Me_2S (C_{2v})	1055.0	-538.1	516.9	1051.1	-3.9	-539.6	-1.5
EtSH (C_s)	1053.7	-499.7	554.0	1050.1	-3.6	-501.5	-1.9
Et_2S (C_{2v})	1053.8	-617.7	436.1	1049.8	-4.0	-619.4	-1.7
MeSSMe (C_1)	1055.4	-665.3	390.1	1051.3	-4.1	-669.7	-4.4
Me_3S^+ (C_1)	1051.4	-679.8	371.7	1047.4	-4.1	-680.3	-0.6
Me_4S (C_{2v})	1048.3	-509.6	538.7	1043.6	-4.7	-510.1	-0.5
Me_5S^- (C_s)	1030.3	-442.7	587.5	1025.5	-4.7	-442.2	0.5
Me_5S^+ (C_s)	1044.7	-607.3	437.4	1042.1	-2.7	-608.9	-1.5
Me_6S (C_i)	1031.6	-370.5	661.2	1030.0	-1.6	-373.2	-2.7
H_2SF_2 (C_{2v})	1044.2	-708.0	336.2	1038.3	-5.8	-707.2	0.7
H_2SO (C_s)	1048.0	-851.2	196.8	1044.9	-3.1	-853.6	-2.4
H_2SO_2 (C_{2v})	1048.2	-845.1	203.0	1045.7	-2.4	-846.8	-1.7
H_4SO (C_{2v})	1041.1	-545.1	496.0	1031.2	-9.9	-537.0	8.1
H_2SF_2O (C_{2v})	1044.1	-796.4	247.7	1038.9	-5.3	-794.2	2.2
Me_2SF_2 (C_{2v})	1046.8	-833.2	213.6	1041.7	-5.1	-832.8	0.4
$CF_3SF_2CF_3$ (C_{2v})	1043.7	-893.0	150.8	1040.1	-3.6	-894.0	-1.0
Me_2SCl_2 (C_{2v})	1051.7	-683.6	368.1	1046.9	-4.9	-684.6	-1.0
Me_2SBr_2 (C_{2v})	1052.5	-647.5	404.9	1047.8	-4.6	-651.5	-4.0
Me_2SO (C_s)	1049.7	-922.4	127.3	1046.4	-3.3	-924.4	-2.0
Me_2SO_2 (C_{2v})	1046.8	-893.7	153.1	1044.1	-2.7	-896.0	-2.3
Me_2SF_2O (C_{2v})	1045.4	-851.0	194.5	1040.7	-4.8	-850.8	0.2
F_2SO (C_s)	1043.4	-1133.9	-90.5	1041.5	-1.9	-1137.9	-4.0
Cl_2SO (C_s)	1051.9	-1224.8	-173.0	1048.5	-3.3	-1229.8	-5.0
F_2SO_2 (C_{2v})	1045.8	-883.8	162.0	1044.2	-1.5	-887.7	-3.9
SF_4 (C_{2v})	1035.9	-1079.9	-44.1	1031.7	-4.1	-1080.8	-0.9
SCl_4 (C_{2v})	1055.7	-1122.4	-66.7	1050.3	-5.4	-1129.3	-6.9
SF_5^- (C_{4v})	1033.0	-999.9	33.1	1027.9	-5.2	-1000.2	-0.3
SF_5^+ (C_{4v})	1038.1	-887.8	150.3	1033.9	-4.2	-889.2	-1.4
HSF_5 (C_{4v})	1032.1	-751.0	281.1	1025.4	-6.8	-748.8	2.2
$MeSF_5$ (C_s)	1033.8	-791.6	242.2	1027.8	-6.0	-790.6	1.0
SF_6 (O_h)	1031.0	-785.6	245.4	1026.3	-4.7	-786.2	-0.6

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Species	$\sigma^{d+p}_{Rlt\text{-}so}$	$\Delta\sigma^{d+p}_{Rlt\text{-}so}$	$\sigma^{so}_{Rlt\text{-}so}$	$\sigma^{t}_{Rlt\text{-}so}$	$\Delta\sigma^{t}_{Rlt\text{-}so}$
H_2S (C_{2v})	692.0	-4.6	17.6	709.6	13.0
HS^- ($C_{\infty v}$)	890.7	-4.9	18.3	909.0	13.4
H_3S^+ (C_{3v})	595.3	-4.5	16.6	611.9	12.2
H_4S (C_{2v})	780.5	-1.9	19.0	799.5	17.1
H_5S^- (C_{4v})	697.4	-3.5	17.9	715.3	14.4
H_5S^+ (C_{4v})	563.8	-1.0	18.1	581.8	17.0
H_6S (O_h)	696.2	0.6	19.8	716.0	20.4
MeS^- (C_s)	597.0	-6.0	19.6	616.6	13.6
MeSH (C_s)	586.7	-5.6	17.9	604.6	12.2
Me_2S (C_{2v})	511.5	-5.4	17.8	529.3	12.5
EtSH (C_s)	548.5	-5.5	17.3	565.9	11.9
Et_2S (C_{2v})	430.4	-5.7	16.7	447.2	11.0
MeSSMe (C_1)	381.6	-8.5	22.2	403.8	13.7
Me_3S^+ (C_1)	367.0	-4.7	17.4	384.4	12.7
Me_4S (C_{2v})	533.5	-5.2	17.8	551.3	12.5
Me_5S^- (C_s)	583.3	-4.2	15.2	598.5	10.9
Me_5S^+ (C_s)	433.2	-4.2	15.9	449.0	11.7
Me_6S (C_i)	656.8	-4.3	16.3	673.1	11.9
H_2SF_2 (C_{2v})	331.1	-5.1	15.5	346.6	10.5
H_2SO (C_s)	191.3	-5.5	16.4	207.7	10.9
H_2SO_2 (C_{2v})	198.9	-4.1	16.8	215.7	12.7
H_4SO (C_{2v})	494.2	-1.8	19.4	513.6	17.7
H_2SF_2O (C_{2v})	244.7	-3.0	19.1	263.8	16.1
Me_2SF_2 (C_{2v})	208.9	-4.7	15.6	224.5	10.9
$CF_3SF_2CF_3$ (C_{2v})	146.1	-4.6	13.8	159.9	9.2
Me_2SCl_2 (C_{2v})	362.3	-5.8	10.8	373.1	5.0
Me_2SBr_2 (C_{2v})	396.3	-8.6	-19.9	376.4	-28.6
Me_2SO (C_s)	122.0	-5.3	17.0	139.0	11.7
Me_2SO_2 (C_{2v})	148.1	-4.9	17.2	165.3	12.3
Me_2SF_2O (C_{2v})	189.9	-4.6	19.2	209.1	14.7
F_2SO (C_s)	-96.4	-5.9	14.2	-82.1	8.4
Cl_2SO (C_s)	-181.3	-8.3	20.7	-160.6	12.3
F_2SO_2 (C_{2v})	156.6	-5.4	19.7	176.2	14.3
SF_4 (C_{2v})	-49.1	-5.0	15.0	-34.1	10.0
SCl_4 (C_{2v})	-79.0	-12.3	19.2	-59.8	6.9
SF_5^- (C_{4v})	27.7	-5.4	13.8	41.5	8.3
SF_5^+ (C_{4v})	144.7	-5.7	30.8	175.5	25.2
HSF_5 (C_{4v})	276.5	-4.6	31.7	308.3	27.2
$MeSF_5$ (C_s)	237.2	-5.0	32.0	269.2	27.0
SF_6 (O_h)	240.0	-5.3	37.7	277.7	32.3

[a] Structures optimized at the MP2 level of Gaussian 03 are employed. [b] σ(S) are denoted by σ in Table. [c] $\Delta\sigma_{Rlt\text{-}so} = \sigma_{Rlt\text{-}so} - \sigma_{Non}$. [d] $\Delta\sigma^{t}_{Rlt\text{-}so} = \sigma^{t}_{Rlt\text{-}so} - \sigma^{d+p}_{Non} = \Delta\sigma^{d+p}_{Rlt\text{-}so} + \sigma^{so}_{Rlt\text{-}so}$.

Table S4. The σ^{d}(Te), σ^{p}(Te), σ^{d+p}(Te), σ^{so}(Te), and σ^{t}(Te) Values Calculated with the QZ4Pae Basis Sets at the Nonrelativistic (Non) and Spin-orbit ZORA Relativistic (Rlt-so) Levels for Various Selenium Species[a-d]

Species	σ^{d}_{Non}	σ^{p}_{Non}	σ^{d+p}_{Non}	σ^{d}_{Rlt-so}	$\Delta\sigma^{d}_{Rlt-so}$	σ^{p}_{Rlt-so}	$\Delta\sigma^{p}_{Rlt-so}$
H_2Te (C_{2v})	5360.1	-1936.3	3423.8	5302.7	-57.4	-2098.6	-162.3
HTe^- ($C_{\infty v}$)	5365.2	-1064.8	4300.4	5308.5	-56.7	-1186.7	-121.9
H_3Te^+ (C_{3v})	5353.8	-2202.1	3151.7	5296.5	-57.3	-2332.1	-130.0
H_4Te (C_{2v})	5356.1	-1813.9	3542.2	5299.1	-57.0	-1940.2	-126.3
H_5Te^- (C_{4v})	5350.0	-1990.3	3359.7	5293.6	-56.4	-2053.6	-63.3
H_5Te^+ (C_{4v})	5351.5	-2374.9	2976.6	5294.1	-57.4	-2471.8	-96.9
H_6Te (O_h)	5343.2	-2149.2	3194.0	5286.3	-56.9	-2215.3	-66.1
$MeTe^-$ (C_s)	5366.0	-2399.5	2966.6	5309.3	-56.7	-2608.8	-209.3
MeTeH (C_s)	5361.3	-2407.3	2954.0	5304.4	-56.9	-2591.4	-184.1
Me_2Te (C_{2v})	5362.6	-2844.2	2518.4	5306.1	-56.5	-3040.4	-196.2
EtTeH (C_s)	5361.0	-2500.5	2860.5	5304.3	-56.7	-2694.0	-193.5
Et_2Te (C_{2v})	5363.1	-3051.0	2312.1	5306.6	-56.5	-3271.6	-220.6
MeTeTeMe (C_2)	5363.9	-2952.7	2411.2	5307.1	-56.8	-3369.4	-416.7
Me_3Te^+ (C_3)	5357.4	-3045.3	2312.1	5300.8	-56.6	-3229.5	-184.2
Me_4Te (C_{2v})	5358.0	-2512.1	2845.9	5301.0	-57.0	-2679.3	-167.2
Me_5Te^- (C_s)	5355.6	-2509.7	2845.9	5297.9	-57.7	-2622.2	-112.5
Me_5Te^+ (C_s)	5353.8	-3005.8	2348.0	5295.1	-58.7	-3149.7	-143.9
Me_6Te (C_i)	5351.0	-2543.8	2807.2	5289.8	-61.2	-2647.5	-103.7
H_2TeF_2 (C_{2v})	5349.7	-3180.4	2169.4	5292.8	-56.9	-3391.5	-211.1
H_2TeO (C_s)	5354.2	-3337.1	2017.1	5297.1	-57.1	-3565.1	-228.0
H_2TeO_2 (C_{2v})	5354.3	-3453.4	1900.9	5296.5	-57.8	-3681.9	-228.5
H_4TeO (C_{2v})	5350.3	-2731.9	2618.3	5292.5	-57.8	-2867.8	-135.9
H_2TeF_2O (C_{2v})	5349.2	-3285.8	2063.4	5292.3	-56.9	-3507.6	-221.8
Me_2TeF_2 (C_{2v})	5351.2	-3588.0	1763.2	5294.8	-56.4	-3845.6	-257.6
$(CF_3)_2TeF_2$ (C_{2v})	5352.2	-3600.9	1751.3	5296.0	-56.2	-3884.4	-283.5
Me_2TeCl_2 (C_{2v})	5354.9	-3260.0	2094.9	5298.3	-56.6	-3484.2	-224.2
Me_2TeBr_2 (C_{2v})	5357.0	-3194.7	2162.3	5300.1	-56.9	-3438.9	-244.2
Me_2TeO (C_s)	5356.6	-3685.2	1671.4	5299.4	-57.2	-3939.5	-254.3
Me_2TeO_2 (C_{2v})	5356.2	-3709.2	1647.0	5299.0	-57.2	-3973.5	-264.3
Me_2TeF_2O (C_{2v})	5351.1	-3535.5	1815.6	5294.3	-56.8	-3787.9	-252.4
F_2TeO (C_s)	5351.6	-4178.8	1172.8	5294.9	-56.7	-4572.0	-393.2
Cl_2TeO (C_s)	5353.7	-4436.6	917.1	5297.9	-55.8	-4854.6	-418.0
F_2TeO_2 (C_{2v})	5351.3	-3514.5	1836.8	5293.6	-57.7	-3782.7	-268.2
TeF_4 (C_{2v})	5346.4	-3728.9	1617.5	5289.6	-56.8	-4056.2	-327.3
$TeCl_4$ (C_{2v})	5349.4	-4379.8	969.6	5295.0	-54.4	-4822.6	-442.8
TeF_5^- (C_{4v})	5341.9	-3499.6	1842.3	5286.0	-55.9	-3803.1	-303.5
TeF_5^+ (C_{4v})	5345.7	-3279.5	2066.2	5288.4	-57.3	-3555.3	-275.8
$HTeF_5$ (C_{4v})	5342.3	-3163.8	2178.5	5283.1	-59.2	-3428.5	-264.7
$MeTeF_5$ (C_s)	5341.8	-3274.4	2067.4	5284.4	-57.4	-3542.0	-267.6
TeF_6 (O_h)	5340.2	-3081.7	2258.5	5284.0	-56.2	-3343.2	-261.5

Continued

Species	$\sigma^{d+p}_{Rlt\text{-}so}$	$\Delta\sigma^{d+p}_{Rlt\text{-}so}$	$\sigma^{so}_{Rlt\text{-}so}$	$\sigma^{t}_{Rlt\text{-}so}$	$\Delta\sigma^{t}_{Rlt\text{-}so}$
H_2Te (C_{2v})	3204.1	-219.7	744.0	3948.1	524.3
HTe^- ($C_{\infty v}$)	4121.8	-178.6	832.5	4954.2	653.8
H_3Te^+ (C_{3v})	2964.4	-187.3	634.8	3599.2	447.5
H_4Te (C_{2v})	3358.9	-183.3	737.5	4096.4	554.2
H_5Te^- (C_{4v})	3240.0	-119.7	558.2	3798.2	438.5
H_5Te^+ (C_{4v})	2822.3	-154.3	642.1	3464.4	487.8
H_6Te (O_h)	3071.0	-123.0	656.5	3727.5	533.5
$MeTe^-$ (C_s)	2700.5	-266.1	912.0	3612.5	645.9
MeTeH (C_s)	2713.0	-241.0	744.6	3457.6	503.6
Me_2Te (C_{2v})	2265.7	-252.7	735.2	3000.8	482.4
EtTeH (C_s)	2610.3	-250.2	721.5	3331.8	471.3
Et_2Te (C_{2v})	2035.0	-277.1	696.2	2731.2	419.1
MeTeTeMe (C_2)	1937.7	-473.5	896.6	2834.4	423.2
Me_3Te^+ (C_3)	2071.3	-240.8	634.5	2705.8	393.7
Me_4Te (C_{2v})	2621.7	-224.2	709.1	3330.8	484.9
Me_5Te^- (C_s)	2675.7	-170.2	562.5	3238.2	392.3
Me_5Te^+ (C_s)	2145.4	-202.6	624.4	2769.7	421.7
Me_6Te (C_i)	2642.3	-164.9	646.6	3289.0	481.8
H_2TeF_2 (C_{2v})	1901.3	-268.1	500.8	2402.1	232.7
H_2TeO (C_s)	1732.0	-285.1	556.9	2288.9	271.8
H_2TeO_2 (C_{2v})	1614.6	-286.3	545.8	2160.4	259.5
H_4TeO (C_{2v})	2424.7	-193.6	593.6	3018.3	400.0
H_2TeF_2O (C_{2v})	1784.7	-278.7	546.0	2330.8	267.4
Me_2TeF_2 (C_{2v})	1449.2	-314.0	497.4	1946.5	183.3
$(CF_3)_2TeF_2$ (C_{2v})	1411.6	-339.7	421.3	1832.9	81.6
Me_2TeCl_2 (C_{2v})	1814.1	-280.8	564.4	2378.5	283.6
Me_2TeBr_2 (C_{2v})	1861.2	-301.1	531.9	2393.1	230.8
Me_2TeO (C_s)	1359.9	-311.5	562.2	1922.2	250.8
Me_2TeO_2 (C_{2v})	1325.5	-321.5	550.1	1875.5	228.5
Me_2TeF_2O (C_{2v})	1506.4	-309.2	541.3	2047.6	232.0
F_2TeO (C_s)	722.9	-449.9	383.2	1106.1	-66.7
Cl_2TeO (C_s)	443.3	-473.8	424.5	867.8	-49.3
F_2TeO_2 (C_{2v})	1510.9	-325.9	506.9	2017.7	180.9
TeF_4 (C_{2v})	1233.4	-384.1	325.0	1558.5	-59.0
$TeCl_4$ (C_{2v})	472.4	-497.2	432.8	905.2	-64.4
TeF_5^- (C_{4v})	1482.9	-359.4	334.2	1817.1	-25.2
TeF_5^+ (C_{4v})	1733.1	-333.1	650.2	2383.3	317.1
$HTeF_5$ (C_{4v})	1854.6	-323.9	632.8	2487.4	308.9
$MeTeF_5$ (C_s)	1742.4	-325.0	601.5	2344.0	276.6
TeF_6 (O_h)	1940.8	-317.7	657.9	2598.6	340.1

[a] Structures optimized at the B3LYP level of Gaussian 03 being employed. [b] σ(Te) are denoted by σ in Table. [c] $\Delta\sigma_{Rlt\text{-}so} = \sigma_{Rlt\text{-}so} - \sigma_{Non}$. [d] $\Delta\sigma^{t}_{Rlt\text{-}so} = \sigma^{t}_{Rlt\text{-}so} - \sigma^{d+p}_{Non} = \Delta\sigma^{d+p}_{Rlt\text{-}so} + \sigma^{so}_{Rlt\text{-}so}$.

