# Can Selenenyl Sulfides be a Substrate of Glutathione Reductase Enzyme? A Theoretical Insight

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# Justification for the methods used

## Functional

A benchmark study was conducted to obtain the standard redox potential of GSSG|2GSH couple which has a value of -0.240 Volts at pH = 7 [1;2]. We have selected three popular functionals B3LYP, $\omega$B97X−D, and M06−2X with 6−311++g(2df,2pd) basis set for this purpose. The redox potential of GSSG|2GSH couple (Eq. 1c in the main text) was calculated from the reaction free energy in solution $\Delta_r G_s^o(A|B)$, where $\sum_i A_i$ = GSSG + 2H$^+$ and $\sum_i B_i$ = 2GSH using the thermodynamic cycle (Fig. 3 in the main text) following the procedure described in the Computational methodology. The calculated redox potentials (in Volts) after correction for pH = 7 (considering pH effect of −59 mV/pH unit [3;4]) along with their deviations from the experimental value are presented in Table S5. Among the functional used, the M06−2X predicts the least deviation of 0.049 V. This level of accuracy in redox potential (within 50 mV, equivalent to free energy of reaction within 5 kJ/mol) to experimental result have been predicted for implicit-solvent model in the literature [5]. Based on these observations, M06−2X/6−311++g(2df,2pd) level of theory was used to calculate the redox potential in this study.

Table S1: Calculated redox potentials (in V) for GSSG|2GSH couple at pH = 7 using the studied functionals with 6−311++g(2df,2pd) basis set [1;2;3;4].

| Functional | $E^o_{rel,SHE}$(GSSG\|2GSH) | Deviation |
|---|---|---|
| B3LYP | −0.010 | −0.230 |
| $\omega$B97X−D | −0.127 | −0.113 |
| M06−2X | −0.289 | 0.049 |
| Experimental | −0.240 | 0 |

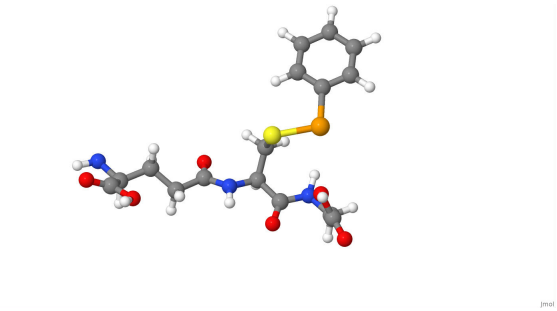
## Solvation energy calculation

As mentioned in the Computational methodology section, the free energy of species in solvent is calculated from the corresponding gas−phase geometries using a single−point calculation. To assess the impact of fully optimizing the geometries in the solvent phase few compounds were optimized fully in the solvent. The results are shown in Table S2 below. The maximum deviation was obtained for GSSG (0.042 V) with a mean absolute deviation (MAD) in the calculated redox potentials by these two methods for the studied compounds of 0.011 V. Thus using single−point geometry optimization in solvent phase it provides a reasonable compromise between the compuational cost and accuracy in the result [6].

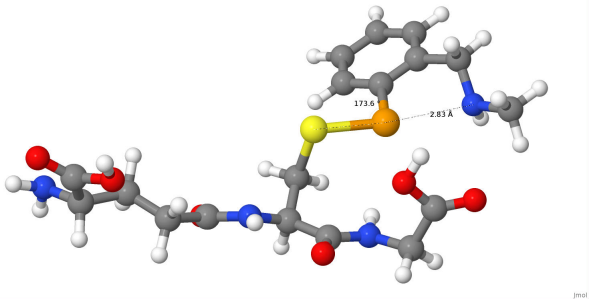
Table S2: Calculated redox potentials, $E^o_{rel,SHE}$(A|B) at pH = 7 in Volts, at M06−2X/6-311++g(2df,2pd) level of theory. Here A|B is either RSeSG|(RSeH + GSH) or GSSG|2GSH couple.

| Compoundd | $E^o_{rel,SHE}$(A\|B)$^a$ | $E^o_{rel,SHE}$(A\|B)$^b$ |
|---|---|---|
| GSSG | −0.289 | −0.247 |
| **1b** | −0.251 | −0.268 |
| **4b** | −0.264 | −0.292 |
| **6b** | −0.396 | −0.435 |
| MAD$^c$ | | 0.011 |

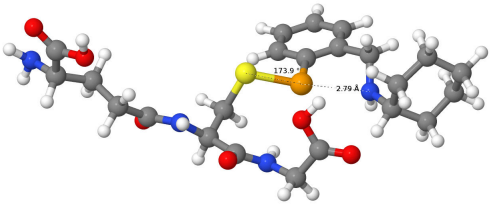
$^a$ Redox potentials were calculated using a single-point method based on gas-phase optimized geometries in the solvent phase. $^b$Redox potentials calculated using full geometry optimization in the solvent phase. $^c$ Mean absolute deviations in $E^o_{rel,SHE}(A|B)^b$ compared to $E^o_{rel,SHE}(A|B)^a$.



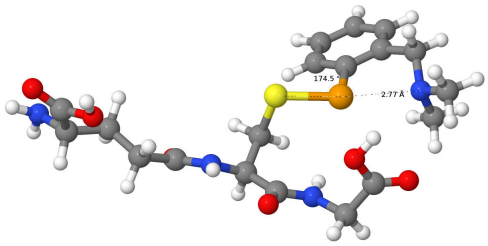
**1b**



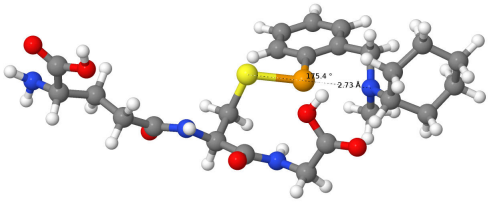

**2b** (2.83) [173.6]



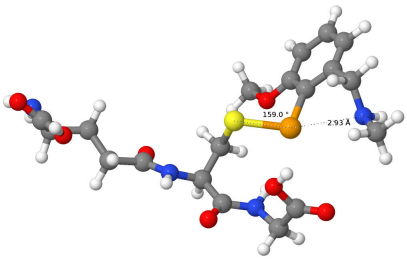

**3b** (2.79) [173.9]




**4b** (2.77) [174.5]

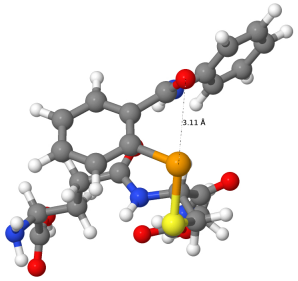



**5b** (2.73) [175.4]

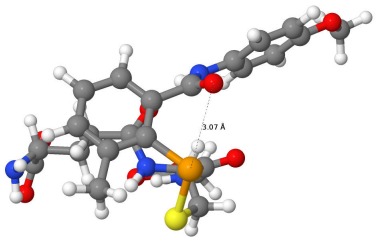



**2'b** (2.93) [159.0]

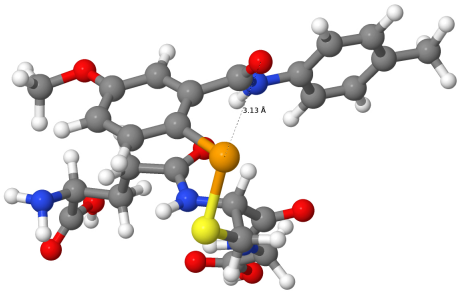
Figure S1: Gas−phase optimized geometries at M06−2X/6-311++g(2df,2pd) level of theory of phenyl selenide based selenenyl sulfide (**1b**) and amine−based selenenyl sulfides **2b** to **5b** and **2'b**. The bond distance $r_{N\cdots Se}$ in Åis given in parentheses and $\angle_{N\cdots Se-S}$ in degrees is given in square brackets. Colour scheme: white − hydrogen, grey − carbon, blue − nitrogen, red − oxygen, yellow − sulfur and orange − selenium



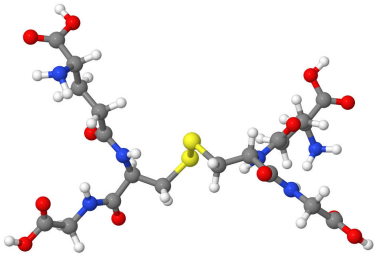

**6b** (3.11)



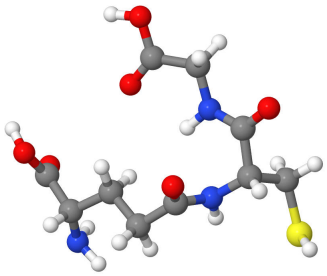

**7b** (3.07)




**8b** (3.13)



GSSG



GSH

Figure S2: Gas−phase optimized geometries at M06−2X/6-311++g(2df,2pd) level of theory of ebselen−based (amide−based) senenyl sulfide **6b** to **8b**, GSSG and GSH. The bond distance $r_{OSe}$ in Åis given in parentheses. Colour scheme: white − hydrogen, grey − carbon, blue − nitrogen, red − oxygen, yellow − sulfur and orange − selenium

## Molecular docking studies

To simulate the interactions between RSeSG (ligand) with the active site of GR, we have emplyoed molecular docking study. M06-2X/6-311++G(2df,2pd) gas−phase optimized geometries of the ligands were docked into GR (PDB ID: 2GH5[7]) using Autodock Vina software[8]. The default Vina force field was applied with an exhaustiveness of 64 for rigid docking. The best docking pose of the ligands at the catalytic site of GR are shown in Figures S3 and S4. The data on binding affinities of the docked compounds along with the distances of closest approach are summerized in Table S3. The binding affinities of the docked compounds ranged from −6.1 to −8.1 kcal $mol^{-1}$, where more negative values indicate stronger binding to the catalytic site. The distance between $S_{CYS-58}$ and $S_{ligand}/Se_{ligand}$ lies between 4.6 to 9.6 Å, while the distance between $N_{HIS-467}$ to $S_{ligand}/Se_{ligand}$ are between 4.1 to 8.0 Å. Usually, the approach to the active site by $S_{ligand}$ is found to be relatively closer than that of the $Se_{ligand}$. The RMSD values around 5 Åfor some of the ligands suggests that these ligands can approch the active site of GR and possibly get reduced.

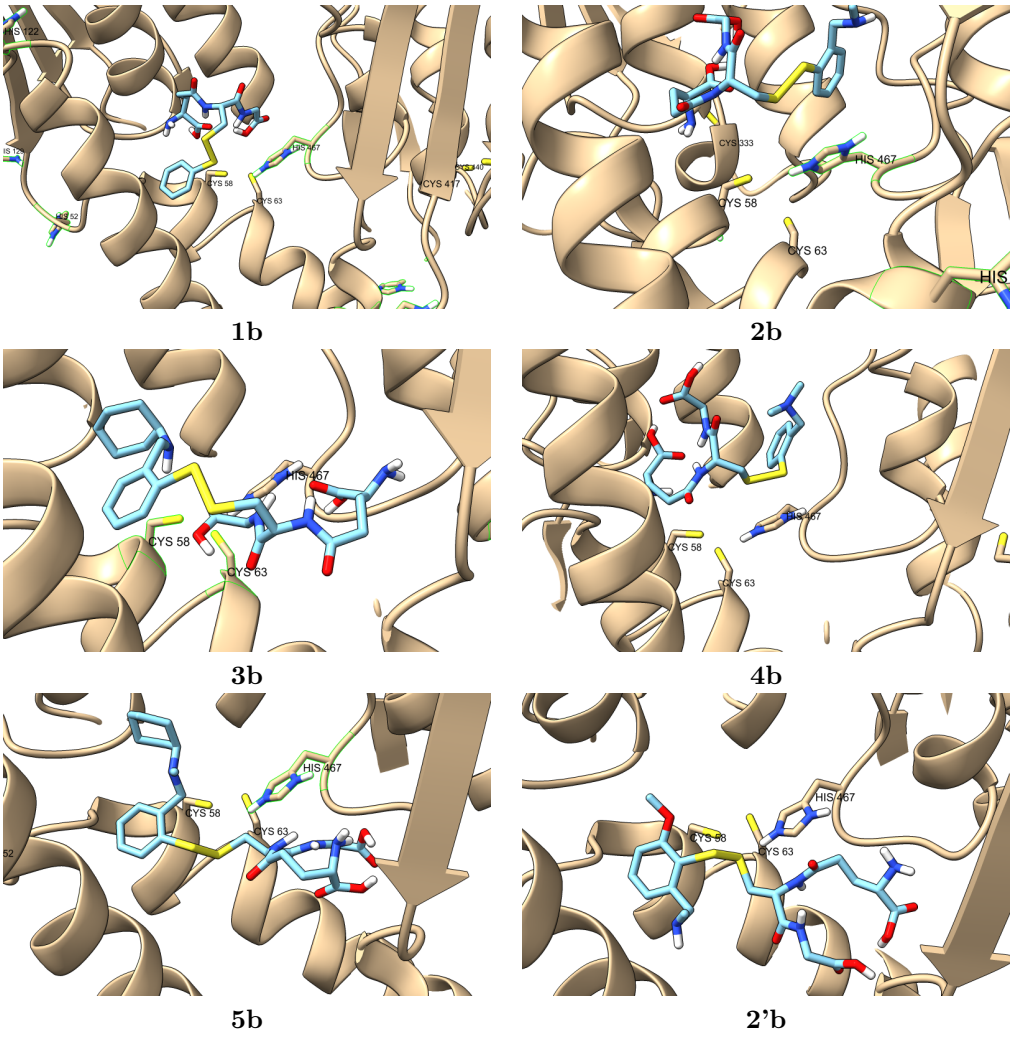



Figure S3: Best pose structure obtained from molecular docking study for (**1b**) and amine−based selenenyl sulfides **2b** to **5b** and **2'b** with glutathione reductase enzyme (PDB: 2GH5).

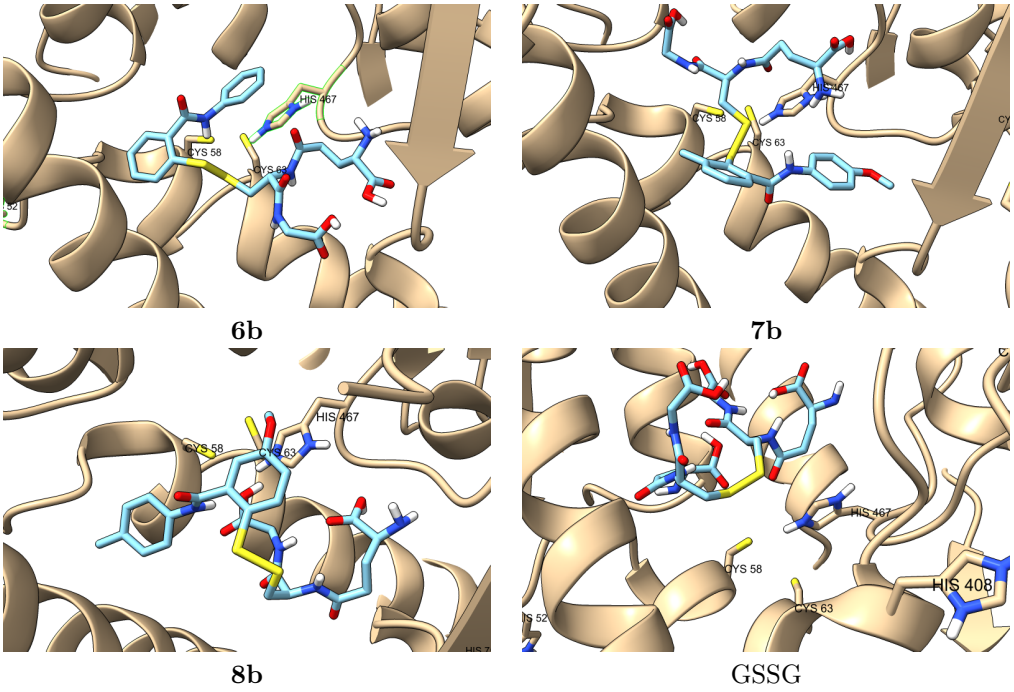



Figure S4: Best pose structure obtained from molecular docking study for ebselen−based (amide−based) senenyl sulfide **6b** to **8b**, and GSSG with glutathione reductase enzyme (PDB: 2GH5).

