

- SUPPLEMENTARY INFORMATION -

Oxidation of organic diselenides and ditellurides by H₂O₂ for bioinspired catalyst design

Marco Bortoli ^a, Francesco Zaccaria ^b, Marco Dalla Tiezza ^a, Matteo Bruschi ^a,
Célia Fonseca Guerra ^{b, c}, F. Matthias Bickelhaupt ^{b, d} and Laura Orian ^a.

^a Dipartimento di Scienze Chimiche Università degli Studi di Padova, Via Marzolo 1, 35131 Padova, Italy

^b Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling (ACMM), Vrije
Universiteit Amsterdam, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands

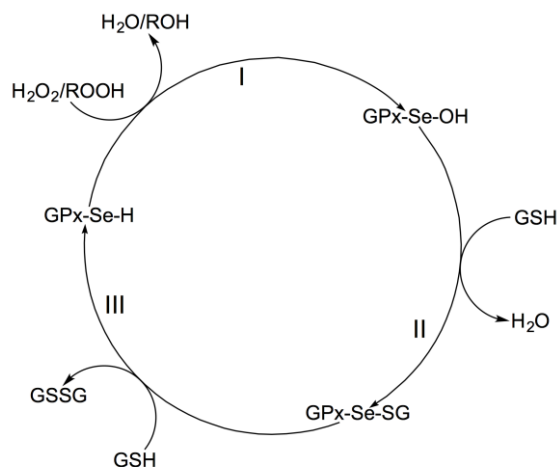
^c Leiden Institute of Chemistry, Leiden University, PO Box 9502, 2300 RA Leiden, The Netherlands

^d Institute for Molecules and Materials (IMM), Radboud University, Heyendaalseweg 135, 6525 AJ Nijmegen,
The Netherlands

Table of Contents

Scheme S1 Organic hydroperoxides reduction mechanism catalyzed by GPx;	3
Table S1 Energies (in kcal mol ⁻¹) and ψ dihedral amplitude ($^{\circ}$) of stationary points and transition states for the oxidation of (PhSe)₂ and (PhTe)₂ in two proposed mechanisms one. Level of theory ZORA-OLYP/TZ2P.	3
Table S2 Energy decomposition analysis (in gas phase, in kcal mol ⁻¹) for the first oxidation of model diphenyldisulphides, diphenyldiselenides and diphenylditellurides; level of theory ZORA-OLYP/TZ2P	3
Table S3 Geometries of the stationary points and transition states for the oxidation of RXXR (X=S,Se,Te; R=H, CH ₃ ,Ph): level of theory ZORA-OLYP/TZ2P	4
Table S4 Geometries of the stationary points and transition states for the oxidation of HXXH (X=S,Se,Te): level of theory ZORA-BLYP-D3(BJ)/TZ2P	10
Table S5 Geometries of the stationary points and transition states for the oxidation of substituted diselenides and ditellurides; level of theory ZORA-OLYP/TZ2P	11
Table S6 Geometries of the stationary points and transition states for the isomerization of the selenoxides and telluroxides. Level of theory ZORA-OLYP/TZ2P	25

Scheme S1 Organic hydroperoxides reduction mechanism catalyzed by GPx;



GSH is glutathione: the selenol form of the enzyme (GPx-Se-H) is oxidized to selenenic acid (GPx-Se-OH) and the hydroperoxide is reduced (oxidative step, I); GPx-Se-OH reacts with one equivalent of GSH and the selenenylsulfide intermediate (GPx-Se-SG) forms (first reductive step, II); GPx-Se-SG reacts with a second equivalent of GSH, GSSG forms and GPx-Se-H is regenerated (second reductive step, III).

Table S1 Energies (in kcal mol⁻¹) and ψ dihedral amplitude ($^{\circ}$) of stationary points and transition states for the oxidation of **(PhSe)₂** and **(PhTe)₂** in two proposed mechanisms one. Level of theory ZORA-OLYP/TZ2P.

	(PhSe)₂				(PhTe)₂			
	cis		trans		cis		trans	
	ψ	ΔE	ψ	ΔE	ψ	ΔE	ψ	ΔE
	82	-2.0	82	-2.0	83	-1.9	83	-1.9
TSox	70	21.0	-169	19.1	72	12.4	-162	13.2
PCox	51	-41.1	-163	-42.3	41	-43.6	-167	-44.7

Table S2 Energy decomposition analysis (in gas phase, in kcal mol⁻¹) for the first oxidation of model diphenyldisulphides, diphenyldiselenides and diphenylditellurides; level of theory ZORA-OLYP/TZ2P

R		S			Se			Te		
		ΔE_{Pauli}	ΔV_{elst}	ΔE_{oi}	ΔE_{Pauli}	ΔV_{elst}	ΔE_{oi}	ΔE_{Pauli}	ΔV_{elst}	ΔE_{oi}
H	RCox	2.4	-2.4	-1.7	2.5	-2.3	-1.7	2.4	-2.1	-1.9
	TSox	186.5	-81.4	-125.2	159.1	-73.1	-112.7	147.6	-72.0	-105.3
CH ₃	RCox	4.0	-3.9	-2.7	4.5	-4.0	-2.9	4.2	-3.7	-2.9
	TSox	169.5	-75.4	-112.6	151.2	-70.1	-106.7	128.1	-62.7	-89.9
Ph	RCox	3.3	-3.3	-2.4	2.9	-2.8	-2.2	2.9	-2.6	-2.3

	TSox	165.1	-72.2	-110.0	146.6	-67.0	-103.9	117.8	-57.2	-80.8
	RCox	-	-	-	3.8	-3.8	-2.8	3.3	-3.3	-2.6
NH ₂	TSox	-	-	-	136.0	-61.9	-97.9	110.4	-53.2	-77.6
	RCox	-	-	-	3.5	-3.2	-2.5	4.1	-4.1	-2.9
CH ₃ O	TSox	-	-	-	138.8	-63.1	-99.4	106.4	-51.5	-72.9
	RCox	-	-	-	3.1	-3.0	-2.3	2.9	-2.7	-2.4
CH ₃ Ph	TSox	-	-	-	143.5	-65.5	-102.2	110.3	-53.6	-75.3
	RCox	-	-	-	2.9	-2.6	-2.1	2.8	-2.4	-2.2
Cl	TSox	-	-	-	149.4	-68.2	-105.3	127.5	-62.0	-88.1
	RCox	-	-	-	2.3	-2.0	-1.7	2.5	-2.1	-2.0
CN	TSox	-	-	-	156.7	-71.9	-109.0	139.8	-68.2	-96.8
	RCox	-	-	-	0.5	-1.9	-0.5	2.5	-1.9	-1.9
NO ₂	TSox	-	-	-	158.2	-72.6	-109.8	142.2	-69.3	-98.5

Table S3 Geometries of the stationary points and transition states for the oxidation of RXXR (X=S,Se,Te; R=H, CH₃,Ph): level of theory ZORA-OLYP/TZ2P

H₂O₂

E = -0.65283 Ha

O	4.983820880	-1.237526390	1.275512280
O	3.761505110	-2.017929120	1.458569200
H	5.511638000	-1.572976630	2.018507700
H	3.822632280	-2.610335940	0.691437620

O	-1.127961000	3.666023000	-0.348506000
H	0.617450000	4.372822000	-0.171427000
H	-1.125435000	2.759547000	0.006713000
H	-2.765988000	0.034177000	0.309668000
H	-0.589613000	0.296896000	-1.907176000

TSox

E = -1.14051 Ha
nimag = -374.08 cm⁻¹

(HS)₂

1

E = -0.52791 Ha

S	-1.445336000	0.006929000	0.586124000
S	-0.757894000	-0.841888000	-1.161505000
H	-2.758403000	0.090011000	0.272027000
H	-0.474996000	0.291385000	-1.843738000

O	6.790000000	-1.839200000	1.521900000
O	7.952400000	-3.460700000	1.490800000
H	7.670900000	-1.659700000	1.144800000
H	7.349100000	-3.990200000	0.946100000
S	5.602000000	-0.728100000	0.642400000
S	4.491100000	1.132200000	0.886400000
H	4.642700000	-1.364800000	1.334300000
H	5.212400000	1.749100000	-0.073600000

PCox

E = -1.25787 Ha

RCox

E = -1.18147 Ha

S	-1.438652000	0.063887000	0.570996000
S	-0.746222000	-0.818948000	-1.159572000
O	0.249084000	3.760093000	-0.828503000

O	5.326263000	-2.051807000	0.937902000
O	8.217089000	-2.007926000	2.248688000
H	7.326540000	-2.270089000	1.974857000
H	8.436329000	-2.619121000	2.961636000
S	5.292924000	-0.810374000	0.123587000

S	4.979389000	0.970908000	1.276656000
H	3.983252000	-0.635797000	-0.296567000
H	6.301569000	1.140591000	1.481657000

(CH₃S)₂

1

E = -1.70070 Ha

S	-1.452841000	0.095999000	0.479812000
S	-0.785347000	-0.911777000	-1.161677000
C	-3.271867000	0.080319000	0.345925000
H	-3.618045000	0.677038000	-0.500594000
H	-3.645057000	-0.942870000	0.271552000
H	-3.634248000	0.532554000	1.275113000
C	-0.640461000	0.348453000	-2.472305000
H	-0.192450000	-0.171601000	-3.325566000
H	-1.617542000	0.738737000	-2.764671000
H	0.017596000	1.160265000	-2.156665000

RCox

E = -2.35627 Ha

S	-1.475976000	0.168458000	0.449816000
S	-0.735240000	-0.888682000	-1.131034000
O	0.118538000	3.886560000	-0.852276000
O	-1.033323000	3.727617000	0.032107000
H	0.763296000	4.256681000	-0.227781000
H	-1.047082000	2.756774000	0.130796000
C	-3.290819000	0.050215000	0.313118000
H	-3.662583000	0.579104000	-0.566475000
H	-3.602571000	-0.995528000	0.294828000
H	-3.682183000	0.531876000	1.215202000
C	-0.699899000	0.275059000	-2.533947000
H	-0.222516000	-0.281689000	-3.347170000
H	-1.706772000	0.562953000	-2.842597000
H	-0.102675000	1.156832000	-2.298050000

TSox

E = -2.31563 Ha

nimag = -335.63 cm⁻¹

S	-1.387336000	-0.497519000	0.754067000
S	-1.155748000	-1.085000000	-1.296662000
O	-0.981181000	-1.166873000	2.482156000
O	-0.415389000	-1.039510000	4.371721000
H	-0.039119000	-1.398855000	2.523933000
H	-1.142738000	-1.599540000	4.681833000
C	-0.090299000	0.769928000	0.711052000
H	-0.355412000	1.527425000	-0.028093000
H	-0.073551000	1.200779000	1.712796000
H	0.879949000	0.327413000	0.472650000
C	-2.673955000	-2.069095000	-1.462042000
H	-3.561659000	-1.458905000	-1.283204000
H	-2.678317000	-2.423766000	-2.496233000
H	-2.656940000	-2.932058000	-0.792864000

PCox

E = -2.43869 Ha

S	-1.555974000	-0.718697000	0.554958000
S	-0.128952000	-0.242916000	-0.972406000
H	-0.198483000	-1.056162000	-3.183109000

C	-0.823123000	-1.258324000	-2.309135000
H	-0.762373000	-2.320843000	-2.066516000
H	-1.852541000	-0.970141000	-2.533824000
C	-0.949961000	0.590244000	1.677664000
H	-1.145091000	1.563520000	1.223951000
H	-1.530350000	0.470174000	2.595203000
H	0.111597000	0.447503000	1.886750000
O	-1.261125000	-2.027985000	1.206125000
O	0.912910000	-2.268826000	3.387473000
H	0.247869000	-2.351493000	2.686182000
H	1.365326000	-3.120303000	3.385656000

(PhS)₂

1

E = -5.37216 Ha

S	-1.518368000	0.229911000	0.409457000
S	-0.816831000	-0.917037000	-1.158743000
C	-3.280250000	-0.063879000	0.495049000
C	-3.805233000	-1.330303000	0.784761000
C	-4.146293000	1.025539000	0.339574000
C	-5.181428000	-1.501933000	0.905528000
C	-5.523338000	0.849757000	0.480870000
C	-6.043838000	-0.412930000	0.758282000
H	-3.135704000	-2.175485000	0.912786000
H	-3.740098000	2.005739000	0.107600000
H	-5.582210000	-2.488083000	1.127758000
H	-6.188524000	1.701556000	0.361453000
H	-7.117315000	-0.550404000	0.860653000
C	-1.119204000	0.034643000	-2.642543000
C	-0.430729000	1.227478000	-2.900880000
C	-2.013911000	-0.468722000	-3.595113000
C	-0.646471000	1.911275000	-4.094302000
C	-2.213179000	0.213272000	-4.795949000
C	-1.534984000	1.405070000	-5.045783000
H	0.269689000	1.615114000	-2.167212000
H	-2.550769000	-1.390888000	-3.393066000
H	-0.110310000	2.837348000	-4.287586000
H	-2.907687000	-0.185353000	-5.531513000
H	-1.695401000	1.938698000	-5.979215000

RCox

E = -6.02775 Ha

S	-1.542611000	0.307859000	0.400690000
S	-0.785513000	-0.831814000	-1.155745000
O	0.452764000	4.098255000	-0.343897000
O	-0.878506000	3.979244000	0.245588000
H	0.967233000	4.337356000	0.444136000
H	-0.993953000	3.012190000	0.225097000
C	-3.295288000	-0.036117000	0.474670000
C	-3.764971000	-1.245466000	1.004573000
C	-4.208083000	0.940034000	0.055901000
C	-5.134578000	-1.475724000	1.104108000
C	-5.578687000	0.707099000	0.170065000
C	-6.043670000	-0.500101000	0.689537000
H	-3.056974000	-1.999016000	1.336317000
H	-3.846455000	1.876779000	-0.357203000
H	-5.493424000	-2.416114000	1.515354000
H	-6.281957000	1.470216000	-0.154055000
H	-7.112245000	-0.681005000	0.774440000
C	-1.132993000	0.066884000	-2.660551000

C	-0.436349000	1.237670000	-2.989044000
C	-2.072701000	-0.457695000	-3.557605000
C	-0.690747000	1.880852000	-4.197500000
C	-2.309501000	0.183104000	-4.773683000
C	-1.623832000	1.354281000	-5.093032000
H	0.296843000	1.645308000	-2.300459000
H	-2.612889000	-1.364058000	-3.300699000
H	-0.152321000	2.792954000	-4.442434000
H	-3.037722000	-0.230912000	-5.466866000
H	-1.814460000	1.856724000	-6.038069000

TSox

E = -5.98657 Ha
nimag = -309.00 cm⁻¹

S	3.667491000	0.983851000	14.275032000
S	5.023148000	0.759873000	15.993809000
C	4.074007000	-0.590116000	13.540476000
C	3.174433000	-1.648498000	13.694240000
C	3.460155000	-2.882517000	13.112685000
C	4.636222000	-3.058278000	12.384694000
C	5.528451000	-1.996374000	12.232503000
C	5.252265000	-0.757658000	12.806444000
C	4.381271000	2.009755000	17.074160000
C	5.128473000	3.176760000	17.297691000
C	4.669526000	4.139182000	18.194806000
C	3.459540000	3.954918000	18.863812000
C	2.709236000	2.799091000	18.638926000
C	3.166052000	1.826905000	17.753593000
H	2.257253000	-1.505171000	14.256879000
H	2.758033000	-3.704245000	13.226445000
H	4.855855000	-4.021427000	11.931360000
H	6.443355000	-2.129194000	11.660925000
H	5.937652000	0.073146000	12.678413000
H	6.066110000	3.320485000	16.769440000
H	5.257018000	5.037787000	18.365561000
H	3.101527000	4.709207000	19.559758000
H	1.767226000	2.650241000	19.160767000
H	2.589711000	0.921628000	17.589978000
O	3.622722000	1.864623000	12.586732000
O	2.657233000	2.510172000	10.994676000
H	3.292886000	2.750958000	12.809330000
H	3.390288000	2.275085000	10.405984000

PCox

E = -6.10923 Ha

S	-2.725169000	-1.103579000	0.606740000
S	-1.521077000	-2.772714000	-0.119809000
O	-2.212331000	-4.073628000	0.095463000
C	-1.763778000	-2.308499000	-1.861638000
C	-2.737524000	-2.955774000	-2.619722000
C	-0.900820000	-1.374734000	-2.439467000
C	-2.863343000	-2.642392000	-3.972653000
C	-1.033790000	-1.071524000	-3.792632000
C	-2.016030000	-1.701992000	-4.558758000
H	-3.377537000	-3.698128000	-2.153529000
H	-0.135642000	-0.885961000	-1.841970000
H	-3.624744000	-3.137903000	-4.569828000
H	-0.366971000	-0.344625000	-4.249268000
H	-2.115761000	-1.464065000	-5.614654000
C	-2.290333000	-1.114012000	2.329472000
C	-2.981446000	-1.938488000	3.229502000

C	-1.288879000	-0.253146000	2.803603000
C	-2.662614000	-1.905003000	4.585623000
C	-0.982694000	-0.221205000	4.162164000
C	-1.666717000	-1.048051000	5.054342000
H	-3.758802000	-2.603721000	2.869707000
H	-0.759421000	0.389832000	2.106913000
H	-3.197005000	-2.553487000	5.275081000
H	-0.207631000	0.450260000	4.523389000
H	-1.424355000	-1.023050000	6.113845000
O	-4.124097000	-5.451983000	2.208314000
H	-3.518976000	-5.102937000	1.537728000
H	-4.426675000	-6.288846000	1.836944000

(HSe)₂

1

E = -5.37216 Ha

Se	-2.742193000	-0.752281000	-0.012941000
Se	-0.584202000	0.170296000	-0.013865000
H	-0.016231000	-0.717263000	1.024854000
H	-3.310999000	0.139063000	1.022063000

RCox

E = -1.12640 Ha

Se	-1.491906000	0.064854000	0.710367000
Se	-0.707937000	-0.903809000	-1.282901000
O	0.265090000	3.840697000	-0.834213000
O	-1.115975000	3.733855000	-0.368630000
H	0.624969000	4.442764000	-0.162833000
H	-1.117089000	2.818160000	-0.036271000
H	-2.917449000	0.141222000	0.320807000
H	-0.423393000	0.366940000	-1.982843000

TSox

E = -1.09168 Ha
nimag = -395.27 cm⁻¹

O	6.798176000	-2.002336000	1.570202000
O	8.062610000	-3.587579000	1.467724000
H	7.738382000	-1.815531000	1.378491000
H	7.837907000	-3.877845000	2.365794000
Se	5.665014000	-0.752192000	0.546651000
Se	4.351687000	1.297315000	0.919046000
H	4.535484000	-1.513180000	1.098343000
H	5.308601000	2.071269000	0.108516000

PCox

E = -1.18139 Ha

O	5.457713000	-2.101569000	1.173534000
O	8.370205000	-2.412259000	2.156370000
H	7.421377000	-2.453988000	1.959451000
H	8.485112000	-3.017887000	2.897781000
Se	5.443608000	-0.829610000	0.122101000
Se	4.686674000	1.229626000	1.213062000
H	4.047801000	-0.879233000	-0.480248000
H	6.082908000	1.576210000	1.534704000

(CH₃Se)₂

1

E = -1.64519 Ha

Se	-5.224537500	2.602743320	-0.901066440
Se	-6.839496350	2.559567210	0.795626350
C	-7.956081120	4.114665070	0.272172670
C	-4.061575390	4.076464340	-0.256184650
H	-8.231619390	4.029417130	-0.779361390
H	-7.418294250	5.046241870	0.455916290
H	-8.852873240	4.079808980	0.897433720
H	-3.796404840	3.902468660	0.787036860
H	-4.567806900	5.036339230	-0.370871050
H	-3.161981460	4.059726220	-0.878103710

RCox

E = -2.30236 Ha

Se	-1.470052000	0.148807000	0.625721000
Se	-0.712542000	-1.004939000	-1.255431000
O	0.163707000	3.931209000	-0.816876000
O	-1.095184000	3.758968000	-0.096148000
H	0.693621000	4.370869000	-0.132401000
H	-1.079821000	2.794895000	0.061591000
C	-3.433317000	0.113073000	0.398719000
H	-3.726634000	0.686414000	-0.480097000
H	-3.772483000	-0.919843000	0.327950000
H	-3.838051000	0.580525000	1.301032000
C	-0.597983000	0.403032000	-2.635310000
H	-0.183823000	-0.102738000	-3.512572000
H	-1.588431000	0.792864000	-2.868316000
H	0.072617000	1.197199000	-2.311110000

TSox

E = -2.26895 Ha

nimag = -314.22 cm⁻¹

Se	-1.443185000	-0.455340000	0.828376000
Se	-1.136743000	-1.119787000	-1.494452000
O	-0.977082000	-1.179168000	2.637623000
O	-0.342336000	-1.029079000	4.539339000
H	-0.022792000	-1.350111000	2.704001000
H	-1.001082000	-1.665818000	4.855394000
C	0.018865000	0.850198000	0.783355000
H	-0.215260000	1.611913000	0.039849000
H	0.044914000	1.277194000	1.786222000
H	0.960875000	0.351980000	0.550899000
C	-2.798979000	-2.160216000	-1.641260000
H	-3.665251000	-1.525528000	-1.454197000
H	-2.821214000	-2.523624000	-2.671040000
H	-2.774756000	-3.009200000	-0.957625000

PCox

E = -2.36543 Ha

Se	-1.642869000	-0.728916000	0.626401000
Se	-0.035694000	-0.169406000	-1.129855000
H	-0.243415000	-1.151560000	-3.408413000
C	-0.853416000	-1.304282000	-2.515462000
H	-0.808987000	-2.351412000	-2.216516000
H	-1.878131000	-0.990483000	-2.716440000
C	-0.892169000	0.620848000	1.874664000
H	-1.035704000	1.612534000	1.443265000
H	-1.464781000	0.503850000	2.796304000

H	0.158803000	0.392664000	2.048368000
O	-1.251416000	-2.184389000	1.313913000
O	0.867084000	-2.224450000	3.448604000
H	0.201763000	-2.341745000	2.748728000
H	1.350306000	-3.058613000	3.457616000

(PhSe)₂**1**

E = -5.31496 Ha

Se	-1.479625000	0.268789000	0.564922000
Se	-0.723366000	-1.051316000	-1.237876000
C	-3.385211000	-0.090490000	0.621032000
C	-3.873618000	-1.250809000	1.232266000
C	-4.279173000	0.852394000	0.101671000
C	-5.248278000	-1.467545000	1.314512000
C	-5.654193000	0.632338000	0.193159000
C	-6.140396000	-0.527152000	0.796494000
H	-3.181301000	-1.980319000	1.641773000
H	-3.901699000	1.753168000	-0.373012000
H	-5.622728000	-2.371097000	1.789873000
H	-6.344602000	1.368710000	-0.211383000
H	-7.211922000	-0.697572000	0.865157000
C	-1.050389000	0.065854000	-2.789577000
C	-0.197413000	1.131520000	-3.098167000
C	-2.114944000	-0.243932000	-3.643023000
C	-0.416020000	1.885856000	-4.249758000
C	-2.322511000	0.509499000	-4.799336000
C	-1.476822000	1.575829000	-5.102733000
H	0.633583000	1.368971000	-2.440713000
H	-2.779025000	-1.069154000	-3.403638000
H	0.248916000	2.713740000	-4.484459000
H	-3.150422000	0.263293000	-5.460018000
H	-1.641759000	2.163524000	-6.002355000

RCox

E = -5.97097 Ha

Se	-1.473578000	0.245765000	0.586995000
Se	-0.700390000	-1.041522000	-1.239219000
O	0.356382000	4.197394000	-0.432735000
O	-1.034650000	3.993412000	-0.035505000
H	0.717358000	4.558435000	0.393138000
H	-1.062813000	3.020364000	0.017212000
C	-3.384898000	-0.083852000	0.613206000
C	-3.888852000	-1.236907000	1.225461000
C	-4.263106000	0.861899000	0.073138000
C	-5.265961000	-1.443080000	1.289833000
C	-5.640539000	0.651140000	0.146628000
C	-6.143353000	-0.500139000	0.751954000
H	-3.207786000	-1.968800000	1.649307000
H	-3.876284000	1.757057000	-0.404057000
H	-5.653503000	-2.340452000	1.766216000
H	-6.319506000	1.389404000	-0.273142000
H	-7.216926000	-0.662216000	0.806554000
C	-1.056543000	0.069429000	-2.786033000
C	-0.218803000	1.143609000	-3.106028000
C	-2.128196000	-0.256620000	-3.625064000
C	-0.461075000	1.892290000	-4.256327000
C	-2.356861000	0.490346000	-4.781163000
C	-1.527139000	1.566101000	-5.096098000
H	0.614454000	1.397812000	-2.458474000