Table S5. The σ^{d}(Se), σ^{p}(Se), σ^{d+p}(Se), σ^{so}(Se), and σ^{t}(Se) Values Calculated with the QZ4Pae Basis Sets at Nonrelativistic (Non) and Spin-orbit ZORA Relativistic (Rlt-so) Levels for Various Selenium Species[a-d]

Species	σ^{d}_{Non}	σ^{p}_{Non}	σ^{d+p}_{Non}	σ^{d}_{Rlt-so}	$\Delta\sigma^{d}_{Rlt-so}$	σ^{p}_{Rlt-so}	$\Delta\sigma^{p}_{Rlt-so}$
H_2Se (C_{2v})	2994.3	-964.3	2030.0	2973.2	-21.1	-996.9	-32.6
HSe^- ($C_{\infty v}$)	3004.5	-524.1	2480.4	2982.8	-21.7	-548.7	-24.6
H_3Se^+ (C_{3v})	2983.0	-1125.5	1857.5	2962.7	-20.3	-1151.3	-25.8
H_4Se (C_{2v})	2980.3	-1043.3	1937.0	2958.9	-21.4	-1067.2	-23.9
H_5Se^- (C_{4v})	2977.0	-1009.1	1967.9	2955.3	-21.7	-1019.2	-10.1
H_5Se^+ (C_{4v})	2971.1	-1216.9	1754.2	2950.9	-20.2	-1231.6	-14.7
H_6Se (O_h)	2958.5	-1065.6	1893.0	2935.1	-23.4	-1068.5	-2.9
$MeSe^-$ (C_s)	3004.0	-1267.1	1736.9	2981.8	-22.2	-1316.5	-49.4
MeSeH (C_s)	2992.6	-1221.4	1771.1	2971.2	-21.4	-1259.5	-38.1
Me_2Se (C_{2v})	2992.2	-1438.8	1553.4	2969.7	-22.5	-1480.0	-41.2
EtSeH (C_s)	2992.7	-1300.1	1692.7	2971.3	-21.4	-1339.2	-39.1
Et_2Se (C_{2v})	2993.4	-1605.8	1387.7	2970.9	-22.5	-1651.5	-45.7
MeSeSeMe (C_2)	2994.7	-1802.2	1192.6	2972.4	-22.3	-1902.6	-100.4
Me_3Se^+ (C_3)	2977.2	-1654.7	1322.5	2954.3	-22.9	-1689.9	-35.2
Me_4Se (C_{2v})	2974.5	-1404.9	1569.6	2951.0	-23.5	-1437.1	-32.2
Me_5Se^- (C_s)	2970.5	-1322.8	1647.7	2946.5	-24.0	-1346.1	-23.3
Me_5Se^+ (C_s)	2968.5	-1586.7	1381.8	2944.4	-24.1	-1608.3	-21.6
Me_6Se (C_i)	2965.0	-1229.5	1735.5	2940.6	-24.4	-1243.4	-13.9
H_2SeF_2 (C_{2v})	2980.1	-1790.7	1189.4	2959.3	-20.8	-1831.3	-40.6
H_2SeO (C_s)	2984.6	-1995.8	988.9	2963.6	-21.0	-2043.7	-47.9
H_2SeO_2 (C_{2v})	2981.8	-2104.4	877.4	2960.6	-21.2	-2150.9	-46.5
H_4SeO (C_{2v})	2971.7	-1505.0	1466.7	2950.8	-20.9	-1528.6	-23.6
H_2SeF_2O (C_{2v})	2973.7	-1992.4	981.3	2953.9	-19.8	-2035.4	-43.0
Me_2SeF_2 (C_{2v})	2974.5	-2105.0	869.5	2951.6	-22.9	-2155.6	-50.6
$(CF_3)_2SeF_2$ (C_{2v})	2977.5	-2239.1	738.4	2956.0	-21.5	-2300.2	-61.1
Me_2SeCl_2 (C_{2v})	2977.0	-1819.5	1157.5	2954.6	-22.4	-1866.0	-46.5
Me_2SeBr_2 (C_{2v})	2982.3	-1751.7	1230.6	2959.7	-22.6	-1807.3	-55.6
Me_2SeO (C_s)	2982.6	-2199.8	782.8	2960.3	-22.3	-2252.1	-52.3
Me_2SeO_2 (C_{2v})	2977.3	-2248.0	729.3	2954.9	-22.4	-2298.8	-50.8
Me_2SeF_2O (C_{2v})	2970.4	-2157.7	812.7	2947.9	-22.5	-2205.0	-47.3
F_2SeO (C_s)	2985.8	-2733.5	252.4	2964.7	-21.1	-2816.5	-83.0
Cl_2SeO (C_s)	2985.7	-2906.6	79.1	2964.4	-21.3	-3003.4	-96.8
F_2SeO_2 (C_{2v})	2985.4	-2256.9	728.6	2964.1	-21.3	-2313.2	-56.3
SeF_4 (C_{2v})	2980.0	-2569.3	410.7	2958.5	-21.5	-2644.2	-74.9
$SeCl_4$ (C_{2v})	2983.9	-2925.1	58.8	2962.0	-21.9	-3039.6	-114.5
SeF_5^- (C_{4v})	2978.3	-2433.8	544.5	2956.5	-21.8	-2511.1	-77.3
SeF_5^+ (C_{4v})	2982.9	-2251.3	731.5	2961.2	-21.7	-2312.8	-61.5
$HSeF_5$ (C_{4v})	2967.2	-2021.1	946.1	2944.6	-22.6	-2076.4	-55.3
$MeSeF_5$ (C_s)	2961.0	-2102.5	858.5	2938.6	-22.4	-2158.9	-56.4
SeF_6 (O_h)	2970.1	-2052.7	917.4	2947.0	-23.1	-2107.6	-54.9

Continued

Species	$\sigma^{d+p}_{Rlt\text{-}so}$	$\Delta\sigma^{d+p}_{Rlt\text{-}so}$	$\sigma^{so}_{Rlt\text{-}so}$	$\sigma^{t}_{Rlt\text{-}so}$	$\Delta\sigma^{t}_{Rlt\text{-}so}$
H_2Se (C_{2v})	1976.3	-53.7	182.6	2158.9	128.9
HSe^- ($C_{\infty v}$)	2434.0	-46.4	198.5	2632.6	152.2
H_3Se^+ (C_{3v})	1811.5	-46.0	163.4	1974.9	117.4
H_4Se (C_{2v})	1891.7	-45.3	171.3	2063.0	126.0
H_5Se^- (C_{4v})	1936.1	-31.8	155.0	2091.1	123.2
H_5Se^+ (C_{4v})	1719.4	-34.8	157.2	1876.6	122.4
H_6Se (O_h)	1866.6	-26.4	161.0	2027.6	134.6
$MeSe^-$ (C_s)	1665.3	-71.6	217.0	1882.3	145.4
MeSeH (C_s)	1711.6	-59.5	184.5	1896.1	125.0
Me_2Se (C_{2v})	1489.7	-63.7	183.2	1672.9	119.5
EtSeH (C_s)	1632.1	-60.6	178.2	1810.3	117.6
Et_2Se (C_{2v})	1319.4	-68.3	172.2	1491.6	103.9
MeSeSeMe (C_2)	1069.8	-122.8	225.0	1294.8	102.2
Me_3Se^+ (C_3)	1264.4	-58.1	164.9	1429.3	106.8
Me_4Se (C_{2v})	1514.0	-55.6	172.4	1686.3	116.7
Me_5Se^- (C_s)	1600.5	-47.2	156.6	1757.1	109.4
Me_5Se^+ (C_s)	1336.2	-45.6	157.4	1493.6	111.8
Me_6Se (C_i)	1697.1	-38.4	163.1	1860.2	124.7
H_2SeF_2 (C_{2v})	1128.1	-61.3	138.0	1266.1	76.7
H_2SeO (C_s)	919.9	-69.0	147.7	1067.6	78.7
H_2SeO_2 (C_{2v})	809.7	-67.7	144.0	953.8	76.4
H_4SeO (C_{2v})	1422.2	-44.5	157.7	1579.9	113.2
H_2SeF_2O (C_{2v})	918.4	-62.9	145.5	1063.9	82.6
Me_2SeF_2 (C_{2v})	796.1	-73.4	135.4	931.4	61.9
$(CF_3)_2SeF_2$ (C_{2v})	655.8	-82.6	115.5	771.2	32.8
Me_2SeCl_2 (C_{2v})	1088.6	-68.9	146.8	1235.5	78.0
Me_2SeBr_2 (C_{2v})	1152.4	-78.2	93.6	1246.0	15.4
Me_2SeO (C_s)	708.2	-74.6	148.4	856.6	73.8
Me_2SeO_2 (C_{2v})	656.1	-73.2	145.6	801.7	72.4
Me_2SeF_2O (C_{2v})	742.9	-69.8	144.6	887.6	74.9
F_2SeO (C_s)	148.2	-104.2	103.6	251.7	-0.7
Cl_2SeO (C_s)	-38.9	-118.0	121.2	82.3	3.2
F_2SeO_2 (C_{2v})	651.0	-77.6	148.4	799.3	70.7
SeF_4 (C_{2v})	314.3	-96.4	92.0	406.3	-4.4
$SeCl_4$ (C_{2v})	-77.6	-136.4	128.8	51.3	-7.5
SeF_5^- (C_{4v})	445.5	-99.0	95.3	540.8	-3.7
SeF_5^+ (C_{4v})	648.4	-83.1	212.7	861.1	129.6
$HSeF_5$ (C_{4v})	868.2	-77.9	194.3	1062.5	116.4
$MeSeF_5$ (C_s)	779.7	-78.8	187.1	966.7	108.2
SeF_6 (O_h)	839.4	-78.0	222.2	1061.6	144.2

[a] Structures optimized at the B3LYP level of Gaussian 03 being employed. [b] σ(Te) are denoted by σ in Table. [c] $\Delta\sigma_{Rlt\text{-}so} = \sigma_{Rlt\text{-}so} - \sigma_{Non}$. [d] $\Delta\sigma^{t}_{Rlt\text{-}so} = \sigma^{t}_{Rlt\text{-}so} - \sigma^{d+p}_{Non} = \Delta\sigma^{d+p}_{Rlt\text{-}so} + \sigma^{so}_{Rlt\text{-}so}$.

Table S6. The σ^{d}(S), σ^{p}(S), σ^{d+p}(S), σ^{so}(S), and σ^{t}(S) Values Calculated with the QZ4Pae Basis Sets at the Nonrelativistic (Non) and Spin-orbit ZORA Relativistic (Rlt-so) Levels for Various Selenium Species[a-d]

Species	σ^{d}_{Non}	σ^{p}_{Non}	σ^{d+p}_{Non}	σ^{d}_{Rlt-so}	$\Delta\sigma^{d}_{Rlt-so}$	σ^{p}_{Rlt-so}	$\Delta\sigma^{p}_{Rlt-so}$
H_2S (C_{2v})	1053.1	-366.7	686.4	1049.4	-3.7	-367.7	-1.0
HS^- ($C_{\infty v}$)	1058.4[e]	-170.4[e]	888.0[e]	1055.9[f]	-2.5	-174.5[f]	-4.1
H_3S^+ (C_{3v})	1046.9	-454.1	592.8	1042.3[f]	-4.6	-454.3[f]	-0.2
H_4S (C_{2v})	1044.9	-281.1	763.8	1037.3	-7.6	-275.8	5.3
H_5S^- (C_{4v})	1047.0	-355.0	692.0	1036.7	-10.3	-348.2	6.8
H_5S^+ (C_{4v})	1041.1	-445.2	595.9	1029.8	-11.3	-434.7	10.5
H_6S (O_h)	1036.8	-344.4	692.4	1031.9	-4.9	-338.8	5.6
MeS^- (C_s)	1059.1	-469.5	589.6	1055.9	-3.2	-472.6	-3.1
MeSH (Cs)	1054.3	-472.9	581.4	1050.9	-3.4	-475.2	-2.3
Me_2S (C_{2v})	1055.0	-552.1	502.9	1051.1	-3.9	-553.8	-1.7
EtSH (Cs)	1053.6	-511.4	542.2	1050.0	-3.6	-513.4	-2.0
Et_2S (C_{2v})	1054.0	-631.5	422.5	1050.1	-3.9	-633.3	-1.8
MeSSMe (C_2)	1055.1	-692.0	363.1	1051.1	-4.0	-696.8	-4.8
Me_3S^+ (C_3)	1052.6	-718.1	334.5	1048.3	-4.3	-718.9	-0.8
Me_4S (C_{2v})	1049.0	-530.0	519.0	1044.5	-4.5	-531.0	-1.0
Me_5S^- (C_s)	1036.2	-484.3	551.9	1031.7	-4.5	-484.3	0.0
Me_5S^+ (C_s)	1046.2	-619.9	426.3	1043.4	-2.8	-621.3	-1.4
Me_6S (C_i)	1034.5	-386.0	648.5	1032.7	-1.8	-388.6	-2.6
H_2SF_2 (C_{2v})	1043.9	-716.0	327.9	1038.2	-5.7	-715.3	0.7
H_2SO (Cs)	1047.7	-862.4	185.3	1044.6	-3.1	-864.9	-2.5
H_2SO_2 (C_{2v})	1047.9	-848.0	199.9	1045.5	-2.4	-849.7	-1.7
H_4SO (C_{2v})	1041.0	-553.4	487.6	1031.6	-9.4	-545.8	7.6
H_2SF_2O (C_{2v})	1044.0	-803.6	240.4	1038.8	-5.2	-801.4	2.2
Me_2SF_2 (C_{2v})	1047.1	-858.6	188.5	1042.0	-5.1	-858.5	0.1
$CF_3SF_2CF_3$ (C_{2v})	1044.0	-932.0	112.0	1040.3	-3.7	-932.9	-0.9
Me_2SCl_2 (C_{2v})	1051.5	-727.3	324.2	1046.9	-4.6	-728.5	-1.2
Me_2SBr_2 (C_{2v})	1052.2	-689.4	362.8	1047.8	-4.4	-692.6	-3.2
Me_2SO (C_s)	1049.9	-940.3	109.6	1046.6	-3.3	-942.4	-2.1
Me_2SO_2 (C_{2v})	1047.0	-899.1	147.9	1044.4	-2.6	-901.5	-2.4
Me_2SF_2O (C_{2v})	1045.8	-866.2	179.6	1041.1	-4.7	-866.1	0.1
F_2SO (C_s)	1043.3	-1141.0	-97.7	1041.4	-1.9	-1145.0	-4.0
Cl_2SO (C_s)	1051.5	-1256.1	-204.6	1048.2	-3.3	-1261.3	-5.2
F_2SO_2 (C_{2v})	1045.7	-886.4	159.3	1044.1	-1.6	-890.3	-3.9
SF_4 (C_{2v})	1035.8	-1102.6	-66.8	1031.6	-4.2	-1103.5	-0.9
SCl_4 (C_{2v})	1054.7	-1224.5	-169.8	1049.6	-5.1	-1232.2	-7.7
SF_5^- (C_{4v})	1033.4	-1034.8	-1.4	1028.3	-5.1	-1035.3	-0.5
SF_5^+ (C_{4v})	1036.6	-915.7	120.9	1031.2	-5.4	-915.8	-0.1
HSF_5 (C_{4v})	1032.4	-766.4	266.0	1025.6	-6.8	-764.2	2.2
$MeSF_5$ (C_s)	1034.1	-811.5	222.6	1028.2	-5.9	-810.6	0.9
SF_6 (O_h)	1031.0	-800.8	230.2	1026.6	-4.4	-801.7	-0.9