Table S3: Docking results of GSSG and RSeSG−type compounds with active site of GR (PDB ID: 2GH5).

| Compound | Affinity (kcal mol$^{-1}$) | Distances between atoms (Å) | | | | |
|---|---|---|---|---|---|---|
| | | $S_{ligand}$-$S_{CYS-58}$ | $Se_{ligand}$-$S_{CYS-58}$ | $S_{ligand}$-$N_{HIS-467}$ | $Se_{ligand}$-$N_{HIS-467}$ | RMSD[a] |
| **1b** | −6.1 | 8.0 | 6.3 | 8.0 | 6.4 | 6.4 |
| **2b** | −6.5 | 5.0 | 7.0 | 4.1 | 5.3 | 4.6 |
| **3b** | −7.5 | 8.0 | 8.9 | 8.2 | 7.5 | 7.8 |
| **4b** | −6.7 | 5.7 | 7.1 | 4.7 | 5.0 | 5.2 |
| **5b** | −7.2 | 5.4 | 6.8 | 5.2 | 6.9 | 5.3 |
| GSSG | −6.2 | 4.6(S1) | 5.7(S2) | 4.8(S1) | 4.5(S2) | 4.6 |
| **6b** | −7.7 | 5.5 | 6.9 | 5.3 | 6.9 | 5.4 |
| **7b** | −8.1 | 4.7 | 5.0 | 4.0 | 5.1 | 4.4 |
| **8b** | −7.3 | 8.9 | 9.6 | 8.0 | 7.9 | 8.4 |
| **2'b** | −6.8 | 4.6 | 6.1 | 4.1 | 6.1 | 4.4 |

[a] Root mean square deviation was calculated using the shortest distance of approach by $S_{ligand}$/$Se_{ligand}$.

Table S4: Elecronic energy in gas−phase ($\epsilon_0, gas$), elecronic energy in solvent ($\epsilon_0, solv$), and thermal correction to free energy ($G_{corr}, gas$) for the phenyl selenide−based RSeSG (**1b**), amine−based RSeSG (**2b** - **5b** and **2'b**), amide−based RSeSG (**6b** - **8b**) and GSSG. All energies are reported in Hartrees

| | **1b** | **2b** | **3b** | **4b** | **5b** |
|---|---|---|---|---|---|
| RSeSG | | | | | |
| $\epsilon_0, gas$ | -4037.72219 | -4171.680053 | -4367.014094 | -4210.982912 | -4406.313896 |
| $\epsilon_0, solv$ | -4037.751136 | -4171.709512 | -4367.043189 | -4211.011396 | -4406.342617 |
| $G_{corr}, gas$ | 0.310989 | 0.381205 | 0.50037 | 0.407874 | 0.527085 |
| RSeH | | | | | |
| $\epsilon_0, gas$ | -2633.765232 | -2767.722042 | -2963.054403 | -2807.024173 | -3002.353443 |
| $\epsilon_0, solv$ | -2633.769912 | -2767.727992 | -2963.059777 | -2807.029143 | -3002.358474 |
| $G_{corr}, gas$ | 0.066898 | 0.136854 | 0.25452 | 0.163726 | 0.282215 |
| | **6b** | **7b** | **8b** | **2'b** | |
| RSeSG | | | | | GSSG |
| $\epsilon_0, gas$ | -4437.469852 | -4591.299047 | -4591.306904 | -4286.199868 | -2809.083253 |
| $\epsilon_0, solv$ | -4437.504439 | -4591.334905 | -4591.340484 | -4286.230895 | -2809.137495 |
| $G_{corr}, gas$ | 0.412982 | 0.4682 | 0.470142 | 0.411504 | 0.475483 |
| RSeH | | | | | GSH |
| $\epsilon_0, gas$ | -3033.497081 | -3187.325562 | -3187.326213 | -2882.243046 | -1405.131377 |
| $\epsilon_0, solv$ | -3033.509365 | -3187.339805 | -3187.340262 | -2882.25082 | -1405.160077 |
| $G_{corr}, gas$ | 0.165675 | 0.221426 | 0.221146 | 0.167039 | 0.238003 |

# Coordinates of optimized geometries in gas phase

Table S5: Coordinates of optimized geometry of GSSG and GSH in gas phase used for benchmark study using B3LYP at 6-311++g(2df,2pd) level of theory.

| | | | |
|---|---|---|---|
| GSSG | | | |
| 7 | -6.097656000 | -1.854773000 | -3.382289000 |
| 6 | -6.105040000 | -2.701522000 | -2.198395000 |
| 6 | -7.485564000 | -3.321897000 | -2.079778000 |
| 8 | -8.507515000 | -2.802072000 | -2.444411000 |
| 8 | -7.450931000 | -4.522805000 | -1.464977000 |
| 6 | -5.780274000 | -2.012999000 | -0.849858000 |
| 6 | -4.347011000 | -1.487734000 | -0.783282000 |
| 6 | -3.994449000 | -0.950387000 | 0.597343000 |
| 8 | -4.423159000 | -1.438880000 | 1.625001000 |
| 7 | -3.145323000 | 0.129365000 | 0.607178000 |
| 6 | -2.529278000 | 0.594025000 | 1.838119000 |
| 6 | -3.316175000 | 1.693270000 | 2.584722000 |
| 8 | -2.901528000 | 2.123716000 | 3.649245000 |
| 6 | -1.106466000 | 1.110126000 | 1.610284000 |
| 16 | 0.095058000 | -0.152564000 | 1.033571000 |
| 7 | -4.443085000 | 2.136036000 | 1.993388000 |
| 6 | -5.301769000 | 3.102944000 | 2.628470000 |
| 6 | -6.484098000 | 3.388784000 | 1.736235000 |
| 8 | -6.680655000 | 2.873624000 | 0.665726000 |
| 8 | -7.305432000 | 4.297963000 | 2.287557000 |
| 7 | 4.443147000 | 2.144960000 | -1.987324000 |
| 6 | 5.300829000 | 3.114408000 | -2.619880000 |
| 6 | 6.482886000 | 3.399149000 | -1.726938000 |
| 8 | 6.680034000 | 2.881396000 | -0.657790000 |

| | | | |
|---|---|---|---|
| 8 | 7.303270000 | 4.310590000 | -2.275939000 |
| 6 | 3.316372000 | 1.703040000 | -2.579546000 |
| 8 | 2.901073000 | 2.136187000 | -3.642721000 |
| 6 | 2.530533000 | 0.601118000 | -1.835792000 |
| 7 | 3.147181000 | 0.133671000 | -0.606207000 |
| 6 | 1.107299000 | 1.115366000 | -1.606389000 |
| 16 | -0.093044000 | -0.149950000 | -1.032984000 |
| 6 | 6.104454000 | -2.709351000 | 2.190869000 |
| 6 | 7.482043000 | -3.335638000 | 2.069253000 |
| 8 | 8.506873000 | -2.820721000 | 2.432767000 |
| 8 | 7.441119000 | -4.535673000 | 1.453133000 |
| 7 | 6.102808000 | -1.863774000 | 3.375630000 |
| 6 | 5.780393000 | -2.018037000 | 0.843594000 |
| 6 | 4.349303000 | -1.486685000 | 0.779927000 |
| 6 | 3.996678000 | -0.945845000 | -0.599338000 |
| 8 | 4.425417000 | -1.431454000 | -1.628334000 |
| 1 | -5.282814000 | -1.259408000 | -3.421675000 |
| 1 | -6.930854000 | -1.279694000 | -3.414512000 |
| 1 | -5.391247000 | -3.516162000 | -2.343119000 |
| 1 | -8.365209000 | -4.828910000 | -1.374560000 |
| 1 | -6.485686000 | -1.193334000 | -0.693695000 |
| 1 | -5.922989000 | -2.720358000 | -0.033176000 |
| 1 | -3.644860000 | -2.302662000 | -0.988031000 |
| 1 | -4.167517000 | -0.719615000 | -1.538205000 |
| 1 | -2.714815000 | 0.397724000 | -0.263730000 |
| 1 | -2.502531000 | -0.246941000 | 2.532529000 |
| 1 | -1.088084000 | 1.947221000 | 0.912510000 |
| 1 | -0.718948000 | 1.464868000 | 2.563851000 |
| 1 | -4.768182000 | 1.717531000 | 1.135961000 |
| 1 | -5.665434000 | 2.746150000 | 3.595903000 |
| 1 | -4.771686000 | 4.036028000 | 2.831867000 |
| 1 | -8.047334000 | 4.435418000 | 1.680462000 |
| 1 | 4.768740000 | 1.724365000 | -1.131107000 |
| 1 | 5.664851000 | 2.760540000 | -3.588255000 |
| 1 | 4.769759000 | 4.047461000 | -2.820823000 |
| 1 | 8.045062000 | 4.447226000 | -1.668525000 |
| 1 | 2.504411000 | -0.238009000 | -2.532445000 |
| 1 | 2.716699000 | 0.399526000 | 0.265489000 |
| 1 | 0.719369000 | 1.472377000 | -2.558941000 |
| 1 | 1.088262000 | 1.950535000 | -0.906328000 |
| 1 | 5.387371000 | -3.521027000 | 2.336002000 |
| 1 | 8.353895000 | -4.845670000 | 1.360823000 |
| 1 | 6.938710000 | -1.292590000 | 3.407114000 |
| 1 | 5.290811000 | -1.264659000 | 3.416854000 |
| 1 | 5.918873000 | -2.725087000 | 0.025922000 |
| 1 | 6.488990000 | -1.201200000 | 0.687102000 |
| 1 | 4.174172000 | -0.718751000 | 1.536080000 |
| 1 | 3.643969000 | -2.298834000 | 0.984858000 |
| | | | |
| GSH | | | |
| 7 | 2.350042000 | 1.142867000 | 0.050373000 |
| 6 | 2.822225000 | 2.484448000 | 0.278874000 |
| 6 | 1.994380000 | 3.455366000 | -0.524893000 |
| 8 | 1.066365000 | 3.153610000 | -1.230695000 |
| 8 | 2.420059000 | 4.719227000 | -0.356695000 |
| 6 | 2.845749000 | 0.095630000 | 0.742371000 |
| 8 | 3.786001000 | 0.183607000 | 1.513807000 |

| | | | |
|---|---|---|---|
| 6 | 2.207536000 | -1.278416000 | 0.463349000 |
| 7 | 0.910363000 | -1.218176000 | -0.191754000 |
| 6 | 3.210885000 | -2.087209000 | -0.369612000 |
| 16 | 2.683004000 | -3.785834000 | -0.807114000 |
| 6 | -4.027515000 | -0.631618000 | -0.361134000 |
| 6 | -5.075538000 | 0.263715000 | 0.274838000 |
| 8 | -5.491315000 | 1.285790000 | -0.204796000 |
| 8 | -5.466121000 | -0.192344000 | 1.483615000 |
| 7 | -4.154879000 | -0.509831000 | -1.806278000 |
| 6 | -2.653750000 | -0.258255000 | 0.247928000 |
| 6 | -1.537294000 | -1.204838000 | -0.187323000 |
| 6 | -0.222014000 | -0.917269000 | 0.525776000 |
| 8 | -0.163564000 | -0.456350000 | 1.649390000 |
| 1 | 1.518790000 | 1.034444000 | -0.509620000 |
| 1 | 2.760792000 | 2.755957000 | 1.336284000 |
| 1 | 3.872689000 | 2.595717000 | 0.000338000 |
| 1 | 1.849917000 | 5.296722000 | -0.884998000 |
| 1 | 2.099157000 | -1.735757000 | 1.448534000 |
| 1 | 0.795295000 | -1.812294000 | -0.999243000 |
| 1 | 4.157412000 | -2.117551000 | 0.161029000 |
| 1 | 3.384830000 | -1.603231000 | -1.331819000 |
| 1 | -4.257825000 | -1.660010000 | -0.071539000 |
| 1 | -6.086856000 | 0.453975000 | 1.850627000 |
| 1 | -4.258494000 | 0.461953000 | -2.072788000 |
| 1 | -3.362385000 | -0.902512000 | -2.293931000 |
| 1 | -2.716558000 | -0.279397000 | 1.335668000 |
| 1 | -2.406435000 | 0.766343000 | -0.039113000 |
| 1 | -1.382105000 | -1.171321000 | -1.267720000 |
| 1 | -1.809267000 | -2.236802000 | 0.059823000 |
| 1 | 2.574925000 | -4.254572000 | 0.447849000 |

Table S6: Coordinates of optimized geometry of GSSG and GSH in gas phase used for benchmark study using wB97-XD at 6-311++g(2df,2pd) level of theory.

| | | | |
|---|---|---|---|
| GSSG | | | |
| 7 | 6.167026000 | -1.939730000 | 3.223699000 |
| 6 | 5.420017000 | -2.844815000 | 2.374658000 |
| 6 | 6.211075000 | -4.130167000 | 2.254133000 |
| 8 | 7.406972000 | -4.205378000 | 2.309277000 |
| 8 | 5.423116000 | -5.189554000 | 2.020055000 |
| 6 | 5.121110000 | -2.352899000 | 0.943937000 |
| 6 | 4.196902000 | -1.147980000 | 0.929597000 |
| 6 | 3.869349000 | -0.680984000 | -0.476559000 |
| 8 | 4.278069000 | -1.224973000 | -1.477823000 |
| 7 | 3.079027000 | 0.436664000 | -0.528341000 |
| 6 | 2.493793000 | 0.885763000 | -1.769459000 |
| 6 | 3.285467000 | 1.993538000 | -2.481169000 |
| 8 | 2.863899000 | 2.490940000 | -3.508348000 |
| 6 | 1.058099000 | 1.366846000 | -1.584148000 |
| 16 | -0.102597000 | 0.084594000 | -1.023219000 |
| 7 | 4.442634000 | 2.356121000 | -1.903782000 |
| 6 | 5.318716000 | 3.313987000 | -2.511940000 |
| 6 | 6.522282000 | 3.513007000 | -1.629994000 |
| 8 | 6.708019000 | 2.946066000 | -0.587745000 |
| 8 | 7.370216000 | 4.402660000 | -2.149768000 |
| 7 | -4.443206000 | 2.356403000 | 1.903369000 |
| 6 | -5.319229000 | 3.314496000 | 2.511250000 |
| 6 | -6.522562000 | 3.513683000 | 1.629024000 |
| 8 | -6.708243000 | 2.946602000 | 0.586839000 |
| 8 | -7.370407000 | 4.403587000 | 2.148511000 |
| 6 | -3.285927000 | 1.994113000 | 2.480713000 |
| 8 | -2.864286000 | 2.491850000 | 3.507701000 |
| 6 | -2.494251000 | 0.886185000 | 1.769241000 |
| 7 | -3.079510000 | 0.436788000 | 0.528244000 |
| 6 | -1.058568000 | 1.367253000 | 1.583785000 |
| 16 | 0.102158000 | 0.084876000 | 1.023204000 |
| 6 | -5.419795000 | -2.845862000 | -2.374001000 |
| 6 | -6.209286000 | -4.132159000 | -2.253286000 |
| 8 | -7.405130000 | -4.208744000 | -2.307674000 |
| 8 | -5.419951000 | -5.190681000 | -2.019932000 |
| 7 | -6.168444000 | -1.941402000 | -3.222262000 |
| 6 | -5.120457000 | -2.353994000 | -0.943352000 |
| 6 | -4.197565000 | -1.148064000 | -0.929328000 |
| 6 | -3.869793000 | -0.680899000 | 0.476722000 |
| 8 | -4.278356000 | -1.224772000 | 1.478114000 |
| 1 | 5.794712000 | -1.002671000 | 3.202900000 |
| 1 | 7.139734000 | -1.915589000 | 2.946651000 |
| 1 | 4.472098000 | -3.087286000 | 2.861319000 |
| 1 | 5.997475000 | -5.953668000 | 1.895397000 |
| 1 | 6.060762000 | -2.105965000 | 0.446657000 |
| 1 | 4.661453000 | -3.157275000 | 0.368909000 |
| 1 | 3.255625000 | -1.379441000 | 1.438302000 |
| 1 | 4.637766000 | -0.302837000 | 1.465568000 |
| 1 | 2.651181000 | 0.744875000 | 0.329481000 |
| 1 | 2.505939000 | 0.041623000 | -2.461913000 |
| 1 | 1.004826000 | 2.211819000 | -0.896261000 |
| 1 | 0.684380000 | 1.706067000 | -2.549050000 |