H	-2.779949000	-1.088377000	-3.374992000
H	0.187110000	2.731538000	-4.495827000
H	-3.189340000	0.232905000	-5.431638000
H	-1.710765000	2.150845000	-5.993982000

TSox

E = -5.93734 Ha
nimag = -286.94 cm⁻¹

O	6.780690000	-2.046856000	1.516744000
O	8.181213000	-3.481094000	1.648677000
H	7.670354000	-1.655432000	1.485582000
H	7.769603000	-3.858370000	2.440842000
Se	5.602097000	-0.786833000	0.472550000
H	1.543266000	-3.350010000	-1.005268000
H	0.979903000	-4.198135000	1.262819000
H	4.377897000	-2.121042000	2.886532000
H	2.400143000	-3.578248000	3.205475000
C	4.054784000	-1.907662000	0.763022000
C	3.750439000	-2.380547000	2.041096000
C	2.639706000	-3.205207000	2.212970000
C	1.842974000	-3.552682000	1.121714000
C	2.156566000	-3.076317000	-0.150697000
C	3.265126000	-2.250715000	-0.336479000
H	3.512397000	-1.885254000	-1.328486000
Se	4.392770000	1.318130000	0.960223000
C	5.751441000	2.536015000	0.346782000
C	5.900725000	2.808934000	-1.019723000
C	6.857997000	3.728801000	-1.444061000
C	7.665813000	4.383363000	-0.513114000
C	7.515985000	4.114789000	0.847513000
C	6.564528000	3.191979000	1.280652000
H	5.267265000	2.308005000	-1.745313000
H	6.969428000	3.936454000	-2.505425000
H	8.409942000	5.101562000	-0.847706000
H	8.142943000	4.621539000	1.576994000
H	6.451390000	2.980914000	2.339660000

PCox

E = -6.03528 Ha

Se	-2.852955000	-0.928661000	0.673063000
Se	-1.580224000	-2.884668000	-0.156751000
O	-2.522615000	-4.242101000	-0.064295000
C	-1.745909000	-2.345178000	-2.049843000
C	-2.645894000	-3.030697000	-2.859446000
C	-0.905598000	-1.358105000	-2.564931000
C	-2.716901000	-2.706045000	-4.214768000
C	-0.982052000	-1.045927000	-3.921995000
C	-1.888293000	-1.716819000	-4.745140000
H	-3.270802000	-3.808642000	-2.430522000
H	-0.202205000	-0.830837000	-1.925291000
H	-3.419922000	-3.231266000	-4.856689000
H	-0.332826000	-0.277903000	-4.334860000
H	-1.945072000	-1.469949000	-5.802208000
C	-2.307171000	-1.028160000	2.520347000
C	-2.911730000	-1.942913000	3.391957000
C	-1.334273000	-0.140469000	2.998827000
C	-2.532169000	-1.970100000	4.733554000
C	-0.973239000	-0.166545000	4.345305000
C	-1.568574000	-1.082589000	5.213147000
H	-3.664060000	-2.635225000	3.029982000
H	-0.865817000	0.567847000	2.322127000

H	-2.996328000	-2.690198000	5.402606000
H	-0.221614000	0.527587000	4.713437000
H	-1.281042000	-1.105155000	6.261323000
O	-3.985406000	-5.419099000	2.356322000
H	-3.511368000	-5.096677000	1.572577000
H	-4.599910000	-6.072927000	2.003364000

(HTe)₂

1

E = -0.41752 Ha

Te	-1.485655000	0.191297000	0.759160000
Te	-0.852858000	-1.372514000	-1.389985000
H	-1.021370000	-0.164315000	-2.536404000
H	-3.131553000	-0.110912000	0.713071000

RCox

E = -1.07279 Ha

Te	-1.565313000	0.111298000	0.882303000
Te	-0.644204000	-0.997447000	-1.442701000
O	0.301504000	3.998564000	-0.894072000
O	-1.069568000	3.928781000	-0.393378000
H	0.695856000	4.585101000	-0.228397000
H	-1.089577000	3.011189000	-0.066104000
H	-3.170634000	0.197270000	0.414858000
H	-0.336000000	0.459627000	-2.203032000

TSox

E = -1.04811 Ha
nimag = -254.07

O	7.050292000	-2.156429000	1.601103000
O	8.170676000	-3.841023000	1.562627000
H	7.974642000	-1.938388000	1.392302000
H	7.895885000	-4.081574000	2.461288000
Te	5.750037000	-0.882755000	0.500456000
Te	4.220724000	1.480260000	0.948892000
H	4.574067000	-1.682875000	1.360994000
H	5.180958000	2.283617000	-0.152702000

PCox

E = -1.13173 Ha

O	5.582668000	-2.280831000	1.325999000
O	8.464252000	-2.776644000	2.013025000
H	7.498664000	-2.724956000	1.906906000
H	8.586222000	-3.234569000	2.852548000
Te	5.526004000	-0.957043000	0.066557000
Te	4.576258000	1.427130000	1.268965000
H	3.930162000	-1.126883000	-0.525735000
H	6.158120000	1.907682000	1.486966000

(CH₃Te)₂

1

E = -1.59683 Ha

Te	-1.517742000	0.244415000	0.780837000
Te	-0.649309000	-1.113039000	-1.399234000
C	-3.675922000	0.126504000	0.498822000

H	-3.964484000	0.691693000	-0.386099000
H	-3.969673000	-0.918563000	0.413828000
H	-4.120160000	0.571873000	1.392649000
C	-0.503805000	0.504063000	-2.853474000
H	-0.070385000	0.060161000	-3.753324000
H	-1.495970000	0.897755000	-3.068842000
H	0.153227000	1.279513000	-2.462765000

RCox

E = -2.25327 Ha

Te	-1.522762000	0.186186000	0.817110000
Te	-0.653916000	-1.107283000	-1.408251000
O	0.211634000	4.059993000	-0.881054000
O	-1.097068000	3.927263000	-0.245678000
H	0.680199000	4.571002000	-0.201446000
H	-1.081573000	2.981573000	0.000341000
C	-3.675538000	0.188284000	0.479083000
H	-3.909581000	0.788555000	-0.398548000
H	-4.016438000	-0.838899000	0.359508000
H	-4.120186000	0.634233000	1.372234000
C	-0.457876000	0.542924000	-2.814104000
H	-0.022458000	0.103825000	-3.715358000
H	-1.439017000	0.959330000	-3.036035000
H	0.208509000	1.298337000	-2.402394000

TSox

E = -2.22996 Ha

O	7.051774000	-2.213677000	1.617695000
O	8.122782000	-3.843157000	1.801351000
H	7.947255000	-1.851130000	1.532017000
H	7.769344000	-4.015927000	2.687569000
Te	5.734189000	-0.874509000	0.491073000
Te	4.296308000	1.499547000	0.999247000
C	4.181375000	-2.162455000	1.234873000
H	3.275822000	-1.988355000	0.656547000
H	4.558330000	-3.175511000	1.092926000
H	4.024893000	-1.958510000	2.293481000
C	5.063094000	2.579827000	-0.724214000
H	6.143082000	2.693164000	-0.639852000
H	4.787117000	2.059931000	-1.640165000
H	4.587258000	3.561845000	-0.689427000

PCox

E = -2.31840 Ha

Te	-1.796357000	-0.750853000	0.740342000
Te	0.115449000	-0.137964000	-1.255297000
H	-0.256029000	-1.203080000	-3.686520000
C	-0.853932000	-1.341535000	-2.783978000
H	-0.840327000	-2.389305000	-2.487615000
H	-1.869078000	-0.986426000	-2.956560000
C	-0.945086000	0.699973000	2.116408000
H	-0.971201000	1.691108000	1.661771000
H	-1.569393000	0.664152000	3.010980000
H	0.069714000	0.379543000	2.351194000
O	-1.312575000	-2.335433000	1.526817000
O	0.982471000	-2.195602000	3.364993000
H	0.236793000	-2.364142000	2.758389000
H	1.557181000	-2.960998000	3.250578000

(PhTe)₂

1

E = -5.26294 Ha

Te	-1.020058000	0.910542000	-1.710152000
Te	1.020058000	-0.910542000	-1.710152000
C	-2.313987000	0.132907000	-0.182432000
C	-2.253667000	0.655953000	1.114445000
C	-3.256999000	-0.855773000	-0.486159000
C	-3.126933000	0.188894000	2.098139000
C	-4.125284000	-1.320943000	0.501931000
C	-4.062195000	-0.800011000	1.794560000
H	-1.526620000	1.424086000	1.360955000
H	-3.315540000	-1.265182000	-1.490293000
H	-3.073163000	0.600170000	3.103566000
H	-4.854037000	-2.090550000	0.257960000
H	-4.741062000	-1.162891000	2.562322000
C	2.313987000	-0.132907000	-0.182432000
C	2.253667000	-0.655953000	1.114445000
C	3.256999000	0.855773000	-0.486159000
C	3.126933000	-0.188894000	2.098139000
C	4.125284000	1.320943000	0.501931000
C	4.062195000	0.800011000	1.794560000
H	1.526620000	-1.424086000	1.360955000
H	3.315540000	1.265182000	-1.490293000
H	3.073163000	-0.600170000	3.103566000
H	4.854037000	2.090550000	0.257960000
H	4.741062000	1.162891000	2.562322000

RCox

E = -5.91889 Ha

Te	-1.461634000	0.279813000	0.784829000
Te	-0.619375000	-1.211748000	-1.354041000
O	0.222084000	4.362474000	-0.738937000
O	-1.166568000	4.129323000	-0.349112000
H	0.538575000	4.843603000	0.042712000
H	-1.144419000	3.169106000	-0.179280000
C	-3.579281000	-0.074163000	0.780838000
C	-4.106350000	-1.174120000	1.467176000
C	-4.441286000	0.818375000	0.133625000
C	-5.485656000	-1.381264000	1.498796000
C	-5.820268000	0.606138000	0.170685000
C	-6.344078000	-0.492697000	0.851106000
H	-3.446036000	-1.870793000	1.975109000
H	-4.045075000	1.675651000	-0.402068000
H	-5.887962000	-2.238835000	2.033065000
H	-6.483992000	1.303440000	-0.335138000
C	-0.988582000	0.109061000	-3.002662000
C	-0.097617000	1.145193000	-3.303884000
C	-2.108077000	-0.103494000	-3.815801000
C	-0.332743000	1.967655000	-4.405322000
C	-2.331950000	0.717558000	-4.922033000
C	-1.447322000	1.754463000	-5.216501000
H	0.773656000	1.319773000	-2.680292000
H	-2.807110000	-0.902673000	-3.587684000
H	0.357767000	2.777961000	-4.625857000
H	-3.203740000	0.547308000	-5.549541000
H	-1.627107000	2.397054000	-6.074773000
H	-7.418614000	-0.655623000	0.877996000

TSox

E = -5.89608 Ha

nimag = -142.59 cm⁻¹

Te	3.477109000	1.025531000	14.124950000
Te	5.241878000	0.659328000	16.331312000
C	3.985990000	-0.859641000	13.261437000
C	3.313710000	-2.007931000	13.690181000
C	3.627378000	-3.243688000	13.124052000
C	4.606015000	-3.333745000	12.134840000
C	5.271599000	-2.184593000	11.709114000
C	4.965963000	-0.943639000	12.268728000
C	4.351200000	2.175174000	17.545307000
C	4.961696000	3.431624000	17.649487000
C	4.407835000	4.411196000	18.474797000
C	3.244225000	4.146585000	19.196282000
C	2.634598000	2.895985000	19.093821000
C	3.184542000	1.910318000	18.274265000
H	2.547348000	-1.947188000	14.457050000
H	3.099748000	-4.134462000	13.455765000
H	4.847257000	-4.297601000	11.693963000
H	6.033802000	-2.248839000	10.936391000
H	5.479459000	-0.052396000	11.925166000
H	5.866437000	3.647577000	17.089414000
H	4.888870000	5.383503000	18.550033000
H	2.814044000	4.911927000	19.837240000
H	1.728268000	2.682176000	19.655345000
H	2.706313000	0.938003000	18.206688000
O	3.543470000	1.892424000	12.081151000
O	2.756826000	2.421522000	10.414331000
H	3.567859000	2.850406000	12.227162000
H	3.341086000	1.836531000	9.908434000

PCox

E = -5.98702 Ha

Te	-2.936008000	-0.742057000	0.736334000
Te	-1.458348000	-2.982121000	-0.208181000
C	-1.697141000	-2.425919000	-2.285612000
C	-2.609702000	-3.150834000	-3.049769000
C	-0.912927000	-1.423414000	-2.860031000
C	-2.747351000	-2.856340000	-4.407272000
C	-1.055888000	-1.138755000	-4.218412000
C	-1.973387000	-1.852927000	-4.990562000
H	-3.198912000	-3.937190000	-2.585279000
H	-0.197602000	-0.859050000	-2.266359000
H	-3.460309000	-3.415308000	-5.008731000
H	-0.449321000	-0.358569000	-4.671824000
H	-2.082027000	-1.628371000	-6.048627000
C	-2.331511000	-0.962504000	2.775795000
C	-2.890280000	-1.966327000	3.576714000
C	-1.403835000	-0.066276000	3.322045000
C	-2.510049000	-2.072338000	4.915339000
C	-1.041774000	-0.173030000	4.665276000
C	-1.591679000	-1.176778000	5.462520000
H	-3.607224000	-2.670988000	3.169103000
H	-0.963878000	0.712002000	2.705754000
H	-2.939532000	-2.861427000	5.527601000
H	-0.324154000	0.528177000	5.084739000
H	-1.303958000	-1.261305000	6.507524000
O	-2.568729000	-4.438775000	-0.139456000
O	-4.031615000	-5.355073000	2.295601000
H	-3.562264000	-5.108753000	1.478170000
H	-4.739652000	-5.934241000	1.991279000

Table S4 Geometries of the stationary points and transition states for the oxidation of HXXH (X=S,Se,Te): level of theory ZORA-BLYP-D3(BJ)/TZ2P

H₂O₂

E = -0.64253 Ha

O	-1.354356000	-0.038163000	0.326995000
O	-0.859342000	-0.665554000	-0.937125000
H	-2.312378000	-0.209750000	0.226691000
H	-0.556422000	0.137567000	-1.406752000

(HS)₂

1

E = -0.51802 Ha

S	-1.443752000	0.074374000	0.594321000
S	-0.738883000	-0.805274000	-1.178787000
H	-2.773932000	0.028911000	0.320549000
H	-0.586419000	0.328129000	-1.912635000

RCox

E = -1.16758 Ha

S	-1.606302000	0.142926000	0.583068000
S	-0.516875000	-0.390759000	-1.151891000
O	-0.080791000	3.064008000	-1.187656000
O	-0.949812000	3.379620000	-0.010539000
H	0.784433000	3.354506000	-0.835175000
H	-1.156725000	2.460981000	0.291850000

H	-2.840032000	0.267730000	0.019585000
H	-0.200547000	0.881825000	-1.528884000

TSox

E = -1.13422 Ha

nimag = -401.09 cm⁻¹

O	6.788400000	-1.865600000	1.547800000
O	7.998300000	-3.485200000	1.484200000
H	7.686100000	-1.718600000	1.171100000
H	7.389300000	-4.019400000	0.937000000
S	5.593800000	-0.740100000	0.637200000
S	4.475300000	1.171400000	0.880900000
H	4.624400000	-1.367800000	1.335700000
H	5.235000000	1.786500000	-0.060100000

PCox

E = -1.23969 Ha

O	5.213022000	-2.191307000	0.835268000
O	7.762842000	-1.513166000	2.071731000
H	6.967960000	-2.049229000	1.865128000
H	8.004658000	-1.755446000	2.981051000
S	5.317447000	-0.885539000	0.094824000
S	5.254506000	0.846659000	1.438289000
H	4.019176000	-0.523731000	-0.274404000
H	6.556625000	0.631914000	1.771982000

(HSe)₂**1**

E = -0.46413 Ha

Se	-2.762077000	-0.760680000	-0.013049000
Se	-0.564318000	0.178694000	-0.013990000
H	-0.001421000	-0.715891000	1.034082000
H	-3.325798000	0.137741000	1.031293000

RCox

E = -1.11611 Ha

Se	-1.594313000	0.036286000	0.777578000
Se	-0.590512000	-0.607850000	-1.301649000
O	-0.051357000	2.987381000	-1.306212000
O	-0.896856000	3.319618000	-0.117683000
H	0.825077000	3.259969000	-0.967099000
H	-1.093786000	2.407172000	0.210613000
H	-2.973994000	0.229404000	0.252346000
H	-0.236486000	0.786451000	-1.691622000

TSox

E = -1.09020 Ha

nimag = -401.876 cm⁻¹

O	6.808011000	-2.036985000	1.589231000
O	8.101765000	-3.620498000	1.451065000
H	7.762615000	-1.870359000	1.401034000
H	7.871119000	-3.934111000	2.347955000
Se	5.668486000	-0.767005000	0.549242000
Se	4.337528000	1.326801000	0.915524000
H	4.527656000	-1.523919000	1.107599000
H	5.328957000	2.101990000	0.130786000

PCox

E = -1.17068 Ha

O	5.363590000	-2.284247000	0.937615000
O	7.648183000	-1.220640000	2.290789000
H	6.907966000	-1.810516000	2.017053000
H	7.740930000	-1.355552000	3.248408000
Se	5.328420000	-0.917197000	-0.035513000
Se	4.979828000	1.093598000	1.381171000
H	3.854244000	-0.788302000	-0.432041000
H	6.374856000	0.898676000	1.856927000

(HTe)₂**1**

E = -0.41580 Ha

Te	-1.490217000	0.202649000	0.774851000
Te	-0.848188000	-1.383920000	-1.405605000
H	-1.021581000	-0.162073000	-2.552261000
H	-3.145343000	-0.106162000	0.719752000

RCox

E = -1.06692 Ha

Te	-1.638138000	0.073264000	0.953289000
Te	-0.569796000	-0.781529000	-1.464294000
O	0.014572000	3.102994000	-1.423771000
O	-0.820449000	3.458379000	-0.234977000
H	0.894369000	3.376604000	-1.094749000
H	-1.019028000	2.553806000	0.112199000
H	-3.206830000	0.294354000	0.380132000
H	-0.172845000	0.778479000	-1.954151000

TSox

E = -1.05195 Ha

nimag = -267.81 cm⁻¹

O	7.064060000	-2.184447000	1.620086000
O	8.199349000	-3.878452000	1.536492000
H	8.003415000	-1.994563000	1.409990000
H	7.919534000	-4.140021000	2.435794000
Te	5.760063000	-0.895155000	0.504639000
Te	4.204889000	1.501471000	0.945397000
H	4.575322000	-1.691561000	1.376710000
H	5.202540000	2.309894000	-0.135772000

PCox

E = -1.12834 Ha

O	5.306218000	-2.479624000	1.136671000
O	7.709727000	-1.452230000	2.089754000
H	6.931939000	-2.062449000	2.038163000
H	7.624929000	-1.011266000	2.952092000
Te	5.501376000	-1.039483000	-0.020091000
Te	4.738198000	1.349944000	1.367234000
H	3.919970000	-0.990678000	-0.703138000
H	6.359381000	1.596578000	1.722628000

Table S5 Geometries of the stationary points and transition states for the oxidation of substituted diselenides and ditellurides; level of theory ZORA-OLYP/TZ2P**(CH₃PhSe)₂****1**

E = -6.48976 Ha

Se	-1.472895000	0.235764000	0.588523000
Se	-0.703236000	-1.053174000	-1.244465000
C	-3.381979000	-0.085278000	0.624627000
C	-3.894498000	-1.227015000	1.250617000

C	-4.265601000	0.848686000	0.076266000
C	-5.270024000	-1.426897000	1.320320000
C	-5.641848000	0.639283000	0.157600000
C	-6.170729000	-0.498219000	0.778805000
H	-3.218865000	-1.960461000	1.680846000
H	-3.885473000	1.737494000	-0.418093000
H	-5.649186000	-2.322255000	1.808753000
H	-6.313449000	1.377119000	-0.275932000
C	-1.038525000	0.065076000	-2.785846000

C	-0.170689000	1.111200000	-3.120483000
C	-2.126386000	-0.214156000	-3.617728000
C	-0.400031000	1.867506000	-4.264725000
C	-2.339252000	0.545479000	-4.768160000
C	-1.486586000	1.600624000	-5.111202000
H	0.679878000	1.338693000	-2.485296000
H	-2.807569000	-1.022678000	-3.369301000
H	0.281120000	2.681719000	-4.502822000
H	-3.189799000	0.312129000	-5.404960000
C	-7.658847000	-0.709496000	0.888207000
H	-8.205900000	-0.108657000	0.156916000
H	-7.926903000	-1.759813000	0.736863000
H	-8.020570000	-0.424572000	1.884546000
C	-1.725564000	2.436867000	-6.341779000
H	-0.831090000	2.478786000	-6.973262000
H	-2.546972000	2.042184000	-6.944928000
H	-1.974563000	3.470062000	-6.071052000

RCox

E = -7.14725 Ha

Se	-1.472895000	0.235764000	0.588523000
Se	-0.703236000	-1.053174000	-1.244465000
O	0.269841000	4.215667000	-0.498867000
O	-1.112868000	3.965013000	-0.099579000
H	0.618991000	4.591161000	0.325627000
H	-1.106461000	2.991828000	-0.036087000
C	-3.381979000	-0.085278000	0.624627000
C	-3.894498000	-1.227015000	1.250617000
C	-4.265601000	0.848686000	0.076266000
C	-5.270024000	-1.426897000	1.320320000
C	-5.641848000	0.639283000	0.157600000
C	-6.170729000	-0.498219000	0.778805000
H	-3.218865000	-1.960461000	1.680846000
H	-3.885473000	1.737494000	-0.418093000
H	-5.649186000	-2.322255000	1.808753000
H	-6.313449000	1.377119000	-0.275932000
C	-1.038525000	0.065076000	-2.785846000
C	-0.170689000	1.111200000	-3.120483000
C	-2.126386000	-0.214156000	-3.617728000
C	-0.400031000	1.867506000	-4.264725000
C	-2.339252000	0.545479000	-4.768160000
C	-1.486586000	1.600624000	-5.111202000
H	0.679878000	1.338693000	-2.485296000
H	-2.807569000	-1.022678000	-3.369301000
H	0.281120000	2.681719000	-4.502822000
H	-3.189799000	0.312129000	-5.404960000
C	-7.658847000	-0.709496000	0.888207000
H	-8.205900000	-0.108657000	0.156916000
H	-7.926903000	-1.759813000	0.736863000
H	-8.020570000	-0.424572000	1.884546000
C	-1.725564000	2.436867000	-6.341779000
H	-0.831090000	2.478786000	-6.973262000
H	-2.546972000	2.042184000	-6.944928000
H	-1.974563000	3.470062000	-6.071052000

TSox

E = -7.11416 Ha

nimag = -277.37 cm⁻¹

O	6.779663000	-2.038046000	1.522573000
O	8.183325000	-3.456689000	1.722421000
H	7.661190000	-1.629479000	1.496637000

H	7.754249000	-3.814476000	2.514184000
Se	5.590597000	-0.792348000	0.456025000
H	1.526693000	-3.352245000	-0.990682000
H	4.372309000	-2.125555000	2.879976000
H	2.409487000	-3.573211000	3.210503000
C	4.049193000	-1.911731000	0.756505000
C	3.745444000	-2.385716000	2.034123000
C	2.637334000	-3.208900000	2.211215000
C	1.816875000	-3.576076000	1.135379000
C	2.142081000	-3.085026000	-0.134809000
C	3.247611000	-2.259792000	-0.331353000
H	3.480585000	-1.896128000	-1.327700000
Se	4.397889000	1.320774000	0.948767000
C	5.757579000	2.537027000	0.344159000
C	5.890309000	2.849772000	-1.014924000
C	6.849886000	3.768730000	-1.429901000
C	7.698483000	4.403878000	-0.512213000
C	7.554765000	4.080129000	0.843201000
C	6.601323000	3.159701000	1.272171000
H	5.242459000	2.376696000	-1.746798000
H	6.938144000	3.995825000	-2.490179000
H	8.201472000	4.550909000	1.580415000
H	6.513519000	2.923491000	2.328462000
C	0.641610000	-4.496402000	1.338513000
H	-0.098531000	-4.387562000	0.541345000
H	0.967768000	-5.544375000	1.343496000
H	0.145533000	-4.308092000	2.295363000
C	8.711766000	5.421500000	-0.967151000
H	9.555825000	5.486087000	-0.275013000
H	9.101126000	5.184253000	-1.961492000
H	8.259540000	6.420154000	-1.025186000