Continued

Species	σ^{d+p}_{Rlt-so}	$\Delta\sigma^{d+p}_{Rlt-so}$	σ^{so}_{Rlt-so}	σ^{t}_{Rlt-so}	$\Delta\sigma^{t}_{Rlt-so}$
H_2S (C_{2v})	681.7	-4.7	17.7	699.4	13.0
HS^- ($C_{\infty v}$)	881.4[f]	-6.6	18.3[f]	899.7[f]	11.7
H_3S^+ (C_{3v})	588.0[f]	-4.8	16.7[f]	604.7[f]	11.9
H_4S (C_{2v})	761.5	-2.3	19.0	780.5	16.7
H_5S^- (C_{4v})	688.5	-3.5	17.8	706.3	14.3
H_5S^+ (C_{4v})	595.1	-0.8	18.6	613.6	17.7
H_6S (O_h)	693.1	0.7	19.8	712.9	20.5
MeS^- (C_s)	583.3	-6.3	19.8	603.1	13.5
MeSH (C_s)	575.7	-5.7	18.0	593.6	12.2
Me_2S (C_{2v})	497.3	-5.6	18.0	515.4	12.5
EtSH (C_s)	536.6	-5.6	17.5	554.1	11.9
Et_2S (C_{2v})	416.8	-5.7	16.9	433.8	11.3
MeSSMe (C_2)	354.3	-8.8	22.6	376.9	13.8
Me_3S^+ (C_3)	329.4	-5.1	17.5	346.9	12.4
Me_4S (C_{2v})	513.5	-5.5	17.9	531.4	12.4
Me_5S^- (C_s)	547.4	-4.5	15.5	562.9	11.0
Me_5S^+ (C_s)	422.1	-4.2	15.9	438.0	11.7
Me_6S (C_i)	644.1	-4.4	16.4	660.4	11.9
H_2SF_2 (C_{2v})	322.9	-5.0	15.4	338.3	10.4
H_2SO (C_s)	179.7	-5.6	16.4	196.2	10.9
H_2SO_2 (C_{2v})	195.8	-4.1	16.8	212.6	12.7
H_4SO (C_{2v})	485.8	-1.8	19.5	505.2	17.6
H_2SF_2O (C_{2v})	237.4	-3.0	19.2	256.6	16.2
Me_2SF_2 (C_{2v})	183.5	-5.0	15.4	199.0	10.5
$CF_3SF_2CF_3$ (C_{2v})	107.4	-4.6	13.7	121.1	9.1
Me_2SCl_2 (C_{2v})	318.4	-5.8	10.2	328.6	4.4
Me_2SBr_2 (C_{2v})	355.2	-7.6	-23.6	331.5	-31.3
Me_2SO (C_s)	104.2	-5.4	17.0	121.2	11.6
Me_2SO_2 (C_{2v})	142.9	-5.0	17.2	160.2	12.3
Me_2SF_2O (C_{2v})	175.0	-4.6	19.3	194.2	14.6
F_2SO (C_s)	-103.6	-5.9	14.2	-89.5	8.2
Cl_2SO (C_s)	-213.1	-8.5	19.7	-193.4	11.2
F_2SO_2 (C_{2v})	153.8	-5.5	19.9	173.7	14.4
SF_4 (C_{2v})	-71.9	-5.1	14.9	-57.1	9.7
SCl_4 (C_{2v})	-182.6	-12.8	15.7	-166.8	3.0
SF_5^- (C_{4v})	-7.0	-5.6	13.3	6.3	7.7
SF_5^+ (C_{4v})	115.4	-5.5	34.7	150.1	29.2
HSF_5 (C_{4v})	261.4	-4.6	32.8	294.3	28.3
$MeSF_5$ (C_s)	217.6	-5.0	33.2	250.8	28.2
SF_6 (O_h)	224.9	-5.3	39.6	264.5	34.3

[a] Structures optimized at the B3LYP level of Gaussian 03 being employed. [b] σ(Te) are denoted by σ in Table. [c] $\Delta\sigma_{Rlt-so} = \sigma_{Rlt-so} - \sigma_{Non}$. [d] $\Delta\sigma^{t}_{Rlt-so} = \sigma^{t}_{Rlt-so} - \sigma^{d+p}_{Non} = \Delta\sigma^{d+p}_{Rlt-so} + \sigma^{so}_{Rlt-so}$. [e] $\sigma^{d}_{Non} = 1058.4$, $\sigma^{p}_{Non} = -172.1$, and $\sigma^{d+p}_{Non} = 886.2$ ppm being predicted as extrapolated values. [f] Extrapolated values.

Figure S1. Relativistic effect on σ(Te) for various tellurium compounds evaluated with QZ4Pae: ■, ■, and ■ stand for the total term ($\Delta\sigma^{t}(Te)_{Rlt\text{-}so} = \Delta\sigma^{d+p}(Te)_{Rlt\text{-}so} + \sigma^{so}(Te)_{Rlt\text{-}so}$), the scalar term ($\Delta\sigma^{d+p}(Te)_{Rlt\text{-}so}$), and the spin-orbit term ($\sigma^{so}(Te)_{Rlt\text{-}so}$), respectively. Values are from Table S4, evaluated on the structures optimized at the B3LYP level.

Figure S2. Relativistic effect on σ(Se) for various selenium compounds evaluated with QZ4Pae: ■, ■, and ■ stand for the total term ($\Delta\sigma^{t}(Se)_{Rlt\text{-}so} = \Delta\sigma^{d+p}(Se)_{Rlt\text{-}so} + \sigma^{so}(Se)_{Rlt\text{-}so}$), the scalar term ($\Delta\sigma^{d+p}(Se)_{Rlt\text{-}so}$), and the spin-orbit term ($\sigma^{so}(Se)_{Rlt\text{-}so}$), respectively. Values are from Table S5, evaluated on the structures optimized at the B3LYP level.

Figure S3. Relativistic effect on σ(S) for various sulfur compounds evaluated with QZ4Pae: ■, ■, and ■ stand for the total term ($\Delta\sigma^{t}(S)_{Rlt\text{-}so} = \Delta\sigma^{d+p}(S)_{Rlt\text{-}so} + \sigma^{so}(S)_{Rlt\text{-}so}$), the scalar term ($\Delta\sigma^{d+p}(S)_{Rlt\text{-}so}$), and the spin-orbit term ($\sigma^{so}(S)_{Rlt\text{-}so}$), respectively. Values are from Table S6, evaluated on the structures optimized at the B3LYP level.

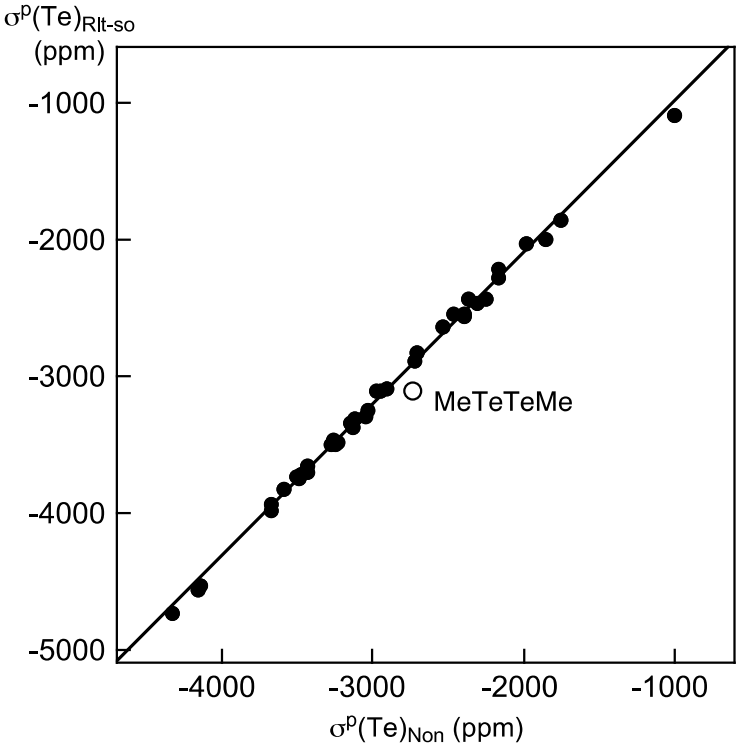

Figure S4. Plot of $\sigma^{p}(Te)_{Rlt\text{-}so}$ versus $\sigma^{p}(Te)_{Non}$ with QZ4Pae. Data for MeTeTeMe being shown by ○.

Table S7. Correlations in σ(Z) or Δσ(Z) (Z = Te, Se, and S) for Various Species Containing Z, Evaluated at Non and Rlt-so Levels with the QZ4Pae Basis Sets[a]

Entry	Correlation	*a*	*b*	R^2	*n*
1	$\sigma^{p}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{p}(Te)_{Non}$	1.103	92.5	0.995	40
1’	$\sigma^{p}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{p}(Te)_{Non}$	1.105	103.2	0.997	39[b]
2	$\Delta\sigma^{p}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{p}(Te)_{Non}$	0.041	-72.5	0.888	7[c]
3	$\Delta\sigma^{p}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{p}(Te)_{Non}$	0.045	-35.5	0.924	4[d]
4	$\Delta\sigma^{p}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{p}(Te)_{Non}$	0.157	-281.4	0.907	28[e]
5	$\sigma^{d+p}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Te)_{Non}$	1.102	-510.9	0.996	40
6	$\sigma^{t}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Te)_{Non}$	1.236	-232.6	0.992	40
7	$\sigma^{t}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Te)_{Rlt\text{-}so}$	1.119	348.3	0.990	40
8	$\sigma^{d+p}(Se)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Se)_{Non}$	1.033	-107.6	0.999	40
9	$\sigma^{t}(Se)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Se)_{Non}$	1.062	14.8	0.998	40
10	$\sigma^{t}(Se)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Se)_{Rlt\text{-}so}$	1.027	125.7	0.998	40
11	$\sigma^{d+p}(S)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(S)_{Non}$	1.004	-6.4	0.9999	40
12	$\sigma^{t}(S)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(S)_{Non}$	1.002	12.3	0.999	40
13	$\sigma^{t}(S)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(S)_{Rlt\text{-}so}$	0.998	18.7	0.998	40
14	$\sigma^{p}(Te)_{Non}$ *vs.* $\sigma^{p}(Se)_{Non}$	1.235	-805.5	0.948	40
15	$\sigma^{p}(S)_{Non}$ *vs.* $\sigma^{p}(Se)_{Non}$	0.459	108.1	0.985	40
16	$\sigma^{d+p}(Te)_{Non}$ *vs.* $\sigma^{d+p}(Se)_{Non}$	1.239	862.3	0.951	40
17	$\sigma^{d+p}(S)_{Non}$ *vs.* $\sigma^{d+p}(Se)_{Non}$	0.460	-215.0	0.987	40
18	$\sigma^{d+p}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Se)_{Rlt\text{-}so}$	1.333	567.0	0.963	40
19	$\sigma^{d+p}(S)_{Rlt\text{-}so}$ *vs.* $\sigma^{d+p}(Se)_{Rlt\text{-}so}$	0.447	-174.1	0.987	40
20	$\sigma^{so}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{so}(Se)_{Rlt\text{-}so}$	4.780	-140.4	0.969	35[c]
21	$\sigma^{so}(S)_{Rlt\text{-}so}$ *vs.* $\sigma^{so}(Se)_{Rlt\text{-}so}$	0.044	10.5	0.299	35[c]
22	$\sigma^{t}(Te)_{Rlt\text{-}so}$ *vs.* $\sigma^{t}(Se)_{Rlt\text{-}so}$	1.460	787.6	0.969	40
23	$\sigma^{t}(S)_{Rlt\text{-}so}$ *vs.* $\sigma^{t}(Se)_{Rlt\text{-}so}$	0.434	-209.6	0.988	40
24	$\Delta\sigma^{d+p}(Te)_{Rlt\text{-}so}$ *vs.* $\Delta\sigma^{d+p}(Se)_{Rlt\text{-}so}$	3.783	-16.3	0.963	40
25	$\Delta\sigma^{d+p}(S)_{Rlt\text{-}so}$ *vs.* $\Delta\sigma^{d+p}(Se)_{Rlt\text{-}so}$	0.071	-0.3	0.604	40
26	$\Delta\sigma^{t}(Te)_{Rlt\text{-}so}$ *vs.* $\Delta\sigma^{t}(Se)_{Rlt\text{-}so}$	4.576	-74.2	0.979	35[f]
27	$\Delta\sigma^{t}(S)_{Rlt\text{-}so}$ *vs.* $\Delta\sigma^{t}(Se)_{Rlt\text{-}so}$	0.040	8.7	0.323	35[f]

[a] The constants (*a*, *b*, R^2) are the correlation constant, the *y*-intercept, and the square of correlation coefficient, respectively, in $y = ax + b$. [b] Neglecting the data of MeTeTeMe. [c] Data for mono- and di-coordinated Te species. [d] Data for R_3Te^+ and R_4Te (R = H and Me). [e] Neglecting the data of MeTeTeMe, mono- and di-coordinated Te species, and R_3Te^+ and R_4Te (R = H and Me). [f] Neglecting the data of Me_2ZBr_2, $MeZF_5$, HZF_5, ZF_5^+, and ZF_6.

Table S8. Correlations in σ(Z) and Δσ(Z) (Z = Te, Se, and S) Evaluated Employing the Optimized Structures at MP2 Levels versus Those and B3LYP for Various Species at Non and Rlt-so Levels with the QZ4Pae Basis Sets[a]

Entry	Correlation	*a*	*b*	R^2	*n*
1	$\sigma^{d+p}(Te)_{Non:B3LYP}$ *vs.* $\sigma^{d+p}(Te)_{Non:MP2}$	1.009	-93.2	0.994	40
2	$\Delta\sigma^{d+p}(Te)_{Rlt\text{-}so:B3LYP}$ *vs.* $\Delta\sigma^{d+p}(Te)_{Rlt\text{-}so:MP2}$	1.036	-4.9	0.991	40
3	$\sigma^{so}(Te)_{Rlt\text{-}so:B3LYP}$ *vs.* $\sigma^{so}(Te)_{Rlt\text{-}so:MP2}$	1.052	-33.6	0.997	40
4	$\sigma^{t}(Te)_{Rlt\text{-}so:B3LYP}$ *vs.* $\sigma^{t}(Te)_{Rlt\text{-}so:MP2}$	1.013	-125.1	0.995	40
5	$\Delta\sigma^{t}(Te)_{Rlt\text{-}so:B3LYP}$ *vs.* $\Delta\sigma^{t}(Te)_{Rlt\text{-}so:MP2}$	1.035	-28.4	0.996	40
6	$\sigma^{d+p}(Se)_{Non:B3LYP}$ *vs.* $\sigma^{d+p}(Se)_{Non:MP2}$	1.022	-73.9	0.995	40
7	$\Delta\sigma^{d+p}(Se)_{Rlt\text{-}so:B3LYP}$ *vs.* $\Delta\sigma^{d+p}(Se)_{Rlt\text{-}so:MP2}$	1.051	0.6	0.994	40
8	$\sigma^{so}(Se)_{Rlt\text{-}so:B3LYP}$ *vs.* $\sigma^{so}(Se)_{Rlt\text{-}so:MP2}$	1.070	-11.0	0.987	40
8’	$\sigma^{so}(Se)_{Rlt\text{-}so:B3LYP}$ *vs.* $\sigma^{so}(Se)_{Rlt\text{-}so:MP2}$	1.074	-10.9	0.997	38[b]
9	$\sigma^{t}(Se)_{Rlt\text{-}so:B3LYP}$ *vs.* $\sigma^{t}(Se)_{Rlt\text{-}so:MP2}$	1.024	-81.4	0.995	40
10	$\Delta\sigma^{t}(Se)_{Rlt\text{-}so:B3LYP}$ *vs.* $\Delta\sigma^{t}(Se)_{Rlt\text{-}so:MP2}$	1.070	-9.2	0.992	40
11	$\sigma^{d+p}(S)_{Non:B3LYP}$ *vs.* $\sigma^{d+p}(S)_{Non:MP2}$	1.028	-28.7	0.995	40
12	$\Delta\sigma^{d+p}(S)_{Rlt\text{-}so:B3LYP}$ *vs.* $\Delta\sigma^{d+p}(S)_{Rlt\text{-}so:MP2}$	1.009	-0.1	0.974	40
12’	$\Delta\sigma^{d+p}(S)_{Rlt\text{-}so:B3LYP}$ *vs.* $\Delta\sigma^{d+p}(S)_{Rlt\text{-}so:MP2}$	1.036	-0.1	0.995	38[c]
13	$\sigma^{so}(S)_{Rlt\text{-}so:B3LYP}$ *vs.* $\sigma^{so}(S)_{Rlt\text{-}so:MP2}$	1.102	-1.8	0.993	40
14	$\sigma^{t}(S)_{Rlt\text{-}so:B3LYP}$ *vs.* $\sigma^{t}(S)_{Rlt\text{-}so:MP2}$	1.029	-29.5	0.995	40
15	$\Delta\sigma^{t}(S)_{Rlt\text{-}so:B3LYP}$ *vs.* $\Delta\sigma^{t}(S)_{Rlt\text{-}so:MP2}$	1.090	-1.3	0.992	40

[a] The constants (*a*, *b*, R^2) are the correlation constant, the *y*-intercept, and the square of correlation coefficient, respectively, in $y = ax + b$. [b] Except for data of SeH_4 and $SeCl_4$. [c] Except for data of HS^- and H_2SBr_2.

