*Supporting Information*

# How Does Non-covalent Se---Se=O Interaction Stabilize Selenoxides at Naphthalene 1,8-Positions: Structural and Theoretical Investigations

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**Table S1** Energies and relative energies for 8-G-1-[MeSe($O_iH_j$)]$C_{10}H_6$ ($i, j$ = 0, 1, and 2)[a]

| Form | L | O | $OH^+$ |
|---|---|---|---|
| **5** (G = H) | –2826.8386: **B** | –2902.0303: **A** | –2902.4017: **A** |
| *Qn*(Se) | 0.344 | 1.309 | 1.307 |
| *Qn*(O) | | –0.968 | –0.837 |
| *Qn*(H) | | | 0.497 |
| +W[b] | –2978.4277 | –2978.4741 | –2978.2198 |
| Δ[c,d] | 121.8 (0.0) | 0.0 | 667.7 (0.0) |
| **6** (G = F) | –2926.1047: **B** | –3001.3000: **A** | –3001.6744: **A** |
| +W[b] | –3077.6938 | –3077.7438 | –3077.4925 |
| Δ[c,d] | 131.3 (9.5) | 0.0 | 659.8 (–7.9) |
| **7** (G = Cl) | –3286.4504: **B** | –3361.6478: **A** | –3362.0250: **A** |
| +W[b] | –3438.0395 | –3438.0916 | –3437.8431 |
| Δ[c,d] | 136.8 (15.0) | 0.0 | 652.4 (–15.2) |
| **8** (G = Br) | –5400.3674: **B** | –5475.5651: **A** | –5475.9442: **A** |
| +W[b] | –5551.9565 | –5552.0089 | –5551.7623 |
| Δ[c,d] | 137.6 (15.7) | 0.0 | 647.4 (–20.2) |
| **1** (G = *trans*-MeSe) | –5267.6906: **CC**[e] | –5342.8896: **AA** | –5343.2854: **AA** |
| +W[b] | –5419.2797 | –5419.3334 | –5419.1035 |
| Δ[c,d] | 141.0 (19.2) | 0.0 | 603.6 (–64.1) |
| **1** (G = *cis*-MeSe) | –5267.6906: **CC**[e] | –5342.8869: **AA** | –5343.2821: **AA** |
| +W[b] | –5419.2797 | –5419.3307 | –5419.1002 |
| Δ[c,d] | 133.9 (12.1) | 0.0 | 605.2 (–62.5) |
| Δ[d,f] | 141.0 (19.2) | 7.1 | 612.3 (–55.4) |

| Form | OH·OH: **A** | OH·OH: **B** | OH·OH: **C** |
|---|---|---|---|
| **5** (G = H) | –2978.4664 | –2978.4683 | –2978.4686 |
| *Qn*(Se) | 1.317 | 1.324 | 1.324 |
| *Qn*(O) | –1.004, –0.992 | –0.991 | –0.996, –0.993 |
| *Qn*(H) | 0.439, 0.429 | 0.432 | 0.433, 0.433 |
| +W[b] | –2978.4664 | –2978.4683 | –2978.4686 |
| Δ[c,g] | 20.2 (5.8) | 15.2 (0.8) | 14.4 (0.0) |
| **6** (G = F) | –3077.7265 | –3077.7354 | –3077.7371 |
| +W[b] | –3077.7265 | –3077.7354 | –3077.7371 |
| Δ[c,g] | 45.4 (31.0) | 22.1 (7.6) | 17.6 (3.2) |
| **7** (G = Cl) | –3438.0676 | –3438.0811 | –3438.0833 |
| +W[b] | –3438.0676 | –3438.0811 | –3438.0833 |
| Δ[c,g] | 63.0 (48.6) | 27.6 (13.1) | 21.8 (7.4) |
| **8** (G = Br) | –5551.9834 | –5551.9983 | –5552.0007 |
| +W[b] | –5551.9834 | –5551.9983 | –5552.0007 |
| Δ[c,g] | 67.0 (52.5) | 27.8 (13.4) | 21.5 (7.1) |
| **1** (G = *trans*-MeSe) | –5419.3063 | –5419.3207 | –5419.3241 |
| +W[b] | –5419.3063 | –5419.3207 | –5419.3241 |
| Δ[c,g] | 71.2 (56.7) | 33.3 (18.9) | 24.4 (10.0) |
| **1** (G = *cis*-MeSe) | –5419.3102 | –5419.3207 | –5419.3214 |
| +W[b] | –5419.3102 | –5419.3207 | –5419.3214 |
| Δ[c,g] | 53.8 (39.4) | 26.3 (11.8) | 24.4 (10.0) |
| Δ[f,g] | 60.9 (46.5) | 33.3 (18.9) | 31.5 (17.1) |