| | | | |
|---|---|---|---|
| 1 | 4.764045000 | 1.891854000 | -1.069978000 |
| 1 | 5.653582000 | 2.987310000 | -3.499797000 |
| 1 | 4.821407000 | 4.274863000 | -2.660571000 |
| 1 | 8.120539000 | 4.482341000 | -1.549569000 |
| 1 | -4.764598000 | 1.891981000 | 1.069646000 |
| 1 | -5.654405000 | 2.987977000 | 3.499057000 |
| 1 | -4.821737000 | 4.275268000 | 2.659918000 |
| 1 | -8.120607000 | 4.483331000 | 1.548167000 |
| 1 | -2.506367000 | 0.042202000 | 2.461885000 |
| 1 | -2.651739000 | 0.744867000 | -0.329663000 |
| 1 | -0.684851000 | 1.706756000 | 2.548586000 |
| 1 | -1.005323000 | 2.212037000 | 0.895663000 |
| 1 | -4.471938000 | -3.087112000 | -2.861393000 |
| 1 | -5.993346000 | -5.955488000 | -1.895083000 |
| 1 | -7.141005000 | -1.918549000 | -2.944589000 |
| 1 | -5.797270000 | -1.003892000 | -3.201382000 |
| 1 | -4.659523000 | -3.158027000 | -0.368860000 |
| 1 | -6.060033000 | -2.108227000 | -0.445358000 |
| 1 | -4.639705000 | -0.303301000 | -1.464854000 |
| 1 | -3.256349000 | -1.378368000 | -1.438662000 |
| | | | |
| GSH | | | |
| 7 | -1.397836000 | -1.605421000 | -0.230379000 |
| 6 | -1.166905000 | -3.019899000 | -0.189323000 |
| 6 | 0.303386000 | -3.291671000 | -0.360729000 |
| 8 | 1.147818000 | -2.447361000 | -0.494233000 |
| 8 | 0.565009000 | -4.600470000 | -0.350629000 |
| 6 | -2.540160000 | -1.073063000 | 0.248004000 |
| 8 | -3.503384000 | -1.735527000 | 0.574802000 |
| 6 | -2.602835000 | 0.459239000 | 0.294097000 |
| 7 | -1.306485000 | 1.093483000 | 0.248285000 |
| 6 | -3.477394000 | 0.915310000 | -0.874101000 |
| 16 | -3.680283000 | 2.715113000 | -1.022610000 |
| 6 | 3.241481000 | 1.586123000 | 0.309691000 |
| 6 | 4.151609000 | 0.594349000 | -0.384446000 |
| 8 | 4.384938000 | 0.592398000 | -1.561300000 |
| 8 | 4.630683000 | -0.330171000 | 0.458114000 |
| 7 | 3.319659000 | 2.841458000 | -0.405573000 |
| 6 | 1.847724000 | 0.931935000 | 0.398745000 |
| 6 | 0.837521000 | 1.791035000 | 1.162868000 |
| 6 | -0.460446000 | 1.030274000 | 1.321484000 |
| 8 | -0.702804000 | 0.335212000 | 2.284711000 |
| 1 | -0.591832000 | -1.017046000 | -0.367670000 |
| 1 | -1.498930000 | -3.443709000 | 0.761614000 |
| 1 | -1.715269000 | -3.551620000 | -0.970467000 |
| 1 | 1.516137000 | -4.712415000 | -0.460183000 |
| 1 | -3.101323000 | 0.689873000 | 1.238093000 |
| 1 | -1.198256000 | 1.858895000 | -0.397175000 |
| 1 | -4.446908000 | 0.432539000 | -0.791890000 |
| 1 | -3.030878000 | 0.607264000 | -1.821080000 |
| 1 | 3.615871000 | 1.731214000 | 1.325249000 |
| 1 | 5.134410000 | -0.963276000 | -0.065865000 |
| 1 | 3.220392000 | 2.694561000 | -1.401350000 |
| 1 | 2.627755000 | 3.504611000 | -0.091864000 |
| 1 | 1.936232000 | -0.035880000 | 0.895403000 |
| 1 | 1.487711000 | 0.741448000 | -0.615838000 |
| 1 | 0.663724000 | 2.736639000 | 0.643764000 |

| | | | |
|---|---|---|---|
| 1 | 1.208332000 | 2.009676000 | 2.163360000 |
| 1 | -4.231965000 | 2.914351000 | 0.181865000 |

Table S7: Coordinates of optimized geometry of GSSG and GSH in gas phase used for benchmark study using M06-2X at 6-311++g(2df,2pd) level of theory.

| GSSH | | | |
|---|---|---|---|
| 7 | -6.443004000 | 1.880325000 | 3.139594000 |
| 6 | -5.739304000 | 2.806307000 | 2.274482000 |
| 6 | -6.617398000 | 4.024064000 | 2.089140000 |
| 8 | -7.812449000 | 4.023082000 | 2.170211000 |
| 8 | -5.905270000 | 5.113574000 | 1.760654000 |
| 6 | -5.382203000 | 2.287303000 | 0.868601000 |
| 6 | -4.380817000 | 1.145696000 | 0.916408000 |
| 6 | -4.020384000 | 0.650288000 | -0.471938000 |
| 8 | -4.535284000 | 1.066065000 | -1.485175000 |
| 7 | -3.075572000 | -0.341097000 | -0.499428000 |
| 6 | -2.499501000 | -0.775738000 | -1.751750000 |
| 6 | -3.291972000 | -1.875814000 | -2.471685000 |
| 8 | -2.893846000 | -2.319474000 | -3.530978000 |
| 6 | -1.070379000 | -1.272688000 | -1.569807000 |
| 16 | 0.098297000 | 0.009923000 | -1.022956000 |
| 7 | -4.410924000 | -2.308448000 | -1.864998000 |
| 6 | -5.265348000 | -3.268542000 | -2.504882000 |
| 6 | -6.449601000 | -3.541060000 | -1.616801000 |
| 8 | -6.640431000 | -3.020654000 | -0.553511000 |
| 8 | -7.273450000 | -4.440640000 | -2.161849000 |
| 7 | 4.410934000 | -2.308458000 | 1.865008000 |
| 6 | 5.265288000 | -3.268642000 | 2.504850000 |
| 6 | 6.449558000 | -3.541155000 | 1.616789000 |
| 8 | 6.640485000 | -3.020630000 | 0.553574000 |
| 8 | 7.273384000 | -4.440756000 | 2.161837000 |
| 6 | 3.291952000 | -1.875857000 | 2.471662000 |
| 8 | 2.893707000 | -2.319662000 | 3.530849000 |
| 6 | 2.499499000 | -0.775768000 | 1.751727000 |
| 7 | 3.075595000 | -0.341104000 | 0.499426000 |
| 6 | 1.070375000 | -1.272705000 | 1.569753000 |
| 16 | -0.098280000 | 0.009926000 | 1.022903000 |
| 6 | 5.739334000 | 2.806330000 | -2.274441000 |
| 6 | 6.617481000 | 4.024049000 | -2.089089000 |
| 8 | 7.812531000 | 4.023017000 | -2.170169000 |
| 8 | 5.905399000 | 5.113588000 | -1.760600000 |
| 7 | 6.442989000 | 1.880329000 | -3.139569000 |
| 6 | 5.382220000 | 2.287323000 | -0.868564000 |
| 6 | 4.380802000 | 1.145745000 | -0.916384000 |
| 6 | 4.020349000 | 0.650337000 | 0.471958000 |
| 8 | 4.535209000 | 1.066140000 | 1.485205000 |
| 1 | -6.040596000 | 0.954542000 | 3.112565000 |
| 1 | -7.417520000 | 1.823432000 | 2.867805000 |
| 1 | -4.820814000 | 3.136471000 | 2.766115000 |
| 1 | -6.529632000 | 5.833051000 | 1.599492000 |
| 1 | -6.292864000 | 1.958492000 | 0.365119000 |
| 1 | -4.964405000 | 3.099580000 | 0.273116000 |
| 1 | -3.462608000 | 1.454990000 | 1.424487000 |
| 1 | -4.774384000 | 0.292571000 | 1.475596000 |
| 1 | -2.582632000 | -0.557582000 | 0.353344000 |
| 1 | -2.502680000 | 0.070894000 | -2.441561000 |
| 1 | -1.024070000 | -2.109154000 | -0.871262000 |
| 1 | -0.705490000 | -1.619374000 | -2.535183000 |

| | | | |
|---|---|---|---|
| 1 | -4.739055000 | -1.878911000 | -1.014275000 |
| 1 | -5.622768000 | -2.909556000 | -3.473165000 |
| 1 | -4.739779000 | -4.205521000 | -2.698709000 |
| 1 | -8.016381000 | -4.571026000 | -1.557758000 |
| 1 | 4.739118000 | -1.878865000 | 1.014332000 |
| 1 | 5.622691000 | -2.909746000 | 3.473172000 |
| 1 | 4.739665000 | -4.205608000 | 2.698588000 |
| 1 | 8.016359000 | -4.571090000 | 1.557789000 |
| 1 | 2.502672000 | 0.070853000 | 2.441552000 |
| 1 | 2.582704000 | -0.557632000 | -0.353365000 |
| 1 | 0.705469000 | -1.619405000 | 2.535117000 |
| 1 | 1.024070000 | -2.109159000 | 0.871193000 |
| 1 | 4.820855000 | 3.136538000 | -2.766064000 |
| 1 | 6.529793000 | 5.833038000 | -1.599439000 |
| 1 | 7.417503000 | 1.823385000 | -2.867782000 |
| 1 | 6.040536000 | 0.954565000 | -3.112554000 |
| 1 | 4.964446000 | 3.099604000 | -0.273069000 |
| 1 | 6.292874000 | 1.958481000 | -0.365089000 |
| 1 | 4.774340000 | 0.292616000 | -1.475585000 |
| 1 | 3.462600000 | 1.455075000 | -1.424454000 |
| | | | |
| GSH | | | |
| 7 | 1.296551000 | 1.605527000 | -0.255726000 |
| 6 | 0.969719000 | 3.002787000 | -0.194486000 |
| 6 | -0.514359000 | 3.173207000 | -0.378721000 |
| 8 | -1.295822000 | 2.274227000 | -0.524815000 |
| 8 | -0.864786000 | 4.462595000 | -0.362440000 |
| 6 | 2.457915000 | 1.157782000 | 0.269426000 |
| 8 | 3.353275000 | 1.891504000 | 0.629748000 |
| 6 | 2.645488000 | -0.362328000 | 0.311031000 |
| 7 | 1.401501000 | -1.094156000 | 0.238118000 |
| 6 | 3.567122000 | -0.734287000 | -0.848787000 |
| 16 | 3.919005000 | -2.511025000 | -0.990281000 |
| 6 | -3.171546000 | -1.684590000 | 0.308877000 |
| 6 | -4.113484000 | -0.700912000 | -0.350264000 |
| 8 | -4.392426000 | -0.704129000 | -1.515393000 |
| 8 | -4.559407000 | 0.225697000 | 0.510388000 |
| 7 | -3.214626000 | -2.917367000 | -0.449330000 |
| 6 | -1.801581000 | -0.985485000 | 0.402931000 |
| 6 | -0.748914000 | -1.841817000 | 1.112722000 |
| 6 | 0.508836000 | -1.018586000 | 1.273910000 |
| 8 | 0.677014000 | -0.254322000 | 2.198871000 |
| 1 | 0.530644000 | 0.965202000 | -0.401503000 |
| 1 | 1.259839000 | 3.428856000 | 0.768955000 |
| 1 | 1.487350000 | 3.584611000 | -0.959941000 |
| 1 | -1.822488000 | 4.513716000 | -0.479093000 |
| 1 | 3.147887000 | -0.557374000 | 1.261318000 |
| 1 | 1.376754000 | -1.901072000 | -0.366812000 |
| 1 | 4.491124000 | -0.171558000 | -0.754288000 |
| 1 | 3.101015000 | -0.463574000 | -1.797137000 |
| 1 | -3.532722000 | -1.868446000 | 1.322993000 |
| 1 | -5.085647000 | 0.860748000 | 0.007450000 |
| 1 | -3.165668000 | -2.722287000 | -1.442265000 |
| 1 | -2.468229000 | -3.547629000 | -0.193861000 |
| 1 | -1.913632000 | -0.045020000 | 0.944954000 |
| 1 | -1.466285000 | -0.740232000 | -0.609054000 |
| 1 | -0.543746000 | -2.754232000 | 0.550200000 |

| | | | |
|---|---|---|---|
| 1 | -1.094424000 | -2.111844000 | 2.109809000 |
| 1 | 4.472207000 | -2.650677000 | 0.220636000 |

Table S8: Coordinates of the optimized geometry of radical of **1b** at M062-X/6-311++g(2df,2pd) level of theory.

| **1b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | 0.764565000 | 1.204825000 | -0.000031000 |
| 6 | 0.068887000 | 0.000168000 | -0.000728000 |
| 6 | 2.151944000 | 1.198754000 | -0.000041000 |
| 1 | 2.686021000 | 2.139064000 | 0.000138000 |
| 6 | 0.764973000 | -1.205123000 | -0.000291000 |
| 6 | 2.850891000 | 0.000236000 | 0.000080000 |
| 1 | 3.931511000 | 0.000241000 | 0.000367000 |
| 6 | 2.151730000 | -1.198890000 | 0.000295000 |
| 1 | 2.686130000 | -2.139011000 | 0.000565000 |
| 1 | 0.228346000 | 2.144736000 | 0.000269000 |
| 34 | -1.831720000 | 0.000000000 | 0.000099000 |
| 1 | 0.228517000 | -2.144862000 | -0.000408000 |

Table S9: Coordinates of the optimized geometry of radical of **2b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **2b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | 1.895284000 | -1.079957000 | 0.202412000 |
| 6 | 0.677456000 | -0.442212000 | -0.016117000 |
| 6 | 3.074729000 | -0.349415000 | 0.220440000 |
| 1 | 4.014788000 | -0.857698000 | 0.385520000 |
| 6 | 0.643324000 | 0.945368000 | -0.198751000 |
| 6 | 3.046001000 | 1.026361000 | 0.047232000 |
| 1 | 3.961397000 | 1.600232000 | 0.076479000 |
| 6 | 1.829482000 | 1.664964000 | -0.152031000 |
| 1 | 1.797399000 | 2.740101000 | -0.279157000 |
| 1 | 1.918320000 | -2.149800000 | 0.360771000 |
| 6 | -0.677581000 | 1.617436000 | -0.449862000 |
| 1 | -0.559253000 | 2.708086000 | -0.438198000 |
| 1 | -1.039705000 | 1.336217000 | -1.444699000 |
| 7 | -1.671051000 | 1.146392000 | 0.501568000 |
| 1 | -1.397372000 | 1.371777000 | 1.449940000 |
| 34 | -0.929165000 | -1.454550000 | -0.093516000 |
| 1 | -3.334153000 | 1.127381000 | -0.740204000 |
| 1 | -3.135920000 | 2.655690000 | 0.135090000 |
| 6 | -3.028279000 | 1.566901000 | 0.209806000 |
| 1 | -3.699024000 | 1.201304000 | 0.984245000 |