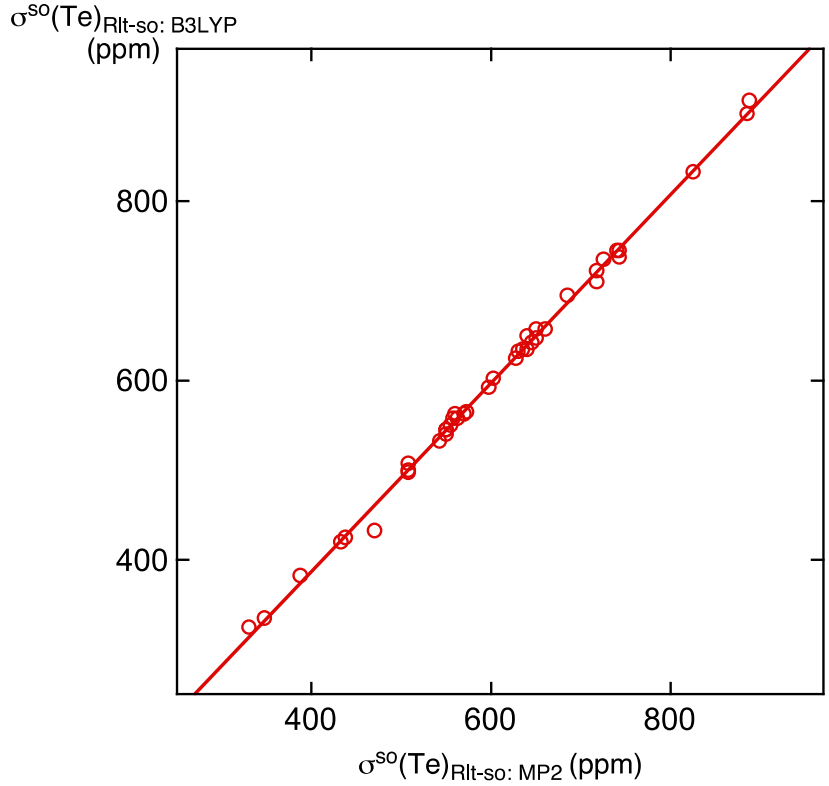

Figure S5. Plot of $\sigma^{so}(Te)_{Rlt\text{-}so:\ B3LYP}$ versus $\sigma^{so}(Te)_{Rlt\text{-}so:\ MP2}$.

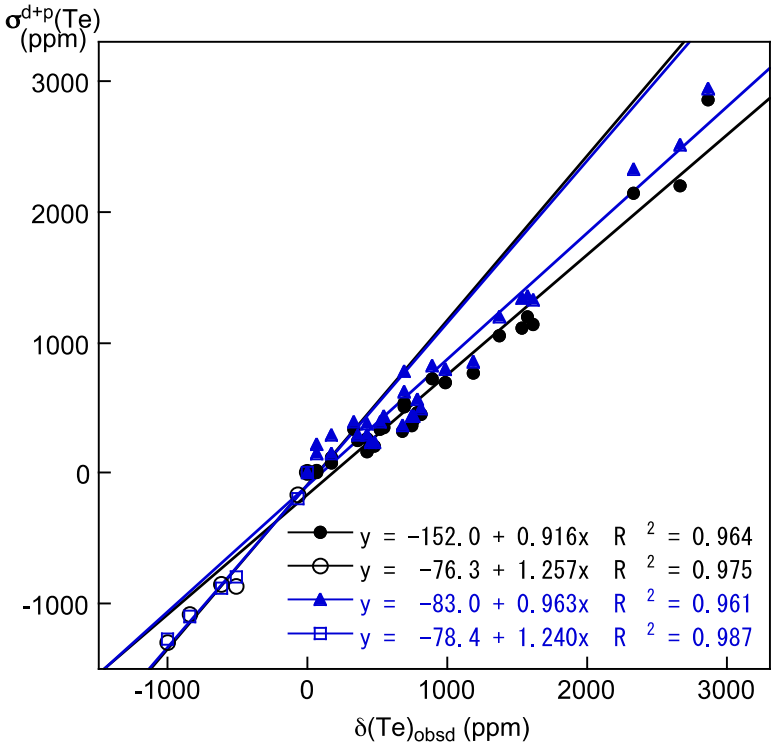

Figure S6. Plots of $\sigma^{d+p}(Te)_{Non:r}$ versus $\delta(Te)_{obsd}$ of which data for **Gr1** ($\delta(Te)_{obsd} \geq 0$) and **Gr2** ($\delta(Te)_{obsd} \leq 0$) are shown by ● and ○ and plots of $\sigma^{d+p}(Te)_{Rlr\text{-}so:r}$ versus $\delta(Te)_{obsd}$ of which data for for **Gr1** ($\delta(Te)_{obsd} \geq 0$) and **Gr2** ($\delta(Te)_{obsd} \leq 0$) are shown by ▲ and □.

Table S9. The σ^{d+p}(Te: M)$_{Non:r}$ values calculated with BLYP$_{Non}$//MP2$_{Non}$ and the σ^{d+p}(Te: M)$_{Rlt\text{-}so:r}$ and $\sigma^{\square}$(Te: M)$_{Rlt\text{-}so:r}$ values with BLYP$_{Rlt\text{-}so}$//MP2$_{Non}$[a]

Compound	σ^{d+p}(Te: **M**)$_{Non:r}$	σ^{d+p}(Te: **M**)$_{Rlt\text{-}so:r}$	$\sigma^{\square}$(Te: **M**)$_{Rlt\text{-}so:r}$
$TeMe_2$ (C_{2v}: **1**)	0.0	0.0	0.0
$TeP(iPr)_3$ (C_1: **2**)	-1301.1	-1272.9	-1360.7
$Te(SiMe_3)_2$ (C_{2v}: **3**)	-1077.3	-1102.9	-1106.5
TeH_2 (C_{2v}: **4**)	-860.3	-881.0	-899.4
$TePMe_3$ (C_1: **5**)	-874.3	-792.6	-881.4
cyclo-$(CMeNMe)_2C$=Te (C_{2v}: **6**)	-317.4	-237.9	-301.6
$TeMe_4$ (C_{2v}: **7**)	-171.1	-195.2	-145.2
MeTeEt (av: **8**)	125.6	144.6	156.2
MeTeEt (C_s: **8a**) (as 0.0)	89.1	98.6	120.0
MeTeEt ($C_{1\text{-}g}$: **8b**) (–2.9)	162.1	190.6	192.3
cyclo-$C_6H_4(CH_2)_2Te$ (C_2: **9**)	104.5	128.7	123.6
EtTeEt (av: **10**)	80.5	287.8	309.1
EtTeEt (C_{2v}: **10a**) (as 0.0)	250.2	214.7	253.6
EtTeEt ($C_{1\text{-}g}$: **10b**) (–2.7)	192.4	301.5	323.8
EtTeEt ($C_{2\text{-}gg}$: **10c**) (–7.1)	262.7	347.3	349.7
MeTeTeMe (C_2: **11**)	15.4	218.6	58.9
spiro-$Te_2C_5H_8O$ (C_1: **12**)	11.9	154.6	51.9
EtTeTeEt (av: **13**)	80.5	289.1	149.2
EtTeTeEt (C_2: **13a**) (as 0.0)	46.2	251.2	118.2
EtTeTeEt ($C_{1\text{-}g}$: **13b**) (–4.4)	80.1	288.5	148.5
EtTeTeEt ($C_{2\text{-}gg}$: **13c**) (–8.6)	115.1	327.6	181.0
cyclo-$Te(CH_2CH_2CH_2)_2Te$ (C_{2v}: **14**)	290.9	364.2	354.1
cyclo-$Te(C(tBu)CH)_2CH_2$ (C_s: **15**)	76.7	125.6	162.1
PhTeMe (C_s: **16**)	332.1	388.4	404.5
cyclo-$C_6H_4TeCH_2CO$ (C_s: **17**)	160.4	188.2	221.4
PhTeTePh (av: **18**)	319.4	562.8	447.4
PhTeTePh (C_2: **18a**) (as 0.0)	478.9	744.1	629.9
PhTeTePh (C_2: **18b**) (–2.1)	159.9	381.5	264.9
cyclo-$Te(C_6H_4)_2O$ (C_s: **19**)	257.6	297.9	355.7
Me_3Te^+ (C_3: **20**)	295.6	236.4	327.7
cyclo-$Te(C(tBu)CH)_2CO$ (C_{2v}: **21**)	164.6	213.1	261.3
cyclo-$Te(C_6H_4)_2CO$ (C_s: **22**)	207.8	237.3	316.6
cyclo-$Te(C_6H_4)_2CH_2$ (C_s: **23**)	336.5	391.5	447.7
TeF_6 (O_h: **24**)	350.4	432.8	508.4
$PhTeCH{=}CH_2$ (C_1: **25**)	470.0	542.8	590.1
PhTePh (C_2: **26**)	541.4	622.3	662.1
$CF_3TeTeCF_3$ (C_2: **27**)	504.4	772.3	664.8
cyclo-$C_6H_4TeCH{=}CH$ (C_1: **28**)	458.9	535.9	590.2
Me_2TeCl_2 (C_{2v}: **29**)	408.7	439.7	592.9
Me_2TeBr_2 (C_{2v}: **30**)	320.7	367.3	550.5
$PhTeCl_2Me$ (C_1: **31**)	445.5	489.1	648.8
$PhTeBr_2Me$ (C_1: **32**)	366.5	428.2	603.0
cyclo-$Te(CH)_4$ (C_{2v}: **33**)	470.7	565.7	623.0
cyclo-$Te(C_6H_4)_2Te$ (C_{2v}: **34**)	717.8	820.1	919.7
$Te(tBu)_2$ (C_2: **35**)	692.2	792.6	831.8
bicyclo-$Te(CH_2CH_2CH_2O)_2$ (C_2: **36**)	750.3	845.1	1027.6
cyclo-$[Te(CH_2CH_2CH_2)Te]^{2+}$ (C_{2v}: **37**)	1215.0	1458.8	1517.6
cyclo-$Te^+(C(tBu)CH)_2CH$ (C_{2v}: **38**)	970.5	1103.8	1220.2
CF_3TeCF_3 (C_{2v}: **39**)	1052.7	1192.0	1279.8
$CF_3TeF_2CF_3$ (C_{2v}: **40**)	764.0	851.7	1144.8
CF_3TeCF_2Cl (C_s: **41**)	1201.4	1359.0	1466.4
cyclo-$F_2CTe_2CF_2$ (C_2: **42**)	2138.0	2320.4	2379.3
cyclo-$C_6H_4(CMe_2)_2C$=Te (C_2: **43**)	2850.1	2941.3	2905.9
$TeCl_6^{2-}$ (O_h: **44**)	1268.8	1524.5	1813.7
$TeBr_6^{2-}$ (O_h: **45**)	1242.9	1615.9	1930.8
cyclo-Te_4^{2+} (C_{2v}: **46**)	2462.1	2796.8	2911.4

[a] σ^{d+p}(Te: **M**)$_r$ = –(σ^{d+p}(Te: **M**) – σ^{d+p}(Te: Me_2Te)) and σ^{t}(Te: **M**)$_r$ = –(σ^{t}(Te: **M**) – σ^{t}(Te: Me_2Te)) in ppm.

Table S 10. Distances for Some Tellurium Compounds Optimized at the Slater-type basis sets of quadruple zeta all electron with four polarization functions (QZ4Pae: 5×1s, 3×2s, 5×2p, 3×3s, 3×3p, 3×3d, 3×4s, 3×4p, 4×4d, 3×4f, 4×5s, 4×5p, and 1×5d for Te) being applied at the BLYP level

		Level		
Compound	Distance[a]	Non	Rlt-sc	Rlt-so
Me_2Te (C_{2v})	*r*(Te, C)	2.1904	2.1929	2.1955
TeH_2 (C_{2v})	*r*(Te, H)	1.6792	1.6754	1.6771
Me_4Te (C_{2v})	*r*(Te, C_e)	2.2247	2.2027	2.2042
	r(Te, C_a)	2.3078	2.3602	2.3590
MeTeTeMe (C_2)	*r*(Te, Te)	2.7557	2.7482	2.7622
	r(Te, C)	2.2038	2.2083	2.2103
Me_3Te^+ (C_3)	*r*(Te, C)	2.1679	2.1730	2.1727
Me_2TeCl_2 (C_{2v})	*r*(Te, C)	2.1716	2.1755	2.1759
	r(Te, Cl)	2.5559	2.5612	2.5627
Me_2TeBr_2 (C_{2v})	*r*(Te, C)	2.1746	2.1786	2.1799
	r(Te, Br)	2.7431	2.7392	2.7424
$C_6H_4(CMe_2)_2C{=}Te$ (C_2)	*r*(Te, C)	2.0222	2.0188	2.0216
$Te(OCH_2CH_2O)_2$ (C_2)	*r*(Te, O_a)	2.0350	2.0486	2.0506
	r(Te, O_e)	1.9995	2.0110	2.0125
$Te(OCMe_2CMe_2O)_2$ (C_2)	*r*(Te, O_a)	2.0347	2.0483	2.0502
	r(Te, O_e)	1.9900	2.0040	2.0042
$CF_3TeTeCF_3$ (C_2)	*r*(Te, C)	2.2398	2.2392	2.2446
$TeCl_6^{2-}$ (O_h)	*r*(Te, Cl)	2.6581	2.6492	2.6501
TeF_6 (O_h)	*r*(Te, F)	1.8714	1.8833	1.8833
$Te{=}PMe_3$ (C_1)	*r*(Te, P)	2.3822	2.3814	2.3878
$Te(SiMe_3)_2$ (C_2)	*r*(Te, Si)	2.5847	2.5790	2.5808

[a] In Å.

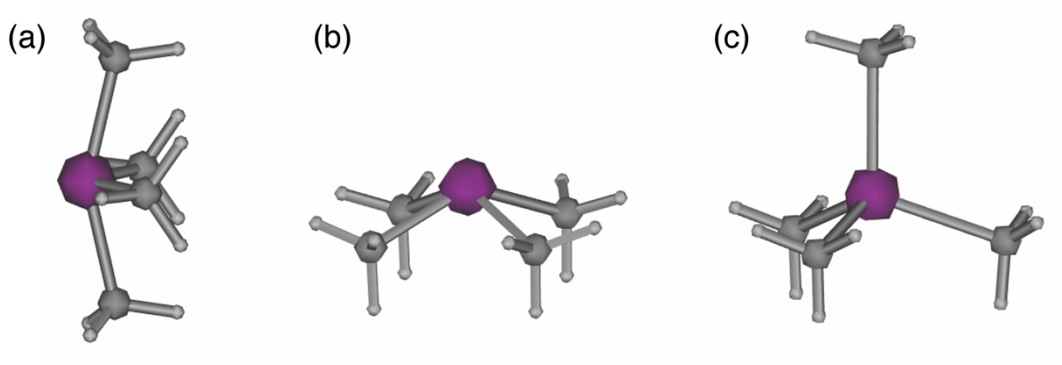

Figure S7. The C_{2v} (a), C_4 (b) and T_d (c) structures of **7**, optimized with $MP2_{Non}$.

Table S11. Effect of Equilibrium on $\sigma^{\square}(Te)_{Rlt\text{-}so:r}$ in TeF_4 and $TeMe_4$ (7), Evaluated with $OPBE_{Non}//OPBE_{Rlt\text{-}so}$ and $BLYP_{Rlt\text{-}so}//MP2_{Non}$

Compound	r(Te, X) (Å)	∠(XTeX) (°)	ΔE kJ mol^{-1}	Population (%)	$\sigma^{\tau}(Te)_{Rlt\text{-}so:r}$ (ppm)
Evaluated with $BLYP_{Rlt\text{-}so}//MP2_{Non}$					
TeF_4 (C_{2v})	1.8547	101.47	0.0[a,b]	99.3	1510.9
	1.9094	161.53			
TeF_4 (C_4)	1.8831	132.70	12.2[a]	0.7	1399.1
TeF_4 (T_d)	1.9530	109.47	208.3[a]	*c*	1524.4
7 (C_{2v})	2.1530	125.08	0.0[a,d]	0.3	–327.4
	2.2035	154.26			
7 (C_4)	2.1723	138.68	–14.3[a]	99.7	–321.5
7 (T_d)	2.4451	109.47	368.4[a]	*c*	1202.3
Evaluated with $OPBE_{Rlt\text{-}so}//OPBE_{Rlt\text{-}so}$					
TeF_4 (C_{2v})	1.8601	100.50	0.0[e,f]	99.7	1644.2
	1.9296	165.12			
TeF_4 (C_{4v})	1.8952	134.79	13.4[e]	0.3	1524.1
TeF_4 (T_d)	1.9564	109.47	107.7[e]	*c*	1607.2
7 (C_{2v})	2.1464	110.88	0.0[e,g]	5.5	–116.0
	2.2860	164.88			
7 (C_4)	2.2077	140.45	–6.5[e]	94.5	–249.4
7 (T_d)	2.4159	109.47	241.6[e]	*c*	1227.8

[a] Based on $MP2_{Non}$ with the Gaussian 03 program. [b] –7010.85230 au. [c] Negligibly small.