PCox

E = -7.21173 Ha

Se	-2.836852000	-0.892312000	0.667340000
Se	-1.592575000	-2.873335000	-0.157422000
O	-2.554551000	-4.216919000	-0.050097000
C	-1.752364000	-2.350448000	-2.050599000
C	-2.656251000	-3.028644000	-2.860558000
C	-0.903237000	-1.380550000	-2.582665000
C	-2.719700000	-2.715618000	-4.217592000
C	-0.977008000	-1.083240000	-3.941248000
C	-1.887616000	-1.740000000	-4.781877000
H	-3.292130000	-3.797756000	-2.431687000
H	-0.189160000	-0.854067000	-1.954084000
H	-3.428759000	-3.247237000	-4.848437000
H	-0.311823000	-0.327628000	-4.353330000
C	-2.312112000	-1.009725000	2.515889000
C	-2.970774000	-1.883223000	3.390878000
C	-1.295812000	-0.182997000	3.008127000
C	-2.604225000	-1.927899000	4.732492000
C	-0.948832000	-0.230709000	4.357087000
C	-1.590559000	-1.104735000	5.243154000
H	-3.759586000	-2.533419000	3.028024000
H	-0.779762000	0.500776000	2.340608000
H	-3.121236000	-2.621015000	5.392393000
H	-0.160782000	0.424110000	4.722492000
O	-3.861565000	-5.504802000	2.399386000
H	-3.428989000	-5.125875000	1.616629000
H	-4.384622000	-6.232656000	2.043939000
C	-1.981126000	-1.388131000	-6.244124000
H	-1.002226000	-1.130278000	-6.659115000

H	-2.394683000	-2.212893000	-6.830640000
H	-2.635577000	-0.519669000	-6.393277000
C	-1.194792000	-1.179377000	6.695038000
H	-2.073849000	-1.201873000	7.347367000
H	-0.622859000	-2.093977000	6.896172000
H	-0.573800000	-0.329233000	6.988832000

(CH₃OPhSe)₂

1

E = -6.92812 Ha

Se	-1.490742030	0.247572350	0.552866090
Se	-0.758485840	-1.079806960	-1.271693620
C	-3.391763500	-0.076240990	0.640359600
C	-3.901869350	-1.211130050	1.289014670
C	-4.287350640	0.855780910	0.111872070
C	-5.269718140	-1.406862980	1.399710940
C	-5.667053510	0.672553140	0.222531930
C	-6.166450750	-0.465422240	0.867795220
H	-3.221538230	-1.945157350	1.710498290
H	-3.911167520	1.740367970	-0.393663020
H	-5.668566510	-2.283653480	1.902054530
H	-6.331034620	1.419318200	-0.197061020
C	-1.034982300	0.043326270	-2.817070910
C	-0.103033680	1.031291400	-3.169593270
C	-2.140643340	-0.164112730	-3.644304900
C	-0.278093630	1.790891270	-4.315814570
C	-2.323884090	0.589742850	-4.805145280
C	-1.390342680	1.575887850	-5.146508320
H	0.765612580	1.204921180	-2.541417900
H	-2.872903610	-0.923850010	-3.387012350
H	0.441591670	2.556066780	-4.592884590
H	-3.192154410	0.397149180	-5.424477420
O	-7.488854100	-0.755439460	1.036710150
C	-8.460682820	0.153644500	0.532010350
H	-8.374762620	1.140871930	1.003304080
H	-8.387034040	0.261290900	-0.557602680
H	-9.429092160	-0.281739320	0.784848730
O	-1.460340650	2.374765440	-6.250267180
C	-2.552220250	2.209694620	-7.148109880
H	-2.569600380	1.202443700	-7.583172500
H	-3.513212870	2.412894710	-6.658748360
H	-2.392381410	2.941051170	-7.942385580

RCox

E = -7.58452 Ha

Se	-1.485016000	0.226586000	0.575726000
Se	-0.730420000	-1.071100000	-1.270778000
O	0.057933000	4.259339000	-0.625255000
O	-1.272691000	3.921280000	-0.126051000
H	0.441817000	4.657832000	0.172569000
H	-1.199546000	2.950263000	-0.063542000
C	-3.390335000	-0.073525000	0.636406000
C	-3.911125000	-1.206249000	1.280527000
C	-4.274884000	0.862143000	0.095764000
C	-5.280619000	-1.395384000	1.377415000
C	-5.655923000	0.684411000	0.192957000
C	-6.167445000	-0.449969000	0.835420000
H	-3.238800000	-1.943327000	1.709468000
H	-3.894115000	1.744862000	-0.408893000
H	-5.688536000	-2.269736000	1.876580000

H	-6.311618000	1.434004000	-0.234299000
C	-1.029875000	0.045495000	-2.812146000
C	-0.105929000	1.036339000	-3.178406000
C	-2.145930000	-0.170602000	-3.623976000
C	-0.298854000	1.790365000	-4.324409000
C	-2.346199000	0.578190000	-4.784429000
C	-1.420461000	1.567400000	-5.140181000
H	0.766592000	1.221581000	-2.559540000
H	-2.871454000	-0.932473000	-3.354522000
H	0.409685000	2.563203000	-4.607691000
H	-3.221498000	0.380746000	-5.392111000
O	-7.491814000	-0.732637000	0.991982000
C	-8.455100000	0.182556000	0.479944000
H	-8.366582000	1.168787000	0.952445000
H	-8.372330000	0.289615000	-0.608920000
H	-9.427566000	-0.247665000	0.725569000
O	-1.507983000	2.362139000	-6.244032000
C	-2.621283000	2.205964000	-7.117115000
H	-2.653067000	1.201000000	-7.556613000
H	-3.569157000	2.411304000	-6.603940000
H	-2.476445000	2.940610000	-7.911149000

TSox

E = -7.55205 Ha

nimag = -270.11

O	6.774821000	-2.019216000	1.562831000
O	8.197444000	-3.402317000	1.829734000
H	7.642946000	-1.583445000	1.553425000
H	7.752340000	-3.754071000	2.615104000
Se	5.568774000	-0.776410000	0.485610000
H	1.458810000	-3.278130000	-0.976185000
H	4.392883000	-2.197854000	2.873201000
H	2.448764000	-3.648086000	3.201477000
C	4.033323000	-1.895751000	0.770185000
C	3.748199000	-2.420087000	2.030000000
C	2.643665000	-3.250156000	2.212801000
C	1.813208000	-3.559268000	1.126717000
C	2.104418000	-3.026845000	-0.140018000
C	3.204903000	-2.203051000	-0.316595000
H	3.421054000	-1.805125000	-1.303466000
Se	4.405303000	1.351466000	1.008266000
C	5.746864000	2.563789000	0.375495000
C	5.833904000	2.901569000	-0.985879000
C	6.775751000	3.816730000	-1.426733000
C	7.659191000	4.422262000	-0.516610000
C	7.579880000	4.091856000	0.842990000
C	6.629951000	3.167815000	1.276540000
H	5.155243000	2.446992000	-1.701138000
H	6.844936000	4.081822000	-2.477778000
H	8.245981000	4.539471000	1.571072000
H	6.578645000	2.918202000	2.332134000
O	8.541085000	5.305882000	-1.057706000
C	9.475187000	5.960090000	-0.202727000
H	8.968954000	6.573989000	0.552384000
H	10.139757000	5.241603000	0.292523000
H	10.065443000	6.605869000	-0.854801000
O	0.713334000	-4.357723000	1.186116000
C	0.358922000	-4.953183000	2.431821000
H	1.152236000	-5.613741000	2.802386000
H	0.127238000	-4.194796000	3.189765000
H	-0.535844000	-5.543812000	2.228827000\

PCox

E = -7.64957 Ha

Se	2.783951000	0.892943000	14.560830000
Se	5.070628000	1.764029000	15.010744000
C	3.445388000	-0.725229000	13.667151000
C	3.387094000	-0.801963000	12.281641000
C	3.792325000	-1.966081000	11.628067000
C	4.251780000	-3.059871000	12.374270000
C	4.297209000	-2.975077000	13.776956000
C	3.895542000	-1.814456000	14.420119000
C	4.615369000	3.176333000	16.226711000
C	4.267912000	4.442759000	15.745162000
C	3.983730000	5.487028000	16.624140000
C	4.050427000	5.274227000	18.007309000
C	4.401115000	4.004175000	18.494839000
C	4.676643000	2.969342000	17.614818000
H	3.018664000	0.046623000	11.712196000
H	3.742017000	-2.004314000	10.546300000
O	4.670777000	-4.244576000	11.849528000
H	4.651898000	-3.831878000	14.342247000
H	3.941337000	-1.764945000	15.505266000
H	4.207302000	4.624031000	14.677261000
H	3.712761000	6.452546000	16.213684000
O	3.799048000	6.217040000	18.958178000
H	4.947469000	1.993177000	18.005931000
O	2.091622000	1.765196000	13.333723000
O	2.493510000	4.592012000	12.236716000
H	2.366559000	3.689267000	12.572383000
H	1.640643000	4.812912000	11.844871000
C	3.433929000	7.530505000	18.543908000
C	4.661821000	-4.412913000	10.434533000
H	4.228839000	8.003018000	17.953764000
H	3.284501000	8.096680000	19.464860000
H	2.501637000	7.526825000	17.965896000
H	5.037870000	-5.422005000	10.258035000
H	5.320334000	-3.689539000	9.938156000
H	3.647827000	-4.328053000	10.024588000
H	4.451291000	3.850517000	19.568975000

(CIPhSe)₂**1**

E = -5.19614 Ha

Se	-1.494166000	0.265835000	0.608015000
Se	-0.692374000	-1.002864000	-1.222576000
C	-3.398987000	-0.079534000	0.613540000
C	-3.904650000	-1.240476000	1.208791000
C	-4.284157000	0.858036000	0.071156000
C	-5.277198000	-1.469044000	1.256416000
C	-5.660011000	0.640522000	0.119310000
C	-6.148224000	-0.524900000	0.709755000
H	-3.227809000	-1.972938000	1.638207000
H	-3.906925000	1.763578000	-0.394022000
H	-5.669266000	-2.369633000	1.717920000
H	-6.346223000	1.368721000	-0.300796000
C	-1.073779000	0.094946000	-2.768384000
C	-0.276603000	1.199478000	-3.088577000
C	-2.124754000	-0.266692000	-3.618590000
C	-0.528597000	1.939784000	-4.240321000
C	-2.376111000	0.460892000	-4.780283000
C	-1.576197000	1.562723000	-5.082509000

H	0.541662000	1.493505000	-2.439085000
H	-2.752030000	-1.119797000	-3.378244000
H	0.085127000	2.801120000	-4.482958000
H	-3.188818000	0.178210000	-5.441530000
Cl	-7.866116000	-0.806047000	0.767860000
Cl	-1.888732000	2.479371000	-6.530475000

RCox

E = -5.85186 Ha

Se	-1.494166000	0.265835000	0.608015000
Se	-0.692374000	-1.002864000	-1.222576000
O	0.534732000	4.061054000	-0.482386000
O	-0.853780000	4.001573000	-0.031741000
H	0.954448000	4.433438000	0.310029000
H	-0.966070000	3.038322000	0.063805000
C	-3.398987000	-0.079534000	0.613540000
C	-3.904650000	-1.240476000	1.208791000
C	-4.284157000	0.858036000	0.071156000
C	-5.277198000	-1.469044000	1.256416000
C	-5.660011000	0.640522000	0.119310000
C	-6.148224000	-0.524900000	0.709755000
H	-3.227809000	-1.972938000	1.638207000
H	-3.906925000	1.763578000	-0.394022000
H	-5.669266000	-2.369633000	1.717920000
H	-6.346223000	1.368721000	-0.300796000
C	-1.073779000	0.094946000	-2.768384000
C	-0.276603000	1.199478000	-3.088577000
C	-2.124754000	-0.266692000	-3.618590000
C	-0.528597000	1.939784000	-4.240321000
C	-2.376111000	0.460892000	-4.780283000
C	-1.576197000	1.562723000	-5.082509000
H	0.541662000	1.493505000	-2.439085000
H	-2.752030000	-1.119797000	-3.378244000
H	0.085127000	2.801120000	-4.482958000
H	-3.188818000	0.178210000	-5.441530000
Cl	-7.866116000	-0.806047000	0.767860000
Cl	-1.888732000	2.479371000	-6.530475000

TSox

E = -5.81726 Ha

nimag = -307.15 cm⁻¹

O	6.766439000	-2.073356000	1.549761000
O	8.160903000	-3.521239000	1.642290000
H	7.667340000	-1.706103000	1.522154000
H	7.767811000	-3.904297000	2.441320000
Se	5.614867000	-0.791105000	0.516319000
H	1.535586000	-3.287795000	-1.037246000
H	4.369118000	-2.185434000	2.891863000
H	2.384732000	-3.639087000	3.166158000
C	4.060079000	-1.903556000	0.772770000
C	3.745923000	-2.413236000	2.034203000
C	2.633806000	-3.236185000	2.189967000
C	1.842878000	-3.543117000	1.081626000
C	2.152737000	-3.036986000	-0.180966000
C	3.266339000	-2.214539000	-0.333090000
H	3.511207000	-1.827013000	-1.317213000
Se	4.409660000	1.327945000	0.999839000
C	5.754032000	2.539142000	0.355529000
C	5.884472000	2.804246000	-1.014499000
C	6.827674000	3.720295000	-1.470986000
C	7.645098000	4.380140000	-0.551365000

C	7.527436000	4.129638000	0.816420000
C	6.584405000	3.208122000	1.264705000
H	5.243462000	2.299350000	-1.730516000
H	6.925922000	3.924847000	-2.532159000
H	8.168110000	4.647333000	1.522930000
H	6.495196000	3.011653000	2.328745000
Cl	8.822377000	5.528665000	-1.118225000
Cl	0.455888000	-4.574697000	1.275349000

PCox

E = -5.91569 Ha

Se	-2.852002000	-0.930168000	0.678142000
Se	-1.569567000	-2.882726000	-0.163373000
O	-2.508052000	-4.242210000	-0.075258000
C	-1.741133000	-2.341246000	-2.052021000
C	-2.628037000	-3.038372000	-2.866108000
C	-0.919745000	-1.341759000	-2.573114000
C	-2.710435000	-2.723135000	-4.221030000
C	-0.995064000	-1.026039000	-3.927528000
C	-1.893631000	-1.718616000	-4.742329000
H	-3.243399000	-3.827008000	-2.442630000
H	-0.222619000	-0.798762000	-1.939963000
H	-3.400299000	-3.255082000	-4.868265000
H	-0.363598000	-0.250381000	-4.348162000
C	-2.308732000	-1.032048000	2.521948000
C	-2.919543000	-1.937876000	3.398635000
C	-1.328252000	-0.156066000	3.005858000
C	-2.547865000	-1.974211000	4.740412000
C	-0.962893000	-0.178105000	4.349352000
C	-1.574307000	-1.091583000	5.209240000
H	-3.678415000	-2.626550000	3.043552000
H	-0.848964000	0.550478000	2.335089000
H	-3.014107000	-2.685083000	5.414677000
H	-0.207250000	0.504163000	4.724973000
O	-3.997800000	-5.356599000	2.373591000
H	-3.525259000	-5.077229000	1.573131000
H	-4.554073000	-6.085442000	2.075254000
Cl	-1.989766000	-1.325695000	-6.435096000
Cl	-1.113596000	-1.129168000	6.888279000

(NH₂PhSe)₂

1

E = -6.17859 Ha

Se	-1.507432000	0.256749000	0.573542000
Se	-0.727918000	-1.037871000	-1.265222000
C	-3.398960000	-0.102046000	0.651198000
C	-3.894480000	-1.236096000	1.307938000
C	-4.314304000	0.805256000	0.102299000
C	-5.261149000	-1.459848000	1.411137000
C	-5.683220000	0.589220000	0.207024000
C	-6.183317000	-0.549515000	0.862889000
H	-3.203814000	-1.951578000	1.744764000
H	-3.953177000	1.692017000	-0.410470000
H	-5.621968000	-2.349902000	1.922933000
H	-6.374799000	1.307908000	-0.228386000
C	-1.029116000	0.076319000	-2.807410000
C	-0.092715000	1.044105000	-3.193977000
C	-2.166293000	-0.109218000	-3.604216000
C	-0.285691000	1.805114000	-4.339405000
C	-2.362909000	0.646948000	-4.753478000
C	-1.426003000	1.620576000	-5.142733000

H	0.796959000	1.204958000	-2.592015000
H	-2.906542000	-0.852679000	-3.323290000
H	0.458795000	2.546536000	-4.622795000
H	-3.250548000	0.479548000	-5.360423000
N	-7.549722000	-0.800257000	0.916252000
H	-8.148856000	0.006609000	0.821507000
H	-7.854250000	-1.420351000	1.652288000
N	-1.588571000	2.336282000	-6.323093000
H	-1.092419000	3.213576000	-6.378232000
H	-2.534057000	2.405842000	-6.669588000

RCox

E = -6.83567 Ha

Se	-1.481807000	0.223794000	0.593954000
Se	-0.703537000	-1.048615000	-1.272171000
O	0.147416000	4.197244000	-0.526713000
O	-1.230872000	3.883297000	-0.159098000
H	0.465487000	4.572810000	0.310226000
H	-1.181329000	2.910967000	-0.802260000
C	-3.381738000	-0.085791000	0.650474000
C	-3.900453000	-1.207831000	1.310241000
C	-4.276075000	0.832070000	0.084513000
C	-5.271005000	-1.408828000	1.402502000
C	-5.648516000	0.637596000	0.178073000
C	-6.173242000	-0.487705000	0.838584000
H	-3.225675000	-1.931541000	1.758209000
H	-3.900740000	1.709508000	-0.433350000
H	-5.650516000	-2.289140000	1.917402000
H	-6.323873000	1.364125000	-0.269226000
C	-1.019254000	0.070679000	-2.802374000
C	-0.099697000	1.059600000	-3.177407000
C	-2.154756000	-0.127165000	-3.599516000
C	-0.309050000	1.830766000	-4.311495000
C	-2.365739000	0.638673000	-4.739034000
C	-1.447930000	1.636244000	-5.114691000
H	0.784834000	1.234659000	-2.572485000
H	-2.881482000	-0.886387000	-3.325714000
H	0.416603000	2.595339000	-4.580420000
H	-3.251484000	0.463956000	-5.346517000
N	-7.542485000	-0.714748000	0.881902000
H	-8.130033000	0.097870000	0.767684000
H	-7.866904000	-1.327434000	1.615369000
N	-1.628606000	2.369936000	-6.279506000
H	-1.148986000	3.257211000	-6.320039000
H	-2.575648000	2.426349000	-6.623968000

TSox

E = -6.80345 Ha

nimag = -259.86 cm⁻¹

O	6.790360000	-2.030932000	1.512443000
O	8.229982000	-3.384982000	1.815030000
H	7.643255000	-1.567240000	1.514947000
H	7.760014000	-3.755742000	2.576597000
Se	5.557940000	-0.804054000	0.431218000
H	1.467607000	-3.335631000	-0.983052000
H	4.397798000	-2.187837000	2.852257000
H	2.449455000	-3.642089000	3.204775000
C	4.034423000	-1.924132000	0.741168000
C	3.751522000	-2.427848000	2.015087000
C	2.651953000	-3.250528000	2.210370000
C	1.803417000	-3.592310000	1.139915000

C	2.099627000	-3.078265000	-0.136218000
C	3.200467000	-2.255585000	-0.331632000
H	3.409915000	-1.875481000	-1.327140000
Se	4.410755000	1.340587000	0.957585000
C	5.764769000	2.545404000	0.350148000
C	5.869451000	2.898378000	-1.004148000
C	6.829778000	3.803764000	-1.431650000
C	7.724920000	4.391337000	-0.517075000
C	7.616697000	4.036772000	0.840856000
C	6.655879000	3.129093000	1.263661000
H	5.190112000	2.461247000	-1.729846000
H	6.887414000	4.065824000	-2.485948000
H	8.292993000	4.479018000	1.569225000
H	6.595900000	2.868628000	2.316207000
N	8.647435000	5.336143000	-0.933463000
H	8.893795000	5.326149000	-1.911666000
H	9.439031000	5.491282000	-0.327624000
N	0.741783000	-4.460429000	1.326734000
H	0.007781000	-4.435679000	0.635523000
H	0.398054000	-4.559794000	2.269703000

PCox

E = -6.90052 Ha

Se	-2.832084000	-0.883585000	0.687890000
Se	-1.581828000	-2.866505000	-0.178154000
O	-2.541587000	-4.213970000	-0.055075000
C	-1.752790000	-2.359844000	-2.060842000
C	-2.653690000	-3.046440000	-2.872256000
C	-0.927543000	-1.374044000	-2.605991000
C	-2.739420000	-2.740782000	-4.224236000
C	-1.010801000	-1.069562000	-3.958262000
C	-1.921588000	-1.746086000	-4.792647000
H	-3.279760000	-3.821600000	-2.439633000
H	-0.219801000	-0.831156000	-1.984034000
H	-3.443612000	-3.282534000	-4.852312000
H	-0.362504000	-0.302642000	-4.376456000
C	-2.314674000	-1.000949000	2.527226000
C	-2.992725000	-1.853256000	3.411882000
C	-1.270046000	-0.208122000	3.025224000
C	-2.634319000	-1.912661000	4.750764000
C	-0.916315000	-0.258482000	4.366821000
C	-1.590458000	-1.115945000	5.256099000
H	-3.796079000	-2.487167000	3.051419000
H	-0.730547000	0.456978000	2.357181000
H	-3.169306000	-2.588386000	5.414407000
H	-0.108680000	0.372354000	4.732490000
O	-3.814109000	-5.504445000	2.387392000
H	-3.383532000	-5.101651000	1.614370000
H	-4.358919000	-6.202997000	2.006751000
N	-1.965645000	-1.482656000	-6.153574000
H	-1.616263000	-0.582594000	-6.446687000
H	-2.813679000	-1.747649000	-6.631965000
N	-1.273467000	-1.133562000	6.606384000
H	-0.349092000	-0.811820000	6.851945000
H	-1.547248000	-1.960808000	7.115566000

(CNPhSe)₂

1

E = -6.22880 Ha

Se	-1.608790000	0.321484000	0.447391000
----	--------------	-------------	-------------

Se	-0.886781000	-1.024527000	-1.297106000
C	-3.502220000	-0.056621000	0.652304000
C	-4.255289000	-0.846753000	-0.216439000
C	-4.111210000	0.535213000	1.766831000
C	-5.609579000	-1.046642000	0.024234000
C	-5.464573000	0.339467000	2.007762000
C	-6.229651000	-0.455705000	1.137381000
H	-3.790274000	-1.313876000	-1.078209000
H	-3.536192000	1.149221000	2.455718000
H	-6.194225000	-1.662640000	-0.652383000
H	-5.933812000	0.798169000	2.872685000
C	-1.077884000	0.052352000	-2.901130000
C	-1.758628000	1.268370000	-2.966725000
C	-0.482516000	-0.480373000	-4.052195000
C	-1.844581000	1.951593000	-4.174109000
C	-0.571061000	0.197941000	-5.260569000
C	-1.253622000	1.424227000	-5.334105000
H	-2.216547000	1.691562000	-2.078968000
H	0.057492000	-1.423307000	-4.014697000
H	-2.373388000	2.898679000	-4.223516000
H	-0.107429000	-0.215986000	-6.150730000
C	-1.342243000	2.126908000	-6.573896000
N	-1.414812000	2.699701000	-7.584788000
C	-7.620922000	-0.661391000	1.383670000
N	-8.755311000	-0.829140000	1.584458000