Table S10: Coordinates of the optimized geometry of radical of **3b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **3b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | 3.472238000 | -0.010096000 | 0.099086000 |
| 6 | 2.091200000 | -0.126291000 | -0.027718000 |
| 6 | 4.072949000 | 1.240842000 | 0.094646000 |
| 1 | 5.147301000 | 1.316823000 | 0.191912000 |
| 6 | 1.308428000 | 1.026811000 | -0.149413000 |
| 6 | 3.299768000 | 2.387084000 | -0.016088000 |
| 1 | 3.763938000 | 3.363056000 | -0.004950000 |
| 6 | 1.920881000 | 2.271984000 | -0.130420000 |
| 1 | 1.308140000 | 3.161679000 | -0.210278000 |
| 1 | 4.076749000 | -0.901046000 | 0.204517000 |
| 6 | -0.181173000 | 0.880256000 | -0.324002000 |
| 1 | -0.664080000 | 1.858926000 | -0.224414000 |
| 1 | -0.373485000 | 0.513239000 | -1.334276000 |
| 7 | -0.667449000 | -0.119712000 | 0.609862000 |
| 1 | -0.417754000 | 0.116205000 | 1.562595000 |
| 34 | 1.260631000 | -1.836250000 | -0.053562000 |
| 6 | -2.533614000 | -0.867542000 | -0.885129000 |
| 6 | -3.172635000 | 0.407189000 | -1.447649000 |
| 6 | -4.193960000 | 1.001826000 | -0.480063000 |
| 6 | -3.561680000 | 1.245367000 | 0.888171000 |
| 6 | -3.021773000 | -0.062453000 | 1.459661000 |
| 6 | -1.995150000 | -0.741134000 | 0.542874000 |
| 1 | -1.744406000 | -1.239693000 | -1.540710000 |
| 1 | -3.301838000 | -1.644581000 | -0.856959000 |
| 1 | -3.647266000 | 0.173394000 | -2.401561000 |
| 1 | -4.601367000 | 1.928129000 | -0.886416000 |
| 1 | -5.033552000 | 0.309201000 | -0.363952000 |
| 1 | -4.289637000 | 1.678529000 | 1.575057000 |
| 1 | -2.750378000 | 1.972977000 | 0.792370000 |
| 1 | -2.576938000 | 0.092675000 | 2.445342000 |
| 1 | -3.856371000 | -0.756285000 | 1.600620000 |
| 1 | -1.846974000 | -1.757917000 | 0.918989000 |
| 1 | -2.414253000 | 1.162123000 | -1.659535000 |

Table S11: Coordinates of the optimized geometry of radical of **4b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **4b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | -2.074232000 | 1.027161000 | 0.266935000 |
| 6 | -0.831956000 | 0.487070000 | -0.056357000 |
| 6 | -3.207862000 | 0.227735000 | 0.265475000 |
| 1 | -4.166541000 | 0.661713000 | 0.514488000 |
| 6 | -0.731480000 | -0.872653000 | -0.367957000 |
| 6 | -3.110469000 | -1.123141000 | -0.035927000 |
| 1 | -3.989891000 | -1.751225000 | -0.023378000 |
| 6 | -1.870266000 | -1.665723000 | -0.342123000 |
| 1 | -1.781871000 | -2.721408000 | -0.568265000 |
| 1 | -2.151341000 | 2.075572000 | 0.522315000 |
| 6 | 0.613683000 | -1.432456000 | -0.744398000 |
| 1 | 0.593315000 | -2.531516000 | -0.718445000 |
| 1 | 0.852498000 | -1.125826000 | -1.766582000 |
| 7 | 1.656470000 | -0.898029000 | 0.117116000 |
| 6 | 1.560507000 | -1.368414000 | 1.486648000 |
| 1 | 1.754065000 | -2.448273000 | 1.555887000 |
| 1 | 2.287452000 | -0.840020000 | 2.100718000 |
| 1 | 0.563870000 | -1.165445000 | 1.875093000 |
| 34 | 0.717998000 | 1.586768000 | -0.082898000 |
| 1 | 3.028110000 | -0.579906000 | -1.417235000 |
| 1 | 3.279733000 | -2.100562000 | -0.525367000 |
| 6 | 2.988479000 | -1.044978000 | -0.433439000 |
| 1 | 3.704938000 | -0.544616000 | 0.216333000 |

Table S12: Coordinates of the optimized geometry of radical of **5b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **5b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | -3.482062000 | 0.117408000 | -0.155345000 |
| 6 | -2.090378000 | 0.161311000 | -0.155174000 |
| 6 | -4.145241000 | -1.101044000 | -0.175428000 |
| 1 | -5.226502000 | -1.119608000 | -0.178299000 |
| 6 | -1.363149000 | -1.032475000 | -0.162473000 |
| 6 | -3.426665000 | -2.287656000 | -0.175038000 |
| 1 | -3.940262000 | -3.238603000 | -0.176415000 |
| 6 | -2.039169000 | -2.244182000 | -0.160688000 |
| 1 | -1.468812000 | -3.165171000 | -0.149785000 |
| 1 | -4.046226000 | 1.040377000 | -0.137265000 |
| 6 | 0.144486000 | -0.971247000 | -0.211683000 |
| 1 | 0.561326000 | -1.959678000 | 0.025364000 |
| 1 | 0.427718000 | -0.719077000 | -1.231446000 |
| 7 | 0.645374000 | 0.072193000 | 0.666294000 |
| 6 | 0.325660000 | -0.153392000 | 2.064353000 |
| 1 | 0.821213000 | -1.046285000 | 2.465630000 |
| 1 | 0.632821000 | 0.713396000 | 2.647916000 |
| 1 | -0.749595000 | -0.278911000 | 2.177482000 |
| 34 | -1.174991000 | 1.826053000 | -0.135372000 |
| 6 | 2.350338000 | 0.845547000 | -1.029389000 |
| 6 | 3.001542000 | -0.383736000 | -1.678409000 |
| 6 | 4.130965000 | -0.956478000 | -0.825884000 |
| 6 | 3.639777000 | -1.238524000 | 0.591166000 |
| 6 | 3.124322000 | 0.048169000 | 1.228117000 |
| 6 | 1.966302000 | 0.694497000 | 0.448487000 |
| 1 | 1.483876000 | 1.181560000 | -1.600544000 |
| 1 | 3.076529000 | 1.661672000 | -1.067867000 |
| 1 | 3.377324000 | -0.099859000 | -2.662403000 |
| 1 | 4.526656000 | -1.861647000 | -1.287714000 |
| 1 | 4.955135000 | -0.238074000 | -0.775919000 |
| 1 | 4.442664000 | -1.657730000 | 1.198840000 |
| 1 | 2.843178000 | -1.988471000 | 0.562499000 |
| 1 | 2.842381000 | -0.111952000 | 2.267764000 |
| 1 | 3.940810000 | 0.776571000 | 1.243388000 |
| 1 | 1.841627000 | 1.705543000 | 0.850479000 |
| 1 | 2.269853000 | -1.174404000 | -1.848806000 |

Table S13: Coordinates of the optimized geometry of radical of **6b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **6b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | -3.539966000 | 0.772777000 | -0.098636000 |
| 6 | -2.325058000 | 0.085861000 | -0.029578000 |
| 6 | -3.581498000 | 2.148575000 | 0.021063000 |
| 1 | -4.532998000 | 2.659450000 | -0.032656000 |
| 6 | -1.141239000 | 0.813135000 | 0.147278000 |
| 6 | -2.412081000 | 2.870980000 | 0.232673000 |
| 1 | -2.444480000 | 3.943225000 | 0.359469000 |
| 6 | -1.206229000 | 2.200120000 | 0.295959000 |
| 1 | -0.308461000 | 2.767549000 | 0.503670000 |
| 1 | -4.457502000 | 0.216841000 | -0.238389000 |
| 6 | 0.144929000 | 0.057646000 | 0.202028000 |
| 8 | 0.156052000 | -1.139833000 | 0.431340000 |
| 7 | 1.275040000 | 0.782148000 | -0.036597000 |
| 1 | 1.138106000 | 1.724667000 | -0.359473000 |
| 6 | 2.614062000 | 0.348054000 | -0.028857000 |
| 6 | 3.016925000 | -0.903308000 | 0.433118000 |
| 6 | 3.570587000 | 1.250848000 | -0.495429000 |
| 1 | 2.286303000 | -1.607962000 | 0.790068000 |
| 1 | 3.256163000 | 2.223231000 | -0.854985000 |
| 6 | 4.366898000 | -1.227023000 | 0.418891000 |
| 6 | 4.911332000 | 0.912716000 | -0.503150000 |
| 1 | 4.671649000 | -2.200156000 | 0.778537000 |
| 1 | 5.637702000 | 1.624821000 | -0.869272000 |
| 6 | 5.319016000 | -0.332962000 | -0.045047000 |
| 1 | 6.365651000 | -0.601323000 | -0.050818000 |
| 34 | -2.359174000 | -1.796801000 | -0.191840000 |

Table S14: Coordinates of the optimized geometry of radical of **7b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **7b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | -4.044468000 | 0.731743000 | -0.118408000 |
| 6 | -2.803272000 | 0.078259000 | -0.017831000 |
| 6 | -4.088405000 | 2.109038000 | 0.039816000 |
| 1 | -5.045785000 | 2.609439000 | -0.031102000 |
| 6 | -1.638483000 | 0.824340000 | 0.206925000 |
| 6 | -2.943999000 | 2.849682000 | 0.304070000 |
| 1 | -3.007090000 | 3.917674000 | 0.454428000 |
| 6 | -1.726006000 | 2.205091000 | 0.385445000 |
| 1 | -0.843845000 | 2.780784000 | 0.632008000 |
| 6 | -0.335370000 | 0.098741000 | 0.276030000 |
| 8 | -0.294407000 | -1.100811000 | 0.498359000 |
| 7 | 0.778473000 | 0.850717000 | 0.059522000 |
| 1 | 0.625702000 | 1.787728000 | -0.271826000 |
| 6 | 2.125200000 | 0.430170000 | 0.066513000 |
| 6 | 2.554534000 | -0.768526000 | 0.641086000 |
| 6 | 3.065722000 | 1.277271000 | -0.502979000 |
| 1 | 1.839832000 | -1.440980000 | 1.083680000 |
| 1 | 2.744074000 | 2.208569000 | -0.953238000 |
| 6 | 3.896991000 | -1.090063000 | 0.629902000 |
| 6 | 4.416236000 | 0.955936000 | -0.512183000 |
| 1 | 4.242109000 | -2.015326000 | 1.069244000 |
| 1 | 5.115922000 | 1.640872000 | -0.965519000 |
| 6 | 4.838788000 | -0.239121000 | 0.056637000 |
| 34 | -2.757889000 | -1.806765000 | -0.193813000 |
| 6 | -5.303050000 | -0.042186000 | -0.384365000 |
| 1 | -5.241235000 | -0.574806000 | -1.335460000 |
| 1 | -5.467435000 | -0.791597000 | 0.392559000 |
| 1 | -6.166226000 | 0.618675000 | -0.416900000 |
| 8 | 6.129992000 | -0.654633000 | 0.100594000 |
| 6 | 7.105811000 | 0.182132000 | -0.474033000 |
| 1 | 6.922009000 | 0.329549000 | -1.540989000 |
| 1 | 7.136701000 | 1.154221000 | 0.024046000 |
| 1 | 8.058132000 | -0.321306000 | -0.339327000 |

Table S15: Coordinates of the optimized geometry of radical of **8b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **8b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | 3.555110000 | 0.495273000 | -0.158753000 |
| 6 | 2.224646000 | 0.889763000 | -0.063176000 |
| 6 | 3.925599000 | -0.839463000 | -0.096315000 |
| 1 | 4.970358000 | -1.099198000 | -0.173904000 |
| 6 | 1.246556000 | -0.101359000 | 0.099796000 |
| 6 | 2.952852000 | -1.816359000 | 0.091145000 |
| 6 | 1.621134000 | -1.435742000 | 0.192202000 |
| 1 | 4.325104000 | 1.245702000 | -0.279284000 |
| 6 | -0.181905000 | 0.327246000 | 0.215773000 |
| 8 | -0.464698000 | 1.460709000 | 0.561708000 |
| 7 | -1.111484000 | -0.616256000 | -0.101261000 |
| 1 | -0.759765000 | -1.468005000 | -0.504863000 |
| 6 | -2.515400000 | -0.512649000 | -0.056290000 |
| 6 | -3.195392000 | 0.565965000 | 0.500156000 |
| 6 | -3.246487000 | -1.576536000 | -0.586912000 |
| 1 | -2.648322000 | 1.396194000 | 0.911870000 |
| 1 | -2.723982000 | -2.421550000 | -1.019195000 |
| 6 | -4.584537000 | 0.559237000 | 0.512931000 |
| 6 | -4.627180000 | -1.561902000 | -0.563583000 |
| 1 | -5.100568000 | 1.404573000 | 0.950437000 |
| 1 | -5.172877000 | -2.399509000 | -0.979994000 |
| 6 | -5.326712000 | -0.489437000 | -0.013301000 |
| 34 | 1.813716000 | 2.735867000 | -0.181605000 |
| 6 | -6.830561000 | -0.473198000 | -0.008887000 |
| 1 | -7.222199000 | -0.338941000 | -1.018259000 |
| 1 | -7.232317000 | -1.410718000 | 0.375230000 |
| 1 | -7.212259000 | 0.337938000 | 0.607979000 |
| 1 | 0.898889000 | -2.216443000 | 0.390484000 |
| 8 | 3.204648000 | -3.143915000 | 0.201397000 |
| 6 | 4.548922000 | -3.564016000 | 0.130776000 |
| 1 | 4.992815000 | -3.306859000 | -0.833513000 |
| 1 | 5.143094000 | -3.120859000 | 0.932966000 |
| 1 | 4.536602000 | -4.643275000 | 0.245247000 |

Table S16: Coordinates of the optimized geometry of radical of **9b** at M06-2X/6-311++g(2df,2pd) level of theory.

| **9b** radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 6 | 1.683309000 | 0.145739000 | 0.032043000 |
| 6 | 0.288303000 | 0.119168000 | -0.100193000 |
| 6 | 2.357005000 | 1.359667000 | 0.089902000 |
| 1 | 3.430645000 | 1.386813000 | 0.196065000 |
| 6 | -0.414785000 | 1.318785000 | -0.193073000 |
| 6 | 1.642965000 | 2.549351000 | 0.014868000 |
| 1 | 2.171981000 | 3.490500000 | 0.066499000 |
| 6 | 0.267172000 | 2.530448000 | -0.123865000 |
| 1 | -0.289433000 | 3.456366000 | -0.184106000 |
| 6 | -1.905746000 | 1.277370000 | -0.386892000 |
| 1 | -2.321809000 | 2.290998000 | -0.327095000 |
| 1 | -2.123398000 | 0.892054000 | -1.389109000 |
| 7 | -2.520884000 | 0.358032000 | 0.554781000 |
| 1 | -2.343890000 | 0.648361000 | 1.508334000 |
| 34 | -0.606623000 | -1.554002000 | -0.155862000 |
| 1 | -4.039359000 | -0.380532000 | -0.653384000 |
| 1 | -4.533217000 | 1.027591000 | 0.302063000 |
| 6 | -3.929562000 | 0.111642000 | 0.313621000 |
| 1 | -4.321001000 | -0.555073000 | 1.078952000 |
| 8 | 2.295552000 | -1.062088000 | 0.084692000 |
| 6 | 3.695627000 | -1.091532000 | 0.238087000 |
| 1 | 4.195263000 | -0.608964000 | -0.604773000 |
| 1 | 4.001271000 | -0.605204000 | 1.167059000 |
| 1 | 3.974178000 | -2.140209000 | 0.270824000 |

Table S17: Coordinates of the optimized geometry of radical of GS at M06-2X/6-311++g(2df,2pd) level of theory.