[d] –6771.05988 au. [e] Based on $OPBE_{Rlt\text{-}so}$ with the ADF 2013 program. [f] –3.05458 au. [g] –5.28518 au.

Cartesian coordinates

Optimized structures given by Cartesian coordinates for examined molecules with the MP2/6-311+G(3df,3pd) method of the Gaussian 03 program except for Te, together with the total energies. Basis sets of the (7433111/743111/7411/2 + 1s1p1d1f) type are employed for Te.

H_2Te (C_{2v})
E = -6613.0414417 au

52	0	0.000000	0.000000	0.042817
1	0	0.000000	1.176333	-1.113253
1	0	0.000000	-1.176333	-1.113253

HTe^- ($C_{\infty v}$)
E = -6612.5087906 au

52	0	0.000000	0.000000	0.031314
1	0	0.000000	0.000000	-1.628312

H_3Te^+ (C_{3v})
E = -6613.3301415 au

52	0	0.000000	0.000000	0.049728
1	0	0.000000	1.380703	-0.861958
1	0	1.195724	-0.690352	-0.861958
1	0	-1.195724	-0.690352	-0.861958

H_4Te (C_{2v})
E = -6614.1274724 au

52	0	0.000000	0.000000	0.041159
1	0	0.000000	1.602811	-0.535067
1	0	0.000000	-1.602811	-0.535067
1	0	-1.602811	0.000000	-0.535067
1	0	1.602811	0.000000	-0.535067

H_5Te^- (C_{4v})
E = -6614.6862295 au

52	0	0.000000	0.000000	0.047301
1	0	0.000000	1.828266	-0.209826
1	0	-1.828266	0.000000	-0.209826
1	0	1.828266	0.000000	-0.209826
1	0	0.000000	-1.828266	-0.209826
1	0	0.000000	0.000000	-1.620366

H_5Te^+ (C_{4v})
E = -6614.3952097 au

52	0	0.000000	0.000000	0.007312
1	0	0.000000	1.663618	0.313441
1	0	-1.663618	0.000000	0.313441
1	0	1.663618	0.000000	0.313441
1	0	0.000000	-1.663618	0.313441
1	0	0.000000	0.000000	-1.633973

H_6Te (O_h)
E = -6615.2428703 au

52	0	0.000000	0.000000	0.000000
1	0	0.000000	0.000000	1.705123
1	0	0.000000	1.705123	0.000000
1	0	0.000000	-1.705123	0.000000
1	0	0.000000	0.000000	-1.705123
1	0	1.705123	0.000000	0.000000
1	0	-1.705123	0.000000	0.000000

$MeTe^-$ (C_s)
E = -6651.7236058 au

52	0	0.000000	0.338305	0.000000
6	0	0.000000	-1.831324	0.000000
1	0	-1.022443	-2.201300	0.000000
1	0	0.511221	-2.201304	0.885460
1	0	0.511221	-2.201304	-0.885460

MeTeH (C_s)
E = -6652.2679691 au

52	0	0.025543	-0.324277	0.000000
6	0	0.025543	1.804666	0.000000
1	0	-1.621725	-0.435398	0.000000
1	0	1.065833	2.115758	0.000000
1	0	-0.462796	2.177014	0.892693
1	0	-0.462796	2.177014	-0.892693

Me_2Te (**1**) (C_{2v})
E = -6691.4965451 au

52	0	0.000000	0.000000	0.396201
6	0	0.000000	1.540131	-1.065523
6	0	0.000000	-1.540131	-1.065523
1	0	0.000000	-2.496586	-0.550903
1	0	0.892029	-1.460284	-1.678589
1	0	-0.892029	-1.460284	-1.678589
1	0	0.000000	2.496586	-0.550903
1	0	-0.892029	1.460284	-1.678589
1	0	0.892029	1.460284	-1.678589

EtTeH (C_s)
E = -6691.4911963 au

52	0	0.000000	0.620283	0.000000
6	0	0.554662	-1.445469	0.000000
6	0	-0.694882	-2.313673	0.000000
1	0	1.157816	-1.624882	0.885142
1	0	-0.420880	-3.367824	0.000000
1	0	-1.305811	-2.124850	0.881498
1	0	1.157816	-1.624882	-0.885142
1	0	-1.305811	-2.124850	-0.881498
1	0	1.558188	1.167431	0.000000

Et_2Te (C_{2v})
E = -6769.9426604 au

52	0	0.000000	0.000000	0.457154
6	0	0.000000	1.557166	-1.001386
6	0	0.000000	-1.557166	-1.001386
6	0	0.000000	-2.931469	-0.347900
6	0	0.000000	2.931469	-0.347900
1	0	-0.884571	-1.416809	-1.618969
1	0	-0.881110	-3.068770	0.277103
1	0	0.000000	-3.713396	-1.106552
1	0	-0.884571	1.416809	-1.618969
1	0	0.000000	3.713396	-1.106552
1	0	-0.881110	3.068770	0.277103
1	0	0.881110	-3.068770	0.277103
1	0	0.884571	-1.416809	-1.618969
1	0	0.884571	1.416809	-1.618969
1	0	0.881110	3.068770	0.277103

MeTeTeMe (C_2)
E = -13303.3993263 au

52	0	1.312820	-0.241468	-0.238484
52	0	-1.312820	0.241468	-0.238484
6	0	-1.312820	1.725671	1.295439

1	0	-0.672923	2.546815	0.992173
1	0	-2.336727	2.073185	1.412692
1	0	-0.962577	1.288182	2.223682
6	0	1.312820	-1.725671	1.295439
1	0	0.672923	-2.546815	0.992173
1	0	2.336727	-2.073185	1.412692
1	0	0.962577	-1.288182	2.223682

Me_3Te^+ (C_3)
E = -6731.0714737 au

52	0	0.000000	0.000000	0.384968
6	0	1.778078	-0.293870	-0.684667
6	0	-0.634540	1.686796	-0.684667
1	0	-1.663733	1.898414	-0.409441
1	0	0.000000	2.524279	-0.409438
1	0	-0.553151	1.470446	-1.745898
1	0	2.475941	0.491628	-0.409441
1	0	2.186090	-1.262139	-0.409438
1	0	1.550019	-0.256180	-1.745898
6	0	-1.143538	-1.392926	-0.684667
1	0	-0.812208	-2.390042	-0.409441
1	0	-2.186090	-1.262139	-0.409438
1	0	-0.996868	-1.214266	-1.745898

Me_4Te (C_{2v})
E = -6771.0598838 au

52	0	0.000000	0.000000	0.318630
6	0	0.000000	1.910379	-0.674205
6	0	0.000000	-1.910379	-0.674205
1	0	0.000000	-2.685365	0.089881
1	0	0.892164	-2.005263	-1.285217
1	0	-0.892164	-2.005263	-1.285217
1	0	0.000000	2.685365	0.089881
1	0	-0.892164	2.005263	-1.285217
1	0	0.892164	2.005263	-1.285217
6	0	2.148202	0.000000	-0.172121
1	0	2.303958	0.000000	-1.251086
1	0	2.604338	0.889096	0.262610
1	0	2.604338	-0.889096	0.262610
6	0	-2.148202	0.000000	-0.172121
1	0	-2.303958	0.000000	-1.251086
1	0	-2.604338	0.889096	0.262610
1	0	-2.604338	-0.889096	0.262610

Me_5Te^- (C_s)
E = -6810.8617886 au

52	0	0.322536	-0.006455	0.000000
6	0	0.035118	-1.553108	1.662994
1	0	0.900431	-1.459109	2.321987
1	0	-0.883562	-1.381956	2.229451
1	0	0.018420	-2.551617	1.219809
6	0	0.035118	1.615592	1.557209
1	0	-0.225083	1.150561	2.510647
1	0	0.977047	2.157941	1.655101
1	0	-0.755507	2.302809	1.249239
6	0	0.035118	-1.553108	-1.662994
1	0	0.900431	-1.459109	-2.321987
1	0	-0.883562	-1.381956	-2.229451
1	0	0.018420	-2.551617	-1.219809
6	0	0.035118	1.615592	-1.557209
1	0	-0.225083	1.150561	-2.510647
1	0	0.977047	2.157941	-1.655101

1	0	-0.755507	2.302809	-1.249239
6	0	-1.847797	-0.086551	0.000000
1	0	-2.131488	-1.137429	0.000000
1	0	-2.229966	0.402668	0.894700
1	0	-2.229966	0.402668	-0.894700

Me_5Te^+ (C_s)
E = -6810.6361731 au

52	0	0.032391	0.001702	0.000000
6	0	0.464323	-1.473248	1.485084
1	0	1.545757	-1.528927	1.601432
1	0	0.013106	-1.170298	2.426031
1	0	0.081839	-2.435864	1.157823
6	0	0.464323	1.487427	1.475649
1	0	0.082332	1.161314	2.438949
1	0	1.545967	1.602635	1.530983
1	0	0.014525	2.428937	1.172213
6	0	0.464323	-1.473248	-1.485084
1	0	1.545757	-1.528927	-1.601432
1	0	0.013106	-1.170298	-2.426031
1	0	0.081839	-2.435864	-1.157823
6	0	0.464323	1.487427	-1.475649
1	0	0.082332	1.161314	-2.438949
1	0	1.545967	1.602635	-1.530983
1	0	0.014525	2.428937	-1.172213
6	0	-2.041633	-0.038518	0.000000
1	0	-2.354566	-1.078662	0.000000
1	0	-2.395386	0.467755	0.893341
1	0	-2.395386	0.467755	-0.893341

Me_6Te (C_i)
E = -6850.6705767 au

52	0	0.000000	0.000000	0.000000
6	0	-0.008063	-0.019100	-2.159983
1	0	0.207981	0.973414	-2.550518
1	0	0.750970	-0.718666	-2.504806
1	0	-0.984814	-0.345141	-2.513419
6	0	0.008063	0.019100	2.159983
1	0	-0.207981	-0.973414	2.550518
1	0	-0.750970	0.718666	2.504806
1	0	0.984814	0.345141	2.513419
6	0	0.019284	2.159987	0.006409
1	0	-0.973364	2.550443	-0.209163
1	0	0.346114	2.514140	0.982636
1	0	0.718289	2.504173	-0.753429
6	0	-0.019284	-2.159987	-0.006409
1	0	0.973364	-2.550443	0.209163
1	0	-0.346114	-2.514140	-0.982636
1	0	-0.718289	-2.504173	0.753429
6	0	-2.160003	-0.006269	-0.017477
1	0	-2.514485	-0.982675	-0.343415
1	0	-2.504727	0.753161	-0.716660
1	0	-2.549618	0.209931	0.975364
6	0	2.160003	0.006269	0.017477
1	0	2.514485	0.982675	0.343415
1	0	2.549618	-0.209931	-0.975364
1	0	2.504727	-0.753161	0.716660

H_2TeF_2 (C_{2v})
E = -6812.5196697 au

52	0	0.000000	0.000000	0.101654
1	0	1.245660	0.000000	-0.974380

1	0	-1.245660	0.000000	-0.974380
9	0	0.000000	1.944152	-0.185404
9	0	0.000000	-1.944152	-0.185404

H_2TeO (C_s)
E = -6688.1103733 au

52	0	-0.037048	-0.221674	0.000000
1	0	1.111436	-0.632333	1.156366
1	0	1.111436	-0.632333	-1.156366
8	0	-0.037048	1.598966	0.000000

H_2TeO_2 (C_{2v})
E = -6763.1871208 au

52	0	0.000000	0.000000	0.163593
1	0	1.265428	0.000000	1.251890
1	0	-1.265428	0.000000	1.251890
8	0	0.000000	1.576324	-0.688163
8	0	0.000000	-1.576324	-0.688163

H_4TeO (C_{2v})
E = -6689.2037338 au

52	0	0.000000	0.000000	0.191673
1	0	0.000000	1.289096	1.268015
1	0	0.000000	-1.289096	1.268015
1	0	1.700276	0.000000	0.244985
1	0	-1.700276	0.000000	0.244985
8	0	0.000000	0.000000	-1.624127

H_2TeF_2O (C_{2v})
E = -6887.5942286 au

52	0	0.000000	0.000000	0.083559
1	0	-1.402727	0.000000	0.941953
1	0	1.402727	0.000000	0.941953
9	0	0.000000	1.883772	0.403968
9	0	0.000000	-1.883772	0.403968
8	0	0.000000	0.000000	-1.687551

Me_2TeF_2 (C_{2v})
E = -6891.0020705 au

52	0	0.000000	0.000000	0.338364
6	0	0.000000	1.565733	-1.031999
6	0	0.000000	-1.565733	-1.031999
1	0	0.000000	-2.512759	-0.502312
1	0	0.901574	-1.473264	-1.628486
1	0	-0.901574	-1.473264	-1.628486
1	0	0.000000	2.512759	-0.502312
1	0	-0.901574	1.473264	-1.628486
1	0	0.901574	1.473264	-1.628486
9	0	-1.972488	0.000000	0.128201
9	0	1.972488	0.000000	0.128201

$(CF_3)_2TeF_2$ (C_{2v})
E = -7485.763307 au

52	0	0.000000	0.000000	0.865925
6	0	0.000000	1.609003	-0.610708
6	0	0.000000	-1.609003	-0.610708
9	0	0.000000	-2.776769	0.037753
9	0	1.075482	-1.546649	-1.374800
9	0	-1.075482	-1.546649	-1.374800
9	0	0.000000	2.776769	0.037753
9	0	-1.075482	1.546649	-1.374800
9	0	1.075482	1.546649	-1.374800

9	0	-1.932727	0.000000	0.617424
9	0	1.932727	0.000000	0.617424

Me_2TeCl_2 (C_{2v})
E = -7610.9547872 au

52	0	0.000000	0.000000	0.312348
6	0	0.000000	1.563371	-1.083374
6	0	0.000000	-1.563371	-1.083374
1	0	0.000000	-2.503790	-0.540812
1	0	0.904032	-1.466119	-1.674635
1	0	-0.904032	-1.466119	-1.674635
1	0	0.000000	2.503790	-0.540812
1	0	-0.904032	1.466119	-1.674635
1	0	0.904032	1.466119	-1.674635
17	0	-2.464958	0.000000	0.133487
17	0	2.464958	0.000000	0.133487

Me_2TeBr_2 (C_{2v})
E = -11836.9944562 au

52	0	0.000000	0.000000	0.268492
6	0	0.000000	1.562278	-1.135314
6	0	0.000000	-1.562278	-1.135314
1	0	0.000000	-2.501903	-0.591087
1	0	0.904373	-1.463800	-1.726026
1	0	-0.904373	-1.463800	-1.726026
1	0	0.000000	2.501903	-0.591087
1	0	-0.904373	1.463800	-1.726026
1	0	0.904373	1.463800	-1.726026
35	0	-2.630449	0.000000	0.110693
35	0	2.630449	0.000000	0.110693

Me_2TeO (C_s)
E = -6766.5908584 au

52	0	-0.338227	-0.111254	0.000000
6	0	0.636974	0.999080	1.503432
6	0	0.636974	0.999080	-1.503432
1	0	0.346265	0.608392	-2.473961
1	0	1.702882	0.849563	-1.347939
1	0	0.375022	2.052159	-1.430665
1	0	0.346265	0.608392	2.473961
1	0	0.375022	2.052159	1.430665
1	0	1.702882	0.849563	1.347939
8	0	0.636974	-1.653000	0.000000

Me_2TeO_2 (C_{2v})
E = -6841.6797424 au

52	0	0.000000	0.000000	0.125400
6	0	0.000000	1.616300	-1.186557
6	0	0.000000	-1.616300	-1.186557
1	0	0.000000	-2.519541	-0.583594
1	0	0.897966	-1.570406	-1.795759
1	0	-0.897966	-1.570406	-1.795759
1	0	0.000000	2.519541	-0.583594
1	0	-0.897966	1.570406	-1.795759
1	0	0.897966	1.570406	-1.795759
8	0	1.568508	0.000000	1.004257
8	0	-1.568508	0.000000	1.004257

Me_2TeF_2O (C_{2v})
E = -6966.0852264 au

52	0	0.000000	0.000000	0.105254
6	0	0.000000	1.763532	-0.973362

6	0	0.000000	-1.763532	-0.973362
1	0	0.000000	-2.565583	-0.239068
1	0	0.903382	-1.802941	-1.569957
1	0	-0.903382	-1.802941	-1.569957
1	0	0.000000	2.565583	-0.239068
1	0	-0.903382	1.802941	-1.569957
1	0	0.903382	1.802941	-1.569957
9	0	-1.918260	0.000000	-0.116422
9	0	1.918260	0.000000	-0.116422
8	0	0.000000	0.000000	1.882587

F_2TeO (C_s)
E = -6886.466944 au

52	0	-0.295865	0.074373	0.000000
9	0	0.591729	-0.930569	1.336037
9	0	0.591729	-0.930569	-1.336037
8	0	0.591729	1.610354	0.000000