RCox

E = -6.88321 Ha

Se	-1.488882000	0.253343000	0.593329000
Se	-0.722363000	-1.028601000	-1.230728000
O	0.492676000	4.153557000	-0.517977000
O	-0.851753000	4.117765000	0.053209000
H	0.973408000	4.585082000	0.207000000
H	-0.952020000	3.160561000	0.196710000
C	-3.399872000	-0.080767000	0.599047000
C	-3.903933000	-1.304541000	1.054697000
C	-4.279464000	0.932611000	0.202446000
C	-5.275301000	-1.518715000	1.107417000
C	-5.654326000	0.727689000	0.261554000
C	-6.161770000	-0.501483000	0.711956000
H	-3.225483000	-2.090770000	1.370768000
H	-3.896292000	1.882685000	-0.156691000
H	-5.667958000	-2.467084000	1.461318000
H	-6.337654000	1.513528000	-0.045376000
C	-1.094934000	0.079402000	-2.776299000
C	-0.425600000	1.290154000	-2.987664000
C	-2.002261000	-0.394182000	-3.731362000
C	-0.668573000	2.028582000	-4.138678000
C	-2.235285000	0.331700000	-4.894864000
C	-1.572583000	1.551736000	-5.104408000
H	0.284609000	1.662830000	-2.257463000
H	-2.529877000	-1.328936000	-3.567765000
H	-0.155165000	2.971677000	-4.298466000
H	-2.936292000	-0.036236000	-5.637808000
C	-1.815789000	2.304601000	-6.294508000
N	-2.013815000	2.916220000	-7.264663000
C	-7.573141000	-0.718686000	0.770268000
N	-8.722072000	-0.897607000	0.818248000

TSox

E = -6.84709 Ha

O	6.758008000	-2.130639000	1.570007000
O	8.110226000	-3.625282000	1.523944000
H	7.681768000	-1.820758000	1.532053000
H	7.758379000	-4.035118000	2.329520000
Se	5.660668000	-0.806577000	0.568967000
H	1.544073000	-3.184532000	-1.069288000
H	4.373560000	-2.225521000	2.903645000
H	2.355933000	-3.638384000	3.137934000
C	4.079004000	-1.898004000	0.788841000
C	3.749806000	-2.424843000	2.039667000
C	2.619911000	-3.223782000	2.170136000
C	1.816598000	-3.498398000	1.050954000
C	2.159537000	-2.965988000	-0.202460000
C	3.289704000	-2.166828000	-0.331653000
H	3.553061000	-1.763690000	-1.304296000
Se	4.432189000	1.311202000	1.030754000
C	5.753912000	2.531704000	0.356318000
C	5.971528000	2.672036000	-1.022104000
C	6.893974000	3.596139000	-1.495449000
C	7.608757000	4.403480000	-0.593448000
C	7.387965000	4.266533000	0.787240000
C	6.470969000	3.333435000	1.256061000
H	5.412664000	2.064448000	-1.726581000
H	7.060805000	3.704041000	-2.562732000
H	7.939900000	4.888265000	1.485363000
H	6.310758000	3.227320000	2.324351000
C	0.654000000	-4.319101000	1.186870000
N	-0.293925000	-4.984625000	1.297748000
C	8.553061000	5.359382000	-1.078879000
N	9.321862000	6.138534000	-1.474312000

PCox

E = -6.94630 Ha

Se	-2.831507000	-0.953265000	0.666072000
Se	-1.558350000	-2.915861000	-0.161615000
O	-2.503189000	-4.268398000	-0.088759000
C	-1.735124000	-2.348110000	-2.049728000
C	-2.633479000	-3.034560000	-2.860905000
C	-0.908492000	-1.347396000	-2.561396000
C	-2.723866000	-2.702796000	-4.208787000
C	-0.992791000	-1.017757000	-3.909277000
C	-1.904622000	-1.692436000	-4.740086000
H	-3.248207000	-3.823739000	-2.437773000
H	-0.204337000	-0.818478000	-1.924612000
H	-3.423724000	-3.223780000	-4.854998000
H	-0.358123000	-0.241025000	-4.324374000
C	-2.296044000	-1.047851000	2.515243000
C	-2.871751000	-1.988574000	3.379543000
C	-1.364725000	-0.122281000	3.006233000
C	-2.509104000	-2.009769000	4.721585000
C	-1.012881000	-0.130882000	4.350485000
C	-1.581059000	-1.079126000	5.218017000
H	-3.595538000	-2.708775000	3.014728000
H	-0.917597000	0.607659000	2.338698000
H	-2.947619000	-2.745720000	5.388352000
H	-0.296029000	0.589153000	4.733016000
O	-4.074211000	-5.275831000	2.379946000
H	-3.600797000	-5.082786000	1.556055000
H	-4.666246000	-6.001528000	2.150625000
C	-1.214671000	-1.093772000	6.599362000

N	-0.914063000	-1.102467000	7.723638000
C	-1.993380000	-1.352401000	-6.125814000
N	-2.065253000	-1.074692000	-7.253495000

(NO₂PhSe)₂

1

E = -6.41724 Ha

Se	-0.773905000	-0.823805000	-2.104415000
Se	0.775463000	0.854157000	-2.139254000
C	-0.124262000	-2.079308000	-0.809648000
C	-0.845526000	-3.276315000	-0.729218000
C	-0.468034000	-4.253594000	0.178844000
C	0.631807000	-4.028440000	1.000637000
C	1.356213000	-2.843864000	0.927080000
C	0.975096000	-1.865947000	0.019224000
C	0.163396000	2.130261000	-0.846506000
C	-0.918602000	1.935205000	0.009301000
C	-1.273731000	2.927991000	0.911518000
C	-0.540978000	4.109008000	0.952378000
C	0.542014000	4.315786000	0.103799000
C	0.893584000	3.323646000	-0.798522000
H	-1.703551000	-3.455548000	-1.375764000
H	-1.014142000	-5.189076000	0.254923000
N	1.036557000	-5.065560000	1.965958000
H	2.210223000	-2.696557000	1.581753000
H	1.539469000	-0.938815000	-0.046077000
H	-1.489608000	1.010689000	-0.030426000
H	-2.113912000	2.795239000	1.586847000
N	-0.918566000	5.162137000	1.911187000
H	1.095366000	5.248703000	0.155125000
H	1.738524000	3.488336000	-1.465848000
O	0.373293000	-6.092747000	1.999581000
O	2.008639000	-4.830862000	2.669990000
O	-0.248278000	6.185321000	1.916035000
O	-1.877013000	4.943815000	2.638784000

RCox

E = -7.07285 Ha

O	9.890848000	-3.645362000	0.526185000
O	10.975130000	-2.943683000	-0.156332000
H	10.374807000	-4.016737000	1.282161000
H	11.108568000	-3.530180000	-0.919349000
Se	5.881636000	-0.615852000	1.841933000
H	6.873309000	3.150447000	-1.487984000
H	8.355969000	-1.179101000	0.437337000
H	9.697180000	-0.077889000	-1.311360000
C	6.833017000	0.371363000	0.470206000
C	8.016409000	-0.233539000	0.024616000
C	8.779429000	0.379002000	-0.961853000
C	8.354418000	1.594976000	-1.495048000
C	7.180690000	2.204878000	-1.056814000
C	6.417007000	1.588795000	-0.071256000
H	5.504748000	2.063793000	0.273338000
Se	4.156720000	0.772116000	2.537791000
C	2.636037000	0.319201000	1.424082000
C	1.427405000	0.928554000	1.790389000
C	0.272278000	0.682001000	1.059486000
C	0.331373000	-0.178489000	-0.035910000
C	1.526242000	-0.790613000	-0.408282000

C	2.681505000	-0.538670000	0.323755000
H	1.376895000	1.595063000	2.647818000
H	-0.669038000	1.144697000	1.331478000
H	1.544892000	-1.454922000	-1.264391000
H	3.611657000	-1.017492000	0.037060000
N	9.165417000	2.251346000	-2.546330000
N	-0.898886000	-0.447330000	-0.815592000
O	-1.933433000	0.116844000	-0.459371000
O	-0.811007000	-1.218049000	-1.771221000
O	8.767151000	3.331417000	-2.982929000
O	10.188032000	1.676513000	-2.919707000

TSox

E = -7.03425 Ha

O	6.764250000	-2.202027000	1.578075000
O	8.088647000	-3.719352000	1.469323000
H	7.696604000	-1.916616000	1.544652000
H	7.743463000	-4.146611000	2.268885000
Se	5.697239000	-0.831132000	0.617056000
H	1.513407000	-3.051753000	-1.100492000
H	4.391929000	-2.336852000	2.889392000
H	2.329630000	-3.721616000	3.057907000
C	4.093918000	-1.901436000	0.793882000
C	3.760514000	-2.480829000	2.020172000
C	2.612434000	-3.261133000	2.118727000
C	1.820459000	-3.447684000	0.989042000
C	2.146847000	-2.878746000	-0.238735000
C	3.294903000	-2.098344000	-0.335005000
H	3.562533000	-1.654706000	-1.288531000
Se	4.500828000	1.290811000	1.133551000
C	5.778150000	2.521760000	0.398203000
C	6.039398000	2.566456000	-0.979614000
C	6.925066000	3.505586000	-1.494677000
C	7.536906000	4.408008000	-0.626328000
C	7.287109000	4.385933000	0.743663000
C	6.411279000	3.434246000	1.255398000
H	5.543108000	1.875351000	-1.652959000
H	7.136331000	3.553241000	-2.556447000
H	7.780657000	5.099418000	1.392976000
H	6.220220000	3.400111000	2.323278000
N	0.588605000	-4.282300000	1.096153000
O	0.329254000	-4.767362000	2.194289000
O	-0.084900000	-4.427174000	0.079155000
N	8.477613000	5.420676000	-1.176925000
O	8.673374000	5.410540000	-2.390613000
O	8.997377000	6.201799000	-0.382628000

PCox

E = -7.13327 Ha

Se	-2.818142000	-0.966222000	0.690374000
Se	-1.577118000	-2.924616000	-0.189674000
O	-2.527625000	-4.272459000	-0.121349000
C	-1.789516000	-2.320619000	-2.064221000
C	-2.716767000	-2.979862000	-2.865612000
C	-0.957802000	-1.324193000	-2.576740000
C	-2.832514000	-2.623316000	-4.206957000
C	-1.066746000	-0.969114000	-3.917904000
C	-2.006242000	-1.622955000	-4.713080000
H	-3.334339000	-3.766887000	-2.443134000
H	-0.230973000	-0.817831000	-1.947367000
H	-3.548665000	-3.111416000	-4.857569000

H	-0.438173000	-0.198857000	-4.348678000
C	-2.251527000	-1.096707000	2.529030000
C	-2.806697000	-2.059157000	3.382973000
C	-1.319159000	-0.172703000	3.021773000
C	-2.421888000	-2.104014000	4.719945000
C	-0.943498000	-0.205262000	4.360536000
C	-1.498667000	-1.174680000	5.192716000
H	-3.532140000	-2.776755000	3.016959000
H	-0.888449000	0.573339000	2.361556000
H	-2.835631000	-2.847804000	5.390556000
H	-0.227198000	0.502856000	4.759888000
O	-4.046243000	-5.313589000	2.373472000
H	-3.596028000	-5.123577000	1.536305000
H	-4.628007000	-6.055058000	2.169821000
N	-2.125883000	-1.242028000	-6.150077000
N	-1.092709000	-1.215468000	6.625422000
O	-1.617210000	-2.066711000	7.339324000
O	-0.258388000	-0.393746000	7.000884000
O	-2.958826000	-1.840552000	-6.825843000
O	-1.383806000	-0.353929000	-6.562910000

(CH₃PhTe)₂

1

E = -6.43895 Ha

Te	-2.521413000	5.175214000	2.865531000
Te	-3.906930000	2.852015000	2.436188000
C	-0.764786000	4.844796000	1.684405000
C	-0.763852000	5.036069000	0.297543000
C	0.401688000	4.830469000	-0.438846000
C	1.598191000	4.438069000	0.179733000
C	2.861666000	4.242987000	-0.622642000
C	1.583833000	4.256428000	1.567818000
C	0.421348000	4.453137000	2.314574000
C	-2.770098000	1.459381000	3.601613000
C	-1.869197000	0.603161000	2.959540000
C	-1.137334000	-0.329766000	3.695913000
C	-1.276572000	-0.433346000	5.084918000
C	-0.496950000	-1.454448000	5.877286000
C	-2.183310000	0.431980000	5.715655000
C	-2.924205000	1.363051000	4.989905000
H	-1.672635000	5.338686000	-0.214354000
H	0.377710000	4.978847000	-1.517257000
H	3.584021000	3.618185000	-0.090572000
H	3.348688000	5.204735000	-0.826595000
H	2.655935000	3.774728000	-1.589990000
H	2.493014000	3.946320000	2.079837000
H	0.443459000	4.289283000	3.387662000
H	-1.725265000	0.664885000	1.885136000
H	-0.438673000	-0.981690000	3.174616000
H	0.364418000	-1.827026000	5.316693000
H	-1.124237000	-2.318950000	6.127642000
H	-0.132255000	-1.037736000	6.821302000
H	-2.314959000	0.378669000	6.795225000
H	-3.616865000	2.017509000	5.510870000

RCox

E = -7.09514 Ha

Te	-1.441226000	0.258485000	0.777337000
Te	-0.628667000	-1.245427000	-1.369787000
O	-0.064831000	4.500335000	-0.764896000

O	-1.420031000	4.093977000	-0.400535000
H	0.178275000	5.007337000	0.026622000
H	-1.282080000	3.143334000	-0.229993000
C	-3.557746000	-0.077726000	0.810274000
C	-4.088635000	-1.151086000	1.533725000
C	-4.430149000	0.794772000	0.151657000
C	-5.467237000	-1.345573000	1.591157000
C	-5.807845000	0.590275000	0.217101000
C	-6.353454000	-0.479740000	0.937067000
H	-3.430192000	-1.842670000	2.051312000
H	-4.044103000	1.633528000	-0.419775000
H	-5.857709000	-2.189355000	2.156602000
H	-6.467738000	1.279516000	-0.305805000
C	-0.935288000	0.097260000	-3.007981000
C	0.019623000	1.069242000	-3.327658000
C	-2.075235000	-0.024343000	-3.808583000
C	-0.173625000	1.908064000	-4.421624000
C	-2.254324000	0.817698000	-4.906356000
C	-1.312809000	1.800841000	-5.231328000
H	0.914505000	1.179622000	-2.722634000
H	-2.828703000	-0.772612000	-3.580504000
H	0.577953000	2.661993000	-4.646263000
H	-3.147978000	0.705441000	-5.516777000
C	-7.844548000	-0.677546000	1.030670000
H	-8.361497000	-0.257506000	0.163353000
H	-8.105527000	-1.737366000	1.104541000
H	-8.247606000	-0.181000000	1.922897000
C	-1.522201000	2.733438000	-6.396248000
H	-0.601057000	2.866163000	-6.972913000
H	-2.298069000	2.366088000	-7.072988000
H	-1.829403000	3.727491000	-6.047563000

TSox

E = -7.07130 Ha
 nimag = -147.26 cm⁻¹

O	6.900247000	-2.464363000	1.599524000
O	7.976498000	-4.018508000	1.740734000
H	7.710068000	-2.001931000	1.863702000
H	7.306093000	-4.483184000	2.264168000
Te	5.734444000	-0.895986000	0.495566000
H	1.349065000	-3.241127000	-1.060171000
H	4.396675000	-2.615157000	2.797106000
H	2.398210000	-4.023078000	3.033540000
C	4.003570000	-2.116530000	0.732197000
C	3.730217000	-2.742558000	1.950904000
C	2.598114000	-3.544875000	2.076977000
C	1.718632000	-3.744695000	1.004896000
C	2.010479000	-3.107012000	-0.207090000
C	3.138723000	-2.301286000	-0.349306000
H	3.335379000	-1.823027000	-1.304288000
Te	4.325753000	1.503898000	1.101878000
C	5.790152000	2.822007000	0.284404000
C	5.837128000	3.080267000	-1.091367000
C	6.772523000	3.974665000	-1.605992000
C	7.681984000	4.640880000	-0.773099000
C	7.623913000	4.373803000	0.599898000
C	6.694549000	3.477875000	1.127300000
H	5.144672000	2.584738000	-1.765150000
H	6.792216000	4.156551000	-2.678623000
H	8.318314000	4.869836000	1.274704000
H	6.679533000	3.291307000	2.196967000
C	0.516019000	-4.641649000	1.143994000

H	-0.275372000	-4.366292000	0.441482000
H	0.785920000	-5.685835000	0.940030000
H	0.103349000	-4.605935000	2.156431000
C	8.669238000	5.629799000	-1.336702000
H	9.519878000	5.776548000	-0.665853000
H	9.052258000	5.304559000	-2.308766000
H	8.196491000	6.609009000	-1.486612000

PCox

E = -7.16341 Ha

Te	-2.916048000	-0.716433000	0.735466000
Te	-1.444169000	-2.961972000	-0.212681000
O	-2.555357000	-4.418047000	-0.128129000
C	-1.691033000	-2.418733000	-2.287315000
C	-2.605948000	-3.139924000	-3.049052000
C	-0.909646000	-1.423534000	-2.879146000
C	-2.746239000	-2.851492000	-4.407170000
C	-1.059229000	-1.149249000	-4.236007000
C	-1.980708000	-1.855230000	-5.024275000
H	-3.198828000	-3.923470000	-2.584358000
H	-0.187369000	-0.854973000	-2.297750000
H	-3.465382000	-3.417879000	-4.994920000
H	-0.446801000	-0.372121000	-4.688749000
C	-2.333003000	-0.944031000	2.776515000
C	-2.910642000	-1.936148000	3.578096000
C	-1.394332000	-0.070593000	3.337626000
C	-2.542549000	-2.047606000	4.917358000
C	-1.047159000	-0.187139000	4.682901000
C	-1.612478000	-1.175517000	5.498099000
H	-3.633293000	-2.633904000	3.168334000
H	-0.928947000	0.700266000	2.730470000
H	-2.993152000	-2.835411000	5.517144000
H	-0.316146000	0.502569000	5.099802000
O	-4.018618000	-5.346864000	2.294844000
H	-3.542828000	-5.087196000	1.484882000
H	-4.731090000	-5.911147000	1.973392000
C	-2.136956000	-1.540276000	-6.489715000
H	-1.174992000	-1.592431000	-7.011694000
H	-2.824766000	-2.233865000	-6.979305000
H	-2.525611000	-0.525106000	-6.634305000
C	-1.253248000	-1.284584000	6.957551000
H	-1.987879000	-0.756573000	7.579269000
H	-1.239561000	-2.326925000	7.289731000
H	-0.273628000	-0.845624000	7.165856000

(CH₃OPhTe)₂

1

E = -6.87601 Ha

Te	-1.497855000	0.363388000	0.709787000
Te	-0.664214000	-1.220769000	-1.371725000
C	-3.592290000	-0.052510000	0.809307000
C	-4.074406000	-1.159106000	1.525016000
C	-4.514557000	0.809108000	0.211307000
C	-5.437005000	-1.396210000	1.633115000
C	-5.889107000	0.583768000	0.316190000
C	-6.358446000	-0.525355000	1.030157000
H	-3.380750000	-1.844304000	2.003289000
H	-4.169763000	1.673426000	-0.348986000
H	-5.811009000	-2.252920000	2.186839000
H	-6.572090000	1.277187000	-0.160802000

C	-0.941444000	0.050445000	-3.067520000
C	0.066556000	0.939580000	-3.470567000
C	-2.108658000	-0.026203000	-3.830670000
C	-0.093044000	1.729676000	-4.599723000
C	-2.280922000	0.762606000	-4.970371000
C	-1.269585000	1.648553000	-5.361211000
H	0.985918000	1.018323000	-2.897868000
H	-2.904981000	-0.706473000	-3.542699000
H	0.686875000	2.418443000	-4.912322000
H	-3.201200000	0.673029000	-5.535961000
O	-7.672573000	-0.850046000	1.202703000
C	-8.667658000	-0.009482000	0.629507000
H	-8.620815000	1.008692000	1.036124000
H	-8.583981000	0.029712000	-0.464003000
H	-9.624182000	-0.460263000	0.900064000
O	-1.320924000	2.467643000	-6.451378000
C	-2.480034000	2.438965000	-7.276469000
H	-2.636451000	1.447802000	-7.720696000
H	-3.379138000	2.736774000	-6.722184000
H	-2.292547000	3.162934000	-8.071484000

RCox

E = -7.53330 Ha

Te	-1.396636000	0.184586000	0.803424000
Te	-0.655290000	-1.301104000	-1.393019000
O	-2.153217000	4.019978000	-1.487840000
O	-1.079294000	3.935442000	-0.503545000
H	-1.655083000	3.854623000	-2.305176000
H	-1.189633000	3.015828000	-0.193756000
C	-3.519838000	-0.041504000	0.844891000
C	-4.104667000	-1.139969000	1.493432000
C	-4.352243000	0.928399000	0.281042000
C	-5.483829000	-1.264102000	1.571109000
C	-5.741971000	0.814589000	0.356559000
C	-6.316660000	-0.286199000	1.003641000
H	-3.480591000	-1.906644000	1.943103000
H	-3.930332000	1.790044000	-0.226805000
H	-5.939119000	-2.113048000	2.073369000
H	-6.354307000	1.589477000	-0.089846000
C	-0.870770000	0.081357000	-3.007436000
C	0.164013000	0.967558000	-3.343823000
C	-2.028448000	0.078078000	-3.789329000
C	0.038070000	1.827997000	-4.425330000
C	-2.165275000	0.934718000	-4.883583000
C	-1.128540000	1.818667000	-5.207802000
H	1.077723000	0.989387000	-2.757377000
H	-2.845411000	-0.596834000	-3.551382000
H	0.840065000	2.512280000	-4.688333000
H	-3.078719000	0.899850000	-5.465831000
O	-7.655387000	-0.504755000	1.141550000
C	-8.565902000	0.448561000	0.603256000
H	-8.438163000	1.435323000	1.065521000
H	-8.460888000	0.538216000	-0.485280000
H	-9.561476000	0.067848000	0.837854000
O	-1.144489000	2.700823000	-6.247136000
C	-2.286570000	2.741890000	-7.097325000
H	-2.450623000	1.780327000	-7.599458000
H	-3.191477000	3.026317000	-6.545867000
H	-2.067197000	3.505483000	-7.845471000

TSox

E = -7.50885 Ha

nimag = -155.89 cm⁻¹

O	6.860850000	-2.492647000	1.678372000
O	7.927960000	-4.040508000	1.875016000
H	7.651526000	-2.024562000	1.986305000
H	7.229805000	-4.510263000	2.355537000
Te	5.716300000	-0.884376000	0.576281000
H	1.262801000	-3.070795000	-1.060239000
H	4.358973000	-2.687227000	2.791239000
H	2.350668000	-4.063449000	2.988571000
C	3.965914000	-2.073687000	0.761424000
C	3.683651000	-2.755330000	1.945192000
C	2.539003000	-3.545707000	2.055429000
C	1.660813000	-3.658499000	0.969928000
C	1.946017000	-2.972451000	-0.221696000
C	3.086021000	-2.189812000	-0.323691000
H	3.287090000	-1.671627000	-1.256572000
Te	4.386887000	1.548093000	1.238770000
C	5.797236000	2.848942000	0.321567000
C	5.756612000	3.105927000	-1.058742000
C	6.651311000	3.990569000	-1.641301000
C	7.613372000	4.648352000	-0.857235000
C	7.661289000	4.401120000	0.520431000
C	6.757801000	3.506152000	1.095943000
H	5.018633000	2.613515000	-1.684597000
H	6.620357000	4.190255000	-2.708663000
H	8.389884000	4.890694000	1.155966000
H	6.811666000	3.326342000	2.165548000
O	8.439054000	5.496188000	-1.531349000
C	9.442145000	6.201429000	-0.806112000
H	9.003001000	6.860785000	-0.047128000
H	10.152952000	5.515251000	-0.329208000
H	9.968118000	6.806121000	-1.546747000
O	0.517487000	-4.397945000	0.960477000
C	0.162632000	-5.132299000	2.128802000
H	0.924578000	-5.879605000	2.382376000
H	-0.002075000	-4.469661000	2.987499000
H	-0.771328000	-5.640116000	1.882466000

PCox

E = -7.60134 Ha

Te	2.727166000	0.896479000	14.464978000
Te	5.360861000	1.804878000	15.081746000
C	3.383090000	-0.933642000	13.545569000
C	3.334614000	-1.027808000	12.158381000
C	3.690901000	-2.215963000	11.518421000
C	4.093978000	-3.321957000	12.278549000
C	4.134986000	-3.223378000	13.680120000
C	3.780806000	-2.038491000	14.307989000
C	4.720509000	3.362364000	16.383334000
C	4.215094000	4.559810000	15.868398000
C	3.816808000	5.591824000	16.718912000
C	3.934748000	5.440080000	18.105976000
C	4.448197000	4.241244000	18.626623000
C	4.830261000	3.214526000	17.775352000
H	3.012126000	-0.171406000	11.571690000
H	3.646182000	-2.262694000	10.436595000
O	4.460526000	-4.530761000	11.769164000
H	4.447122000	-4.089074000	14.257116000
H	3.822844000	-1.986728000	15.393506000
H	4.107722000	4.702930000	14.798329000
H	3.416487000	6.498112000	16.280130000