| GS radical | | | |
|---|---|---|---|
| 0 | 2 | | |
| 7 | -1.397836000 | -1.605421000 | -0.230379000 |
| 6 | -1.166905000 | -3.019899000 | -0.189323000 |
| 6 | 0.303386000 | -3.291671000 | -0.360729000 |
| 8 | 1.147818000 | -2.447361000 | -0.494233000 |
| 8 | 0.565009000 | -4.600470000 | -0.350629000 |
| 6 | -2.540160000 | -1.073063000 | 0.248004000 |
| 8 | -3.503384000 | -1.735527000 | 0.574802000 |
| 6 | -2.602835000 | 0.459239000 | 0.294097000 |
| 7 | -1.306485000 | 1.093483000 | 0.248285000 |
| 6 | -3.477394000 | 0.915310000 | -0.874101000 |
| 16 | -3.680283000 | 2.715113000 | -1.022610000 |
| 6 | 3.241481000 | 1.586123000 | 0.309691000 |
| 6 | 4.151609000 | 0.594349000 | -0.384446000 |
| 8 | 4.384938000 | 0.592398000 | -1.561300000 |
| 8 | 4.630683000 | -0.330171000 | 0.458114000 |
| 7 | 3.319659000 | 2.841458000 | -0.405573000 |
| 6 | 1.847724000 | 0.931935000 | 0.398745000 |
| 6 | 0.837521000 | 1.791035000 | 1.162868000 |
| 6 | -0.460446000 | 1.030274000 | 1.321484000 |
| 8 | -0.702804000 | 0.335212000 | 2.284711000 |
| 1 | -0.591832000 | -1.017046000 | -0.367670000 |
| 1 | -1.498930000 | -3.443709000 | 0.761614000 |
| 1 | -1.715269000 | -3.551620000 | -0.970467000 |
| 1 | 1.516137000 | -4.712415000 | -0.460183000 |
| 1 | -3.101323000 | 0.689873000 | 1.238093000 |
| 1 | -1.198256000 | 1.858895000 | -0.397175000 |
| 1 | -4.446908000 | 0.432539000 | -0.791890000 |
| 1 | -3.030878000 | 0.607264000 | -1.821080000 |
| 1 | 3.615871000 | 1.731214000 | 1.325249000 |
| 1 | 5.134410000 | -0.963276000 | -0.065865000 |
| 1 | 3.220392000 | 2.694561000 | -1.401350000 |
| 1 | 2.627755000 | 3.504611000 | -0.091864000 |
| 1 | 1.936232000 | -0.035880000 | 0.895403000 |
| 1 | 1.487711000 | 0.741448000 | -0.615838000 |
| 1 | 0.663724000 | 2.736639000 | 0.643764000 |
| 1 | 1.208332000 | 2.009676000 | 2.163360000 |
| 1 | -4.231965000 | 2.914351000 | 0.181865000 |

Table S18: Coordinates of the optimized geometry of selenenyl sulfide **1b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| | | | |
|---|---|---|---|
| **1b** RSeSG | | | |
| 6 | -2.945805000 | -2.949385000 | 0.057848000 |
| 6 | -3.740990000 | -1.847167000 | 0.329863000 |
| 6 | -3.543213000 | -4.168216000 | -0.238959000 |
| 1 | -2.919433000 | -5.026413000 | -0.448325000 |
| 6 | -5.127885000 | -1.960603000 | 0.305067000 |
| 6 | -4.924259000 | -4.288814000 | -0.267139000 |
| 1 | -5.382912000 | -5.239499000 | -0.499148000 |
| 6 | -5.714885000 | -3.180348000 | 0.006728000 |
| 1 | -6.792874000 | -3.263525000 | -0.008930000 |
| 1 | -1.868437000 | -2.864686000 | 0.088314000 |
| 34 | -3.050868000 | -0.093385000 | 0.735640000 |
| 16 | -0.898281000 | -0.427792000 | 0.745570000 |
| 8 | 2.414942000 | -0.867418000 | -2.040017000 |
| 8 | 0.371769000 | 3.124400000 | -0.639917000 |
| 8 | 5.855395000 | 0.405778000 | 1.699110000 |
| 8 | 7.542432000 | -1.044178000 | 1.830834000 |
| 8 | -2.067417000 | 2.899121000 | 1.241267000 |
| 8 | -2.407394000 | 5.068720000 | 0.814211000 |
| 7 | 1.664549000 | 0.837503000 | -0.777327000 |
| 7 | 6.947189000 | -2.199494000 | -0.519763000 |
| 7 | -1.597937000 | 2.325078000 | -1.363593000 |
| 6 | 4.778346000 | -1.087309000 | -0.474897000 |
| 6 | 4.010025000 | 0.221613000 | -0.605379000 |
| 6 | 0.368676000 | 0.853773000 | -1.410762000 |
| 6 | 6.283350000 | -0.945308000 | -0.220810000 |
| 6 | 2.638219000 | -0.004767000 | -1.211325000 |
| 6 | -0.455849000 | -0.377068000 | -1.029908000 |
| 6 | -0.279116000 | 2.198658000 | -1.078999000 |
| 6 | 6.638943000 | -0.569348000 | 1.204017000 |
| 6 | -2.253443000 | 3.568083000 | -1.042234000 |
| 6 | -2.236157000 | 3.950240000 | 0.428586000 |
| 1 | 4.664970000 | -1.634707000 | -1.410489000 |
| 1 | 4.341560000 | -1.716987000 | 0.301805000 |
| 1 | 3.921584000 | 0.739752000 | 0.346297000 |
| 1 | 4.538854000 | 0.895101000 | -1.287476000 |
| 1 | 0.504419000 | 0.819658000 | -2.498543000 |
| 1 | 6.650640000 | -0.098374000 | -0.823277000 |
| 1 | 1.898714000 | 1.653585000 | -0.230791000 |
| 1 | -1.365542000 | -0.465121000 | -1.620971000 |
| 1 | 0.153992000 | -1.253774000 | -1.238972000 |
| 1 | 7.867227000 | -2.233452000 | -0.100427000 |
| 1 | 7.026966000 | -2.340766000 | -1.516754000 |
| 1 | -2.164262000 | 1.497506000 | -1.454275000 |
| 1 | -3.296215000 | 3.507268000 | -1.350496000 |
| 1 | -1.789781000 | 4.394368000 | -1.576380000 |
| 1 | 6.177342000 | 0.606010000 | 2.588037000 |
| 1 | -2.063985000 | 3.227948000 | 2.149924000 |
| 1 | -5.750972000 | -1.101329000 | 0.520683000 |
| | | | |
| **1b** RSeSH | | | |
| 6 | 0.807381000 | 1.211852000 | -0.004697000 |
| 6 | 0.098784000 | 0.015847000 | 0.003985000 |

| | | | |
|---|---|---|---|
| 6 | 2.194537000 | 1.193278000 | -0.003929000 |
| 1 | 2.737132000 | 2.128741000 | -0.007900000 |
| 6 | 0.785477000 | -1.193706000 | 0.008851000 |
| 6 | 2.883010000 | -0.011463000 | -0.001667000 |
| 1 | 3.963635000 | -0.021257000 | -0.003010000 |
| 6 | 2.172329000 | -1.203282000 | 0.003079000 |
| 1 | 2.696977000 | -2.148824000 | 0.006211000 |
| 1 | 0.282623000 | 2.157280000 | -0.013778000 |
| 34 | -1.811322000 | -0.043016000 | -0.006139000 |
| 1 | -1.984951000 | 1.399891000 | 0.172889000 |
| 1 | 0.240416000 | -2.128438000 | 0.020565000 |

Table S19: Coordinates of the optimized geometry of selenenyl sulfide **2b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **2b** RSeSG | | | |
|---|---|---|---|
| 6 | 2.338687000 | 2.854799000 | -0.576109000 |
| 6 | 3.119207000 | 1.882849000 | 0.031583000 |
| 6 | 2.864760000 | 4.114012000 | -0.832138000 |
| 1 | 2.245618000 | 4.863274000 | -1.305696000 |
| 6 | 4.440023000 | 2.167654000 | 0.397246000 |
| 6 | 4.174101000 | 4.404955000 | -0.485105000 |
| 1 | 4.588949000 | 5.382535000 | -0.686278000 |
| 6 | 4.951270000 | 3.430607000 | 0.124785000 |
| 1 | 5.973889000 | 3.650986000 | 0.404378000 |
| 1 | 1.311217000 | 2.641210000 | -0.834726000 |
| 6 | 5.278554000 | 1.126335000 | 1.086724000 |
| 1 | 6.290075000 | 1.513220000 | 1.264125000 |
| 1 | 4.842096000 | 0.908778000 | 2.067689000 |
| 7 | 5.261574000 | -0.116546000 | 0.334036000 |
| 1 | 5.691496000 | 0.017955000 | -0.572638000 |
| 34 | 2.437537000 | 0.106879000 | 0.394487000 |
| 1 | 5.254178000 | -1.456753000 | 1.923797000 |
| 1 | 6.886298000 | -1.047688000 | 1.366902000 |
| 6 | 5.856581000 | -1.239120000 | 1.040645000 |
| 1 | 5.837735000 | -2.123822000 | 0.409235000 |
| 16 | 0.274126000 | 0.510912000 | 0.515851000 |
| 8 | -3.240666000 | 0.606034000 | -2.094697000 |
| 8 | -0.963376000 | -3.183149000 | -0.522699000 |
| 8 | -6.364107000 | -0.445679000 | 1.979278000 |
| 8 | -8.092539000 | 0.954824000 | 2.107324000 |
| 8 | 1.614080000 | -2.860546000 | 1.198440000 |
| 8 | 3.580076000 | -3.634677000 | 0.463289000 |
| 7 | -2.341783000 | -0.957695000 | -0.748866000 |
| 7 | -7.703903000 | 1.919041000 | -0.369223000 |
| 7 | 0.927112000 | -2.369341000 | -1.454438000 |
| 6 | -5.495420000 | 0.885311000 | -0.384995000 |
| 6 | -4.690361000 | -0.405504000 | -0.462768000 |
| 6 | -1.085342000 | -0.978470000 | -1.455823000 |
| 6 | -6.972996000 | 0.718051000 | -0.012977000 |
| 6 | -3.371940000 | -0.188355000 | -1.181464000 |
| 6 | -0.284077000 | 0.304321000 | -1.213964000 |
| 6 | -0.372421000 | -2.279077000 | -1.071986000 |
| 6 | -7.216069000 | 0.456688000 | 1.460202000 |
| 6 | 1.737794000 | -3.502139000 | -1.079188000 |
| 6 | 2.435153000 | -3.342189000 | 0.260950000 |
| 1 | -5.466782000 | 1.354933000 | -1.368113000 |
| 1 | -5.029363000 | 1.591364000 | 0.304066000 |
| 1 | -4.517886000 | -0.838346000 | 0.519461000 |
| 1 | -5.239979000 | -1.149775000 | -1.047905000 |
| 1 | -1.288501000 | -1.026458000 | -2.532480000 |
| 1 | -7.347780000 | -0.189858000 | -0.513483000 |
| 1 | -2.501542000 | -1.719909000 | -0.106713000 |
| 1 | 0.578316000 | 0.376535000 | -1.875000000 |
| 1 | -0.941466000 | 1.139862000 | -1.447992000 |
| 1 | -8.596260000 | 1.956472000 | 0.105909000 |
| 1 | -7.852029000 | 1.972004000 | -1.367022000 |
| 1 | 1.413243000 | -1.524327000 | -1.707032000 |

| | | | |
|---|---|---|---|
| 1 | 2.502894000 | -3.687661000 | -1.827208000 |
| 1 | 1.085318000 | -4.372645000 | -1.009060000 |
| 1 | -6.615617000 | -0.576254000 | 2.903135000 |
| 1 | 2.119841000 | -2.751149000 | 2.014726000 |
| | | | |
| **2b** RSeH | | | |
| 6 | 1.964926000 | -0.951187000 | 0.246526000 |
| 6 | 0.707446000 | -0.421058000 | -0.019383000 |
| 6 | 3.082825000 | -0.130446000 | 0.271753000 |
| 1 | 4.054677000 | -0.558505000 | 0.475447000 |
| 6 | 0.562775000 | 0.949782000 | -0.253423000 |
| 6 | 2.949748000 | 1.231223000 | 0.047845000 |
| 1 | 3.815572000 | 1.877667000 | 0.074081000 |
| 6 | 1.692814000 | 1.759182000 | -0.207314000 |
| 1 | 1.579342000 | 2.821525000 | -0.384152000 |
| 1 | 2.071536000 | -2.009898000 | 0.439666000 |
| 6 | -0.788972000 | 1.537550000 | -0.550407000 |
| 1 | -0.687608000 | 2.608167000 | -0.774322000 |
| 1 | -1.199551000 | 1.058143000 | -1.445336000 |
| 7 | -1.714857000 | 1.268855000 | 0.537443000 |
| 1 | -1.373605000 | 1.687924000 | 1.393388000 |
| 34 | -0.837475000 | -1.559381000 | -0.066371000 |
| 1 | -3.462953000 | 1.094582000 | -0.574020000 |
| 1 | -3.151249000 | 2.751306000 | -0.032550000 |
| 6 | -3.073061000 | 1.693264000 | 0.250484000 |
| 1 | -3.703783000 | 1.518348000 | 1.119685000 |
| 1 | -0.055231000 | -2.722154000 | -0.513869000 |

Table S20: Coordinates of the optimized geometry of selenenyl sulfide **3b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **3b** RSeSG | | | |
|---|---|---|---|
| 6 | 2.118874000 | 2.806745000 | -0.629397000 |
| 6 | 2.893470000 | 1.888042000 | 0.065666000 |
| 6 | 2.656713000 | 4.024135000 | -1.023129000 |
| 1 | 2.038762000 | 4.729333000 | -1.561480000 |
| 6 | 4.222795000 | 2.191961000 | 0.379791000 |
| 6 | 3.976610000 | 4.328203000 | -0.731797000 |
| 1 | 4.403446000 | 5.271202000 | -1.042866000 |
| 6 | 4.747819000 | 3.410034000 | -0.034923000 |
| 1 | 5.779034000 | 3.639889000 | 0.202355000 |
| 1 | 1.084308000 | 2.586705000 | -0.849682000 |
| 6 | 5.057873000 | 1.240861000 | 1.194506000 |
| 1 | 6.104696000 | 1.581657000 | 1.209829000 |
| 1 | 4.695672000 | 1.257915000 | 2.227027000 |
| 7 | 4.943219000 | -0.126224000 | 0.720563000 |
| 6 | 5.540809000 | -0.319306000 | -0.588566000 |
| 1 | 6.628207000 | -0.150486000 | -0.571056000 |
| 1 | 5.348525000 | -1.339067000 | -0.918884000 |
| 1 | 5.097122000 | 0.373137000 | -1.303709000 |
| 34 | 2.190897000 | 0.155850000 | 0.582659000 |
| 1 | 4.906519000 | -0.973621000 | 2.626609000 |
| 1 | 6.526180000 | -0.905013000 | 1.902032000 |
| 6 | 5.459446000 | -1.073813000 | 1.691329000 |
| 1 | 5.332022000 | -2.085321000 | 1.312495000 |
| 16 | 0.021426000 | 0.571872000 | 0.559697000 |
| 8 | -3.410899000 | 0.568615000 | -2.107512000 |
| 8 | -1.054827000 | -3.148742000 | -0.454757000 |
| 8 | -6.527097000 | -0.498524000 | 1.970235000 |
| 8 | -8.269400000 | 0.885216000 | 2.092787000 |
| 8 | 1.770710000 | -2.973849000 | 1.129468000 |
| 8 | 3.689808000 | -3.328547000 | 0.034967000 |
| 7 | -2.494171000 | -0.969248000 | -0.744987000 |
| 7 | -7.887215000 | 1.847150000 | -0.385628000 |
| 7 | 0.787639000 | -2.340081000 | -1.483866000 |
| 6 | -5.668494000 | 0.835382000 | -0.395985000 |
| 6 | -4.850905000 | -0.447850000 | -0.470076000 |
| 6 | -1.231467000 | -0.968497000 | -1.438967000 |
| 6 | -7.144867000 | 0.654377000 | -0.025525000 |
| 6 | -3.533545000 | -0.218694000 | -1.186804000 |
| 6 | -0.453461000 | 0.326600000 | -1.188172000 |
| 6 | -0.495492000 | -2.252951000 | -1.048335000 |
| 6 | -7.387236000 | 0.394161000 | 1.447992000 |
| 6 | 1.615422000 | -3.481640000 | -1.175934000 |
| 6 | 2.492060000 | -3.255797000 | 0.041957000 |
| 1 | -5.643168000 | 1.303108000 | -1.380105000 |
| 1 | -5.210163000 | 1.547217000 | 0.292310000 |
| 1 | -4.676246000 | -0.877207000 | 0.513277000 |
| 1 | -5.392322000 | -1.198088000 | -1.055163000 |
| 1 | -1.423651000 | -1.020252000 | -2.517275000 |
| 1 | -7.509897000 | -0.258430000 | -0.524337000 |
| 1 | -2.637402000 | -1.716272000 | -0.081690000 |
| 1 | 0.435748000 | 0.397845000 | -1.812927000 |
| 1 | -1.109520000 | 1.150440000 | -1.464778000 |