Cl_2TeO (C_s)
E = -7606.4131695 au

52	0	0.430902	-0.330782	0.000000
17	0	-0.533498	0.937599	1.702088
17	0	-0.533498	0.937599	-1.702088
8	0	-0.533498	-1.834715	0.000000

F_2TeO_2 (C_{2v})
E = -6961.5285549 au

52	0	0.000000	0.000000	0.131674
9	0	0.000000	1.337597	-1.158791
9	0	0.000000	-1.337597	-1.158791
8	0	-1.603916	0.000000	0.875699
8	0	1.603916	0.000000	0.875699

TeF_4 (C_{2v})
E = -7010.8522956 au

52	0	0.000000	0.000000	0.302805
9	0	0.000000	1.435950	-0.871077
9	0	0.000000	-1.435950	-0.871077
9	0	-1.884681	0.000000	-0.003694
9	0	1.884681	0.000000	-0.003694

$TeCl_4$ (C_s)
E = -8450.734914 au

52	0	0.407217	-0.214847	0.000000
17	0	-0.873884	0.461069	1.771912
17	0	-0.873884	0.461069	-1.771912
17	0	-0.873884	-2.264649	0.000000
17	0	1.376049	1.999692	0.000000

TeF_5^- (C_s)
E = -7110.7243404 au

52	0	0.000034	0.281568	0.000000
9	0	0.000034	-0.005752	1.935883
9	0	1.935882	-0.005948	0.000000
9	0	-1.935911	-0.005443	0.000000
9	0	0.000034	-0.005752	-1.935883
9	0	-0.000235	-1.603941	0.000000

TeF_5^+ (C_{4v})
E = -7110.1754938 au

52	0	0.000000	0.000000	0.024719
9	0	0.000000	1.770097	0.406658

9	0	-1.770097	0.000000	0.406658
9	0	1.770097	0.000000	0.406658
9	0	0.000000	-1.770097	0.406658
9	0	0.000000	0.000000	-1.769453

$HTeF_5$ (C_{4v})
E = -7111.1853602 au

52	0	0.000000	0.000000	0.167942
1	0	0.000000	0.000000	1.803778
9	0	0.000000	1.851028	0.124503
9	0	0.000000	-1.851028	0.124503
9	0	0.000000	0.000000	-1.668764
9	0	1.851028	0.000000	0.124503
9	0	-1.851028	0.000000	0.124503

$MeTeF_5$ (C_s)
E = -7150.4329743 au

52	0	0.000969	-0.001724	0.000000
9	0	-0.080685	1.308553	1.317613
9	0	-1.838535	-0.002047	0.000000
9	0	-0.080685	-1.319153	-1.310303
9	0	-0.080685	1.308553	-1.317613
9	0	-0.080685	-1.319153	1.310303
6	0	2.044836	0.030365	0.000000
1	0	2.389821	-0.476640	-0.893990
1	0	2.389821	-0.476640	0.893990
1	0	2.352413	1.069975	0.000000

TeF_6 (O_h)
E = -7210.355713 au

52	0	0.000000	0.000000	0.000000
9	0	0.000000	0.000000	1.831470
9	0	0.000000	1.831470	0.000000
9	0	0.000000	-1.831470	0.000000
9	0	0.000000	0.000000	-1.831470
9	0	1.831470	0.000000	0.000000
9	0	-1.831470	0.000000	0.000000

MeTeEt (C_s)
E = -6730.7195781 au

52	0	0.000000	0.536733	0.000000
6	0	2.108600	0.276708	0.000000
1	0	2.571726	1.259174	0.000000
1	0	2.408569	-0.263725	0.892125
1	0	2.408569	-0.263725	-0.892125
6	0	-0.378640	-1.562076	0.000000
1	0	0.103561	-1.973154	0.884413
1	0	0.103561	-1.973154	-0.884413
6	0	-1.870526	-1.860476	0.000000
1	0	-2.043230	-2.936074	0.000000
1	0	-2.354679	-1.442191	0.881182
1	0	-2.354679	-1.442191	-0.881182

MeTeEt (C_1-*g*)
E = -6730.72069 au

52	0	0.546103	-0.328351	-0.059690
6	0	-1.483776	-0.361150	0.589878
6	0	0.708585	1.781441	0.131175
6	0	-2.446957	0.326337	-0.364611
1	0	0.076503	2.278395	-0.596786
1	0	-1.501545	0.096318	1.577566
1	0	-3.465264	0.285132	0.024218

1	0	-2.187542	1.375109	-0.500384
1	0	0.431703	2.070988	1.140491
1	0	-1.731941	-1.414414	0.710914
1	0	-2.431105	-0.150667	-1.342459
1	0	1.744698	2.053630	-0.048342

EtTeEt (C_1-*g*)
E = -6769.9436978 au

52	0	0.041197	-0.630456	-0.057330
6	0	-1.782382	0.273526	0.579616
6	0	1.179778	1.154124	0.211416
6	0	2.660200	0.911004	-0.044689
6	0	-2.323139	1.316996	-0.385309
1	0	0.787983	1.904420	-0.470899
1	0	2.830697	0.561975	-1.062132
1	0	3.225850	1.831955	0.092800
1	0	-1.588709	0.696924	1.563798
1	0	-3.247509	1.750768	-0.001308
1	0	-1.611394	2.128191	-0.529866
1	0	3.059615	0.163688	0.638975
1	0	1.007217	1.484051	1.234135
1	0	-2.485325	-0.547971	0.708211
1	0	-2.527387	0.875832	-1.358745

EtTeEt (C_2-*gg*)
E = -6769.9453759 au

52	0	0.000000	0.000000	0.794558
6	0	-0.962185	-1.232517	-0.656910
6	0	0.962185	1.232517	-0.656910
6	0	0.000000	1.886141	-1.635134
6	0	0.000000	-1.886141	-1.635134
1	0	1.498758	1.979848	-0.074236
1	0	-0.725413	2.506246	-1.111831
1	0	0.542895	2.511984	-2.344554
1	0	-1.704009	-0.622763	-1.167618
1	0	-0.542895	-2.511984	-2.344554
1	0	0.550378	-1.140868	-2.208000
1	0	-0.550378	1.140868	-2.208000
1	0	1.704009	0.622763	-1.167618
1	0	-1.498758	-1.979848	-0.074236
1	0	0.725413	-2.506246	-1.111831

PhTePh (C_2)
E = -7074.1619196 au

52	0	0.000000	0.000000	1.490514
6	0	0.000016	1.526765	0.054907
6	0	0.853475	2.625316	0.195869
6	0	-0.857862	1.457327	-1.048392
6	0	0.844532	3.644878	-0.755274
6	0	-0.844372	2.467126	-2.006741
6	0	0.000811	3.566675	-1.860454
1	0	1.534472	2.679163	1.035715
1	0	-1.525189	0.612374	-1.164352
1	0	1.508366	4.491707	-0.637084
1	0	-1.504864	2.399766	-2.861889
1	0	0.003051	4.353288	-2.603217
6	0	-0.000016	-1.526765	0.054907
6	0	-0.853475	-2.625316	0.195869
6	0	0.857862	-1.457327	-1.048392
6	0	-0.844532	-3.644878	-0.755274
6	0	0.844372	-2.467126	-2.006741
6	0	-0.000811	-3.566675	-1.860454

1	0	-1.534472	-2.679163	1.035715
1	0	1.525189	-0.612374	-1.164352
1	0	-1.508366	-4.491707	-0.637084
1	0	1.504864	-2.399766	-2.861889
1	0	-0.003051	-4.353288	-2.603217

EtTeTeEt (C_2)
E = -13381.8481395 au

52	0	0.239544	1.312543	-0.418918
52	0	-0.239544	-1.312543	-0.418918
6	0	-1.159623	1.841222	1.118619
1	0	-2.130131	1.479489	0.789546
1	0	-0.866152	1.300640	2.014699
6	0	-1.159623	3.345549	1.342853
1	0	-1.441561	3.878822	0.435944
1	0	-1.871487	3.610980	2.124077
1	0	-0.176637	3.700006	1.650619
6	0	1.159623	-1.841222	1.118619
1	0	0.866152	-1.300640	2.014699
1	0	2.130131	-1.479489	0.789546
6	0	1.159623	-3.345549	1.342853
1	0	1.441561	-3.878822	0.435944
1	0	1.871487	-3.610980	2.124077
1	0	0.176637	-3.700006	1.650619

EtTeTeEt (C_1-*g*)
E = -13381.8498126 au

52	0	-1.076485	0.248874	-0.615511
52	0	1.315327	-0.749829	0.022756
6	0	-2.092956	-0.334518	1.181367
1	0	-1.573755	0.142726	2.008439
1	0	-1.975977	-1.411646	1.265670
6	0	-3.556236	0.075893	1.121999
1	0	-4.069263	-0.221813	2.036168
1	0	-3.660674	1.154916	1.015155
1	0	-4.064201	-0.396768	0.282407
6	0	2.043473	0.982194	1.056085
1	0	1.337610	1.182966	1.858785
1	0	2.983441	0.657462	1.503114
6	0	2.233632	2.186637	0.152955
1	0	1.291863	2.460259	-0.321593
1	0	2.583136	3.043660	0.730120
1	0	2.960542	1.976661	-0.629442

EtTeTeEt (C_2-*gg*)
E = -13381.8514258 au

52	0	0.604969	1.190187	-0.334511
52	0	-0.604969	-1.190187	-0.334511
6	0	-0.604969	2.082910	1.194445
1	0	-0.116545	3.034048	1.408008
1	0	-0.510459	1.448300	2.072699
6	0	-2.053416	2.271434	0.783363
1	0	-2.627296	2.707922	1.601837
1	0	-2.131135	2.927174	-0.081842
1	0	-2.505419	1.313901	0.527042
6	0	0.604969	-2.082910	1.194445
1	0	0.510459	-1.448300	2.072699
1	0	0.116545	-3.034048	1.408008
6	0	2.053416	-2.271434	0.783363
1	0	2.505419	-1.313901	0.527042
1	0	2.627296	-2.707922	1.601837
1	0	2.131135	-2.927174	-0.081842

PhTeTePh (C_2)
E = -13686.0683983 au

52	0	0.504748	1.228923	-1.221161
52	0	-0.504748	-1.228923	-1.221161
6	0	-0.565174	2.026966	0.409872
6	0	-1.267822	1.233821	1.317548
6	0	-1.915223	1.825390	2.401168
6	0	-1.856826	3.203856	2.592866
6	0	-1.150012	3.994545	1.688694
6	0	-0.504748	3.411961	0.600549
1	0	-1.323636	0.160810	1.176431
1	0	-2.460659	1.201825	3.098154
1	0	-2.359022	3.658114	3.436473
1	0	-1.102712	5.067438	1.824509
1	0	0.032567	4.041250	-0.099381
6	0	0.565174	-2.026966	0.409872
6	0	1.267822	-1.233821	1.317548
6	0	1.915223	-1.825390	2.401168
6	0	1.856826	-3.203856	2.592866
6	0	1.150012	-3.994545	1.688694
6	0	0.504748	-3.411961	0.600549
1	0	1.323636	-0.160810	1.176431
1	0	2.460659	-1.201825	3.098154
1	0	2.359022	-3.658114	3.436473
1	0	1.102712	-5.067438	1.824509
1	0	-0.032567	-4.041250	-0.099381

PhTeMe (C_s)
E = -6882.8282506 au

6	0	0.227189	0.672296	0.000000
6	0	0.232891	2.775510	1.205430
6	0	0.232891	1.381879	1.206645
6	0	0.232335	3.474035	0.000000
6	0	0.232891	2.775510	-1.205430
6	0	0.232891	1.381879	-1.206645
1	0	0.236661	3.312711	2.145099
1	0	0.238800	0.842824	2.145257
1	0	0.234419	4.556103	0.000000
1	0	0.236661	3.312711	-2.145099
1	0	0.238800	0.842824	-2.145257
52	0	0.174903	-1.425595	0.000000
6	0	-1.953264	-1.493269	0.000000
1	0	-2.254526	-2.537522	0.000000
1	0	-2.326363	-1.002870	0.892835
1	0	-2.326363	-1.002870	-0.892835

PhTeCl$_2$Me (C_1)
E = -7802.2838203 au

6	0	1.037747	-0.035477	-0.088437
6	0	1.618404	-1.020307	0.709847
6	0	3.004698	-1.049692	0.843166
6	0	3.800681	-0.126314	0.169175
6	0	3.206561	0.841963	-0.637170
6	0	1.821210	0.900131	-0.765273
1	0	1.008892	-1.762655	1.206345
1	0	3.461789	-1.803659	1.470758
1	0	4.876843	-0.161760	0.271566
1	0	3.819637	1.560454	-1.165157
1	0	1.363647	1.675763	-1.364105
52	0	-1.040993	0.067992	-0.286510
17	0	-0.854933	2.470420	0.258227

17	0	-1.076389	-2.394095	-0.458410
6	0	-1.584851	-0.150381	1.728179
1	0	-2.441629	0.493957	1.898508
1	0	-0.739336	0.199079	2.313919
1	0	-1.812420	-1.193815	1.912880

$PhTeBr_2Me$ (C_1)
E = -12028.3235804 au

6	0	-0.137255	1.234975	-0.067251
6	0	0.595284	1.936151	0.889103
6	0	0.409098	3.311705	1.004701
6	0	-0.477312	3.978356	0.161447
6	0	-1.190743	3.264853	-0.799204
6	0	-1.031778	1.886449	-0.916433
1	0	1.312747	1.429833	1.520606
1	0	0.965862	3.862065	1.751911
1	0	-0.610638	5.047843	0.252189
1	0	-1.878590	3.778476	-1.457942
1	0	-1.614461	1.331203	-1.639249
52	0	0.089672	-0.834439	-0.256425
35	0	-2.517120	-1.039597	0.066793
35	0	2.699769	-0.489075	-0.230098
6	0	0.196738	-1.333097	1.783264
1	0	-0.269545	-2.307296	1.895634
1	0	-0.384189	-0.582489	2.311414
1	0	1.238972	-1.341653	2.081437

cyclo-$Te(CH)_4$ (C_{2v})
E = -6766.3363629 au

52	0	0.000000	0.000000	0.766412
6	0	0.000000	1.342723	-0.757468
1	0	0.000000	2.411765	-0.613574
6	0	0.000000	-1.342723	-0.757468
1	0	0.000000	-2.411765	-0.613574
6	0	0.000000	0.709799	-1.977904
1	0	0.000000	1.275683	-2.900914
6	0	0.000000	-0.709799	-1.977904
1	0	0.000000	-1.275683	-2.900914

23 (C_s)
E = -7112.212253 au

52	0	-1.595103	0.229723	0.000000
6	0	1.389272	1.276654	0.000000
1	0	0.697403	2.129698	0.000000
1	0	2.408157	1.663742	0.000000
6	0	-0.144427	-0.051798	1.478682
6	0	1.132752	0.478632	1.247447
6	0	2.135609	0.251727	2.193221
6	0	1.869338	-0.455172	3.362442
6	0	0.588920	-0.958164	3.590996
6	0	-0.416850	-0.769712	2.647176
1	0	3.128429	0.648257	2.014161
1	0	2.654458	-0.613557	4.089767
1	0	0.376820	-1.512475	4.496151
1	0	-1.399563	-1.192499	2.812425
6	0	-0.144427	-0.051798	-1.478682
6	0	1.132752	0.478632	-1.247447
6	0	2.135609	0.251727	-2.193221
6	0	1.869338	-0.455172	-3.362442
6	0	0.588920	-0.958164	-3.590996
6	0	-0.416850	-0.769712	-2.647176
1	0	3.128429	0.648257	-2.014161

1	0	2.654458	-0.613557	-4.089767
1	0	0.376820	-1.512475	-4.496151
1	0	-1.399563	-1.192499	-2.812425

19 (C_s)
E = -7148.0889915 au

52	0	1.616657	-0.207924	0.000000
8	0	-1.439631	-1.043104	0.000000
6	0	0.154752	0.070337	1.456216
6	0	-1.134613	-0.386925	1.177660
6	0	-2.159059	-0.254717	2.110602
6	0	-1.891841	0.331028	3.344041
6	0	-0.611319	0.800203	3.634476
6	0	0.403050	0.681409	2.688681
1	0	-3.144016	-0.622492	1.855916
1	0	-2.685183	0.426881	4.073281
1	0	-0.403622	1.264507	4.589093
1	0	1.392446	1.061526	2.909907
6	0	0.154752	0.070337	-1.456216
6	0	-1.134613	-0.386925	-1.177660
6	0	-2.159059	-0.254717	-2.110602
6	0	-1.891841	0.331028	-3.344041
6	0	-0.611319	0.800203	-3.634476
6	0	0.403050	0.681409	-2.688681
1	0	-3.144016	-0.622492	-1.855916
1	0	-2.685183	0.426881	-4.073281
1	0	-0.403622	1.264507	-4.589093
1	0	1.392446	1.061526	-2.909907