O	3.584059000	6.378373000	19.030214000
H	5.216496000	2.292818000	18.200221000
O	2.173174000	1.820631000	12.979474000
O	2.058442000	4.779927000	12.747543000
H	2.066421000	3.806030000	12.799171000
H	1.973505000	4.959453000	11.804192000
C	3.045309000	7.617792000	18.578618000
C	4.443555000	-4.716743000	10.356519000
H	3.762320000	8.166296000	17.955266000
H	2.839761000	8.194038000	19.482388000
H	2.111778000	7.473229000	18.021099000
H	4.769198000	-5.745414000	10.193328000
H	5.137136000	-4.033374000	9.851213000
H	3.435135000	-4.586978000	9.944590000
H	4.534522000	4.131393000	19.703955000

(CIPhTe)₂

1

E = -5.14431 Ha

Te	4.251082000	0.532369000	2.324575000
Te	5.741092000	2.818709000	2.126422000
C	4.032611000	0.322079000	4.447674000
C	5.000834000	-0.352168000	5.200038000
C	4.837417000	-0.532365000	6.572518000
C	3.692597000	-0.036077000	7.196027000
C	2.714698000	0.634945000	6.462472000
C	2.889517000	0.810520000	5.090325000
C	4.224495000	4.335138000	2.140820000
C	3.953439000	5.043437000	3.316770000
C	3.000324000	6.061391000	3.331109000
C	2.311627000	6.369332000	2.158484000
C	2.570814000	5.676442000	0.975714000
C	3.529314000	4.664766000	0.972018000
H	5.893798000	-0.743309000	4.721689000
H	5.591264000	-1.055703000	7.152110000
Cl	3.480054000	-0.260628000	8.911528000
H	1.826691000	1.015713000	6.956985000
H	2.123706000	1.334596000	4.526297000
H	4.481705000	4.805873000	4.235406000
H	2.793320000	6.608018000	4.245673000
Cl	1.113821000	7.635804000	2.169282000
H	2.032191000	5.927155000	0.067354000
H	3.727830000	4.133027000	0.046289000

RCox

E = -5.79992 Ha

Te	-1.467010000	0.277211000	0.787509000
Te	-0.642199000	-1.211340000	-1.363334000
O	0.194926000	4.348267000	-0.806361000
O	-1.200883000	4.112873000	-0.443859000
H	0.472327000	4.901627000	-0.058392000
H	-1.165389000	3.166613000	-0.211847000
C	-3.580019000	-0.085137000	0.810248000
C	-4.097252000	-1.174573000	1.519979000
C	-4.460377000	0.785406000	0.158354000
C	-5.471562000	-1.399507000	1.574077000
C	-5.836993000	0.569926000	0.206856000
C	-6.334387000	-0.524309000	0.914230000
H	-3.432472000	-1.860559000	2.036454000
H	-4.083935000	1.639213000	-0.396774000

H	-5.868817000	-2.246197000	2.124816000
H	-6.516847000	1.246878000	-0.300571000
C	-0.964192000	0.128088000	-3.002595000
C	-0.037822000	1.133479000	-3.300434000
C	-2.084195000	-0.035583000	-3.825878000
C	-0.227180000	1.969831000	-4.398155000
C	-2.278260000	0.790448000	-4.932172000
C	-1.346731000	1.790399000	-5.210463000
H	0.837608000	1.280131000	-2.675618000
H	-2.816955000	-0.807829000	-3.611414000
H	0.488018000	2.755451000	-4.618844000
H	-3.147033000	0.660398000	-5.569583000
Cl	-1.583456000	2.828593000	-6.589440000
Cl	-8.053527000	-0.800859000	0.976409000

TSox

E = -5.77499 Ha

nimag = -152.61

Te	5.217124000	1.525450000	5.364568000
Te	7.886352000	1.805849000	4.378925000
Cl	3.656063000	7.849333000	4.004204000
Cl	9.193094000	-4.700988000	3.747884000
C	4.740155000	3.559598000	4.942640000
C	4.805804000	4.532195000	5.943682000
C	4.472451000	5.854294000	5.656067000
C	4.074681000	6.198846000	4.364183000
C	4.005065000	5.235251000	3.358042000
C	4.338237000	3.914758000	3.651956000
C	8.256375000	-0.286339000	4.193864000
C	7.806818000	-0.998533000	3.074503000
C	8.090123000	-2.355456000	2.934615000
C	8.833071000	-3.006438000	3.920085000
C	9.291338000	-2.313437000	5.040435000
C	9.000116000	-0.956828000	5.173269000
H	5.103715000	4.268433000	6.952417000
H	4.521293000	6.611273000	6.432150000
H	3.688051000	5.511094000	2.357651000
H	4.275768000	3.170507000	2.863810000
H	7.234581000	-0.498840000	2.299001000
H	7.739789000	-2.902432000	2.065157000
H	9.868787000	-2.827687000	5.802002000
H	9.360005000	-0.425197000	6.048839000
O	4.153432000	1.754984000	7.268507000
O	2.567154000	1.606298000	8.391061000
H	4.380133000	0.967376000	7.786643000
H	2.608330000	2.541353000	8.643565000

PCox

E = -5.86762 Ha

Te	-2.918551000	-0.725265000	0.736434000
Te	-1.433871000	-2.964621000	-0.213747000
O	-2.543271000	-4.420882000	-0.143766000
C	-1.685047000	-2.411214000	-2.287682000
C	-2.597633000	-3.140656000	-3.047335000
C	-0.913611000	-1.407945000	-2.877140000
C	-2.753474000	-2.859495000	-4.403787000
C	-1.062309000	-1.123227000	-4.233212000
C	-1.984846000	-1.851423000	-4.987061000
H	-3.182073000	-3.929853000	-2.581319000
H	-0.194582000	-0.833846000	-2.297579000
H	-3.463905000	-3.419488000	-5.003577000

H	-0.468695000	-0.344596000	-4.701167000
C	-2.332430000	-0.953200000	2.776514000
C	-2.908938000	-1.946423000	3.578066000
C	-1.397353000	-0.073152000	3.335511000
C	-2.547630000	-2.064284000	4.919264000
C	-1.042549000	-0.177608000	4.679160000
C	-1.619717000	-1.176653000	5.463257000
H	-3.632430000	-2.644867000	3.171301000
H	-0.937955000	0.701502000	2.729069000
H	-2.988282000	-2.842830000	5.533546000
H	-0.320663000	0.507859000	5.111446000
O	-4.058083000	-5.264828000	2.296914000
H	-3.580923000	-5.057889000	1.473712000
H	-4.715812000	-5.916747000	2.029116000
Cl	-2.174018000	-1.498364000	-6.681407000
Cl	-1.173213000	-1.316504000	7.141479000

(NH₂PhTe)₂

1

E = -6.12641 Ha

Te	-1.496030000	0.349194000	0.738202000
Te	-0.636168000	-1.186111000	-1.377923000
C	-3.583868000	-0.083742000	0.818937000
C	-4.065722000	-1.184859000	1.538821000
C	-4.512811000	0.758308000	0.193838000
C	-5.428859000	-1.440459000	1.629072000
C	-5.877909000	0.509589000	0.282314000
C	-6.362635000	-0.596558000	1.002002000
H	-3.371724000	-1.855400000	2.037356000
H	-4.171653000	1.621195000	-0.370888000
H	-5.775863000	-2.305848000	2.190467000
H	-6.577968000	1.177731000	-0.215734000
C	-0.938967000	0.103249000	-3.050011000
C	0.067810000	0.981462000	-3.471772000
C	-2.132691000	0.060594000	-3.782228000
C	-0.110867000	1.793794000	-4.585278000
C	-2.317816000	0.870936000	-4.896577000
C	-1.309502000	1.754898000	-5.319351000
H	1.004641000	1.038531000	-2.925038000
H	-2.932873000	-0.609356000	-3.481113000
H	0.689250000	2.463816000	-4.893992000
H	-3.253086000	0.815092000	-5.450351000
N	-7.722804000	-0.882438000	1.042031000
H	-8.340801000	-0.100773000	0.880712000
H	-8.027472000	-1.459893000	1.811905000
N	-1.467869000	2.522227000	-6.467959000
H	-0.886267000	3.344938000	-6.530017000
H	-2.420791000	2.703582000	-6.747188000

RCox

E = -6.78331 Ha

Te	-1.443568000	0.248047000	0.778396000
Te	-0.630266000	-1.250210000	-1.393157000
O	-0.207025000	4.510607000	-0.824538000
O	-1.533302000	4.034378000	-0.439736000
H	0.032324000	5.009150000	-0.026527000
H	-1.345906000	3.091044000	-0.270744000
C	-3.551026000	-0.074893000	0.829755000
C	-4.088817000	-1.147513000	1.553176000
C	-4.433015000	0.801165000	0.183465000

C	-5.462599000	-1.342226000	1.628168000
C	-5.808044000	0.611791000	0.255923000
C	-6.350255000	-0.464774000	0.980015000
H	-3.431654000	-1.843429000	2.066699000
H	-4.051336000	1.643391000	-0.385769000
H	-5.854087000	-2.185870000	2.193206000
H	-6.471213000	1.305055000	-0.257743000
C	-0.919229000	0.091981000	-3.019302000
C	0.077528000	1.006496000	-3.385202000
C	-2.101601000	0.057938000	-3.770740000
C	-0.102513000	1.865683000	-4.461010000
C	-2.285707000	0.913782000	-4.850053000
C	-1.290771000	1.839046000	-5.212542000
H	1.003773000	1.059350000	-2.820770000
H	-2.893288000	-0.638734000	-3.510905000
H	0.684430000	2.570644000	-4.720623000
H	-3.212191000	0.867026000	-5.419005000
N	-7.720771000	-0.689962000	1.004468000
H	-8.303848000	0.112885000	0.819782000
H	-8.063342000	-1.248103000	1.772428000
N	-1.451608000	2.664085000	-6.318594000
H	-0.890779000	3.503549000	-6.323221000
H	-2.404998000	2.838628000	-6.600735000

TSox

E = -6.76032 Ha

nimag = -158.26 cm⁻¹

O	6.713174000	-2.540959000	1.918222000
O	7.608370000	-4.083178000	2.635364000
H	7.402848000	-2.062626000	2.402325000
H	7.820196000	-4.433215000	1.756984000
Te	5.764610000	-0.920847000	0.652484000
H	1.213447000	-2.458433000	-1.368762000
H	4.459436000	-3.298076000	2.289119000
H	2.423479000	-4.655508000	2.138400000
C	3.993851000	-2.091164000	0.558072000
C	3.746846000	-3.099624000	1.496581000
C	2.594457000	-3.869968000	1.405314000
C	1.654929000	-3.654623000	0.381194000
C	1.916472000	-2.639873000	-0.558564000
C	3.070460000	-1.873167000	-0.471495000
H	3.241070000	-1.098527000	-1.213398000
Te	4.568335000	1.533407000	1.422847000
C	5.762039000	2.808262000	0.215905000
C	5.441263000	3.047438000	-1.128312000
C	6.201947000	3.914892000	-1.900727000
C	7.316538000	4.578532000	-1.354508000
C	7.635591000	4.338749000	-0.005594000
C	6.871728000	3.468985000	0.762456000
H	4.587148000	2.553010000	-1.581243000
H	5.927619000	4.087262000	-2.939445000
H	8.488854000	4.841550000	0.444879000
H	7.146691000	3.304471000	1.800081000
N	8.041943000	5.488286000	-2.107134000
H	7.981087000	5.392158000	-3.109583000
H	8.976956000	5.691497000	-1.787189000
N	0.533625000	-4.460938000	0.262264000
H	-0.240536000	-4.080280000	-0.260739000
H	0.243358000	-4.949320000	1.096041000

PCox

E = -6.85191 Ha

Te	-2.895613000	-0.686642000	0.747463000
Te	-1.438016000	-2.947483000	-0.229123000
O	-2.555999000	-4.399009000	-0.116902000
C	-1.695480000	-2.430161000	-2.295550000
C	-2.623887000	-3.148961000	-3.050243000
C	-0.921947000	-1.441019000	-2.909552000
C	-2.785900000	-2.875740000	-4.402559000
C	-1.081284000	-1.166579000	-4.262199000
C	-2.019181000	-1.878613000	-5.033943000
H	-3.217541000	-3.925394000	-2.574656000
H	-0.191410000	-0.867998000	-2.342843000
H	-3.511394000	-3.444235000	-4.980982000
H	-0.471447000	-0.396132000	-4.729200000
C	-2.338826000	-0.927581000	2.782718000
C	-2.985486000	-1.869704000	3.596015000
C	-1.339673000	-0.124286000	3.350159000
C	-2.638812000	-2.006496000	4.933724000
C	-0.998483000	-0.252820000	4.691197000
C	-1.641142000	-1.199538000	5.509343000
H	-3.753662000	-2.518010000	3.187714000
H	-0.819007000	0.610751000	2.743351000
H	-3.149347000	-2.751894000	5.539684000
H	-0.224923000	0.387459000	5.110430000
O	-3.916520000	-5.436837000	2.309933000
H	-3.461953000	-5.116891000	1.508498000
H	-4.569314000	-6.058941000	1.969049000
N	-2.139179000	-1.646052000	-6.395942000
H	-1.824937000	-0.745682000	-6.725508000
H	-3.004951000	-1.938858000	-6.823598000
N	-1.340566000	-1.295688000	6.861018000
H	-0.433653000	-0.952465000	7.140473000
H	-1.579625000	-2.169626000	7.305746000

(CNPhTe)₂

1

E = -6.17634 Ha

Te	-1.531490000	0.419279000	0.708585000
Te	-0.616520000	-1.173665000	-1.308041000
C	-3.623822000	-0.067476000	0.738920000
C	-4.070387000	-1.364582000	1.017571000
C	-4.558661000	0.954382000	0.533833000
C	-5.430642000	-1.642119000	1.079662000
C	-5.922656000	0.687907000	0.607924000
C	-6.369359000	-0.615315000	0.877555000
H	-3.359019000	-2.166533000	1.188176000
H	-4.229746000	1.964324000	0.307426000
H	-5.773799000	-2.649890000	1.293713000
H	-6.644553000	1.483089000	0.448046000
C	-0.988257000	0.070668000	-3.021166000
C	-0.031412000	1.004705000	-3.435773000
C	-2.168659000	-0.082447000	-3.758102000
C	-0.251189000	1.782889000	-4.567299000
C	-2.396369000	0.691385000	-4.891646000
C	-1.437890000	1.631633000	-5.303664000
H	0.890610000	1.130745000	-2.876713000
H	-2.918156000	-0.805226000	-3.450807000
H	0.492051000	2.507283000	-4.886507000
H	-3.313277000	0.572013000	-5.460902000
C	-1.667076000	2.429527000	-6.467212000
N	-1.852916000	3.080539000	-7.413845000

C	-7.768617000	-0.896829000	0.945657000
N	-8.908232000	-1.127180000	1.000255000

RCox

E = -6.83159 Ha

Te	-1.467313000	0.298874000	0.800994000
Te	-0.621343000	-1.192963000	-1.329078000
O	0.440125000	4.266829000	-0.738666000
O	-0.951330000	4.220165000	-0.294617000
H	0.823347000	4.816602000	-0.036104000
H	-1.020203000	3.282861000	-0.038954000
C	-3.583319000	-0.074531000	0.769372000
C	-4.104576000	-1.217847000	1.386538000
C	-4.451421000	0.845513000	0.169877000
C	-5.476083000	-1.446340000	1.399306000
C	-5.825329000	0.625570000	0.181014000
C	-6.347207000	-0.524431000	0.795082000
H	-3.443329000	-1.937187000	1.859669000
H	-4.063428000	1.737137000	-0.312714000
H	-5.878694000	-2.334174000	1.877451000
H	-6.497064000	1.339745000	-0.285504000
C	-1.025338000	0.107941000	-2.987999000
C	-0.303754000	1.291499000	-3.180578000
C	-1.993882000	-0.273977000	-3.924481000
C	-0.553226000	2.092399000	-4.289002000
C	-2.237338000	0.514155000	-5.044997000
C	-1.519893000	1.706391000	-5.233029000
H	0.453071000	1.601541000	-2.467904000
H	-2.567433000	-1.185163000	-3.783659000
H	0.000273000	3.015821000	-4.428617000
H	-2.987296000	0.215599000	-5.771201000
C	-1.772764000	2.522417000	-6.378909000
N	-1.979003000	3.185317000	-7.313009000
C	-7.757556000	-0.756547000	0.806562000
N	-8.905550000	-0.947255000	0.815721000

TSox

E = -6.80529 Ha

nimag = -186.86 cm⁻¹

O	6.873976000	-2.443882000	1.527852000
O	8.022598000	-4.057465000	1.468274000
H	7.772816000	-2.101713000	1.658281000
H	7.495675000	-4.515424000	2.141488000
Te	5.764110000	-0.910121000	0.491404000
H	1.222366000	-3.067719000	-0.910979000
H	4.544972000	-2.746868000	2.769557000
H	2.523345000	-4.134155000	3.055003000
C	4.017602000	-2.108648000	0.772218000
C	3.818103000	-2.805185000	1.967501000
C	2.682567000	-3.592202000	2.127883000
C	1.738043000	-3.688098000	1.093187000
C	1.946844000	-2.988749000	-0.106494000
C	3.083315000	-2.203183000	-0.263858000
H	3.233483000	-1.672690000	-1.198908000
Te	4.321068000	1.483403000	1.126834000
C	5.804170000	2.808036000	0.349672000
C	5.920188000	3.026470000	-1.030045000
C	6.860509000	3.923257000	-1.524405000
C	7.698658000	4.623013000	-0.640138000
C	7.580993000	4.408813000	0.742828000
C	6.641893000	3.506113000	1.230286000

H	5.272451000	2.501716000	-1.725041000
H	6.947158000	4.089683000	-2.593818000
H	8.227033000	4.948357000	1.428658000
H	6.564618000	3.348013000	2.301369000
C	0.569476000	-4.494474000	1.259588000
N	-0.383433000	-5.148155000	1.396043000
C	8.663423000	5.548458000	-1.144950000
N	9.449076000	6.302144000	-1.556148000

PCox

E = -6.89846 Ha

Te	-2.864940000	-0.732329000	0.713923000
Te	-1.408553000	-3.000259000	-0.211287000
O	-2.537629000	-4.439005000	-0.152385000
C	-1.672364000	-2.417679000	-2.283943000
C	-2.603355000	-3.132263000	-3.036128000
C	-0.895484000	-1.414420000	-2.867540000
C	-2.773286000	-2.832705000	-4.384289000
C	-1.059520000	-1.113659000	-4.215538000
C	-2.002750000	-1.820776000	-4.981081000
H	-3.187682000	-3.919980000	-2.567759000
H	-0.164188000	-0.857179000	-2.287585000
H	-3.498819000	-3.378860000	-4.979540000
H	-0.462884000	-0.334897000	-4.680471000
C	-2.317825000	-0.956866000	2.768491000
C	-2.882334000	-1.973434000	3.549957000
C	-1.428980000	-0.041760000	3.348611000
C	-2.550831000	-2.079559000	4.897068000
C	-1.108263000	-0.135904000	4.698361000
C	-1.665855000	-1.159484000	5.482445000
H	-3.573022000	-2.692230000	3.122986000
H	-0.983379000	0.747710000	2.751531000
H	-2.981343000	-2.874998000	5.497599000
H	-0.423110000	0.576146000	5.148249000
O	-4.077429000	-5.169494000	2.322880000
H	-3.612582000	-5.036405000	1.478746000
H	-4.722775000	-5.860150000	2.133477000
C	-1.331649000	-1.261944000	6.868412000
N	-1.056860000	-1.342520000	7.996442000
C	-2.173927000	-1.511088000	-6.366291000
N	-2.312827000	-1.257394000	-7.493385000

(NO₂PhTe)₂

1

E = -6.36503 Ha

Te	-3.839485000	-1.505898000	1.149516000
Te	-2.820084000	-3.448132000	-0.427810000
C	-1.873851000	-2.368323000	-2.026384000
C	-1.333120000	-3.148050000	-3.058118000
C	-1.774289000	-0.976626000	-2.084186000
C	-0.698990000	-2.543020000	-4.137493000
C	-1.142244000	-0.364439000	-3.161898000
C	-0.609866000	-1.152992000	-4.179529000
H	-1.399938000	-4.233120000	-3.036293000
H	-2.190503000	-0.358887000	-1.294686000
H	-0.277953000	-3.134981000	-4.941678000
H	-1.058760000	0.714737000	-3.219011000
C	-2.253637000	-1.097050000	2.539873000
C	-0.956465000	-1.600511000	2.420524000
C	-2.578648000	-0.258526000	3.615010000

C	0.010687000	-1.273519000	3.365650000
C	-1.616207000	0.075034000	4.561494000
C	-0.327423000	-0.437738000	4.427740000
H	-0.690216000	-2.254523000	1.596317000
H	-3.583059000	0.141098000	3.731855000
H	1.020857000	-1.658149000	3.285224000
H	-1.855559000	0.720814000	5.398189000
N	0.063180000	-0.502316000	-5.329099000
N	0.702166000	-0.088051000	5.435681000
O	1.830079000	-0.555777000	5.282975000
O	0.364453000	0.648220000	6.362308000
O	0.519344000	-1.232020000	-6.209034000
O	0.123518000	0.726791000	-5.332152000

RCox

E = -7.01873 Ha

Te	-1.453419000	0.266950000	0.791853000
Te	-0.649953000	-1.201343000	-1.366114000
O	0.213133000	4.377761000	-0.687945000
O	-1.129646000	4.265682000	-0.122344000
H	0.634854000	4.934062000	-0.013089000
H	-1.138783000	3.320886000	0.112991000
C	-3.574181000	-0.089942000	0.780758000
C	-4.096072000	-1.220907000	1.420142000
C	-4.440630000	0.829556000	0.177598000
C	-5.470674000	-1.438173000	1.453341000
C	-5.817551000	0.621128000	0.207278000
C	-6.314414000	-0.512240000	0.844969000
H	-3.435205000	-1.938980000	1.895459000
H	-4.051522000	1.711371000	-0.321498000
H	-5.889814000	-2.308632000	1.944336000
H	-6.500881000	1.323217000	-0.256002000
C	-1.024744000	0.120962000	-3.015087000
C	-0.442305000	1.390901000	-3.095389000
C	-1.824778000	-0.345138000	-4.066271000
C	-0.663796000	2.194719000	-4.209126000
C	-2.036338000	0.445717000	-5.192895000
C	-1.454936000	1.709336000	-5.248548000
H	0.186005000	1.767085000	-2.295589000
H	-2.294722000	-1.322667000	-4.012537000
H	-0.225081000	3.183174000	-4.278147000
H	-2.652138000	0.098119000	-6.014082000
N	-7.786592000	-0.739652000	0.880034000
O	-8.190037000	-1.748704000	1.454494000
O	-8.502205000	0.095872000	0.332352000
N	-1.684030000	2.560508000	-6.447008000
O	-2.403669000	2.107466000	-7.335769000
O	-1.138457000	3.661769000	-6.473748000

TSox

E = -6.99263 Ha

nimag = -202.77 cm⁻¹

O	6.868316000	-2.559188000	1.322037000
O	7.971294000	-4.193610000	1.063921000
H	7.788557000	-2.264382000	1.416450000
H	7.489187000	-4.687014000	1.745791000
Te	5.763866000	-0.926511000	0.459884000
H	1.059998000	-2.799097000	-0.852050000
H	4.619138000	-2.954729000	2.612444000
H	2.553737000	-4.309246000	2.874944000
C	3.993003000	-2.093474000	0.730004000

C	3.843455000	-2.906645000	1.857062000
C	2.691083000	-3.673686000	2.008013000
C	1.704941000	-3.616557000	1.027513000
C	1.842042000	-2.814880000	-0.102265000
C	2.995160000	-2.049521000	-0.249045000
H	3.106801000	-1.427354000	-1.131348000
Te	4.436796000	1.460645000	1.325584000
C	5.840833000	2.802544000	0.439789000
C	5.901927000	2.971798000	-0.950810000
C	6.791936000	3.882871000	-1.510945000
C	7.613113000	4.630906000	-0.670332000
C	7.565721000	4.484893000	0.713416000
C	6.679396000	3.564420000	1.265779000
H	5.250463000	2.400019000	-1.603672000
H	6.848983000	4.023091000	-2.584052000
H	8.217872000	5.080804000	1.341151000
H	6.646760000	3.442095000	2.343725000
N	0.470006000	-4.435646000	1.190246000
O	0.378822000	-5.125594000	2.202618000
O	-0.375982000	-4.365006000	0.301926000
N	8.562069000	5.611181000	-1.265593000
O	9.268300000	6.256315000	-0.493540000
O	8.577645000	5.711906000	-2.490670000