| | | | |
|---|---|---|---|
| 1 | -8.780379000 | 1.877025000 | 0.088518000 |
| 1 | -8.034751000 | 1.896181000 | -1.383710000 |
| 1 | 1.250350000 | -1.503105000 | -1.797453000 |
| 1 | 2.267325000 | -3.715220000 | -2.012813000 |
| 1 | 0.953645000 | -4.323415000 | -0.975467000 |
| 1 | -6.777948000 | -0.628951000 | 2.894293000 |
| 1 | 2.379366000 | -2.772329000 | 1.853249000 |
| | | | |
| **3b** RSeH | | | |
| 6 | 2.199869000 | -0.738267000 | 0.331420000 |
| 6 | 0.895080000 | -0.436906000 | -0.044089000 |
| 6 | 3.183262000 | 0.238930000 | 0.301540000 |
| 1 | 4.194104000 | -0.012024000 | 0.592067000 |
| 6 | 0.566062000 | 0.861036000 | -0.443608000 |
| 6 | 2.865962000 | 1.531544000 | -0.087714000 |
| 1 | 3.625394000 | 2.300457000 | -0.104029000 |
| 6 | 1.561706000 | 1.831733000 | -0.450607000 |
| 1 | 1.302685000 | 2.839402000 | -0.751309000 |
| 1 | 2.448549000 | -1.740470000 | 0.652907000 |
| 6 | -0.839149000 | 1.196511000 | -0.866147000 |
| 1 | -0.894097000 | 2.255752000 | -1.164700000 |
| 1 | -1.095672000 | 0.594044000 | -1.742031000 |
| 7 | -1.803193000 | 0.883562000 | 0.175876000 |
| 6 | -1.656461000 | 1.752307000 | 1.328221000 |
| 1 | -1.859330000 | 2.806201000 | 1.078105000 |
| 1 | -2.351278000 | 1.443251000 | 2.107609000 |
| 1 | -0.643524000 | 1.680944000 | 1.721929000 |
| 34 | -0.463464000 | -1.793078000 | -0.011038000 |
| 1 | -3.253406000 | 0.173239000 | -1.143544000 |
| 1 | -3.453541000 | 1.888154000 | -0.713994000 |
| 6 | -3.159316000 | 0.896965000 | -0.334123000 |
| 1 | -3.850709000 | 0.617464000 | 0.459706000 |
| 1 | 0.508855000 | -2.869832000 | -0.257901000 |

Table S21: Coordinates of the optimized geometry of selenenyl sulfide **4b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **4b** RSeSG | | | |
|---|---|---|---|
| 6 | 1.171017000 | 3.252406000 | -0.608268000 |
| 6 | 2.062126000 | 2.280465000 | -0.182106000 |
| 6 | 1.589771000 | 4.569845000 | -0.745306000 |
| 1 | 0.886270000 | 5.320022000 | -1.078965000 |
| 6 | 3.386577000 | 2.619783000 | 0.119682000 |
| 6 | 2.899852000 | 4.917136000 | -0.459271000 |
| 1 | 3.230570000 | 5.940303000 | -0.569213000 |
| 6 | 3.788725000 | 3.940177000 | -0.031048000 |
| 1 | 4.814178000 | 4.203208000 | 0.196795000 |
| 1 | 0.143259000 | 2.990445000 | -0.817348000 |
| 6 | 4.345462000 | 1.560583000 | 0.602785000 |
| 1 | 5.335205000 | 2.005601000 | 0.760285000 |
| 1 | 3.992345000 | 1.198464000 | 1.570675000 |
| 7 | 4.311693000 | 0.450464000 | -0.332039000 |
| 1 | 4.571515000 | 0.760527000 | -1.260106000 |
| 34 | 1.542747000 | 0.426799000 | 0.024229000 |
| 6 | 4.751860000 | -1.288962000 | 1.421177000 |
| 6 | 5.846456000 | -0.733768000 | 2.339814000 |
| 6 | 7.241366000 | -0.983545000 | 1.770656000 |
| 6 | 7.353015000 | -0.414523000 | 0.358319000 |
| 6 | 6.311436000 | -1.059701000 | -0.551377000 |
| 6 | 4.872459000 | -0.878325000 | -0.049716000 |
| 1 | 3.758825000 | -1.023004000 | 1.792169000 |
| 1 | 4.804001000 | -2.380083000 | 1.439258000 |
| 1 | 5.751769000 | -1.194910000 | 3.324001000 |
| 1 | 7.997207000 | -0.546280000 | 2.423989000 |
| 1 | 7.434348000 | -2.060255000 | 1.735540000 |
| 1 | 8.353133000 | -0.580757000 | -0.043870000 |
| 1 | 7.202968000 | 0.668845000 | 0.388192000 |
| 1 | 6.386800000 | -0.672390000 | -1.570446000 |
| 1 | 6.513395000 | -2.133671000 | -0.610536000 |
| 1 | 4.247372000 | -1.575568000 | -0.615139000 |
| 1 | 5.722810000 | 0.340015000 | 2.489846000 |
| 16 | -0.631281000 | 0.638302000 | 0.342466000 |
| 8 | -4.335655000 | 0.608629000 | -2.006605000 |
| 8 | -1.705491000 | -3.082473000 | -0.802574000 |
| 8 | -7.087174000 | -0.880413000 | 2.201994000 |
| 8 | -8.879223000 | 0.399704000 | 2.541223000 |
| 8 | 0.942878000 | -2.599971000 | 0.762424000 |
| 8 | 2.760258000 | -3.637270000 | -0.025842000 |
| 7 | -3.237265000 | -0.945128000 | -0.804516000 |
| 7 | -8.721734000 | 1.545253000 | 0.116846000 |
| 7 | 0.065672000 | -2.087069000 | -1.785576000 |
| 6 | -6.464494000 | 0.653421000 | -0.117371000 |
| 6 | -5.592321000 | -0.576884000 | -0.332992000 |
| 6 | -2.036206000 | -0.844586000 | -1.596514000 |
| 6 | -7.900044000 | 0.371171000 | 0.339976000 |
| 6 | -4.346178000 | -0.233548000 | -1.127526000 |
| 6 | -1.309257000 | 0.480649000 | -1.348892000 |
| 6 | -1.212393000 | -2.108099000 | -1.328746000 |
| 6 | -8.023500000 | -0.000139000 | 1.804361000 |
| 6 | 0.954816000 | -3.193771000 | -1.541279000 |

| | | | |
|---|---|---|---|
| 6 | 1.669977000 | -3.168364000 | -0.200755000 |
| 1 | -6.532730000 | 1.183004000 | -1.067555000 |
| 1 | -5.993599000 | 1.343897000 | 0.584095000 |
| 1 | -5.323044000 | -1.055113000 | 0.605372000 |
| 1 | -6.138611000 | -1.318313000 | -0.924746000 |
| 1 | -2.313021000 | -0.860641000 | -2.657697000 |
| 1 | -8.256413000 | -0.523752000 | -0.196090000 |
| 1 | -3.300883000 | -1.747205000 | -0.195217000 |
| 1 | -0.507326000 | 0.644909000 | -2.067068000 |
| 1 | -2.038382000 | 1.276273000 | -1.490331000 |
| 1 | -9.579435000 | 1.496341000 | 0.651058000 |
| 1 | -8.941871000 | 1.654065000 | -0.862967000 |
| 1 | 0.485573000 | -1.197998000 | -2.004277000 |
| 1 | 1.717459000 | -3.247164000 | -2.313302000 |
| 1 | 0.370037000 | -4.113884000 | -1.567783000 |
| 1 | -7.265752000 | -1.086588000 | 3.129050000 |
| 1 | 1.462681000 | -2.611158000 | 1.577508000 |
| | | | |
| **4b** RSeH | | | |
| 6 | 3.468359000 | 0.210472000 | 0.104811000 |
| 6 | 2.109986000 | -0.043570000 | -0.042294000 |
| 6 | 3.947196000 | 1.512431000 | 0.075425000 |
| 1 | 5.007202000 | 1.693838000 | 0.188183000 |
| 6 | 1.214953000 | 1.016800000 | -0.213885000 |
| 6 | 3.067992000 | 2.571623000 | -0.085798000 |
| 1 | 3.433107000 | 3.588870000 | -0.100353000 |
| 6 | 1.711371000 | 2.315302000 | -0.224075000 |
| 1 | 1.016750000 | 3.136460000 | -0.350764000 |
| 1 | 4.156508000 | -0.611439000 | 0.248361000 |
| 6 | -0.259474000 | 0.756585000 | -0.389946000 |
| 1 | -0.769392000 | 1.710495000 | -0.575774000 |
| 1 | -0.389738000 | 0.138128000 | -1.280704000 |
| 7 | -0.751135000 | 0.012015000 | 0.753595000 |
| 1 | -0.562440000 | 0.511314000 | 1.613090000 |
| 34 | 1.447465000 | -1.844979000 | -0.009026000 |
| 6 | -2.561474000 | -1.105374000 | -0.574615000 |
| 6 | -3.190512000 | -0.019705000 | -1.455475000 |
| 6 | -4.248836000 | 0.780085000 | -0.698260000 |
| 6 | -3.668082000 | 1.358181000 | 0.590100000 |
| 6 | -3.144293000 | 0.235519000 | 1.481002000 |
| 6 | -2.072342000 | -0.624171000 | 0.796022000 |
| 1 | -1.748197000 | -1.613492000 | -1.096001000 |
| 1 | -3.324724000 | -1.864157000 | -0.382269000 |
| 1 | -3.631258000 | -0.489377000 | -2.336167000 |
| 1 | -4.645629000 | 1.573394000 | -1.332910000 |
| 1 | -5.088961000 | 0.125609000 | -0.444810000 |
| 1 | -4.422778000 | 1.937562000 | 1.123578000 |
| 1 | -2.855328000 | 2.049132000 | 0.347804000 |
| 1 | -2.740597000 | 0.632502000 | 2.415517000 |
| 1 | -3.980823000 | -0.415640000 | 1.754891000 |
| 1 | -1.939532000 | -1.519347000 | 1.411434000 |
| 1 | -2.430958000 | 0.670844000 | -1.824063000 |
| 1 | 2.711854000 | -2.394601000 | -0.525383000 |

Table S22: Coordinates of the optimized geometry of selenenyl sulfide **5b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **5b** RSeSG | | | |
|---|---|---|---|
| 6 | 1.081027000 | 3.339599000 | -0.318912000 |
| 6 | 1.984447000 | 2.333246000 | -0.013520000 |
| 6 | 1.509178000 | 4.657398000 | -0.414956000 |
| 1 | 0.794509000 | 5.433019000 | -0.652974000 |
| 6 | 3.334220000 | 2.638888000 | 0.196614000 |
| 6 | 2.842706000 | 4.972130000 | -0.211865000 |
| 1 | 3.181806000 | 5.995405000 | -0.290848000 |
| 6 | 3.744995000 | 3.960303000 | 0.086768000 |
| 1 | 4.791121000 | 4.195744000 | 0.238543000 |
| 1 | 0.037035000 | 3.100880000 | -0.465157000 |
| 6 | 4.320946000 | 1.547107000 | 0.546155000 |
| 1 | 5.339432000 | 1.961691000 | 0.526188000 |
| 1 | 4.112176000 | 1.229379000 | 1.566760000 |
| 7 | 4.139223000 | 0.409075000 | -0.331892000 |
| 6 | 4.369724000 | 0.714186000 | -1.728928000 |
| 1 | 5.413830000 | 0.976395000 | -1.946735000 |
| 1 | 4.101951000 | -0.151940000 | -2.335405000 |
| 1 | 3.742686000 | 1.551214000 | -2.035375000 |
| 34 | 1.453355000 | 0.476278000 | 0.130749000 |
| 6 | 4.387497000 | -1.264121000 | 1.546522000 |
| 6 | 5.551679000 | -0.826226000 | 2.446323000 |
| 6 | 6.904005000 | -1.268897000 | 1.893477000 |
| 6 | 7.070103000 | -0.797794000 | 0.451524000 |
| 6 | 5.953518000 | -1.372891000 | -0.414091000 |
| 6 | 4.549859000 | -0.952849000 | 0.052704000 |
| 1 | 3.443634000 | -0.852837000 | 1.909861000 |
| 1 | 4.298798000 | -2.352047000 | 1.612061000 |
| 1 | 5.397859000 | -1.239003000 | 3.444433000 |
| 1 | 7.708421000 | -0.887152000 | 2.523166000 |
| 1 | 6.970681000 | -2.360857000 | 1.916813000 |
| 1 | 8.041206000 | -1.101525000 | 0.058679000 |
| 1 | 7.043999000 | 0.296167000 | 0.416850000 |
| 1 | 6.098273000 | -1.115444000 | -1.462707000 |
| 1 | 5.994518000 | -2.464894000 | -0.358624000 |
| 1 | 3.842156000 | -1.601119000 | -0.478102000 |
| 1 | 5.570768000 | 0.258379000 | 2.563994000 |
| 16 | -0.732025000 | 0.677552000 | 0.408939000 |
| 8 | -4.385408000 | 0.649533000 | -2.009546000 |
| 8 | -1.736794000 | -3.040805000 | -0.855708000 |
| 8 | -7.172803000 | -0.934969000 | 2.135240000 |
| 8 | -8.995506000 | 0.305069000 | 2.459395000 |
| 8 | 0.865425000 | -2.560358000 | 0.776756000 |
| 8 | 2.545707000 | -3.849512000 | 0.060648000 |
| 7 | -3.288392000 | -0.915594000 | -0.820828000 |
| 7 | -8.828188000 | 1.472871000 | 0.046301000 |
| 7 | 0.046764000 | -1.998828000 | -1.760582000 |
| 6 | -6.551371000 | 0.625343000 | -0.165287000 |
| 6 | -5.655930000 | -0.587421000 | -0.384346000 |
| 6 | -2.074426000 | -0.782785000 | -1.588269000 |
| 6 | -7.987157000 | 0.312860000 | 0.271212000 |
| 6 | -4.400539000 | -0.211377000 | -1.148947000 |
| 6 | -1.369512000 | 0.546102000 | -1.299492000 |