22 (C_s)
E = -7186.1328805843 au

52	0	0.000144	-1.648224	0.000000
6	0	-0.000867	1.848016	0.000000
8	0	-0.001702	3.075350	0.000000
6	0	0.000130	-0.252348	1.522220
6	0	-0.000330	1.137346	1.315164
6	0	-0.000311	1.979530	2.443225
6	0	0.000130	1.471147	3.729760
6	0	0.000556	0.087835	3.926418
6	0	0.000555	-0.760517	2.831304
1	0	-0.000662	3.045758	2.265164
1	0	0.000142	2.144107	4.576614
1	0	0.000901	-0.326918	4.926087
1	0	0.000905	-1.832525	2.990774
6	0	0.000130	-0.252348	-1.522220
6	0	-0.000330	1.137346	-1.315164
6	0	-0.000311	1.979530	-2.443225
6	0	0.000130	1.471147	-3.729760
6	0	0.000556	0.087835	-3.926418
6	0	0.000555	-0.760517	-2.831304
1	0	-0.000662	3.045758	-2.265164
1	0	0.000142	2.144107	-4.576614
1	0	0.000901	-0.326918	-4.926087
1	0	0.000905	-1.832525	-2.990774

34 (C_{2v})
E = -13684.859073 au

52	0	0.000000	1.774390	-0.684532
52	0	0.000000	-1.774390	-0.684532
6	0	1.541354	0.702017	0.233449
6	0	1.541354	-0.702017	0.233449
6	0	2.592440	-1.393441	0.852160

6	0	3.653912	-0.697500	1.420180
6	0	3.653912	0.697500	1.420180
6	0	2.592440	1.393441	0.852160
1	0	2.577139	-2.475446	0.885741
1	0	4.469498	-1.242516	1.877352
1	0	4.469498	1.242516	1.877352
1	0	2.577139	2.475446	0.885741
6	0	-1.541354	0.702017	0.233449
6	0	-1.541354	-0.702017	0.233449
6	0	-2.592440	-1.393441	0.852160
6	0	-3.653912	-0.697500	1.420180
6	0	-3.653912	0.697500	1.420180
6	0	-2.592440	1.393441	0.852160
1	0	-2.577139	-2.475446	0.885741
1	0	-4.469498	-1.242516	1.877352
1	0	-4.469498	1.242516	1.877352
1	0	-2.577139	2.475446	0.885741

43 (C_2)
E = -7115.7856622 au

6	0	-0.000002	0.697481	-1.764008
6	0	0.000002	-0.697481	-1.764008
6	0	-0.000002	1.405149	-2.963432
6	0	0.000002	0.698563	-4.166414
6	0	-0.000002	-0.698563	-4.166414
6	0	0.000002	-1.405149	-2.963432
1	0	0.000000	2.489152	-2.968680
1	0	0.000007	1.235266	-5.106350
1	0	-0.000007	-1.235266	-5.106350
1	0	0.000000	-2.489152	-2.968680
6	0	-0.000021	1.256061	-0.364395
6	0	1.251016	2.104113	-0.103236
1	0	1.259266	2.967744	-0.770510
1	0	1.247097	2.453342	0.930251
1	0	2.155256	1.520602	-0.276143
6	0	-1.251116	2.104027	-0.103258
1	0	-2.155315	1.520459	-0.276184
1	0	-1.247237	2.453254	0.930230
1	0	-1.259409	2.967659	-0.770530
6	0	0.000021	-1.256061	-0.364395
6	0	-1.251016	-2.104113	-0.103236
1	0	-1.259266	-2.967744	-0.770510
1	0	-1.247097	-2.453342	0.930251
1	0	-2.155256	-1.520602	-0.276143
6	0	1.251116	-2.104027	-0.103258
1	0	2.155315	-1.520459	-0.276184
1	0	1.247237	-2.453254	0.930230
1	0	1.259409	-2.967659	-0.770530
6	0	0.000000	0.000000	0.491412
52	0	0.000000	0.000000	2.447005

$CF_3TeTeCF_3$ (C_2)
E = -13898.1920679 au

52	0	1.183946	-0.601103	-0.692219
52	0	-1.183946	0.601103	-0.692219
6	0	-0.671184	2.068755	0.820052
9	0	0.340482	2.853940	0.449174
9	0	-1.744211	2.845373	1.019420
9	0	-0.340482	1.514927	1.984191
6	0	0.671184	-2.068755	0.820052
9	0	-0.340482	-2.853940	0.449174
9	0	1.744211	-2.845373	1.019420

9	0	0.340482	-1.514927	1.984191

CF_3TeCF_3 (C_{2v})
E = -7286.2869086 au

52	0	0.000000	0.000000	0.988860
6	0	0.000000	1.542702	-0.519957
9	0	0.000000	2.727618	0.100596
9	0	-1.073560	1.486515	-1.305332
9	0	1.073560	1.486515	-1.305332
6	0	0.000000	-1.542702	-0.519957
9	0	0.000000	-2.727618	0.100596
9	0	1.073560	-1.486515	-1.305332
9	0	-1.073560	-1.486515	-1.305332

$(TeCF_2)_2$ (D_{2h})
E = -13698.6611145 au

52	0	1.665070	0.000000	0.000000
6	0	0.000000	1.385664	0.000000
9	0	0.000000	2.203484	1.074725
9	0	0.000000	2.203484	-1.074725
52	0	-1.665070	0.000000	0.000000
6	0	0.000000	-1.385664	0.000000
9	0	0.000000	-2.203484	1.074725
9	0	0.000000	-2.203484	-1.074725

Te=P(*i*Pr)$_3$ (C_1)
E = -7307.6044163470 au

52	0	-1.895771	0.169071	-0.069006
15	0	0.429498	0.042888	0.024561
6	0	1.152570	1.677546	0.466383
1	0	0.659653	1.900650	1.416530
6	0	0.745667	2.755029	-0.536049
1	0	-0.333758	2.779037	-0.671518
1	0	1.076351	3.727970	-0.170542
1	0	1.216618	2.590197	-1.505938
6	0	2.667132	1.667994	0.664622
1	0	3.182295	1.534237	-0.286275
1	0	2.979992	2.630597	1.071352
1	0	3.000308	0.891962	1.352656
6	0	1.252101	-0.461044	-1.554941
1	0	1.417906	0.494000	-2.062945
6	0	0.352180	-1.314544	-2.445760
1	0	-0.597139	-0.821643	-2.639824
1	0	0.861286	-1.498885	-3.393098
1	0	0.136992	-2.276301	-1.981323
6	0	2.603065	-1.152799	-1.352394
1	0	3.079682	-1.287049	-2.324257
1	0	3.285821	-0.589209	-0.721248
1	0	2.470481	-2.141060	-0.913546
6	0	1.013742	-1.115266	1.326458
1	0	2.100326	-1.168784	1.226244
6	0	0.654430	-0.590457	2.715085
1	0	-0.421879	-0.430164	2.788075
1	0	0.945472	-1.328059	3.463955
1	0	1.161308	0.344295	2.950178
6	0	0.414507	-2.504536	1.116560
1	0	0.655412	-2.919929	0.139483
1	0	0.799041	-3.182733	1.879531
1	0	-0.670885	-2.455660	1.202602

Te(SiMe$_3$)$_2$ (C_2)
E = -7429.0038386 au

52	0	0.000000	0.000000	1.163324
14	0	0.000000	1.890575	-0.479076
6	0	-0.514548	3.395442	0.503869
1	0	0.167621	3.567254	1.336178
1	0	-0.506259	4.282174	-0.132629
1	0	-1.518227	3.271167	0.908632
6	0	-1.220860	1.588116	-1.865175
1	0	-1.259819	2.467715	-2.511492
1	0	-0.936850	0.734947	-2.479845
1	0	-2.220058	1.407716	-1.470223
6	0	1.715359	2.147859	-1.177424
1	0	1.718493	2.999441	-1.861112
1	0	2.425286	2.347714	-0.375371
1	0	2.061838	1.270413	-1.721114
14	0	0.000000	-1.890575	-0.479076
6	0	0.514548	-3.395442	0.503869
1	0	-0.167621	-3.567254	1.336178
1	0	0.506259	-4.282174	-0.132629
1	0	1.518227	-3.271167	0.908632
6	0	1.220860	-1.588116	-1.865175
1	0	1.259819	-2.467715	-2.511492
1	0	0.936850	-0.734947	-2.479845
1	0	2.220058	-1.407716	-1.470223
6	0	-1.715359	-2.147859	-1.177424
1	0	-2.061838	-1.270413	-1.721114
1	0	-1.718493	-2.999441	-1.861112
1	0	-2.425286	-2.347714	-0.375371

$Te{=}PMe_3$ (C_1)
E = -7072.2590895 au

52	0	-1.265259	0.000000	0.000000
15	0	1.053981	0.000000	0.000000
6	0	1.805534	1.643660	-0.083969
1	0	1.467295	2.135750	-0.993330
1	0	1.467337	2.225840	0.770540
1	0	2.893407	1.571934	-0.080331
6	0	1.805535	-0.894549	-1.381466
1	0	1.467318	-1.928130	-1.352931
1	0	1.467316	-0.445631	-2.312904
1	0	2.893408	-0.855512	-1.321184
6	0	1.805534	-0.749111	1.465435
1	0	1.467319	-0.207606	2.346275
1	0	1.467314	-1.780218	1.542381
1	0	2.893407	-0.716425	1.401487

$Te_2C_5H_8O$ (**12**) (C_1)
E = -13493.7642466 au

52	0	-1.001072	-1.333067	-0.070733
52	0	-0.899638	1.396719	-0.037658
6	0	0.911845	-1.274653	0.899070
1	0	0.758277	-1.180719	1.972936
1	0	1.382373	-2.232709	0.679093
6	0	1.115830	1.215268	0.693953
1	0	1.685645	2.020311	0.230451
1	0	1.090929	1.358647	1.772596
6	0	1.716015	-0.128403	0.341698
6	0	2.147054	-0.213351	-1.128970
1	0	2.087123	-1.226144	-1.535655
1	0	1.695366	0.500285	-1.817661
6	0	3.242323	-0.131457	0.603383
1	0	3.628523	-1.109931	0.901752
1	0	3.636221	0.645660	1.258621

8	0	3.509258	0.138790	-0.785072

(tBu)$_2$Te (C_2)
E = -6926.852667 au

52	0	0.000000	0.000000	0.873417
6	0	0.000000	1.709535	-0.452019
6	0	1.026409	1.575531	-1.568154
6	0	-1.388568	1.959129	-1.030556
6	0	0.384730	2.879990	0.451326
1	0	2.024123	1.387803	-1.172642
1	0	0.773070	0.776768	-2.263462
1	0	1.051248	2.510945	-2.136250
1	0	-2.123832	2.097003	-0.238852
1	0	-1.362433	2.867999	-1.640416
1	0	-1.721777	1.138644	-1.662686
1	0	0.352821	3.802363	-0.135822
1	0	-0.310665	2.988676	1.285003
1	0	1.390758	2.760652	0.852709
6	0	0.000000	-1.709535	-0.452019
6	0	-1.026409	-1.575531	-1.568154
6	0	1.388568	-1.959129	-1.030556
6	0	-0.384730	-2.879990	0.451326
1	0	-2.024123	-1.387803	-1.172642
1	0	-0.773070	-0.776768	-2.263462
1	0	-1.051248	-2.510945	-2.136250
1	0	2.123832	-2.097003	-0.238852
1	0	1.362433	-2.867999	-1.640416
1	0	1.721777	-1.138644	-1.662686
1	0	-0.352821	-3.802363	-0.135822
1	0	0.310665	-2.988676	1.285003
1	0	-1.390758	-2.760652	0.852709

CF_3TeCF_2Cl (C_s)
E = -7646.2513407 au

52	0	-0.951641	-0.221150	0.000000
6	0	0.553104	-1.770674	0.000000
9	0	-0.072203	-2.954026	0.000000
9	0	1.338922	-1.718192	1.073721
9	0	1.338922	-1.718192	-1.073721
6	0	0.544450	1.329276	0.000000
17	0	-0.273611	2.889461	0.000000
9	0	1.338922	1.252281	1.075191
9	0	1.338922	1.252281	-1.075191

$TeCl_6^{2-}$ (O_h)
E = -9370.2966513 au

52	0	0.000000	0.000000	0.000000
17	0	0.000000	0.000000	2.560967
17	0	0.000000	2.560967	0.000000
17	0	0.000000	0.000000	-2.560967
17	0	2.560967	0.000000	0.000000
17	0	-2.560967	0.000000	0.000000
17	0	0.000000	-2.560967	0.000000

$TeCl_6^{2-}$ $(D_{4h})_{obsd}$
E = -9370.2952465 au

52	0	0.000000	0.000000	0.000000
17	0	0.000000	2.524000	0.000000
17	0	2.524000	0.000000	0.000000
17	0	0.000000	-2.524000	0.000000
17	0	0.000000	0.000000	2.529000
17	0	0.000000	0.000000	-2.529000

17	0	-2.524000	0.000000	0.000000

$TeBr_6^{2-}$ (O_h)
E = -22048.2675267 au

52	0	0.000000	0.000000	0.000000
35	0	0.000000	0.000000	2.496885
35	0	0.000000	2.496885	0.000000
35	0	0.000000	0.000000	-2.496885
35	0	2.496885	0.000000	0.000000
35	0	-2.496885	0.000000	0.000000
35	0	0.000000	-2.496885	0.000000

$TeBr_6^{2-}$ $(D_{4h})_{obsd}$
E = -22048.4429501 au

52	0	0.000000	0.000000	0.000000
35	0	0.000000	0.000000	2.693000
35	0	0.000000	2.706000	0.000000
35	0	0.000000	0.000000	-2.693000
35	0	2.706000	0.000000	0.000000
35	0	-2.706000	0.000000	0.000000
35	0	0.000000	-2.706000	0.000000

$TeBr_6^{2-}$ $(D_{2h})_{obsd}$
E = -22048.4427812 au

52	0	0.000000	0.000000	0.000000
35	0	0.000000	0.000000	2.687000
35	0	-2.710000	0.000000	0.000000
35	0	0.000000	0.000000	-2.687000
35	0	0.000000	2.696000	0.000000
35	0	0.000000	-2.696000	0.000000
35	0	2.710000	0.000000	0.000000

cyclic-Te_4^{2+} (C_{2h})
E = -26446.8870009 au

52	0	-1.354575	1.354578	0.000000
52	0	-1.354575	-1.354593	0.000000
52	0	1.354575	-1.354578	0.000000
52	0	1.354575	1.354593	0.000000

cyclic-Te_4^{2+} $(C_{2h})_{obsd}$
E = -26446.885622 au

52	0	1.332118	-1.339528	0.000000
52	0	1.332118	1.331077	0.000000
52	0	-1.332118	1.339528	0.000000
52	0	-1.332118	-1.331077	0.000000

H_2S (C_{2v})
E = -398.8992401 au

16	0	0.000000	0.000000	0.102585
1	0	0.000000	0.960553	-0.820680
1	0	0.000000	-0.960553	-0.820680

HS^- ($C_{\infty v}$)
E = -398.3327815 au

16	0	0.000000	0.000000	0.078716
1	0	0.000000	0.000000	-1.259463

H_3S^+ (C_{3v})
E = -399.17734 au

16	0	0.000000	0.000000	0.113133
1	0	0.000000	1.140342	-0.603377
1	0	0.987565	-0.570171	-0.603377

1	0	-0.987565	-0.570171	-0.603377

H_4S (C_{2v})
E = -399.9518102 au

16	0	0.000000	0.000000	0.053811
1	0	0.000000	1.354354	-0.215247
1	0	0.000000	-1.354354	-0.215247
1	0	-1.354355	0.000000	-0.215245
1	0	1.354355	0.000000	-0.215245

H_5S^- (C_{4v})
E = -400.4812501 au

16	0	0.000000	0.000000	0.083909
1	0	0.000000	1.585352	-0.029487
1	0	-1.585352	0.000000	-0.029487
1	0	1.585352	0.000000	-0.029487
1	0	0.000000	-1.585352	-0.029487
1	0	0.000000	0.000000	-1.224590

H_5S^+ (C_{4v})
E = -400.2181826 au

16	0	0.000000	0.000000	0.025715
1	0	0.000000	1.372282	0.226713
1	0	-1.372282	0.000000	0.226713
1	0	1.372282	0.000000	0.226713
1	0	0.000000	-1.372282	0.226713
1	0	0.000000	0.000000	-1.318296

H_6S (O_h)
E = -401.0534084 au

16	0	0.000000	0.000000	0.000000
1	0	0.000000	0.000000	1.395475
1	0	0.000000	1.395475	0.000000
1	0	0.000000	-1.395475	0.000000
1	0	0.000000	0.000000	-1.395475
1	0	1.395475	0.000000	0.000000
1	0	-1.395475	0.000000	0.000000

MeS^- (C_s)
E = -437.5387288 au

16	0	0.000000	0.705049	0.000000
6	0	0.000000	-1.118738	0.000000
1	0	-1.016420	-1.522785	0.000000
1	0	0.508209	-1.522783	0.880246
1	0	0.508209	-1.522783	-0.880246