PCox

E = -7.08556 Ha

Te	-2.833717000	-0.752991000	0.741526000
Te	-1.420284000	-3.020707000	-0.249657000
O	-2.563292000	-4.447994000	-0.202426000

C	-1.720006000	-2.381772000	-2.302505000
C	-2.679181000	-3.061495000	-3.051729000
C	-0.938375000	-1.376008000	-2.876001000
C	-2.874169000	-2.722969000	-4.389143000
C	-1.126384000	-1.035684000	-4.212939000
C	-2.095297000	-1.713820000	-4.949632000
H	-3.266698000	-3.851902000	-2.592361000
H	-0.185354000	-0.846512000	-2.298081000
H	-3.616530000	-3.230380000	-4.994189000
H	-0.536548000	-0.258436000	-4.684269000
C	-2.249002000	-1.000337000	2.783573000
C	-2.788986000	-2.032284000	3.562603000
C	-1.364070000	-0.077557000	3.358445000
C	-2.437542000	-2.145529000	4.905776000
C	-1.021769000	-0.178978000	4.703670000
C	-1.562644000	-1.215324000	5.460533000
H	-3.477568000	-2.755445000	3.139754000
H	-0.937690000	0.723013000	2.762296000
H	-2.841621000	-2.943452000	5.517691000
H	-0.341953000	0.528138000	5.164225000
O	-4.065479000	-5.177745000	2.299179000
H	-3.622504000	-5.053492000	1.442346000
H	-4.728879000	-5.856381000	2.129850000
N	-2.300617000	-1.348775000	-6.381078000
N	-1.194535000	-1.328704000	6.899308000
O	-1.703886000	-2.241665000	7.544873000
O	-0.404103000	-0.500580000	7.348796000
O	-3.159421000	-1.967069000	-7.004721000
O	-1.597565000	-0.452635000	-6.842406000

Table S6 Geometries of the stationary points and transition states for the isomerization of the selenoxides and telluroxides. Level of theory ZORA-OLYP/TZ2P

(HSe)₂

2

E = -0.66076 Ha

O	6.458149000	-1.435216000	1.610933000
Se	5.581201000	-0.812504000	0.367952000
Se	4.435381000	1.269947000	1.011516000
H	4.203535000	-1.453271000	0.508610000
H	5.590452000	2.060197000	0.548443000

TSiso

E = -0.58830 Ha

nimag = -351.64 cm⁻¹

Se	-1.524100000	-0.727800000	1.051700000
Se	-0.624300000	-0.236100000	-1.266000000
H	-1.316200000	-1.510000000	-1.717400000
H	-2.884800000	-0.151500000	0.828800000
O	-0.500400000	0.718800000	0.598500000

3

E = -0.64555 Ha

Se	0.016185000	1.596437000	-0.179880000
Se	-0.016185000	-1.596437000	-0.179880000
O	0.000000000	0.000000000	-1.105657000
H	-1.449973000	1.686156000	0.028662000
H	1.449973000	-1.686156000	0.028662000

(CH₃Se)₂

2

E = -1.84325 Ha

Se	-2.130297000	-0.491947000	1.087751000
Se	-0.432242000	-0.950405000	-0.631562000
H	-1.276730000	-1.570339000	-2.910722000
C	-1.827855000	-1.291844000	-2.010892000
H	-2.448709000	-2.119248000	-1.668000000
H	-2.408809000	-0.381912000	-2.170539000
C	-0.849858000	-0.078763000	2.524574000
H	-0.221537000	-0.946832000	2.723662000
H	-0.250660000	0.795860000	2.269365000
H	-1.461128000	0.140799000	3.402569000
O	0.248402000	-2.429792000	-0.372938000

TSiso

E = -1.77250 Ha

nimag = -299.52 cm⁻¹

Se	-1.572322000	-0.706937000	1.053297000
Se	-0.608197000	-0.257550000	-1.286293000
O	-0.530238000	0.703538000	0.552584000
C	-3.339673000	0.140505000	1.076758000
H	-3.545257000	0.580006000	0.101435000
H	-4.067411000	-0.640178000	1.316863000

H	-3.333013000	0.903090000	1.858849000
C	-1.325174000	-1.985910000	-2.025519000
H	-0.990588000	-1.921416000	-3.071269000
H	-0.867891000	-2.853913000	-1.550267000
H	-2.414033000	-2.031614000	-1.987431000

3

E = -1.82849 Ha

Se	-1.982904000	-0.518461000	1.145853000
Se	-0.136643000	-1.634137000	-1.208105000
H	1.454954000	-0.041179000	-2.247719000
C	0.478143000	0.128728000	-1.783239000
H	-0.212759000	0.546166000	-2.516865000
H	0.594585000	0.787856000	-0.921386000
C	-2.040543000	-2.209885000	2.121733000
H	-2.217017000	-1.936779000	3.167203000
H	-2.863514000	-2.825566000	1.756363000
H	-1.083821000	-2.727859000	2.037067000
O	-1.808738000	-1.173110000	-0.572722000

(PhSe)₂

2

E = -5.51356 Ha

Se	-2.666148000	-0.729703000	0.630441000
Se	-1.634217000	-2.871745000	-0.110275000
O	-2.711436000	-4.100714000	0.102148000
C	-1.813250000	-2.391121000	-2.022253000
C	-2.821055000	-3.000456000	-2.762931000
C	-0.890252000	-1.530414000	-2.616328000
C	-2.916038000	-2.726668000	-4.127873000
C	-0.992548000	-1.266788000	-3.982302000
C	-2.005509000	-1.861890000	-4.736294000
H	-3.510694000	-3.681891000	-2.272525000
H	-0.102169000	-1.063064000	-2.030896000
H	-3.702387000	-3.193297000	-4.716271000
H	-0.280034000	-0.596119000	-4.456124000
H	-2.081988000	-1.653572000	-5.800442000
C	-2.300512000	-0.910490000	2.514361000
C	-3.130347000	-1.700274000	3.320891000
C	-1.232891000	-0.209063000	3.089838000
C	-2.886310000	-1.788459000	4.690818000
C	-1.002771000	-0.294866000	4.462543000
C	-1.826487000	-1.085282000	5.264433000
H	-3.958605000	-2.243474000	2.877313000
H	-0.588734000	0.403595000	2.466291000
H	-3.530677000	-2.406902000	5.310886000
H	-0.175572000	0.255828000	4.903928000
H	-1.643361000	-1.152583000	6.333863000

TSiso

E = -5.44626 Ha

nimag = -289.91 cm⁻¹

Se	-1.838265000	-0.756328000	0.932025000
Se	-0.554306000	-0.353407000	-1.324727000
O	-0.671929000	0.581099000	0.564234000
C	-3.526135000	0.163113000	0.950300000
C	-4.663783000	-0.556949000	1.339387000
C	-3.619240000	1.515860000	0.613208000
C	-5.899181000	0.084337000	1.381279000

C	-4.860230000	2.147679000	0.674117000
C	-6.001274000	1.437787000	1.051543000
H	-4.591762000	-1.607634000	1.612475000
H	-2.728175000	2.057502000	0.313027000
H	-6.783071000	-0.473929000	1.680019000
H	-4.935009000	3.202150000	0.418936000
H	-6.966245000	1.936220000	1.090843000
C	-1.311808000	-1.957234000	-2.159492000
C	-2.521413000	-1.887007000	-2.866552000
C	-0.586820000	-3.157777000	-2.146308000
C	-2.986505000	-2.997956000	-3.567684000
C	-1.056130000	-4.266853000	-2.849219000
C	-2.256200000	-4.188710000	-3.558129000
H	-3.089128000	-0.960761000	-2.873042000
H	0.347448000	-3.216591000	-1.594449000
H	-3.918659000	-2.934855000	-4.124530000
H	-0.484758000	-5.192276000	-2.843963000
H	-2.622926000	-5.055212000	-4.102986000

3

E = -5.49865 Ha

Se	-1.185930000	-0.902809000	-1.218254000
Se	1.298742000	1.098538000	-1.611080000
C	-0.147315000	-2.496367000	-0.937412000
C	-0.124180000	-3.057447000	0.345574000
C	0.551012000	-4.258119000	0.567587000
C	1.236692000	-4.880486000	-0.474702000
C	1.231602000	-4.306363000	-1.748279000
C	0.528752000	-3.128383000	-1.988671000
C	0.339477000	2.705165000	-1.170691000
C	0.329756000	3.153582000	0.156464000
C	-0.311408000	4.349223000	0.483054000
C	-0.968640000	5.082979000	-0.503606000
C	-0.973753000	4.627576000	-1.824457000
C	-0.310509000	3.451147000	-2.163756000
H	-0.623103000	-2.555205000	1.170061000
H	0.558561000	-4.693118000	1.564153000
H	1.776470000	-5.806952000	-0.296444000
H	1.764778000	-4.787980000	-2.564626000
H	0.507686000	-2.698208000	-2.985231000
H	0.816875000	2.566590000	0.929576000
H	-0.310301000	4.696781000	1.513356000
H	-1.477582000	6.008370000	-0.245684000
H	-1.483549000	5.199648000	-2.595983000
H	-0.296146000	3.108963000	-3.194166000
O	-0.072841000	0.061961000	-2.330609000

(CH₃PhSe)₂

2

E = -6.68982 Ha

Se	-2.677315000	-0.739435000	0.634919000
Se	-1.631707000	-2.875618000	-0.115242000
O	-2.700938000	-4.113136000	0.093825000
C	-1.809401000	-2.394281000	-2.022202000
C	-2.805784000	-3.006677000	-2.773857000
C	-0.895004000	-1.527184000	-2.619522000
C	-2.895718000	-2.730403000	-4.137391000
C	-0.996748000	-1.264423000	-3.983625000
C	-1.999609000	-1.855785000	-4.765710000
H	-3.493389000	-3.697631000	-2.293901000

H	-0.108339000	-1.053492000	-2.037050000
H	-3.677305000	-3.210317000	-4.722433000
H	-0.281174000	-0.588261000	-4.446438000
C	-2.305627000	-0.909403000	2.515606000
C	-3.152839000	-1.658702000	3.342061000
C	-1.217031000	-0.238850000	3.085427000
C	-2.905987000	-1.733892000	4.710029000
C	-0.986348000	-0.316623000	4.457497000
C	-1.821476000	-1.066039000	5.295585000
H	-4.002903000	-2.181213000	2.914772000
H	-0.554334000	0.350188000	2.458285000
H	-3.575915000	-2.321935000	5.333829000
H	-0.138950000	0.218271000	4.880986000
C	-2.120068000	-1.539584000	-6.234302000
H	-1.138258000	-1.409287000	-6.699369000
H	-2.651623000	-2.328297000	-6.773337000
H	-2.676921000	-0.605954000	-6.386216000
C	-1.552107000	-1.173484000	6.774274000
H	-2.481853000	-1.185161000	7.351320000
H	-1.016746000	-2.103332000	7.005951000
H	-0.937539000	-0.343678000	7.133569000

TSiso

E = -6.62261 Ha

nimag = -289.40 cm⁻¹

Se	-1.877976000	-0.769080000	0.919150000
Se	-0.560294000	-0.363846000	-1.329879000
O	-0.693120000	0.556825000	0.573507000
C	-3.546539000	0.178572000	0.964206000
C	-4.693399000	-0.509713000	1.381590000
C	-3.631556000	1.527070000	0.612566000
C	-5.913781000	0.154728000	1.437860000
C	-4.860352000	2.178486000	0.690252000
C	-6.023210000	1.511975000	1.098726000
H	-4.641247000	-1.558904000	1.665233000
H	-2.741554000	2.054813000	0.285476000
H	-6.797220000	-0.393024000	1.759154000
H	-4.913640000	3.230601000	0.418095000
C	-1.285124000	-1.969422000	-2.173997000
C	-2.502134000	-1.932255000	-2.871451000
C	-0.540304000	-3.156967000	-2.177379000
C	-2.944026000	-3.048312000	-3.573797000
C	-0.990703000	-4.269650000	-2.884334000
C	-2.198442000	-4.237978000	-3.594751000
H	-3.098027000	-1.023681000	-2.867444000
H	0.397997000	-3.205636000	-1.631146000
H	-3.885371000	-2.995828000	-4.117510000
C	-7.343105000	2.231703000	1.200319000
H	-8.176792000	1.587295000	0.904347000
H	-7.534921000	2.554586000	2.232006000
H	-7.363111000	3.125231000	0.570384000
H	-0.393288000	-5.179104000	-2.881071000
C	-2.673500000	-5.432965000	-4.378645000
H	-2.414180000	-5.327835000	-5.440265000
H	-2.215443000	-6.358756000	-4.020530000
H	-3.760840000	-5.543477000	-4.323120000

3

E = -6.67492 Ha

Se	5.062710000	1.369142000	4.789228000
Se	8.222573000	1.879041000	5.162284000

C	4.595813000	3.194356000	4.417241000
C	4.570592000	3.644454000	3.093073000
C	4.171597000	4.949631000	2.803076000
C	3.819849000	5.844001000	3.819309000
C	3.866978000	5.383120000	5.145401000
C	4.233638000	4.076744000	5.445182000
C	8.748654000	0.080693000	4.741129000
C	9.102538000	-0.244287000	3.427501000
C	9.542906000	-1.531398000	3.117617000
C	9.609247000	-2.530812000	4.093941000
C	9.235279000	-2.193664000	5.405160000
C	8.825601000	-0.906957000	5.733302000
H	4.866093000	2.977582000	2.288206000
H	4.151264000	5.278347000	1.766348000
H	3.596468000	6.055675000	5.957066000
H	4.242267000	3.738198000	6.477037000
H	9.030481000	0.505626000	2.644906000
H	9.821624000	-1.762067000	2.091745000
H	9.281158000	-2.949093000	6.187152000
H	8.561870000	-0.666020000	6.758847000
O	6.540107000	1.593386000	5.893897000
C	3.402300000	7.258872000	3.512235000
H	3.424068000	7.461822000	2.438721000
H	2.385662000	7.457263000	3.871653000
H	4.062231000	7.981950000	4.005621000
C	10.053836000	-3.930557000	3.757108000
H	10.847758000	-4.268747000	4.432260000
H	9.224269000	-4.641200000	3.857639000
H	10.428804000	-3.999223000	2.732926000

(CH₃OPhSe)₂

2

E = -7.12734 Ha

Se	-2.710061000	-0.839657000	0.647433000
Se	-1.558569000	-2.914896000	-0.146237000
O	-2.571492000	-4.204656000	0.037501000
C	-1.735522000	-2.427381000	-2.043127000
C	-2.676856000	-3.091135000	-2.818957000
C	-0.870304000	-1.494020000	-2.622718000
C	-2.776101000	-2.820118000	-4.184152000
C	-0.961338000	-1.221566000	-3.979217000
C	-1.917442000	-1.880968000	-4.771325000
H	-3.328503000	-3.826946000	-2.355502000
H	-0.127388000	-0.972227000	-2.024350000
H	-3.518910000	-3.347450000	-4.771082000
H	-0.300350000	-0.499076000	-4.448991000
C	-2.288409000	-0.983679000	2.514009000
C	-3.099562000	-1.734553000	3.370623000
C	-1.188603000	-0.297491000	3.055061000
C	-2.829267000	-1.806592000	4.736916000
C	-0.914466000	-0.358968000	4.412698000
C	-1.732408000	-1.115351000	5.267888000
H	-3.952471000	-2.274003000	2.970683000
H	-0.547466000	0.292806000	2.407239000
H	-3.479448000	-2.400903000	5.368072000
H	-0.067049000	0.173931000	4.834455000
O	-1.372608000	-1.106203000	6.582569000
C	-2.151400000	-1.851295000	7.513568000
H	-3.186540000	-1.489932000	7.554807000
H	-2.146584000	-2.922830000	7.278206000
H	-1.677176000	-1.694232000	8.483907000

O	-1.918354000	-1.536168000	-6.089548000
C	-2.857364000	-2.157201000	-6.962326000
H	-2.708305000	-3.243125000	-7.009001000
H	-3.890554000	-1.941452000	-6.663178000
H	-2.670638000	-1.726063000	-7.947318000

TSiso

E = -7.06081 Ha
 nimag = -289.16 cm⁻¹

Se	-1.981131000	-0.783259000	0.870920000
Se	-0.597141000	-0.391834000	-1.372347000
O	-0.758125000	0.511624000	0.557968000
C	-3.604108000	0.228814000	0.970130000
C	-4.771585000	-0.405156000	1.426376000
C	-3.644357000	1.577985000	0.618878000
C	-5.957336000	0.303869000	1.520673000
C	-4.832598000	2.299904000	0.728838000
C	-5.999472000	1.666253000	1.175295000
H	-4.757785000	-1.453827000	1.715842000
H	-2.741045000	2.065505000	0.266567000
H	-6.866274000	-0.175829000	1.872132000
H	-4.832137000	3.349210000	0.457461000
C	-1.236590000	-2.021812000	-2.207000000
C	-2.475752000	-2.071651000	-2.874134000
C	-0.422237000	-3.162312000	-2.228454000
C	-2.865842000	-3.206115000	-3.563133000
C	-0.800494000	-4.311651000	-2.920407000
C	-2.030164000	-4.339026000	-3.593694000
H	-3.129724000	-1.204229000	-2.856609000
H	0.530060000	-3.148699000	-1.704937000
H	-3.813063000	-3.243239000	-4.094159000
H	-0.136582000	-5.168381000	-2.926259000
O	-7.217130000	2.266507000	1.313520000
C	-7.339414000	3.648912000	0.996572000
H	-6.694775000	4.268192000	1.632916000
H	-7.107828000	3.844156000	-0.058108000
H	-8.383616000	3.902494000	1.187829000
O	-2.511828000	-5.397288000	-4.299372000
C	-1.733306000	-6.588814000	-4.378315000
H	-0.766649000	-6.406497000	-4.863400000
H	-1.569882000	-7.029195000	-3.387207000
H	-2.317868000	-7.279748000	-4.987914000

3

E = -7.11296 Ha

Se	2.785031000	1.340311000	14.012210000
Se	5.528868000	1.919822000	15.622480000
C	3.282254000	-0.353491000	13.269005000
C	3.638956000	-0.467704000	11.920666000
C	3.980022000	-1.700217000	11.368075000
C	3.952256000	-2.851834000	12.168379000
C	3.588611000	-2.747057000	13.520643000
C	3.266065000	-1.512391000	14.063079000
C	4.791692000	3.187916000	16.854986000
C	5.019441000	4.559461000	16.695723000
C	4.493497000	5.485714000	17.593721000
C	3.735217000	5.040603000	18.686589000
C	3.510116000	3.665375000	18.859121000
C	4.025383000	2.754151000	17.949737000
H	3.652559000	0.417554000	11.291610000
H	4.253881000	-1.749833000	10.320711000

O	4.254113000	-4.108908000	11.739050000
H	3.573512000	-3.646459000	14.129581000
H	2.997996000	-1.442139000	15.112884000
H	5.613139000	4.911949000	15.857373000
H	4.687066000	6.540297000	17.436060000
O	3.178004000	5.848019000	19.631813000
H	3.832488000	1.694378000	18.085902000
O	4.438371000	2.186646000	14.137166000
C	3.348384000	7.257941000	19.522185000
C	4.639047000	-4.299799000	10.380987000
H	2.914360000	7.646032000	18.592407000
H	4.406262000	7.542839000	19.579954000
H	2.814745000	7.684125000	20.373463000
H	4.832574000	-5.369022000	10.279314000
H	5.552147000	-3.742473000	10.137866000
H	3.837860000	-4.010497000	9.689606000
H	2.919583000	3.334467000	19.708677000

(ClPhSe)₂

2

E = -5.39405 Ha

Se	-2.635894000	-0.699619000	0.632703000
Se	-1.613946000	-2.850681000	-0.112858000
O	-2.696191000	-4.071570000	0.114951000
C	-1.809597000	-2.383819000	-2.023342000
C	-2.817932000	-3.004595000	-2.753688000
C	-0.900743000	-1.524131000	-2.639710000
C	-2.933826000	-2.752410000	-4.119217000
C	-1.010165000	-1.270422000	-4.005285000
C	-2.029384000	-1.885883000	-4.735189000
H	-3.501986000	-3.686478000	-2.255887000
H	-0.107663000	-1.042575000	-2.072984000
H	-3.717250000	-3.226402000	-4.701834000
H	-0.312177000	-0.602540000	-4.499415000
C	-2.292419000	-0.901145000	2.515004000
C	-3.128820000	-1.698614000	3.306952000
C	-1.232073000	-0.210905000	3.116191000
C	-2.907121000	-1.810448000	4.677231000
C	-1.010640000	-0.308803000	4.487821000
C	-1.849853000	-1.111608000	5.261154000
H	-3.954414000	-2.238159000	2.854152000
H	-0.576284000	0.410583000	2.514049000
H	-3.553161000	-2.432756000	5.287965000
H	-0.191669000	0.230856000	4.952274000
Cl	-2.168289000	-1.571403000	-6.442053000
Cl	-1.574717000	-1.241292000	6.976124000

TSiso

E = -5.32751 Ha
 nimag = -288.36 Ha

Se	-1.859131000	-0.770023000	0.922752000
Se	-0.562831000	-0.350904000	-1.334951000
O	-0.694642000	0.569162000	0.566010000
C	-3.539016000	0.157555000	0.953487000
C	-4.684465000	-0.547414000	1.346548000
C	-3.627094000	1.511393000	0.619178000
C	-5.916084000	0.096889000	1.396631000
C	-4.856376000	2.161677000	0.683234000
C	-5.995853000	1.451903000	1.065713000
H	-4.628110000	-1.598729000	1.620269000

H	-2.735688000	2.050979000	0.316073000
H	-6.806982000	-0.444553000	1.697794000
H	-4.931195000	3.214812000	0.431424000
C	-1.301639000	-1.953203000	-2.176466000
C	-2.510528000	-1.897646000	-2.886501000
C	-0.577801000	-3.154579000	-2.158227000
C	-2.978857000	-3.008137000	-3.582002000
C	-1.035590000	-4.273134000	-2.849477000
C	-2.237432000	-4.192508000	-3.556268000
H	-3.086069000	-0.976431000	-2.903954000
H	0.356976000	-3.214035000	-1.607458000
H	-3.907518000	-2.959921000	-4.141925000
H	-0.468600000	-5.198701000	-2.843050000
Cl	-7.535563000	2.263257000	1.133523000
Cl	-2.821836000	-5.587630000	-4.416517000

3

E = -5.37980 Ha

Se	-1.176921000	-0.898749000	-1.196941000
Se	1.314815000	1.105108000	-1.571662000
C	-0.150949000	-2.500526000	-0.934494000
C	0.001417000	-3.005293000	0.362491000
C	0.672166000	-4.207713000	0.580088000
C	1.225503000	-4.886745000	-0.504417000
C	1.101323000	-4.384025000	-1.802244000
C	0.398801000	-3.202664000	-2.015055000
C	0.350007000	2.712231000	-1.156180000
C	0.265663000	3.147235000	0.172467000
C	-0.387956000	4.337001000	0.488714000
C	-0.984226000	5.079109000	-0.530273000
C	-0.921994000	4.652693000	-1.859481000
C	-0.243670000	3.478560000	-2.168704000
H	-0.398285000	-2.458866000	1.212070000
H	0.782875000	-4.601588000	1.585217000
H	1.534889000	-4.923597000	-2.638193000
H	0.282211000	-2.825415000	-3.026438000
H	0.708180000	2.554451000	0.967477000
H	-0.447952000	4.676112000	1.517845000
H	-1.387100000	5.243072000	-2.642355000
H	-0.177790000	3.156176000	-3.203420000
O	-0.050221000	0.067175000	-2.300350000
Cl	-1.818737000	6.557813000	-0.143337000
Cl	2.085671000	-6.378377000	-0.238878000

(NH₂PhSe)₂

2

E = -6.37798 Ha

Se	-2.802661000	-0.846111000	0.680397000
Se	-1.547876000	-2.843232000	-0.178198000
O	-2.484784000	-4.191968000	-0.005434000
C	-1.756722000	-2.351121000	-2.065754000
C	-2.649417000	-3.072076000	-2.855979000
C	-0.961678000	-1.355192000	-2.636410000
C	-2.757657000	-2.791016000	-4.211860000
C	-1.067370000	-1.074491000	-3.992637000
C	-1.970255000	-1.786631000	-4.805304000
H	-3.250796000	-3.855294000	-2.402540000
H	-0.259809000	-0.786060000	-2.031389000