| | | | |
|---|---|---|---|
| 6 | -1.242067000 | -2.044063000 | -1.337389000 |
| 6 | -8.122027000 | -0.071631000 | 1.731204000 |
| 6 | 0.927203000 | -3.116555000 | -1.542617000 |
| 6 | 1.548988000 | -3.218850000 | -0.159237000 |
| 1 | -6.616982000 | 1.165265000 | -1.109785000 |
| 1 | -6.100633000 | 1.315215000 | 0.549879000 |
| 1 | -5.396622000 | -1.076742000 | 0.551148000 |
| 1 | -6.179240000 | -1.327328000 | -0.998369000 |
| 1 | -2.332379000 | -0.778506000 | -2.654402000 |
| 1 | -8.319878000 | -0.584561000 | -0.275782000 |
| 1 | -3.353846000 | -1.732173000 | -0.231421000 |
| 1 | -0.553614000 | 0.733630000 | -1.996083000 |
| 1 | -2.105076000 | 1.335310000 | -1.442841000 |
| 1 | -9.691079000 | 1.403935000 | 0.569858000 |
| 1 | -9.038753000 | 1.584443000 | -0.935301000 |
| 1 | 0.471216000 | -1.099810000 | -1.923715000 |
| 1 | 1.744536000 | -3.098018000 | -2.259355000 |
| 1 | 0.365048000 | -4.038377000 | -1.694803000 |
| 1 | -7.358945000 | -1.150998000 | 3.058553000 |
| 1 | 1.326504000 | -2.671580000 | 1.619325000 |
| | | | |
| **5b** RSeH | | | |
| 6 | 3.407368000 | -0.304994000 | -0.239563000 |
| 6 | 2.018044000 | -0.282066000 | -0.172444000 |
| 6 | 4.119371000 | 0.860360000 | -0.477897000 |
| 1 | 5.198695000 | 0.825406000 | -0.532542000 |
| 6 | 1.328915000 | 0.922559000 | -0.330013000 |
| 6 | 3.446780000 | 2.062906000 | -0.634202000 |
| 1 | 3.994343000 | 2.977699000 | -0.812021000 |
| 6 | 2.062919000 | 2.083170000 | -0.553596000 |
| 1 | 1.530142000 | 3.019239000 | -0.667158000 |
| 1 | 3.936208000 | -1.238300000 | -0.102163000 |
| 6 | -0.177619000 | 0.977808000 | -0.272469000 |
| 1 | -0.493617000 | 2.009805000 | -0.488322000 |
| 1 | -0.574626000 | 0.338993000 | -1.060554000 |
| 7 | -0.695715000 | 0.507587000 | 1.005591000 |
| 6 | -0.249762000 | 1.374486000 | 2.085823000 |
| 1 | -0.636146000 | 2.401898000 | 1.996993000 |
| 1 | -0.572877000 | 0.965350000 | 3.041117000 |
| 1 | 0.837700000 | 1.427478000 | 2.091644000 |
| 34 | 1.039879000 | -1.901809000 | 0.142003000 |
| 6 | -2.582899000 | -1.095377000 | 0.510940000 |
| 6 | -2.857733000 | -1.155879000 | -0.991648000 |
| 6 | -3.837745000 | -0.060033000 | -1.404525000 |
| 6 | -3.318314000 | 1.320247000 | -1.007175000 |
| 6 | -3.036731000 | 1.403064000 | 0.497123000 |
| 6 | -2.152003000 | 0.272110000 | 1.064273000 |
| 1 | -1.845696000 | -1.840077000 | 0.807612000 |
| 1 | -3.517594000 | -1.354369000 | 1.018839000 |
| 1 | -3.267309000 | -2.137065000 | -1.237528000 |
| 1 | -4.025641000 | -0.097845000 | -2.478254000 |
| 1 | -4.797635000 | -0.237125000 | -0.908192000 |
| 1 | -4.049302000 | 2.085801000 | -1.273116000 |
| 1 | -2.419680000 | 1.541964000 | -1.584214000 |
| 1 | -2.605346000 | 2.373613000 | 0.753326000 |
| 1 | -3.997956000 | 1.351975000 | 1.016705000 |
| 1 | -2.355552000 | 0.227355000 | 2.135009000 |

| | | | |
|---|---|---|---|
| 1 | -1.931753000 | -1.065808000 | -1.562553000 |
| 1 | 2.084210000 | -2.737767000 | -0.469612000 |

Table S23: Coordinates of the optimized geometry of selenenyl sulfide **6b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **6b** RSeSG | | | |
|---|---|---|---|
| 7 | 1.492668000 | -1.802761000 | -1.686110000 |
| 6 | 2.022478000 | -3.135037000 | -1.768701000 |
| 6 | 3.459074000 | -3.130423000 | -1.320308000 |
| 8 | 4.051622000 | -2.164723000 | -0.923814000 |
| 8 | 4.005482000 | -4.345268000 | -1.418500000 |
| 6 | 0.153775000 | -1.606053000 | -1.673983000 |
| 8 | -0.646475000 | -2.491439000 | -1.880581000 |
| 6 | -0.321499000 | -0.164088000 | -1.467419000 |
| 7 | 0.651238000 | 0.655665000 | -0.778045000 |
| 6 | -0.663318000 | 0.408812000 | -2.838912000 |
| 16 | -1.205608000 | 2.150984000 | -2.837222000 |
| 6 | 4.584360000 | 1.376696000 | 1.482487000 |
| 6 | 5.849004000 | 0.630924000 | 1.115159000 |
| 8 | 6.599507000 | 0.957706000 | 0.240686000 |
| 8 | 6.006956000 | -0.483131000 | 1.844056000 |
| 7 | 4.768878000 | 2.768169000 | 1.128634000 |
| 6 | 3.423411000 | 0.642104000 | 0.784777000 |
| 6 | 2.059471000 | 1.257397000 | 1.112353000 |
| 6 | 0.985275000 | 0.384914000 | 0.510907000 |
| 8 | 0.527973000 | -0.583150000 | 1.098173000 |
| 1 | 2.120599000 | -1.077401000 | -1.375060000 |
| 1 | 1.454326000 | -3.820843000 | -1.135542000 |
| 1 | 1.972655000 | -3.538991000 | -2.782103000 |
| 1 | 4.922619000 | -4.287458000 | -1.120188000 |
| 1 | -1.237788000 | -0.248538000 | -0.879786000 |
| 1 | 0.846991000 | 1.572771000 | -1.152055000 |
| 1 | -1.431773000 | -0.215012000 | -3.287954000 |
| 1 | 0.215404000 | 0.400482000 | -3.488554000 |
| 1 | 4.444353000 | 1.290040000 | 2.562191000 |
| 1 | 6.782543000 | -0.946784000 | 1.502412000 |
| 1 | 5.195739000 | 2.845279000 | 0.213039000 |
| 1 | 3.899949000 | 3.282477000 | 1.138350000 |
| 1 | 3.425376000 | -0.405250000 | 1.091441000 |
| 1 | 3.597679000 | 0.665265000 | -0.294877000 |
| 1 | 1.981566000 | 2.275024000 | 0.727059000 |
| 1 | 1.901051000 | 1.278622000 | 2.189726000 |
| 6 | -1.140995000 | 3.599372000 | 0.257732000 |
| 6 | -1.965489000 | 2.482282000 | 0.179827000 |
| 6 | -0.431720000 | 3.863170000 | 1.419287000 |
| 1 | 0.192163000 | 4.745073000 | 1.477072000 |
| 6 | -2.077715000 | 1.625865000 | 1.272292000 |
| 6 | -0.534028000 | 3.006492000 | 2.508443000 |
| 1 | 0.013400000 | 3.213216000 | 3.417762000 |
| 6 | -1.347698000 | 1.888130000 | 2.429208000 |
| 1 | -1.431614000 | 1.211493000 | 3.269696000 |
| 1 | -1.057244000 | 4.261730000 | -0.593294000 |
| 6 | -3.024671000 | 0.457061000 | 1.221282000 |
| 8 | -4.195646000 | 0.625362000 | 0.949459000 |
| 7 | -2.434432000 | -0.735492000 | 1.495526000 |
| 1 | -1.420579000 | -0.733136000 | 1.538990000 |
| 6 | -3.033833000 | -2.011185000 | 1.476251000 |
| 6 | -4.406992000 | -2.207590000 | 1.594957000 |

| | | | |
|---|---|---|---|
| 6 | -2.179763000 | -3.105928000 | 1.352420000 |
| 1 | -5.067500000 | -1.361153000 | 1.680164000 |
| 1 | -1.115958000 | -2.934567000 | 1.242086000 |
| 6 | -4.906290000 | -3.502819000 | 1.590883000 |
| 6 | -2.693444000 | -4.389964000 | 1.351761000 |
| 1 | -5.973369000 | -3.652605000 | 1.681929000 |
| 1 | -2.022951000 | -5.231841000 | 1.248908000 |
| 6 | -4.061782000 | -4.595966000 | 1.471281000 |
| 1 | -4.464610000 | -5.598869000 | 1.466870000 |
| 34 | -2.914199000 | 2.106715000 | -1.462073000 |
| | | | |
| **6b** RSeH | | | |
| 6 | -3.497919000 | 0.841526000 | -0.139360000 |
| 6 | -2.309748000 | 0.118585000 | -0.036688000 |
| 6 | -3.513451000 | 2.215905000 | 0.019380000 |
| 1 | -4.450709000 | 2.749201000 | -0.060502000 |
| 6 | -1.119827000 | 0.812508000 | 0.211766000 |
| 6 | -2.339436000 | 2.902586000 | 0.297154000 |
| 1 | -2.349422000 | 3.972101000 | 0.449193000 |
| 6 | -1.154507000 | 2.196182000 | 0.389198000 |
| 1 | -0.243249000 | 2.723577000 | 0.640003000 |
| 1 | -4.424153000 | 0.320165000 | -0.336007000 |
| 6 | 0.168606000 | 0.057614000 | 0.330273000 |
| 8 | 0.196061000 | -1.078809000 | 0.755733000 |
| 7 | 1.277020000 | 0.743763000 | -0.081301000 |
| 1 | 1.106733000 | 1.620191000 | -0.545599000 |
| 6 | 2.621415000 | 0.329570000 | -0.061323000 |
| 6 | 3.057447000 | -0.841000000 | 0.556756000 |
| 6 | 3.548820000 | 1.165042000 | -0.685859000 |
| 1 | 2.348681000 | -1.493966000 | 1.035476000 |
| 1 | 3.208852000 | 2.074374000 | -1.166696000 |
| 6 | 4.410366000 | -1.152121000 | 0.538365000 |
| 6 | 4.892863000 | 0.840116000 | -0.695513000 |
| 1 | 4.740490000 | -2.062378000 | 1.019779000 |
| 1 | 5.596113000 | 1.499509000 | -1.184896000 |
| 6 | 5.333537000 | -0.324740000 | -0.081656000 |
| 1 | 6.382866000 | -0.582430000 | -0.088223000 |
| 34 | -2.333322000 | -1.782806000 | -0.242944000 |
| 1 | -3.679870000 | -1.751441000 | -0.834137000 |

Table S24: Coordinates of the optimized geometry of selenenyl sulfide **7b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **7b** RSeSG | | | |
|---|---|---|---|
| 7 | 1.011649000 | 2.190692000 | 1.737822000 |
| 6 | 1.007098000 | 3.621802000 | 1.854415000 |
| 6 | 2.334328000 | 4.163712000 | 1.396082000 |
| 8 | 3.237590000 | 3.497797000 | 0.970597000 |
| 8 | 2.389588000 | 5.492499000 | 1.521989000 |
| 6 | -0.155827000 | 1.506762000 | 1.719297000 |
| 8 | -1.227597000 | 2.021893000 | 1.952888000 |
| 6 | -0.051594000 | -0.000575000 | 1.466852000 |
| 7 | 1.138343000 | -0.357994000 | 0.725560000 |
| 6 | -0.095891000 | -0.699787000 | 2.822732000 |
| 16 | 0.181288000 | -2.500488000 | 2.775844000 |
| 6 | 4.978937000 | 0.447772000 | -1.636336000 |
| 6 | 5.917579000 | 1.568427000 | -1.245109000 |
| 8 | 6.762083000 | 1.482704000 | -0.399939000 |
| 8 | 5.656552000 | 2.701318000 | -1.913192000 |
| 7 | 5.644966000 | -0.807827000 | -1.361951000 |
| 6 | 3.657070000 | 0.698682000 | -0.884902000 |
| 6 | 2.584378000 | -0.338866000 | -1.228899000 |
| 6 | 1.292987000 | 0.059706000 | -0.558736000 |
| 8 | 0.484456000 | 0.806316000 | -1.087265000 |
| 1 | 1.859739000 | 1.760685000 | 1.400976000 |
| 1 | 0.214634000 | 4.060478000 | 1.243251000 |
| 1 | 0.826944000 | 3.954797000 | 2.878764000 |
| 1 | 3.256923000 | 5.787481000 | 1.215024000 |
| 1 | -0.949352000 | -0.261984000 | 0.903373000 |
| 1 | 1.671257000 | -1.152628000 | 1.049005000 |
| 1 | -1.052232000 | -0.481183000 | 3.290406000 |
| 1 | 0.701253000 | -0.328828000 | 3.471696000 |
| 1 | 4.784266000 | 0.530759000 | -2.707793000 |
| 1 | 6.235558000 | 3.388295000 | -1.558147000 |
| 1 | 6.097822000 | -0.776367000 | -0.456208000 |
| 1 | 5.008474000 | -1.591239000 | -1.392508000 |
| 1 | 3.285402000 | 1.693815000 | -1.135389000 |
| 1 | 3.861245000 | 0.688135000 | 0.189637000 |
| 1 | 2.881908000 | -1.338264000 | -0.907403000 |
| 1 | 2.404419000 | -0.358294000 | -2.302824000 |
| 6 | 0.731142000 | -3.895255000 | -0.454611000 |
| 6 | -0.439726000 | -3.149977000 | -0.262475000 |
| 6 | 1.387712000 | -3.775476000 | -1.680151000 |
| 1 | 2.284177000 | -4.359922000 | -1.846331000 |
| 6 | -0.944250000 | -2.346574000 | -1.288553000 |
| 6 | 0.912354000 | -2.950531000 | -2.685913000 |
| 1 | 1.441163000 | -2.882289000 | -3.626882000 |
| 6 | -0.257292000 | -2.234183000 | -2.491134000 |
| 1 | -0.656414000 | -1.603094000 | -3.274059000 |
| 6 | -2.287416000 | -1.680367000 | -1.141453000 |
| 8 | -3.268120000 | -2.336611000 | -0.852430000 |
| 7 | -2.273664000 | -0.344231000 | -1.373379000 |
| 1 | -1.362940000 | 0.095182000 | -1.452400000 |
| 6 | -3.369246000 | 0.539291000 | -1.236505000 |
| 6 | -4.690115000 | 0.142218000 | -1.445491000 |
| 6 | -3.097033000 | 1.856173000 | -0.899667000 |

| | | | |
|---|---|---|---|
| 1 | -4.911644000 | -0.882199000 | -1.696703000 |
| 1 | -2.072984000 | 2.155682000 | -0.715335000 |
| 6 | -5.708976000 | 1.064456000 | -1.314511000 |
| 6 | -4.120500000 | 2.785192000 | -0.771409000 |
| 1 | -6.738853000 | 0.775172000 | -1.468863000 |
| 1 | -3.876102000 | 3.799824000 | -0.497819000 |
| 6 | -5.436088000 | 2.388499000 | -0.977987000 |
| 34 | -1.398664000 | -3.203800000 | 1.419352000 |
| 6 | 1.291397000 | -4.829031000 | 0.582337000 |
| 1 | 1.838286000 | -4.287698000 | 1.354607000 |
| 1 | 0.496097000 | -5.379954000 | 1.082201000 |
| 1 | 1.973233000 | -5.538312000 | 0.118029000 |
| 8 | -6.511586000 | 3.212767000 | -0.872142000 |
| 6 | -6.273348000 | 4.551912000 | -0.510778000 |
| 1 | -5.794853000 | 4.618485000 | 0.469261000 |
| 1 | -5.647637000 | 5.056975000 | -1.250849000 |
| 1 | -7.244655000 | 5.035683000 | -0.471165000 |
| | | | |
| **7b** RSeH | | | |
| 6 | -4.022747000 | 0.749830000 | -0.151165000 |
| 6 | -2.794499000 | 0.082901000 | -0.024805000 |
| 6 | -4.053790000 | 2.129861000 | 0.034741000 |
| 1 | -5.003391000 | 2.641155000 | -0.056669000 |
| 6 | -1.640428000 | 0.812948000 | 0.287293000 |
| 6 | -2.916819000 | 2.853428000 | 0.349876000 |
| 1 | -2.974340000 | 3.920542000 | 0.509929000 |
| 6 | -1.710504000 | 2.189415000 | 0.477942000 |
| 1 | -0.820097000 | 2.734256000 | 0.763307000 |
| 6 | -0.331434000 | 0.106973000 | 0.488649000 |
| 8 | -0.268038000 | -0.956503000 | 1.070854000 |
| 7 | 0.747226000 | 0.765715000 | -0.024580000 |
| 1 | 0.541237000 | 1.576322000 | -0.584737000 |
| 6 | 2.106631000 | 0.395519000 | 0.028214000 |
| 6 | 2.589564000 | -0.659785000 | 0.806459000 |
| 6 | 3.004269000 | 1.141110000 | -0.724152000 |
| 1 | 1.907747000 | -1.252859000 | 1.391344000 |
| 1 | 2.640937000 | 1.960443000 | -1.332588000 |
| 6 | 3.941655000 | -0.940435000 | 0.813628000 |
| 6 | 4.363386000 | 0.859388000 | -0.716225000 |
| 1 | 4.327958000 | -1.754695000 | 1.410359000 |
| 1 | 5.027987000 | 1.462426000 | -1.315364000 |
| 6 | 4.839821000 | -0.191215000 | 0.058369000 |
| 34 | -2.648193000 | -1.816597000 | -0.264844000 |
| 6 | -5.305878000 | 0.033800000 | -0.463309000 |
| 1 | -5.311798000 | -0.350720000 | -1.485077000 |
| 1 | -5.452748000 | -0.814880000 | 0.205033000 |
| 1 | -6.150983000 | 0.710197000 | -0.358996000 |
| 8 | 6.145334000 | -0.555282000 | 0.139816000 |
| 6 | 7.077201000 | 0.182026000 | -0.615034000 |
| 1 | 6.861145000 | 0.116521000 | -1.684175000 |
| 1 | 7.088541000 | 1.232360000 | -0.313754000 |
| 1 | 8.049136000 | -0.259239000 | -0.416943000 |
| 1 | -3.820282000 | -1.897821000 | -1.143149000 |