MeSH (C_s)
E = -438.1157526 au

16	0	0.047492	-0.661627	0.000000
6	0	0.047492	1.145988	0.000000
1	0	-1.275598	-0.820167	0.000000
1	0	1.090762	1.449129	0.000000
1	0	-0.429990	1.540573	0.891027
1	0	-0.429990	1.540573	-0.891027

Me_2S (C_{2v})
E = -477.3372851 au

16	0	0.000000	0.000000	0.662316
6	0	0.000000	1.358554	-0.513176
6	0	0.000000	-1.358554	-0.513176
1	0	0.000000	-2.283848	0.057536
1	0	0.890227	-1.329696	-1.138505

1	0	-0.890227	-1.329696	-1.138505
1	0	0.000000	2.283848	0.057536
1	0	-0.890227	1.329696	-1.138505
1	0	0.890227	1.329696	-1.138505

EtSH (C_s)
E = -477.3399271 au

16	0	-0.754438	-0.821558	0.000000
6	0	0.000000	0.829526	0.000000
6	0	1.511323	0.662845	0.000000
1	0	-0.322809	1.372991	0.884867
1	0	1.996507	1.637181	0.000000
1	0	1.840113	0.116546	0.882390
1	0	-0.322809	1.372991	-0.884867
1	0	1.840113	0.116546	-0.882390
1	0	-2.028039	-0.425552	0.000000

EtSEt (C_{2v})
E = -555.7854972 au

16	0	0.000000	0.000000	0.547413
6	0	0.000000	1.374964	-0.620648
6	0	0.000000	-1.374964	-0.620648
6	0	0.000000	-2.690747	0.142417
6	0	0.000000	2.690747	0.142417
1	0	-0.884166	-1.299344	-1.254584
1	0	-0.882086	-2.769540	0.775315
1	0	0.000000	-3.529819	-0.551383
1	0	-0.884166	1.299344	-1.254584
1	0	0.000000	3.529819	-0.551383
1	0	-0.882086	2.769540	0.775315
1	0	0.882086	-2.769540	0.775315
1	0	0.884166	-1.299344	-1.254584
1	0	0.884166	1.299344	-1.254584
1	0	0.882086	2.769540	0.775315

MeSSMe (C_1)
E = -6691.4965452 au

52	0	0.000000	0.396201	0.000000
6	0	-1.540131	-1.065523	0.000000
6	0	1.540131	-1.065523	0.000000
1	0	2.496586	-0.550903	-0.000003
1	0	1.460282	-1.678590	-0.892028
1	0	1.460285	-1.678587	0.892030
1	0	-2.496586	-0.550903	-0.000007
1	0	-1.460287	-1.678585	0.892032
1	0	-1.460278	-1.678593	-0.892026

Me_3S^+ (C_1)
E = -516.9043243 au

16	0	-0.000024	0.000003	-0.526882
6	0	-0.947031	-1.288435	0.266798
6	0	-0.642282	1.464379	0.266798
1	0	-0.041081	2.305858	-0.068668
1	0	-1.668571	1.592032	-0.068613
1	0	-0.592691	1.351397	1.346878
1	0	-1.976393	-1.188510	-0.068606
1	0	-0.544451	-2.241038	-0.068675
1	0	-0.873922	-1.189041	1.346878
6	0	1.589350	-0.175948	0.266688
1	0	2.017470	-1.117351	-0.068783
1	0	2.213019	0.649010	-0.068790
1	0	1.466788	-0.162376	1.346777

Me_4S (C_{2v})
E = -556.8544625 au

16	0	0.000000	0.000000	0.400182
6	0	0.000000	1.441488	-0.676107
6	0	0.000000	-1.441488	-0.676107
1	0	0.000000	-2.315016	-0.026794
1	0	0.896202	-1.440507	-1.286934
1	0	-0.896202	-1.440507	-1.286934
1	0	0.000000	2.315016	-0.026794
1	0	-0.896202	1.440507	-1.286934
1	0	0.896202	1.440507	-1.286934
6	0	2.019675	0.000000	0.367212
1	0	2.515053	0.000000	-0.607792
1	0	2.319434	0.886636	0.930181
1	0	2.319434	-0.886636	0.930181
6	0	-2.019675	0.000000	0.367212
1	0	-2.515053	0.000000	-0.607792
1	0	-2.319434	0.886636	0.930181
1	0	-2.319434	-0.886636	0.930181

Me_5S^- (C_s)
E = -596.6226016 au

16	0	0.309524	0.008842	0.000000
6	0	0.255266	-1.440694	1.565927
1	0	1.209888	-1.280829	2.070863
1	0	-0.572130	-1.304985	2.270712
1	0	0.219282	-2.434894	1.115104
6	0	0.255266	1.485333	1.417710
1	0	0.052841	1.035114	2.391336
1	0	1.259401	1.912176	1.395112
1	0	-0.482622	2.257226	1.183278
6	0	0.255266	-1.440694	-1.565927
1	0	1.209888	-1.280829	-2.070863
1	0	-0.572130	-1.304985	-2.270712
1	0	0.219282	-2.434894	-1.115104
6	0	0.255266	1.485333	-1.417710
1	0	0.052841	1.035114	-2.391336
1	0	1.259401	1.912176	-1.395112
1	0	-0.482622	2.257226	-1.183278
6	0	-1.491076	-0.106472	0.000000
1	0	-1.752767	-1.161128	0.000000
1	0	-1.876428	0.377604	0.895743
1	0	-1.876428	0.377604	-0.895743

Me_5S^+ (C_s)
E = -596.4234006 au

16	0	0.049607	0.000984	0.000000
6	0	0.409750	-1.288838	1.316033
1	0	1.487496	-1.275576	1.478536
1	0	-0.101451	-1.010469	2.231819
1	0	0.097486	-2.271441	0.982677
6	0	0.409750	1.314697	1.295187
1	0	0.077839	0.984225	2.272691
1	0	1.490581	1.454903	1.300207
1	0	-0.076978	2.241959	1.011979
6	0	0.409750	-1.288838	-1.316033
1	0	1.487496	-1.275576	-1.478536
1	0	-0.101451	-1.010469	-2.231819
1	0	0.097486	-2.271441	-0.982677
6	0	0.409750	1.314697	-1.295187
1	0	0.077839	0.984225	-2.272691

1	0	1.490581	1.454903	-1.300207
1	0	-0.076978	2.241959	-1.011979
6	0	-1.730550	-0.058887	0.000000
1	0	-2.021144	-1.105212	0.000000
1	0	-2.086602	0.442642	0.895083
1	0	-2.086602	0.442642	-0.895083

Me_6S (C_i)
E = -636.4218043 au

16	0	0.000000	0.000000	0.000000
6	0	-0.012489	-0.025308	-1.908086
1	0	0.190289	0.965041	-2.308806
1	0	0.748948	-0.719874	-2.253714
1	0	-0.984903	-0.365032	-2.257571
6	0	0.012489	0.025308	1.908086
1	0	-0.190289	-0.965041	2.308806
1	0	-0.748948	0.719874	2.253714
1	0	0.984903	0.365032	2.257571
6	0	0.025466	1.908093	0.010996
1	0	-0.964983	2.308736	-0.191445
1	0	0.365864	2.258319	0.982908
1	0	0.719552	2.253060	-0.751177
6	0	-0.025466	-1.908093	-0.010996
1	0	0.964983	-2.308736	0.191445
1	0	-0.365864	-2.258319	-0.982908
1	0	-0.719552	-2.253060	0.751177
6	0	-1.908116	-0.010895	-0.023877
1	0	-2.258670	-0.982997	-0.363396
1	0	-2.253628	0.750869	-0.718140
1	0	-2.307925	0.192160	0.966783
6	0	1.908116	0.010895	0.023877
1	0	2.258670	0.982997	0.363396
1	0	2.307925	-0.192160	-0.966783
1	0	2.253628	-0.750869	0.718140

H_2SF_2 (C_{2v})
E = -598.3162338 au

16	0	0.000000	0.000000	0.127099
1	0	1.009938	0.000000	-0.734455
1	0	-1.009938	0.000000	-0.734455
9	0	0.000000	1.709210	-0.031371
9	0	0.000000	-1.709210	-0.031371

H_2SO (C_s)
E = -473.9665139 au

16	0	-0.067946	-0.422593	0.000000
1	0	0.815346	-0.864377	0.943080
1	0	0.815346	-0.864377	-0.943080
8	0	-0.067946	1.061281	0.000000

H_2SO_2 (C_{2v})
E = -549.1013079 au

16	0	0.000000	0.000000	0.268960
1	0	1.028463	0.000000	1.141678
1	0	-1.028463	0.000000	1.141678
8	0	0.000000	1.260759	-0.411669
8	0	0.000000	-1.260759	-0.411669

H_4SO (C_{2v})
E = -475.0570164 au

16	0	0.000000	0.000000	0.352988
1	0	0.000000	0.975827	1.305322

1	0	0.000000	-0.975827	1.305322
1	0	1.383611	0.000000	0.373728
1	0	-1.383611	0.000000	0.373728
8	0	0.000000	0.000000	-1.125739

H_2SF_2O (C_{2v})
E = -673.413398 au

16	0	0.000000	0.000000	0.108930
1	0	-1.126587	0.000000	0.814086
1	0	1.126587	0.000000	0.814086
9	0	0.000000	1.636935	0.397115
9	0	0.000000	-1.636935	0.397115
8	0	0.000000	0.000000	-1.314891

Me_2SF_2 (C_{2v})
E = -676.7777749 au

16	0	0.000000	0.000000	0.428999
6	0	0.000000	1.387205	-0.694992
6	0	0.000000	-1.387205	-0.694992
1	0	0.000000	-2.290461	-0.092266
1	0	0.903106	-1.337672	-1.292112
1	0	-0.903106	-1.337672	-1.292112
1	0	0.000000	2.290461	-0.092266
1	0	-0.903106	1.337672	-1.292112
1	0	0.903106	1.337672	-1.292112
9	0	-1.747235	0.000000	0.379384
9	0	1.747235	0.000000	0.379384

$CF_3SF_2CF_3$ (C_{2v})
E = -1271.5436033 au

16	0	0.000000	0.000000	0.946794
6	0	0.000000	1.448689	-0.258291
6	0	0.000000	-1.448689	-0.258291
9	0	0.000000	-2.539162	0.493563
9	0	1.069047	-1.434952	-1.019156
9	0	-1.069047	-1.434952	-1.019156
9	0	0.000000	2.539162	0.493563
9	0	-1.069047	1.434952	-1.019156
9	0	1.069047	1.434952	-1.019156
9	0	-1.692798	0.000000	0.875348
9	0	1.692798	0.000000	0.875348

Me_2SCl_2 (C_{2v})
E = -1396.7355138 au

16	0	0.000000	0.000000	0.288225
6	0	0.000000	1.382680	-0.864846
6	0	0.000000	-1.382680	-0.864846
1	0	0.000000	-2.285814	-0.260713
1	0	0.903986	-1.321584	-1.459946
1	0	-0.903986	-1.321584	-1.459946
1	0	0.000000	2.285814	-0.260713
1	0	-0.903986	1.321584	-1.459946
1	0	0.903986	1.321584	-1.459946
17	0	-2.262881	0.000000	0.356699
17	0	2.262881	0.000000	0.356699

Me_2SBr_2 (C_{2v})
E = -5622.4219469 au

16	0	0.000000	0.000000	0.132146
6	0	0.000000	1.380513	-1.028997
6	0	0.000000	-1.380513	-1.028997
1	0	0.000000	-2.285648	-0.427514

1	0	0.903677	-1.317793	-1.625243
1	0	-0.903677	-1.317793	-1.625243
1	0	0.000000	2.285648	-0.427514
1	0	-0.903677	1.317793	-1.625243
1	0	0.903677	1.317793	-1.625243
35	0	-2.444823	0.000000	0.251280
35	0	2.444823	0.000000	0.251280

Me_2SO (C_s)
E = -552.4368594 au

16	0	-0.257068	0.425531	0.000000
6	0	-0.257068	-0.776356	1.330632
6	0	-0.257068	-0.776356	-1.330632
1	0	-0.203984	-0.217476	-2.261068
1	0	-1.174686	-1.361066	-1.297837
1	0	0.621954	-1.409842	-1.225048
1	0	-0.203984	-0.217476	2.261068
1	0	0.621954	-1.409842	1.225048
1	0	-1.174686	-1.361066	1.297837
8	0	1.088916	1.060567	0.000000

Me_2SO_2 (C_{2v})
E = -627.5825177 au

16	0	0.000000	0.000000	0.188933
6	0	0.000000	1.384611	-0.907180
6	0	0.000000	-1.384611	-0.907180
1	0	0.000000	-2.263686	-0.267294
1	0	0.899424	-1.362656	-1.515357
1	0	-0.899424	-1.362656	-1.515357
1	0	0.000000	2.263686	-0.267294
1	0	-0.899424	1.362656	-1.515357
1	0	0.899424	1.362656	-1.515357
8	0	1.251565	0.000000	0.903703
8	0	-1.251565	0.000000	0.903703

Me_2SF_2O (C_{2v})
E = -751.8804141 au

16	0	0.000000	0.000000	0.150012
6	0	0.000000	1.507375	-0.792795
6	0	0.000000	-1.507375	-0.792795
1	0	0.000000	-2.284882	-0.030837
1	0	0.903954	-1.562416	-1.383207
1	0	-0.903954	-1.562416	-1.383207
1	0	0.000000	2.284882	-0.030837
1	0	-0.903954	1.562416	-1.383207
1	0	0.903954	1.562416	-1.383207
9	0	-1.698303	0.000000	0.002138
9	0	1.698303	0.000000	0.002138
8	0	0.000000	0.000000	1.583671

F_2SO (C_s)
E = -672.2817036 au

16	0	-0.245975	0.359519	0.000000
9	0	-0.245975	-0.744456	1.155170
9	0	-0.245975	-0.744456	-1.155170
8	0	1.045392	0.955987	0.000000

Cl_2SO (C_s)
E = -1392.2167367 au

16	0	-0.176053	0.715973	0.000000
17	0	-0.176053	-0.661842	1.555754
17	0	-0.176053	-0.661842	-1.555754

8	0	1.100332	1.380882	0.000000

F_2SO_2 (C_{2v})
E = -747.4082379 au

16	0	0.000000	0.000000	0.167649
9	0	0.000000	1.140404	-0.873371
9	0	0.000000	-1.140404	-0.873371
8	0	-1.249301	0.000000	0.814893
8	0	1.249301	0.000000	0.814893

SF_4 (C_{2v})
E = -796.5730669 au

16	0	0.000000	0.000000	0.376335
9	0	0.000000	1.201910	-0.606844
9	0	0.000000	-1.201910	-0.606844
9	0	-1.649458	0.000000	0.272324
9	0	1.649458	0.000000	0.272324

SCl_4 (C_{2v})
E = -2236.4515908 au

16	0	0.000000	0.000000	0.453264
17	0	0.000000	1.573360	-0.777604
17	0	0.000000	-1.573360	-0.777604
17	0	-2.236658	0.000000	0.564304
17	0	2.236658	0.000000	0.564304

SF_5^- (C_{4v})
E = -896.3932748 au

16	0	0.000000	0.000000	0.319354
9	0	0.000000	1.725750	0.177138
9	0	-1.725750	0.000000	0.177138
9	0	1.725750	0.000000	0.177138
9	0	0.000000	-1.725750	0.177138
9	0	0.000000	0.000000	-1.276293

SF_5^+ (C_{4v})
E = -895.8964594 au

16	0	0.000000	0.000000	0.031857
9	0	0.000000	1.487699	0.347061
9	0	-1.487699	0.000000	0.347061
9	0	1.487699	0.000000	0.347061
9	0	0.000000	-1.487699	0.347061
9	0	0.000000	0.000000	-1.444878

HSF_5 (C_{4v})
E = -896.8974633 au

16	0	0.000000	0.000000	0.209114
1	0	0.000000	0.000000	1.527338
9	0	0.000000	1.583446	0.204535
9	0	0.000000	-1.583446	0.204535
9	0	0.000000	0.000000	-1.359602
9	0	1.583446	0.000000	0.204535
9	0	-1.583446	0.000000	0.204535

$MeSF_5$ (C_s)
E = -936.1260725 au

16	0	0.012963	0.003720	0.000000
9	0	0.066676	-1.119476	1.132541
9	0	1.595173	0.003183	0.000000
9	0	0.066676	1.135765	-1.123727
9	0	0.066676	-1.119476	-1.132541
9	0	0.066676	1.135765	1.123727

6	0	-1.774030	-0.037953	0.000000
1	0	-2.125084	0.462585	-0.892759
1	0	-2.125084	0.462585	0.892759
1	0	-2.069960	-1.078830	0.000000

SF_6 (O_h)
E = -996.03527 au

16	0	0.000000	0.000000	0.000000
9	0	0.000000	0.000000	1.564790
9	0	0.000000	1.564790	0.000000
9	0	0.000000	-1.564790	0.000000
9	0	0.000000	0.000000	-1.564790
9	0	1.564790	0.000000	0.000000
9	0	-1.564790	0.000000	0.000000