H	-3.454834000	-3.360053000	-4.823482000
H	-0.442636000	-0.299174000	-4.430867000
C	-2.314428000	-0.996454000	2.526748000
C	-3.039386000	-1.826027000	3.395138000
C	-1.245748000	-0.253997000	3.049885000
C	-2.706132000	-1.912337000	4.740020000
C	-0.912927000	-0.333140000	4.395900000
C	-1.636092000	-1.166997000	5.268100000
H	-3.867484000	-2.414158000	3.011938000
H	-0.669435000	0.394959000	2.396955000
H	-3.284011000	-2.562789000	5.393283000
H	-0.084435000	0.259176000	4.778923000
N	-2.034226000	-1.547739000	-6.171097000
H	-1.714083000	-0.641963000	-6.479909000
H	-2.883212000	-1.838280000	-6.632872000
N	-1.341575000	-1.206364000	6.624416000
H	-0.406703000	-0.927875000	6.883229000
H	-1.652791000	-2.027953000	7.121164000

TSiso

E = -6.31239 Ha

nimag = -295.73 cm⁻¹

Se	-1.854532000	-0.741352000	0.959511000
Se	-0.561361000	-0.374718000	-1.348135000
O	-0.692387000	0.586654000	0.574288000
C	-3.544828000	0.172629000	0.981848000
C	-4.678196000	-0.547531000	1.386066000
C	-3.626993000	1.515843000	0.627563000
C	-5.902887000	0.114396000	1.419470000
C	-4.863369000	2.179703000	0.675575000
C	-6.005027000	1.459455000	1.072093000
H	-4.610430000	-1.593014000	1.674980000
H	-2.726810000	2.037875000	0.315948000
H	-6.795494000	-0.424254000	1.729536000
H	-6.972552000	1.955129000	1.103915000
C	-1.289254000	-1.950067000	-2.188215000
C	-2.502364000	-1.899531000	-2.900762000
C	-0.586528000	-3.169182000	-2.163431000
C	-2.973129000	-3.002357000	-3.593108000
C	-1.049112000	-4.278557000	-2.852465000
C	-2.254269000	-4.216539000	-3.582449000
H	-3.074752000	-0.976149000	-2.914787000
H	0.342160000	-3.237844000	-1.603150000
H	-3.902183000	-2.933241000	-4.155607000
H	-0.477300000	-5.204337000	-2.836522000
N	-2.695032000	-5.301573000	-4.309489000
H	-3.663792000	-5.315335000	-4.587713000
H	-2.319474000	-6.206629000	-4.073037000
N	-4.965457000	3.509546000	0.271414000
H	-4.106698000	4.039202000	0.315689000
H	-5.745055000	4.020723000	0.659456000

3

E = -6.36416 Ha

Se	5.049011000	1.380386000	4.781993000
Se	8.230350000	1.866230000	5.154553000
C	4.575713000	3.195497000	4.415442000
C	4.852477000	3.766673000	3.163966000
C	4.479056000	5.072740000	2.876268000
C	3.824685000	5.860728000	3.840854000
C	3.554034000	5.289342000	5.099752000

C	3.918665000	3.980315000	5.376422000
C	8.764755000	0.079902000	4.733354000
C	8.791559000	-0.360438000	3.401452000
C	9.204490000	-1.647340000	3.082444000
C	9.590817000	-2.547466000	4.092111000
C	9.557981000	-2.106642000	5.429707000
C	9.158381000	-0.815617000	5.740394000
H	5.364341000	3.179271000	2.407558000
H	4.704651000	5.494570000	1.898900000
H	3.050534000	5.880714000	5.861946000
H	3.692120000	3.556888000	6.350668000
H	8.483299000	0.313067000	2.607353000
H	9.224152000	-1.964154000	2.041611000
H	9.860141000	-2.783327000	6.226531000
H	9.146049000	-0.495145000	6.778121000
O	6.537820000	1.589301000	5.884277000
N	3.505128000	7.183785000	3.579838000
H	2.788400000	7.595577000	4.158220000
H	3.426583000	7.444239000	2.608356000
N	10.050190000	-3.816819000	3.775784000
H	9.769995000	-4.182940000	2.878238000
H	10.004914000	-4.505313000	4.512004000

(CNPhSe)₂

2

E = -6.42503 Ha

Se	-2.728418000	-0.842160000	0.646169000
Se	-1.483160000	-2.846036000	-0.158373000
O	-2.424266000	-4.182976000	0.024437000
C	-1.734679000	-2.338305000	-2.057638000
C	-2.664099000	-3.052837000	-2.807346000
C	-0.925779000	-1.361233000	-2.638654000
C	-2.803966000	-2.774269000	-4.162909000
C	-1.060384000	-1.083270000	-3.994253000
C	-2.003393000	-1.787576000	-4.763333000
H	-3.263273000	-3.823305000	-2.330125000
H	-0.195591000	-0.811977000	-2.050046000
H	-3.527462000	-3.318481000	-4.762175000
H	-0.440492000	-0.325382000	-4.462993000
C	-2.272339000	-1.016435000	2.509292000
C	-2.860671000	-2.014866000	3.297928000
C	-1.385077000	-0.101761000	3.092923000
C	-2.557728000	-2.104377000	4.651299000
C	-1.092277000	-0.177116000	4.449459000
C	-1.674242000	-1.183048000	5.238991000
H	-3.553986000	-2.721784000	2.854307000
H	-0.924218000	0.671644000	2.486489000
H	-3.008858000	-2.881532000	5.260490000
H	-0.409245000	0.535328000	4.901714000
C	-1.369641000	-1.266897000	6.632582000
N	-1.119921000	-1.333924000	7.767356000
C	-2.142022000	-1.502246000	-6.157280000
N	-2.253845000	-1.268434000	-7.291674000

TSiso

E = -6.35919 Ha

nimag = -288.40 cm⁻¹

Se	-1.771527000	-0.728612000	0.949654000
Se	-0.518696000	-0.340848000	-1.312881000
O	-0.657848000	0.638964000	0.549888000

C	-3.489597000	0.122918000	0.921200000
C	-4.613960000	-0.640610000	1.267772000
C	-3.619937000	1.477548000	0.598961000
C	-5.869190000	-0.050426000	1.283517000
C	-4.875190000	2.070126000	0.628409000
C	-6.011679000	1.313083000	0.965364000
H	-4.517747000	-1.691976000	1.528666000
H	-2.740984000	2.055203000	0.332513000
H	-6.744423000	-0.636153000	1.546856000
H	-4.984883000	3.122786000	0.385781000
C	-1.340695000	-1.921471000	-2.139671000
C	-2.446431000	-1.762352000	-2.987854000
C	-0.774114000	-3.194192000	-1.974360000
C	-2.967213000	-2.850817000	-3.678653000
C	-1.291729000	-4.289189000	-2.654098000
C	-2.394589000	-4.123647000	-3.512234000
H	-2.894799000	-0.781239000	-3.114653000
H	0.083592000	-3.324679000	-1.320565000
H	-3.815683000	-2.725533000	-4.344669000
H	-0.846952000	-5.272630000	-2.534750000
C	-7.302432000	1.922146000	0.984899000
N	-8.356159000	2.417170000	0.999350000
C	-2.931335000	-5.247835000	-4.211743000
N	-3.369235000	-6.164568000	-4.779735000

3

E = -6.36898 Ha

Te	-2.620606000	-0.237818000	0.977994000
Te	-1.546836000	-3.294569000	-0.446176000
O	-2.971484000	-2.101132000	0.315762000
C	-1.774408000	-2.731249000	-2.480345000
C	-3.002874000	-2.281495000	-2.981734000
C	-0.676861000	-2.851670000	-3.344490000
C	-3.129373000	-1.944781000	-4.323409000
C	-0.806578000	-2.542998000	-4.693111000
C	-2.034341000	-2.079201000	-5.195036000
H	-3.865038000	-2.192811000	-2.328366000
H	0.292154000	-3.173971000	-2.971961000
H	-4.080957000	-1.589830000	-4.707814000
H	0.045409000	-2.640143000	-5.359143000
C	-2.240231000	-0.731798000	3.007318000
C	-2.811472000	-1.862761000	3.605059000
C	-1.430821000	0.120378000	3.771892000
C	-2.568062000	-2.144371000	4.943324000
C	-1.207733000	-0.142253000	5.117993000
C	-1.769795000	-1.282783000	5.716157000
H	-3.448855000	-2.526888000	3.029950000
H	-0.956517000	0.989157000	3.322500000
H	-3.007069000	-3.025192000	5.402354000
H	-0.582601000	0.522087000	5.706887000
C	-1.529826000	-1.565576000	7.094886000
N	-1.334234000	-1.796016000	8.219227000
C	-2.167369000	-1.743404000	-6.576364000
N	-2.275664000	-1.468865000	-7.702589000

(NO₂PhSe)₂

2

E = -6.61220 Ha

Se	-2.679920000	-0.837024000	0.668988000
Se	-1.492684000	-2.852606000	-0.189863000

O	-2.453867000	-4.174537000	-0.008100000
C	-1.779428000	-2.303198000	-2.073720000
C	-2.749217000	-2.975856000	-2.811186000
C	-0.954534000	-1.340681000	-2.657180000
C	-2.914821000	-2.667933000	-4.159251000
C	-1.114094000	-1.032834000	-4.005074000
C	-2.095192000	-1.700430000	-4.735933000
H	-3.360081000	-3.736712000	-2.333743000
H	-0.192835000	-0.825395000	-2.078034000
H	-3.663921000	-3.168445000	-4.761522000
H	-0.492355000	-0.289723000	-4.490036000
C	-2.199984000	-1.047029000	2.522681000
C	-2.749173000	-2.082041000	3.292798000
C	-1.337558000	-0.115862000	3.118311000
C	-2.430000000	-2.192516000	4.642252000
C	-1.029517000	-0.211209000	4.471498000
C	-1.577033000	-1.252669000	5.216863000
H	-3.425682000	-2.799716000	2.840962000
H	-0.906486000	0.684626000	2.525441000
H	-2.841744000	-2.989366000	5.250314000
H	-0.368236000	0.502975000	4.947766000
N	-2.267177000	-1.371938000	-6.180313000
N	-1.243148000	-1.362433000	6.663003000
O	-1.746435000	-2.290671000	7.292298000
O	-0.484772000	-0.517552000	7.135289000
O	-3.134857000	-1.982202000	-6.799592000
O	-1.529675000	-0.511786000	-6.656157000

TSiso

E = -6.54659 Ha
nimag = -288.12 cm⁻¹

Se	-1.678251000	-0.654576000	1.002205000
Se	-0.492747000	-0.360502000	-1.294305000
O	-0.623801000	0.726322000	0.499193000
C	-3.431188000	0.117704000	0.927177000
C	-4.518635000	-0.676492000	1.320827000
C	-3.620906000	1.445345000	0.529852000
C	-5.800091000	-0.142725000	1.309488000
C	-4.902485000	1.982249000	0.530454000
C	-5.979370000	1.183993000	0.915671000
H	-4.374859000	-1.706225000	1.639273000
H	-2.769995000	2.046622000	0.227814000
H	-6.656770000	-0.736284000	1.605680000
H	-5.076525000	3.009458000	0.232046000
C	-1.397833000	-1.909819000	-2.091852000
C	-2.184351000	-1.673421000	-3.228635000
C	-1.183019000	-3.227078000	-1.659825000
C	-2.719884000	-2.738720000	-3.950115000
C	-1.730621000	-4.294189000	-2.358856000
C	-2.491402000	-4.036019000	-3.501701000
H	-2.377341000	-0.655480000	-3.554919000
H	-0.569596000	-3.421605000	-0.784790000
H	-3.321324000	-2.572103000	-4.836219000
H	-1.563314000	-5.318393000	-2.046407000
N	-7.346800000	1.757051000	0.908087000
O	-8.271047000	1.026846000	1.265195000
O	-7.471204000	2.926177000	0.545041000
N	-3.074124000	-5.178012000	-4.256444000
O	-2.864177000	-6.309529000	-3.822656000
O	-3.727818000	-4.917642000	-5.264592000

3

E = -6.60140 Ha

Se	-1.104600000	-0.962753000	-0.983878000
Se	1.261414000	1.151983000	-1.234479000
C	-0.093324000	-2.585908000	-0.897301000
C	-0.391459000	-3.470580000	0.150074000
C	0.254094000	-4.698008000	0.229866000
C	1.217210000	-5.023112000	-0.724255000
C	1.533862000	-4.145842000	-1.760977000
C	0.868609000	-2.929762000	-1.855207000
C	0.274098000	2.780609000	-1.041114000
C	0.757337000	3.714021000	-0.111650000
C	0.130536000	4.945624000	0.028570000
C	-0.996060000	5.227261000	-0.743051000
C	-1.495410000	4.301873000	-1.658909000
C	-0.851960000	3.080697000	-1.817643000
H	-1.118041000	-3.203623000	0.913153000
H	0.034668000	-5.392969000	1.031752000
H	2.283892000	-4.427436000	-2.490818000
H	1.095249000	-2.254848000	-2.673327000
H	1.615715000	3.482519000	0.513764000
H	0.491947000	5.678029000	0.740688000
H	-2.370619000	4.549958000	-2.247974000
H	-1.223393000	2.367975000	-2.545783000
O	-0.002145000	0.075172000	-2.038404000
N	-1.676407000	6.532914000	-0.584146000
O	-1.202064000	7.326923000	0.228343000
O	-2.673159000	6.743636000	-1.275081000
N	1.919412000	-6.323876000	-0.632318000
O	2.766551000	-6.575652000	-1.489173000
O	1.611576000	-7.072795000	0.294970000

(HTe)₂

2

E = -0.60962 Ha

O	5.591413000	-2.289255000	1.313054000
Te	5.526979000	-0.962475000	0.066656000
Te	4.574212000	1.433482000	1.270455000
H	3.931075000	-1.107873000	-0.547559000
H	6.156411000	1.903695000	1.509420000

TSiso

E = -0.56259 Ha
nimag = -230.50 cm⁻¹

Te	-1.579452000	-0.761374000	1.189860000
Te	-0.570200000	-0.209035000	-1.406907000
H	-1.328097000	-1.643493000	-1.973984000
H	-3.110740000	-0.074152000	0.987319000
O	-0.475241000	0.775207000	0.626989000

3

E = -0.60156 Ha

Te	0.018343000	1.771070000	-0.178856000
Te	-0.018345000	-1.771070000	-0.178859000
O	0.000011000	0.000003000	-1.124280000
H	-1.642047000	1.856432000	0.044650000
H	1.642042000	-1.856445000	0.044670000

(CH₃Te)₂

2

E = -1.79496 Ha

O	7.107630000	-1.056654000	1.540805000
Te	5.644572000	-0.973779000	0.451751000
Te	4.299133000	1.478853000	0.958029000
C	4.173177000	-2.090349000	1.609512000
H	3.181019000	-1.968968000	1.171932000
H	4.490657000	-3.133917000	1.570014000
H	4.212278000	-1.719880000	2.633904000
C	5.681488000	2.643825000	-0.248769000
H	6.682532000	2.569351000	0.173464000
H	5.656500000	2.303171000	-1.283164000
H	5.328441000	3.674700000	-0.190196000

TSiso

E = -1.74916 Ha

nimag = -182.89 cm⁻¹

Te	-1.614482000	-0.736312000	1.201140000
Te	-0.541140000	-0.230693000	-1.419506000
O	-0.514304000	0.778432000	0.568803000
C	-3.550949000	0.222440000	1.153192000
H	-3.727587000	0.610274000	0.151265000
H	-4.302555000	-0.524294000	1.422128000
H	-3.538560000	1.026986000	1.890788000
C	-1.345235000	-2.126938000	-2.244970000
H	-1.021336000	-2.097405000	-3.293400000
H	-0.902120000	-2.989648000	-1.748263000
H	-2.433600000	-2.150401000	-2.194643000

3

E = -1.78696 Ha

Te	-2.146224000	-0.493533000	1.255678000
Te	-0.059650000	-1.742760000	-1.312681000
H	2.558739000	-1.452686000	-0.836860000
C	1.714980000	-0.866708000	-0.460721000
H	1.804765000	0.167509000	-0.793251000
H	1.676070000	-0.935865000	0.626821000
C	-3.746300000	-1.857566000	0.785341000
H	-4.344661000	-1.955813000	1.695877000
H	-4.356222000	-1.438875000	-0.015241000
H	-3.335277000	-2.829177000	0.509585000
O	-1.363635000	-0.393577000	-0.592706000

(PhTe)₂

2

E = -5.46234 Ha

Te	-0.420733000	-0.654016000	-1.124021000
Te	-1.963970000	-0.927554000	1.268355000
H	-4.129523000	-5.564839000	0.242940000
H	-2.183345000	-6.948851000	0.929723000
H	-0.105703000	-5.854908000	1.741881000
O	-3.696715000	-0.540292000	0.844251000
H	0.037205000	-3.391760000	1.860336000
C	-1.975517000	-3.091393000	1.110271000
C	-3.149049000	-3.695231000	0.662122000

C	-3.218068000	-5.087759000	0.595572000
C	-2.125112000	-5.864493000	0.981231000
C	-0.957318000	-5.251234000	1.437352000
C	-0.878191000	-3.859532000	1.505088000
H	-3.996971000	-3.078633000	0.374229000
C	-0.179004000	1.461111000	-0.928943000
C	-1.211730000	2.324146000	-1.316914000
C	-1.039072000	3.705119000	-1.218228000
C	0.161705000	4.232719000	-0.743887000
C	1.192715000	3.374512000	-0.362209000
C	1.025415000	1.991918000	-0.450054000
H	-2.148680000	1.923294000	-1.690496000
H	-1.847890000	4.367886000	-1.516464000
H	0.293700000	5.309372000	-0.672129000
H	2.131725000	3.778638000	0.008688000
H	1.831773000	1.331285000	-0.146090000

TSiso

E = -5.41871 Ha

nimag = -173.13 cm⁻¹

Te	-0.682459000	-0.322656000	1.559539000
Te	-0.550147000	-0.491580000	-1.358968000
O	0.443866000	0.656355000	0.269974000
H	-2.878725000	4.413951000	1.235236000
H	-4.568685000	4.021093000	3.016184000
H	-4.651123000	1.823761000	4.179009000
H	-3.058810000	0.041673000	3.583086000
C	-2.075694000	1.216959000	2.044240000
C	-2.025524000	2.447256000	1.385123000
C	-2.921372000	3.454033000	1.744694000
C	-3.869782000	3.234281000	2.744466000
C	-3.916983000	2.001366000	3.396761000
C	-3.017346000	0.992311000	3.055143000
H	-1.292012000	2.615714000	0.602585000
C	-2.039354000	-2.083508000	-1.436748000
C	-3.408870000	-1.787716000	-1.476941000
C	-4.346224000	-2.809922000	-1.626573000
C	-3.925572000	-4.137085000	-1.732590000
C	-2.564343000	-4.439751000	-1.691123000
C	-1.624779000	-3.418496000	-1.538988000
H	-3.745421000	-0.757563000	-1.396031000
H	-5.406592000	-2.569562000	-1.663860000
H	-4.657522000	-4.932967000	-1.847178000
H	-2.231653000	-5.472087000	-1.775418000
H	-0.566295000	-3.663197000	-1.504293000

3

E = -5.45457 Ha

Te	0.363951000	-3.319198000	0.681635000
Te	1.090083000	-0.022505000	-0.432474000
H	3.522269000	0.565641000	1.465990000
O	-0.199870000	-1.492141000	0.045041000
C	1.371057000	0.776803000	1.520873000
C	0.274613000	1.198657000	2.285681000
C	0.474474000	1.731836000	3.557719000
C	1.767241000	1.877995000	4.064903000
C	2.861327000	1.472574000	3.301791000
C	2.666027000	0.909419000	2.039534000
H	-0.733158000	1.109849000	1.890733000
H	-0.382087000	2.048176000	4.148533000
H	1.919788000	2.305601000	5.052744000
H	3.870305000	1.577231000	3.693864000

C	0.591911000	-4.248628000	-1.220091000
C	-0.492234000	-4.341594000	-2.104165000
C	-0.334346000	-4.967055000	-3.339592000
C	0.894311000	-5.529444000	-3.691521000
C	1.971756000	-5.450678000	-2.810230000
C	1.827690000	-4.800758000	-1.583295000
H	-1.457347000	-3.926335000	-1.829276000
H	-1.177907000	-5.028031000	-4.023303000
H	1.010303000	-6.027243000	-4.651080000
H	2.932587000	-5.881899000	-3.081386000
H	2.679747000	-4.718112000	-0.914591000

(CH₃PhTe)₂

2

E = -6.63993 Ha

Te	-2.874167000	-0.680766000	0.718441000
Te	-1.387851000	-2.944076000	-0.211288000
O	-2.464613000	-4.410672000	-0.055637000
C	-1.702861000	-2.421097000	-2.287554000
C	-2.623943000	-3.172992000	-3.012992000
C	-0.961752000	-1.419099000	-2.916480000
C	-2.810979000	-2.907883000	-4.369231000
C	-1.158071000	-1.166702000	-4.272926000
C	-2.087155000	-1.902054000	-5.022512000
H	-3.183505000	-3.963840000	-2.519425000
H	-0.232608000	-0.828759000	-2.365981000
H	-3.532521000	-3.500188000	-4.928211000
H	-0.575262000	-0.384679000	-4.755214000
C	-2.353714000	-0.945955000	2.771704000
C	-3.035007000	-1.879848000	3.562029000
C	-1.352535000	-0.163527000	3.358122000
C	-2.712116000	-2.025289000	4.909520000
C	-1.044901000	-0.313810000	4.709898000
C	-1.716385000	-1.244752000	5.511673000
H	-3.813282000	-2.500229000	3.128472000
H	-0.807657000	0.564176000	2.764031000
H	-3.249576000	-2.763235000	5.501556000
H	-0.262434000	0.305337000	5.143811000
C	-2.314942000	-1.601232000	-6.481621000
H	-1.391893000	-1.283990000	-6.975885000
H	-2.706807000	-2.471496000	-7.015079000
H	-3.043146000	-0.788729000	-6.601829000
C	-1.400393000	-1.385931000	6.978390000
H	-2.101074000	-0.798677000	7.585944000
H	-1.481399000	-2.426205000	7.307775000
H	-0.391987000	-1.031806000	7.209196000

TSiso

E = -6.59477 Ha

nimag = -172.54 cm⁻¹

Te	-1.859646000	-0.819042000	1.104886000
Te	-0.479723000	-0.293301000	-1.431762000
O	-0.643055000	0.643523000	0.583282000
C	-3.709423000	0.235000000	1.075904000
C	-4.864673000	-0.389538000	1.557727000
C	-3.776288000	1.549087000	0.609705000
C	-6.075894000	0.298626000	1.561946000
C	-4.992654000	2.228135000	0.634230000
C	-6.164246000	1.620691000	1.105711000
H	-4.836783000	-1.410764000	1.932904000

H	-2.884096000	2.039203000	0.232004000
H	-6.966480000	-0.204113000	1.933294000
H	-5.028583000	3.253061000	0.270319000
C	-1.275914000	-2.089599000	-2.365053000
C	-2.507680000	-2.073075000	-3.033288000
C	-0.521472000	-3.269874000	-2.383069000
C	-2.961092000	-3.202322000	-3.711514000
C	-0.981063000	-4.396042000	-3.064864000
C	-2.207582000	-4.384738000	-3.741850000
H	-3.118047000	-1.173781000	-3.027065000
H	0.433062000	-3.313388000	-1.864704000
H	-3.918940000	-3.162843000	-4.227230000
C	-7.468842000	2.373803000	1.149770000
H	-8.325746000	1.701649000	1.047480000
H	-7.582389000	2.903151000	2.104882000
H	-7.526553000	3.123552000	0.355381000
H	-0.374286000	-5.299695000	-3.067155000
C	-2.689969000	-5.593410000	-4.501391000
H	-2.391394000	-5.534059000	-5.556270000
H	-2.269667000	-6.518208000	-4.096313000
H	-3.780879000	-5.673910000	-4.479009000