[a] Calculated with the B3LYP/6-311+G(d) method. [b] Energies evaluated for 8-G-1-[MeSe($O_iH_j$)]-$C_{10}H_6$ + $O_kH_l$ ($i + k = j + l = 2$) with the calculated values of $E(O_2H_2)$ = –151.5891 au, $E(OH_2)$ = –76.4438 au, and $E(OH^-)$ = –75.8181 au. [c] Energies relative to that of the corresponding species of ***n*** (O): **A**. [d] Energies relative to the same structure of **5** (G = H) being given in parenthesis. [e] Corresponding to the observed structure. [f] Energies relative to that of the corresponding species of **1** (G = *trans*-MeSe; O): **A**. [g] Energies relative to **5** (OH·OH): **C** being given in parenthesis.

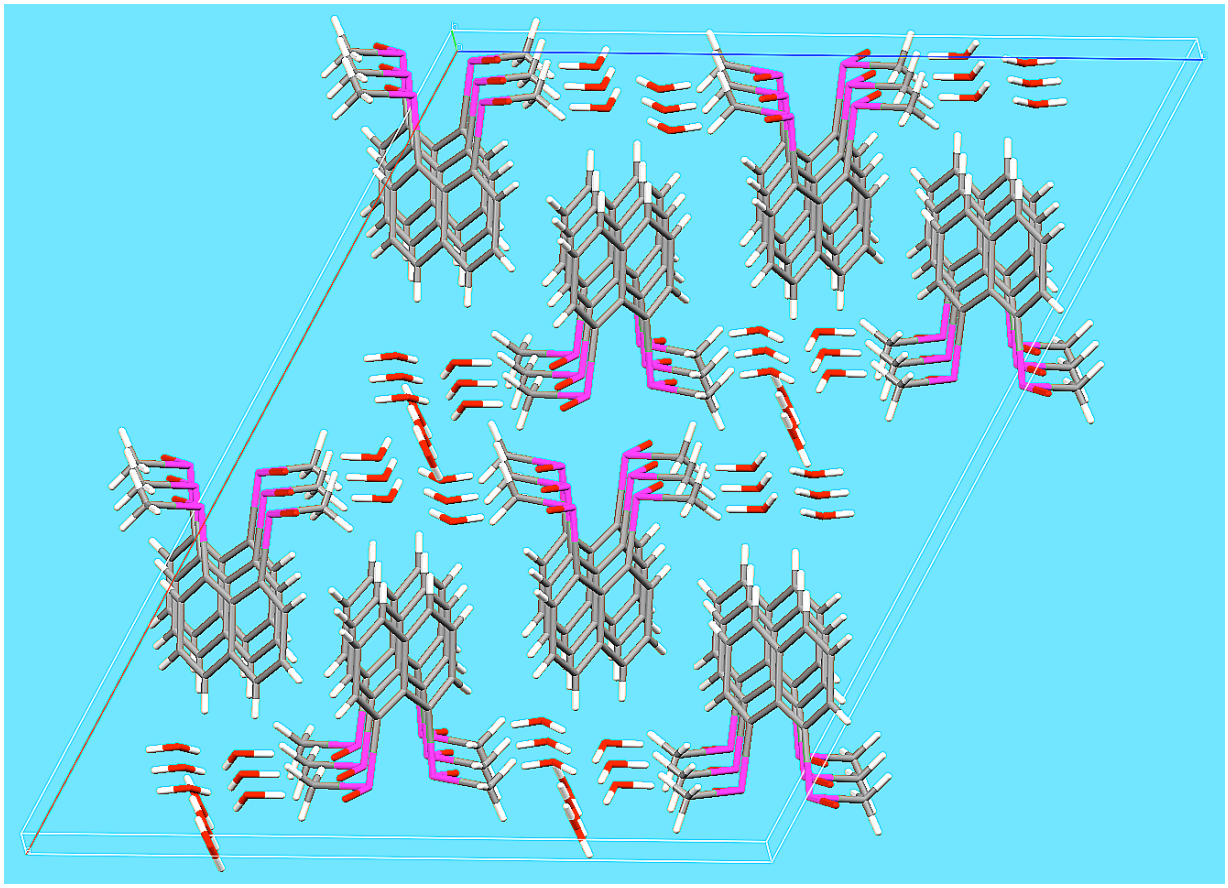

**Fig. S1** The packing structures of **1** (OO): red line; *a* axis, green line; *b* axis, blue line; *c* axis.

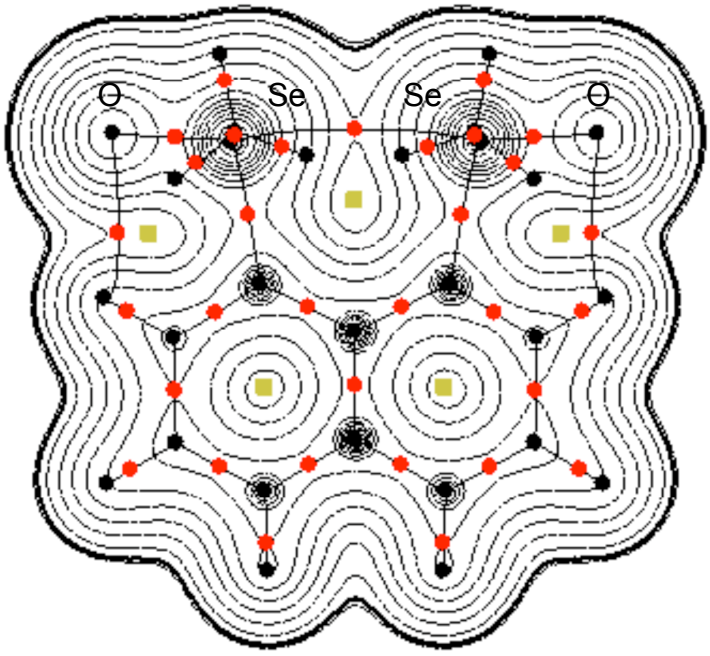


**Fig. S2** Contour map of $\rho_b(r_c)$ of **1** (OO) in the $SeSeC_9$ plane, together with BCPs (●), ring critical points (■), and bond paths. The contours [$ea_o^{-3}$] are at $2^l$ ($l$= ±8, ±7, …0), and 0.0047 (heavy line).

## Optimized Structures

Optimized structures given by Cartesian coordinates for Optimized structures given by Cartesian coordinates for 8-G-1-[MeSe(X)]$C_{10}H_6$ [G = MeSe (**1**), H (**5**), F (**6**), Cl (**7**), and Br (**8**) with X = lone pair (L), O (O), $OH^+$ ($OH^+$), and $O_2H_2$ (OH·OH)], together with the total energies. QC calculations were employed the 6-311+G(d) basis sets of the Gaussian 98 program.[28] Calculations are performed at the density functional theory (DFT) level of the Becke three parameter hybrid functionals with the Lee-Yang-Parr correlation functional (B3LYP).[29,30]