Table S25: Coordinates of the optimized geometry of selenenyl sulfide **8b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **8b** RSeSG | | | |
|---|---|---|---|
| 7 | 0.787234000 | 2.414288000 | 1.972592000 |
| 6 | 0.940461000 | 3.838794000 | 1.859655000 |
| 6 | 2.278219000 | 4.159531000 | 1.246424000 |
| 8 | 3.111306000 | 3.346728000 | 0.953062000 |
| 8 | 2.451379000 | 5.477316000 | 1.110810000 |
| 6 | -0.426765000 | 1.842630000 | 1.760164000 |
| 8 | -1.460261000 | 2.469762000 | 1.715032000 |
| 6 | -0.438565000 | 0.313011000 | 1.696363000 |
| 7 | 0.797846000 | -0.229044000 | 1.169029000 |
| 6 | -0.722087000 | -0.208820000 | 3.101897000 |
| 16 | -0.719856000 | -2.024535000 | 3.274217000 |
| 6 | 4.874988000 | -0.108461000 | -1.115110000 |
| 6 | 5.939240000 | 0.964593000 | -0.992823000 |
| 8 | 6.895467000 | 0.907448000 | -0.272165000 |
| 8 | 5.702719000 | 1.995956000 | -1.815391000 |
| 7 | 5.386211000 | -1.341575000 | -0.543055000 |
| 6 | 3.586111000 | 0.423878000 | -0.471002000 |
| 6 | 2.440851000 | -0.583186000 | -0.600998000 |
| 6 | 1.155346000 | 0.043400000 | -0.116210000 |
| 8 | 0.526910000 | 0.837351000 | -0.796721000 |
| 1 | 1.615434000 | 1.863295000 | 1.800269000 |
| 1 | 0.141700000 | 4.253881000 | 1.242575000 |
| 1 | 0.886951000 | 4.347698000 | 2.825231000 |
| 1 | 3.327840000 | 5.627641000 | 0.733063000 |
| 1 | -1.279223000 | 0.064720000 | 1.044972000 |
| 1 | 1.148100000 | -1.072830000 | 1.600904000 |
| 1 | -1.676026000 | 0.193484000 | 3.433186000 |
| 1 | 0.057830000 | 0.123037000 | 3.791520000 |
| 1 | 4.690488000 | -0.227325000 | -2.187506000 |
| 1 | 6.396549000 | 2.651875000 | -1.669773000 |
| 1 | 6.164229000 | -1.132794000 | 0.072391000 |
| 1 | 4.684162000 | -1.826225000 | -0.002877000 |
| 1 | 3.289527000 | 1.349253000 | -0.964744000 |
| 1 | 3.777504000 | 0.661027000 | 0.578665000 |
| 1 | 2.637188000 | -1.502161000 | -0.046311000 |
| 1 | 2.299180000 | -0.840657000 | -1.651155000 |
| 6 | -0.001234000 | -3.710007000 | 0.394012000 |
| 6 | -1.117416000 | -2.894707000 | 0.296269000 |
| 6 | 0.887862000 | -3.843055000 | -0.665307000 |
| 1 | 1.756540000 | -4.474330000 | -0.553846000 |
| 6 | -1.358160000 | -2.208837000 | -0.896200000 |
| 6 | 0.658759000 | -3.135816000 | -1.841675000 |
| 6 | -0.464373000 | -2.319312000 | -1.948874000 |
| 1 | 0.185445000 | -4.253694000 | 1.310311000 |
| 6 | -2.596475000 | -1.364269000 | -1.037809000 |
| 8 | -3.686966000 | -1.822914000 | -0.766155000 |
| 7 | -2.355595000 | -0.096468000 | -1.462028000 |
| 1 | -1.384290000 | 0.191361000 | -1.498140000 |
| 6 | -3.299449000 | 0.946363000 | -1.583067000 |
| 6 | -4.649279000 | 0.720878000 | -1.823231000 |
| 6 | -2.826455000 | 2.252149000 | -1.470277000 |
| 1 | -5.023418000 | -0.286600000 | -1.901347000 |

| | | | |
|---|---|---|---|
| 1 | -1.778366000 | 2.417542000 | -1.253494000 |
| 6 | -5.505181000 | 1.806662000 | -1.953919000 |
| 6 | -3.695092000 | 3.317482000 | -1.605431000 |
| 1 | -6.555276000 | 1.622574000 | -2.143043000 |
| 1 | -3.316024000 | 4.326708000 | -1.502265000 |
| 6 | -5.052663000 | 3.115718000 | -1.848710000 |
| 34 | -2.257066000 | -2.656621000 | 1.837806000 |
| 6 | -5.991980000 | 4.284610000 | -1.968380000 |
| 1 | -6.119585000 | 4.781965000 | -1.005730000 |
| 1 | -5.610001000 | 5.025502000 | -2.670819000 |
| 1 | -6.974097000 | 3.965796000 | -2.312485000 |
| 1 | -0.621523000 | -1.765884000 | -2.865316000 |
| 8 | 1.462263000 | -3.184620000 | -2.929082000 |
| 6 | 2.722345000 | -3.806700000 | -2.796277000 |
| 1 | 3.328588000 | -3.319368000 | -2.027605000 |
| 1 | 2.625091000 | -4.868089000 | -2.560125000 |
| 1 | 3.216983000 | -3.705528000 | -3.757184000 |
| | | | |
| **8b** RSeH | | | |
| 6 | -3.535389000 | -0.436090000 | -0.231607000 |
| 6 | -2.221756000 | -0.859613000 | -0.080879000 |
| 6 | -3.890455000 | 0.902842000 | -0.142891000 |
| 1 | -4.926675000 | 1.179967000 | -0.262988000 |
| 6 | -1.239490000 | 0.110737000 | 0.155995000 |
| 6 | -2.914198000 | 1.857301000 | 0.115446000 |
| 6 | -1.594164000 | 1.448861000 | 0.261786000 |
| 1 | -4.312983000 | -1.164224000 | -0.416249000 |
| 6 | 0.188878000 | -0.308834000 | 0.341061000 |
| 8 | 0.468229000 | -1.370801000 | 0.858143000 |
| 7 | 1.112282000 | 0.584558000 | -0.119571000 |
| 1 | 0.749285000 | 1.365505000 | -0.640501000 |
| 6 | 2.516358000 | 0.495719000 | -0.069915000 |
| 6 | 3.204782000 | -0.498455000 | 0.618200000 |
| 6 | 3.239460000 | 1.482538000 | -0.742020000 |
| 1 | 2.663061000 | -1.268385000 | 1.139724000 |
| 1 | 2.710021000 | 2.261282000 | -1.277876000 |
| 6 | 4.594086000 | -0.486077000 | 0.618629000 |
| 6 | 4.620292000 | 1.475061000 | -0.727982000 |
| 1 | 5.116973000 | -1.265062000 | 1.159125000 |
| 1 | 5.159657000 | 2.251792000 | -1.255835000 |
| 6 | 5.328199000 | 0.486274000 | -0.046917000 |
| 34 | -1.785339000 | -2.721182000 | -0.207184000 |
| 6 | 6.832153000 | 0.475417000 | -0.052517000 |
| 1 | 7.216956000 | 0.219342000 | -1.040745000 |
| 1 | 7.233075000 | 1.454320000 | 0.210208000 |
| 1 | 7.221813000 | -0.252351000 | 0.656504000 |
| 1 | -0.857794000 | 2.204697000 | 0.500780000 |
| 8 | -3.148063000 | 3.185556000 | 0.247180000 |
| 6 | -4.480713000 | 3.630636000 | 0.127541000 |
| 1 | -4.884359000 | 3.406371000 | -0.862357000 |
| 1 | -5.117710000 | 3.176747000 | 0.889861000 |
| 1 | -4.456380000 | 4.706161000 | 0.271389000 |
| 1 | -3.048984000 | -3.023805000 | -0.895972000 |

Table S26: Coordinates of the optimized geometry of selenenyl sulfide **9b** (RSeSG) and its corresponding selenol (RSeH) at M06-2X/6-311++g(2df,2pd) level of theory.

| **9b** RSeSG | | | |
|---|---|---|---|
| 6 | -2.674860000 | -2.613589000 | -0.620003000 |
| 6 | -3.162549000 | -1.602299000 | 0.215892000 |
| 6 | -3.250765000 | -3.881681000 | -0.581677000 |
| 1 | -2.872107000 | -4.673979000 | -1.208401000 |
| 6 | -4.269012000 | -1.849279000 | 1.030983000 |
| 6 | -4.330671000 | -4.124337000 | 0.252301000 |
| 1 | -4.775774000 | -5.109395000 | 0.269796000 |
| 6 | -4.850279000 | -3.112261000 | 1.040730000 |
| 1 | -5.709881000 | -3.295668000 | 1.671179000 |
| 6 | -4.850948000 | -0.730686000 | 1.853476000 |
| 1 | -5.696324000 | -1.101968000 | 2.446019000 |
| 1 | -4.095894000 | -0.367568000 | 2.557140000 |
| 7 | -5.200276000 | 0.387906000 | 0.990449000 |
| 1 | -5.939587000 | 0.120244000 | 0.352957000 |
| 34 | -2.377206000 | 0.157184000 | 0.259931000 |
| 1 | -4.650968000 | 1.942494000 | 2.252649000 |
| 1 | -6.346152000 | 1.465151000 | 2.444247000 |
| 6 | -5.537259000 | 1.600365000 | 1.715218000 |
| 1 | -5.815711000 | 2.383373000 | 1.013910000 |
| 16 | -0.227844000 | -0.283768000 | 0.466759000 |
| 8 | 3.375175000 | -0.639880000 | -2.005282000 |
| 8 | 1.153763000 | 3.304626000 | -0.754856000 |
| 8 | 6.373148000 | 0.647748000 | 2.108868000 |
| 8 | 7.997174000 | -0.833947000 | 2.472761000 |
| 8 | -1.434791000 | 3.115817000 | 0.928601000 |
| 8 | -3.340883000 | 3.999779000 | 0.159560000 |
| 7 | 2.482775000 | 1.036822000 | -0.796921000 |
| 7 | 7.654200000 | -2.038565000 | 0.096904000 |
| 7 | -0.736913000 | 2.469325000 | -1.666769000 |
| 6 | 5.518329000 | -0.884234000 | -0.136163000 |
| 6 | 4.802693000 | 0.435406000 | -0.397358000 |
| 6 | 1.244415000 | 1.040222000 | -1.537030000 |
| 6 | 6.987039000 | -0.764547000 | 0.286423000 |
| 6 | 3.500282000 | 0.211796000 | -1.143007000 |
| 6 | 0.403442000 | -0.204109000 | -1.244318000 |
| 6 | 0.553583000 | 2.377838000 | -1.254899000 |
| 6 | 7.184287000 | -0.357144000 | 1.733007000 |
| 6 | -1.527872000 | 3.641242000 | -1.380664000 |
| 6 | -2.224197000 | 3.608000000 | -0.030285000 |
| 1 | 5.500298000 | -1.460220000 | -1.061290000 |
| 1 | 4.979006000 | -1.477017000 | 0.604446000 |
| 1 | 4.624860000 | 0.990315000 | 0.520154000 |
| 1 | 5.420641000 | 1.068264000 | -1.042011000 |
| 1 | 1.478089000 | 1.018969000 | -2.608523000 |
| 1 | 7.439335000 | 0.058770000 | -0.290310000 |
| 1 | 2.644762000 | 1.834628000 | -0.200294000 |
| 1 | -0.438939000 | -0.301925000 | -1.924543000 |
| 1 | 1.043249000 | -1.071354000 | -1.396249000 |
| 1 | 8.519831000 | -2.076928000 | 0.619147000 |
| 1 | 7.844171000 | -2.206945000 | -0.880802000 |
| 1 | -1.235510000 | 1.620166000 | -1.879119000 |
| 1 | -2.292279000 | 3.779500000 | -2.139580000 |

| | | | |
|---|---|---|---|
| 1 | -0.863113000 | 4.505431000 | -1.382589000 |
| 1 | 6.592564000 | 0.863905000 | 3.024797000 |
| 1 | -1.942940000 | 3.083119000 | 1.749816000 |
| 8 | -1.659228000 | -2.289964000 | -1.451557000 |
| 6 | -1.071671000 | -3.312501000 | -2.227260000 |
| 1 | -0.676706000 | -4.107549000 | -1.592348000 |
| 1 | -1.787111000 | -3.731840000 | -2.937293000 |
| 1 | -0.254588000 | -2.846997000 | -2.771302000 |
| | | | |
| **9b** RSeSH | | | |
| 6 | 1.684950000 | 0.237221000 | 0.045299000 |
| 6 | 0.301537000 | 0.096352000 | -0.135725000 |
| 6 | 2.256171000 | 1.504708000 | 0.088906000 |
| 1 | 3.319729000 | 1.620917000 | 0.228313000 |
| 6 | -0.493367000 | 1.233110000 | -0.276125000 |
| 6 | 1.455087000 | 2.630190000 | -0.040853000 |
| 1 | 1.906308000 | 3.611689000 | -0.001368000 |
| 6 | 0.091199000 | 2.495947000 | -0.219905000 |
| 1 | -0.535188000 | 3.371692000 | -0.325439000 |
| 6 | -1.978057000 | 1.100002000 | -0.481084000 |
| 1 | -2.410027000 | 2.088272000 | -0.689514000 |
| 1 | -2.164178000 | 0.473255000 | -1.359211000 |
| 7 | -2.600546000 | 0.438833000 | 0.654179000 |
| 1 | -2.442708000 | 0.977892000 | 1.496248000 |
| 34 | -0.509182000 | -1.637176000 | -0.170373000 |
| 1 | -4.129883000 | -0.540226000 | -0.357093000 |
| 1 | -4.593458000 | 1.076345000 | 0.196591000 |
| 6 | -4.014406000 | 0.179470000 | 0.454761000 |
| 1 | -4.438043000 | -0.260372000 | 1.355393000 |
| 1 | 0.689930000 | -2.290715000 | -0.708270000 |
| 8 | 2.405878000 | -0.904741000 | 0.163291000 |
| 6 | 3.796259000 | -0.798265000 | 0.366564000 |
| 1 | 4.282323000 | -0.299355000 | -0.474519000 |
| 1 | 4.020071000 | -0.256565000 | 1.287892000 |
| 1 | 4.167900000 | -1.815152000 | 0.447044000 |

## Notes and references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