3

E = -6.63096 Ha

Te	3.541736000	1.724838000	12.324902000
Te	5.557498000	3.484749000	14.672175000
C	3.011242000	0.157393000	13.660265000
C	1.924440000	0.303814000	14.530306000
C	1.561068000	-0.735806000	15.387303000
C	2.277933000	-1.936855000	15.417282000
C	3.370722000	-2.069773000	14.546806000
C	3.728801000	-1.047747000	13.673689000
C	5.699054000	5.288348000	13.555471000
C	6.771246000	5.508658000	12.678446000
C	6.863173000	6.699810000	11.966298000
C	5.909791000	7.718271000	12.120355000
C	4.851065000	7.493296000	13.006489000
C	4.735833000	6.292285000	13.707797000
H	1.359639000	1.231516000	14.546003000
H	0.709357000	-0.601087000	16.050700000
C	1.904555000	-3.051767000	16.359774000
H	3.945277000	-2.994100000	14.542902000
H	4.569493000	-1.188286000	13.000519000
H	7.536342000	4.748248000	12.551526000
H	7.700908000	6.846374000	11.287110000
C	6.026338000	9.004777000	11.344532000
H	4.093895000	8.261949000	13.146142000
H	3.888994000	6.139948000	14.370912000
H	1.831486000	-4.009796000	15.833607000
H	0.947483000	-2.861038000	16.851650000
H	2.663503000	-3.173592000	17.142510000
H	5.278162000	9.735899000	11.660663000
H	5.890001000	8.829524000	10.270379000
H	7.016545000	9.456433000	11.471325000
O	5.325173000	2.202233000	13.135802000

(CH₃OPhTe)₂

2

E = -7.07734 Ha

Te	2.668867000	0.776774000	14.623685000
----	-------------	-------------	--------------

Te	5.327609000	1.685600000	15.213893000
C	3.384284000	-0.944686000	13.539900000
C	3.338430000	-0.900452000	12.150096000
C	3.740028000	-2.002416000	11.393523000
C	4.187759000	-3.162873000	12.038740000
C	4.224575000	-3.206237000	13.442926000
C	3.824218000	-2.105491000	14.186858000
C	4.715461000	3.367370000	16.365849000
C	4.375576000	4.567987000	15.735762000
C	4.005519000	5.691217000	16.476767000
C	3.976469000	5.624970000	17.875238000
C	4.318817000	4.422647000	18.514238000
C	4.681194000	3.310165000	17.768307000
H	2.982398000	-0.001469000	11.652582000
H	3.696268000	-1.940718000	10.312346000
O	4.603270000	-4.298172000	11.409565000
H	4.570129000	-4.113615000	13.929916000
H	3.863038000	-2.163795000	15.272329000
H	4.390509000	4.638974000	14.652636000
H	3.745025000	6.601612000	15.949765000
O	3.636149000	6.653888000	18.702504000
H	4.940872000	2.390678000	18.284309000
O	2.041798000	1.813856000	13.256267000
C	3.274091000	7.905568000	18.127456000
C	4.600252000	-4.335632000	9.985504000
H	4.099589000	8.337938000	17.548231000
H	3.045372000	8.560031000	18.970349000
H	2.386657000	7.815489000	17.488704000
H	4.969368000	-5.327248000	9.718196000
H	5.266703000	-3.575050000	9.560141000
H	3.589265000	-4.204980000	9.579980000
H	4.293476000	4.380195000	19.599479000

TSiso

E = -7.03232 Ha
 nimag = -170.02 cm⁻¹

Te	-1.919920000	-0.834247000	1.082318000
Te	-0.492551000	-0.317775000	-1.446045000
O	-0.654744000	0.594898000	0.585672000
C	-3.720399000	0.294370000	1.089859000
C	-4.874938000	-0.243060000	1.678314000
C	-3.765296000	1.576476000	0.544424000
C	-6.053073000	0.487949000	1.707729000
C	-4.942567000	2.324539000	0.584648000
C	-6.097565000	1.781618000	1.162316000
H	-4.866107000	-1.235279000	2.124824000
H	-2.876799000	2.004928000	0.090833000
H	-6.951563000	0.078193000	2.160219000
H	-4.942268000	3.321171000	0.158576000
C	-1.236732000	-2.123602000	-2.379762000
C	-2.502302000	-2.174838000	-2.989781000
C	-0.423607000	-3.260259000	-2.450615000
C	-2.928111000	-3.311926000	-3.658557000
C	-0.834897000	-4.412005000	-3.124341000
C	-2.096351000	-4.443091000	-3.732458000
H	-3.161439000	-1.311926000	-2.945371000
H	0.555451000	-3.255544000	-1.978185000
H	-3.902260000	-3.348141000	-4.138897000
H	-0.169295000	-5.266758000	-3.163566000
O	-2.612865000	-5.505489000	-4.412810000
C	-1.833194000	-6.691281000	-4.530349000
H	-0.893616000	-6.505603000	-5.065561000

H	-1.614374000	-7.129936000	-3.548783000
H	-2.444010000	-7.387823000	-5.107298000
O	-7.303439000	2.413500000	1.250843000
C	-7.425873000	3.733169000	0.730566000
H	-8.460185000	4.027179000	0.917506000
H	-6.753299000	4.433473000	1.241595000
H	-7.231968000	3.761955000	-0.349058000

3

E = -7.06914 Ha

Te	2.388626000	0.694008000	14.323520000
Te	5.585562000	2.069862000	15.101292000
C	3.146312000	-1.086848000	13.458145000
C	3.149185000	-1.263766000	12.069628000
C	3.645180000	-2.430219000	11.488487000
C	4.141294000	-3.455901000	12.305058000
C	4.136691000	-3.292197000	13.699481000
C	3.650365000	-2.122325000	14.264239000
C	4.885819000	3.536049000	16.463780000
C	4.835517000	4.886452000	16.098682000
C	4.385010000	5.861609000	16.987846000
C	3.983597000	5.491641000	18.278908000
C	4.035503000	4.140743000	18.658019000
C	4.476143000	3.179380000	17.760388000
H	2.761755000	-0.481642000	11.423175000
H	3.632877000	-2.526297000	10.409012000
O	4.643777000	-4.639940000	11.855608000
H	4.525300000	-4.093424000	14.321796000
H	3.664811000	-2.011045000	15.344336000
H	5.150153000	5.190857000	15.104679000
H	4.358797000	6.895916000	16.665051000
O	3.533615000	6.351795000	19.235010000
H	4.500575000	2.138872000	18.070154000
O	3.947135000	1.915383000	13.933395000
C	3.446932000	7.739831000	18.927367000
C	4.689839000	-4.880352000	10.452458000
H	4.430185000	8.162202000	18.685527000
H	3.063688000	8.216536000	19.831227000
H	2.753556000	7.927351000	18.098151000
H	5.128019000	-5.873526000	10.339900000
H	5.321653000	-4.146127000	9.937400000
H	3.686544000	-4.875881000	10.008594000
H	3.720311000	3.866078000	19.660754000

(ClPhTe)₂

2

E = -5.34336 Ha

Te	-2.856655000	-0.660059000	0.717296000
Te	-1.359244000	-2.919382000	-0.209596000
O	-2.434877000	-4.384369000	-0.047749000
C	-1.688793000	-2.407524000	-2.288664000
C	-2.609560000	-3.174642000	-2.999923000
C	-0.960375000	-1.402971000	-2.928444000
C	-2.816141000	-2.931897000	-4.357054000
C	-1.159959000	-1.155301000	-4.285515000
C	-2.089479000	-1.922672000	-4.990258000
H	-3.160679000	-3.964238000	-2.494748000
H	-0.235005000	-0.799444000	-2.387774000
H	-3.532926000	-3.522241000	-4.919110000
H	-0.600123000	-0.375758000	-4.792134000

C	-2.340788000	-0.944677000	2.769176000
C	-3.002795000	-1.908710000	3.539839000
C	-1.364905000	-0.141581000	3.372190000
C	-2.690769000	-2.075139000	4.887986000
C	-1.053025000	-0.295090000	4.722058000
C	-1.717593000	-1.264781000	5.472862000
H	-3.764745000	-2.540586000	3.094437000
H	-0.839303000	0.612166000	2.793834000
H	-3.202824000	-2.827387000	5.479428000
H	-0.297785000	0.331585000	5.185576000
Cl	-2.339816000	-1.618226000	-6.684523000
Cl	-1.328753000	-1.464682000	7.156865000

TSiso

E = -5.30010 Ha

nimag = -171.00 cm⁻¹

Te	-1.861964000	-0.822813000	1.099884000
Te	-0.483359000	-0.288581000	-1.435352000
O	-0.648339000	0.641131000	0.579929000
C	-3.709466000	0.235371000	1.054023000
C	-4.876971000	-0.393533000	1.500727000
C	-3.755726000	1.561171000	0.617691000
C	-6.088323000	0.294029000	1.502248000
C	-4.961983000	2.258143000	0.630027000
C	-6.123189000	1.619947000	1.067709000
H	-4.863515000	-1.421979000	1.855558000
H	-2.852060000	2.054323000	0.272586000
H	-6.995927000	-0.192756000	1.844359000
H	-5.000740000	3.290530000	0.297016000
C	-1.283763000	-2.086739000	-2.367162000
C	-2.516285000	-2.066723000	-3.034109000
C	-0.531377000	-3.269017000	-2.379557000
C	-2.986234000	-3.193074000	-3.706774000
C	-0.987383000	-4.403893000	-3.048965000
C	-2.216581000	-4.357854000	-3.707546000
H	-3.121063000	-1.163900000	-3.037414000
H	0.426194000	-3.312154000	-1.867273000
H	-3.938107000	-3.169063000	-4.228269000
H	-0.396382000	-5.314480000	-3.060367000
Cl	-7.633946000	2.487768000	1.074946000
Cl	-2.799600000	-5.772863000	-4.541303000

3

E = -5.33605 Ha

Te	4.908284000	1.337765000	4.621921000
Te	8.396660000	1.919391000	5.029483000
Cl	3.173370000	7.724330000	3.850975000
Cl	10.242299000	-4.413071000	4.090055000
C	4.380660000	3.384727000	4.385201000
C	4.350935000	3.962901000	3.109316000
C	3.969195000	5.292929000	2.937116000
C	3.638119000	6.057643000	4.054897000
C	3.674201000	5.504716000	5.336557000
C	4.032241000	4.168543000	5.494036000
C	8.964713000	-0.108635000	4.732918000
C	9.261105000	-0.578057000	3.446545000
C	9.666258000	-1.896765000	3.243805000
C	9.751952000	-2.759397000	4.335768000
C	9.449239000	-2.315147000	5.624450000
C	9.070025000	-0.989633000	5.818276000
H	4.632203000	3.379883000	2.237181000

H	3.943147000	5.734820000	1.946158000
H	3.411082000	6.109721000	6.198414000
H	4.038678000	3.739424000	6.491599000
H	9.171592000	0.082053000	2.588715000
H	9.898965000	-2.254466000	2.245894000
H	9.523198000	-2.995735000	6.466693000
H	8.854659000	-0.645603000	6.825542000
O	6.548690000	1.592917000	5.763571000

(NH₂PhTe)₂

2

E = -6.32795 Ha

Te	-2.838194000	-0.640526000	0.728291000
Te	-1.406582000	-2.942136000	-0.233045000
O	-2.517576000	-4.384574000	-0.070870000
C	-1.705194000	-2.423997000	-2.299889000
C	-2.647929000	-3.149933000	-3.029497000
C	-0.949150000	-1.436795000	-2.937984000
C	-2.841805000	-2.885946000	-4.379662000
C	-1.140120000	-1.170975000	-4.288729000
C	-2.093070000	-1.890372000	-5.034225000
H	-3.228060000	-3.925187000	-2.534843000
H	-0.207285000	-0.858285000	-2.391760000
H	-3.578481000	-3.460153000	-4.938144000
H	-0.543656000	-0.401557000	-4.774566000
C	-2.344329000	-0.917090000	2.776573000
C	-3.094615000	-1.786292000	3.581421000
C	-1.286228000	-0.211282000	3.366013000
C	-2.795196000	-1.948313000	4.928376000
C	-0.986423000	-0.366693000	4.714338000
C	-1.735170000	-1.240533000	5.522595000
H	-3.918271000	-2.349911000	3.154079000
H	-0.685872000	0.469241000	2.769347000
H	-3.393551000	-2.629540000	5.529926000
H	-0.163607000	0.198136000	5.148042000
N	-2.245085000	-1.666431000	-6.395792000
H	-1.946115000	-0.763944000	-6.734133000
H	-3.122698000	-1.960867000	-6.797800000
N	-1.475175000	-1.354925000	6.882178000
H	-0.544342000	-1.100127000	7.177542000
H	-1.803288000	-2.200651000	7.324702000

TSiso

E = -6.28321 Ha

nimag = -178.05 cm⁻¹

Te	-1.854498000	-0.806617000	1.144373000
Te	-0.475671000	-0.305712000	-1.417801000
O	-0.638568000	0.648185000	0.612400000
C	-3.712448000	0.237117000	1.089090000
C	-4.865992000	-0.406844000	1.552390000
C	-3.753669000	1.548005000	0.626507000
C	-6.070886000	0.294981000	1.531626000
C	-4.968075000	2.255436000	0.617747000
C	-6.130468000	1.607595000	1.073750000
H	-4.838757000	-1.426632000	1.927476000
H	-2.843014000	2.022914000	0.271227000
H	-6.979451000	-0.187464000	1.885081000
H	-7.081544000	2.135210000	1.064381000
C	-1.281299000	-2.060591000	-2.373982000

C	-2.503011000	-2.017036000	-3.066051000
C	-0.568830000	-3.271101000	-2.376537000
C	-2.982033000	-3.123366000	-3.753899000
C	-1.038110000	-4.383946000	-3.061701000
C	-2.256722000	-4.330724000	-3.765040000
H	-3.088807000	-1.101581000	-3.071178000
H	0.373316000	-3.344484000	-1.839227000
H	-3.923734000	-3.056623000	-4.295779000
H	-0.456745000	-5.304227000	-3.060935000
N	-2.703158000	-5.419397000	-4.495344000
H	-3.686943000	-5.442829000	-4.717262000
H	-2.331192000	-6.320900000	-4.237358000
N	-5.027224000	3.548470000	0.104198000
H	-4.151582000	4.051376000	0.096932000
H	-5.789352000	4.117061000	0.443710000

3

E = -6.32025 Ha

Te	4.882029000	1.350855000	4.663253000
Te	8.386012000	1.896412000	5.071608000
C	4.370828000	3.387478000	4.404927000
C	4.643398000	4.053694000	3.199630000
C	4.295510000	5.386633000	3.020928000
C	3.666683000	6.108922000	4.051369000
C	3.396367000	5.443936000	5.262445000
C	3.738116000	4.109266000	5.430033000
C	8.972595000	-0.110680000	4.751266000
C	8.970341000	-0.667404000	3.462538000
C	9.365826000	-1.981514000	3.247044000
C	9.772349000	-2.794103000	4.320923000
C	9.773376000	-2.238431000	5.614376000
C	9.385427000	-0.921946000	5.820635000
H	5.135089000	3.524661000	2.388500000
H	4.521062000	5.879617000	2.077327000
H	2.913111000	5.981716000	6.075831000
H	3.509955000	3.621371000	6.373263000
H	8.651513000	-0.067759000	2.614985000
H	9.359423000	-2.386569000	2.237000000
H	10.090277000	-2.844809000	6.460650000
H	9.400131000	-0.520065000	6.829618000
O	6.531772000	1.576222000	5.805827000
N	3.372944000	7.455207000	3.899700000
H	2.669096000	7.832880000	4.515994000
H	3.289320000	7.792334000	2.952488000
N	10.218281000	-4.089161000	4.104603000
H	9.912278000	-4.530298000	3.250284000
H	10.188925000	-4.710328000	4.899214000

(CNPhTe)₂

2

E = -6.37537 Ha

Te	-2.713756000	-0.573831000	0.678076000
Te	-1.299025000	-2.904654000	-0.199770000
O	-2.419010000	-4.321487000	0.047305000
C	-1.698874000	-2.435364000	-2.284466000
C	-2.697673000	-3.171316000	-2.920475000
C	-0.945884000	-1.492060000	-2.987253000
C	-2.959472000	-2.954377000	-4.269593000
C	-1.202097000	-1.272620000	-4.336943000
C	-2.213380000	-2.002501000	-4.985018000

H	-3.262292000	-3.913101000	-2.361007000
H	-0.159836000	-0.920369000	-2.500005000
H	-3.737614000	-3.518629000	-4.774814000
H	-0.624509000	-0.541129000	-4.893746000
C	-2.327605000	-0.943309000	2.747051000
C	-3.004676000	-1.969718000	3.419355000
C	-1.427087000	-0.131830000	3.449831000
C	-2.777939000	-2.189275000	4.773732000
C	-1.205973000	-0.338982000	4.807146000
C	-1.878563000	-1.372856000	5.479197000
H	-3.708547000	-2.603302000	2.889734000
H	-0.893291000	0.664691000	2.940990000
H	-3.299341000	-2.989277000	5.290398000
H	-0.509873000	0.293193000	5.349959000
C	-1.648817000	-1.591817000	6.872620000
N	-1.460608000	-1.769523000	8.007290000
C	-2.477818000	-1.778082000	-6.372045000
N	-2.692096000	-1.593693000	-7.500845000

TSiso

E = -6.33235 Ha

nimag = -170.04 cm⁻¹

Te	-1.790155000	-0.808260000	1.120512000
Te	-0.471017000	-0.260933000	-1.422544000
O	-0.616027000	0.680360000	0.590380000
C	-3.667311000	0.196344000	1.053658000
C	-4.827841000	-0.486168000	1.439812000
C	-3.733273000	1.537871000	0.666855000
C	-6.053890000	0.166983000	1.429237000
C	-4.956607000	2.196995000	0.666997000
C	-6.128029000	1.516927000	1.043577000
H	-4.791972000	-1.527263000	1.752699000
H	-2.831705000	2.064611000	0.369644000
H	-6.956516000	-0.359965000	1.723004000
H	-5.012919000	3.240477000	0.371827000
C	-1.309932000	-2.056936000	-2.347748000
C	-2.541838000	-2.008090000	-3.015150000
C	-0.580215000	-3.253927000	-2.349862000
C	-3.035667000	-3.126756000	-3.678023000
C	-1.062780000	-4.379829000	-3.009445000
C	-2.297996000	-4.323403000	-3.677231000
H	-3.121417000	-1.089228000	-3.024737000
H	0.376495000	-3.310640000	-1.837862000
H	-3.987182000	-3.082387000	-4.199823000
H	-0.491022000	-5.303242000	-3.013443000
C	-7.386265000	2.192508000	1.036045000
N	-8.412285000	2.742354000	1.029117000
C	-2.802398000	-5.478000000	-4.351434000
N	-3.214141000	-6.419292000	-4.898490000

3

E = -6.36898 Ha

Te	-2.620606000	-0.237818000	0.977994000
Te	-1.546836000	-3.294569000	-0.446176000
O	-2.971484000	-2.101132000	0.315762000
C	-1.774408000	-2.731249000	-2.480345000
C	-3.002874000	-2.281495000	-2.981734000
C	-0.676861000	-2.851670000	-3.344490000
C	-3.129373000	-1.944781000	-4.323409000
C	-0.806578000	-2.542998000	-4.693111000
C	-2.034341000	-2.079201000	-5.195036000

H	-3.865038000	-2.192811000	-2.328366000
H	0.292154000	-3.173971000	-2.971961000
H	-4.080957000	-1.589830000	-4.707814000
H	0.045409000	-2.640143000	-5.359143000
C	-2.240231000	-0.731798000	3.007318000
C	-2.811472000	-1.862761000	3.605059000
C	-1.430821000	0.120378000	3.771892000
C	-2.568062000	-2.144371000	4.943324000
C	-1.207733000	-0.142253000	5.117993000
C	-1.769795000	-1.282783000	5.716157000
H	-3.448855000	-2.526888000	3.029950000
H	-0.956517000	0.989157000	3.322500000
H	-3.007069000	-3.025192000	5.402354000
H	-0.582601000	0.522087000	5.706887000
C	-1.529826000	-1.565576000	7.094886000
N	-1.334234000	-1.796016000	8.219227000
C	-2.167369000	-1.743404000	-6.576364000
N	-2.275664000	-1.468865000	-7.702589000

(NO₂PhTe)₂

2

E = -6.56265 Ha

Te	-2.636648000	-0.552650000	0.704819000
Te	-1.250833000	-2.874960000	-0.237406000
O	-2.364084000	-4.292125000	0.033755000
C	-1.720257000	-2.377882000	-2.302409000
C	-2.745135000	-3.099817000	-2.912604000
C	-0.984389000	-1.430065000	-3.017757000
C	-3.052673000	-2.863026000	-4.250539000
C	-1.285443000	-1.189873000	-4.356175000
C	-2.318607000	-1.909800000	-4.952331000
H	-3.295741000	-3.845512000	-2.344762000
H	-0.177745000	-0.870466000	-2.550763000
H	-3.847270000	-3.406003000	-4.749022000
H	-0.733067000	-0.459503000	-4.935546000
C	-2.234439000	-0.964286000	2.762605000
C	-2.840150000	-2.056625000	3.398972000
C	-1.399953000	-0.108680000	3.494718000
C	-2.607570000	-2.297427000	4.750181000
C	-1.174430000	-0.336207000	4.849311000
C	-1.779891000	-1.431327000	5.460327000
H	-3.493767000	-2.723742000	2.846768000
H	-0.920079000	0.737214000	3.012723000
H	-3.065554000	-3.140730000	5.253695000
H	-0.533707000	0.318300000	5.428481000
N	-2.644032000	-1.653616000	-6.384954000
N	-1.536584000	-1.680810000	6.907281000
O	-2.099553000	-2.646311000	7.418866000
O	-0.787321000	-0.905010000	7.497960000
O	-3.559946000	-2.304043000	-6.882009000
O	-1.975216000	-0.807825000	-6.974770000

TSiso

E = -6.51977 Ha

nimag = -170.17 cm⁻¹

Te	-1.783970000	-0.792270000	1.129348000
Te	-0.458895000	-0.262830000	-1.406563000
O	-0.608213000	0.694073000	0.601205000
C	-3.661700000	0.208053000	1.048733000
C	-4.824874000	-0.484346000	1.410620000

C	-3.725007000	1.555590000	0.681395000
C	-6.053412000	0.166250000	1.396173000
C	-4.950945000	2.212743000	0.676690000
C	-6.102296000	1.510716000	1.030156000
H	-4.790031000	-1.530125000	1.707294000
H	-2.821564000	2.088916000	0.402554000
H	-6.965719000	-0.351473000	1.667990000
H	-5.023223000	3.257998000	0.399350000
C	-1.302895000	-2.062894000	-2.326211000
C	-2.526188000	-2.009190000	-3.009037000
C	-0.580875000	-3.264573000	-2.310279000
C	-3.020615000	-3.130074000	-3.671419000
C	-1.063609000	-4.393674000	-2.967660000
C	-2.281383000	-4.310859000	-3.639190000
H	-3.099082000	-1.086574000	-3.033065000
H	0.369512000	-3.324434000	-1.787309000
H	-3.961218000	-3.098323000	-4.209151000
H	-0.511343000	-5.326344000	-2.966888000
N	-7.411803000	2.210330000	1.019074000
O	-8.405666000	1.560977000	1.342492000
O	-7.420170000	3.394716000	0.687029000
N	-2.805823000	-5.515080000	-4.341288000
O	-2.134913000	-6.543730000	-4.281829000
O	-3.876988000	-5.404704000	-4.934497000

3

E = -6.55762 Ha

Te	-1.213897000	-1.054134000	-0.765884000
Te	1.438984000	1.271082000	-0.947213000
C	-0.120800000	-2.866292000	-0.883605000
C	-0.440689000	-3.900031000	0.009422000
C	0.217715000	-5.121477000	-0.065856000
C	1.214002000	-5.298483000	-1.025108000
C	1.551216000	-4.278277000	-1.913424000
C	0.874829000	-3.065280000	-1.848731000
C	0.309335000	3.064369000	-0.991295000
C	0.693449000	4.121022000	-0.152094000
C	0.007750000	5.329358000	-0.186238000
C	-1.079468000	5.469556000	-1.047739000
C	-1.481033000	4.426100000	-1.880591000
C	-0.777981000	3.226878000	-1.859579000
H	-1.195913000	-3.761339000	0.779242000
H	-0.020204000	-5.928021000	0.617683000
H	2.326375000	-4.445246000	-2.652342000
H	1.123542000	-2.279914000	-2.554873000
H	1.520675000	4.010133000	0.544699000
H	0.294337000	6.153360000	0.456593000
H	-2.326624000	4.564803000	-2.544276000
H	-1.077931000	2.423545000	-2.524407000
O	0.066872000	0.086499000	-1.806939000
N	-1.822285000	6.750285000	-1.076657000
O	-1.432908000	7.651690000	-0.333755000
O	-2.782950000	6.834703000	-1.842036000
N	1.928018000	-6.593475000	-1.099615000
O	2.803759000	-6.713030000	-1.956719000
O	1.601539000	-7.470952000	-0.299852000