**5** (G = H: L): **B**; HF=-2826.8386 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.489034 | -0.718514 | 0.000000 |
| 6 | 0 | 1.906527 | -0.933803 | 0.000000 |
| 6 | 0 | 0.000000 | 0.629510 | 0.000000 |
| 6 | 0 | 2.785749 | 0.180423 | 0.000000 |
| 6 | 0 | -0.360276 | -1.856285 | 0.000000 |
| 6 | 0 | 2.401781 | -2.264260 | 0.000000 |
| 6 | 0 | 0.888409 | 1.683473 | 0.000000 |
| 6 | 0 | 2.284062 | 1.456497 | 0.000000 |
| 6 | 0 | 0.152543 | -3.132296 | 0.000000 |
| 6 | 0 | 1.549321 | -3.341398 | 0.000000 |
| 1 | 0 | 3.857396 | 0.006280 | 0.000000 |
| 1 | 0 | -1.436903 | -1.723771 | 0.000000 |
| 1 | 0 | 3.477322 | -2.416276 | 0.000000 |
| 1 | 0 | 0.536087 | 2.707282 | 0.000000 |
| 1 | 0 | 2.955272 | 2.309655 | 0.000000 |
| 1 | 0 | -0.520211 | -3.983825 | 0.000000 |
| 1 | 0 | 1.944558 | -4.352139 | 0.000000 |
| 34 | 0 | -1.917077 | 0.895772 | 0.000000 |
| 6 | 0 | -2.007691 | 2.857281 | 0.000000 |
| 1 | 0 | -1.548940 | 3.269946 | 0.897081 |
| 1 | 0 | -1.548940 | 3.269946 | -0.897081 |
| 1 | 0 | -3.071771 | 3.092893 | 0.000000 |

**6** (G = F: L): **B**; HF=-2926.1047 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.655962 | -0.552447 | 0.000000 |
| 6 | 0 | 2.094719 | -0.601075 | 0.000000 |
| 6 | 0 | 0.000000 | 0.727536 | 0.000000 |
| 6 | 0 | 2.833241 | 0.609119 | 0.000000 |
| 6 | 0 | 0.005054 | -1.812186 | 0.000000 |
| 6 | 0 | 2.764185 | -1.853116 | 0.000000 |
| 6 | 0 | 0.774056 | 1.872225 | 0.000000 |
| 6 | 0 | 2.183317 | 1.815137 | 0.000000 |
| 6 | 0 | 0.656324 | -3.015551 | 0.000000 |
| 6 | 0 | 2.065524 | -3.034091 | 0.000000 |
| 1 | 0 | 3.917354 | 0.561038 | 0.000000 |
| 9 | 0 | -1.353275 | -1.842114 | 0.000000 |
| 1 | 0 | 3.849469 | -1.857225 | 0.000000 |
| 1 | 0 | 0.308869 | 2.848460 | 0.000000 |
| 1 | 0 | 2.747040 | 2.742723 | 0.000000 |
| 1 | 0 | 0.074506 | -3.929778 | 0.000000 |
| 1 | 0 | 2.587314 | -3.984943 | 0.000000 |
| 34 | 0 | -1.935924 | 0.851972 | 0.000000 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.159976 | 2.804527 | 0.000000 |
| 1 | 0 | -1.739103 | 3.257327 | 0.896879 |
| 1 | 0 | -1.739103 | 3.257327 | -0.896879 |
| 1 | 0 | -3.239887 | 2.956579 | 0.000000 |

**7** (G = Cl: L): **B**; HF=-3286.4504 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 2.638746 | -1.525504 | 0.001235 |
| 6 | 0 | 1.309314 | -1.168413 | -0.000058 |
| 6 | 0 | 0.867019 | 0.192732 | -0.000248 |
| 6 | 0 | 1.930862 | 1.175214 | 0.000223 |
| 6 | 0 | 3.291829 | 0.776842 | 0.001518 |
| 6 | 0 | 3.645791 | -0.545576 | 0.002176 |
| 1 | 0 | 2.900594 | -2.576417 | 0.001341 |
| 6 | 0 | -0.492650 | 0.685136 | -0.000906 |
| 6 | 0 | 1.632367 | 2.560931 | -0.000663 |
| 1 | 0 | 4.051879 | 1.551573 | 0.001924 |
| 1 | 0 | 4.687994 | -0.846084 | 0.003215 |
| 6 | 0 | 0.334314 | 2.988760 | -0.002004 |
| 6 | 0 | -0.714313 | 2.050711 | -0.002060 |
| 1 | 0 | 2.454572 | 3.269114 | -0.000339 |
| 1 | 0 | 0.098162 | 4.048050 | -0.002910 |
| 1 | 0 | -1.723221 | 2.436541 | -0.002964 |
| 17 | 0 | 0.190182 | -2.532512 | -0.002203 |
| 34 | 0 | -2.057206 | -0.479704 | 0.000513 |
| 6 | 0 | -3.504325 | 0.855717 | 0.002560 |
| 1 | 0 | -4.415050 | 0.255239 | 0.004797 |
| 1 | 0 | -3.490250 | 1.472137 | -0.895502 |
| 1 | 0 | -3.486498 | 1.473204 | 0.899818 |

**8** (G = Br: L): **B**; HF=-5400.3674 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.000000 | 1.007805 | 0.000000 |
| 6 | 0 | 0.269973 | 2.431190 | 0.000000 |
| 6 | 0 | -1.390318 | 0.667727 | 0.000000 |
| 6 | 0 | -2.391874 | 1.611119 | 0.000000 |
| 6 | 0 | -2.091814 | 2.982386 | 0.000000 |
| 6 | 0 | -0.783837 | 3.377330 | 0.000000 |
| 1 | 0 | -3.420945 | 1.286604 | 0.000000 |
| 1 | 0 | -2.894551 | 3.706227 | 0.000000 |
| 1 | 0 | -0.524394 | 4.427224 | 0.000000 |
| 6 | 0 | 1.142082 | 0.121456 | 0.000000 |
| 6 | 0 | 2.413635 | 0.662775 | 0.000000 |
| 6 | 0 | 2.652175 | 2.047310 | 0.000000 |
| 6 | 0 | 1.600355 | 2.916093 | 0.000000 |
| 1 | 0 | 3.273538 | 0.015399 | 0.000000 |
| 1 | 0 | 3.671350 | 2.408795 | 0.000000 |
| 1 | 0 | 1.758595 | 3.985772 | 0.000000 |
| 35 | 0 | -2.055037 | -1.134465 | 0.000000 |
| 34 | 0 | 1.010271 | -1.818746 | 0.000000 |
| 6 | 0 | 2.911096 | -2.316154 | 0.000000 |
| 1 | 0 | 2.889448 | -3.404126 | 0.000000 |
| 1 | 0 | 3.417603 | -1.968238 | 0.896176 |
| 1 | 0 | 3.417603 | -1.968238 | -0.896176 |

**1** (G = *t*-MeSe and *c*-MeSe: LL): **CC**; HF=-5267.6906 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.000000 | 0.000000 | 1.059487 |
| 6 | 0 | 0.000000 | 0.000000 | 2.503537 |
| 6 | 0 | 0.000000 | 1.282972 | 0.412172 |
| 6 | 0 | -0.104049 | 1.218486 | 3.222430 |
| 6 | 0 | 0.000000 | -1.282972 | 0.412172 |
| 6 | 0 | 0.104049 | -1.218486 | 3.222430 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.140072 | 2.437776 | 1.156218 |
| 6 | 0 | -0.200878 | 2.414573 | 2.563166 |
| 6 | 0 | 0.140072 | -2.437776 | 1.156218 |
| 6 | 0 | 0.200878 | -2.414573 | 2.563166 |
| 1 | 0 | -0.111363 | 1.180546 | 4.307412 |
| 1 | 0 | 0.111363 | -1.180546 | 4.307412 |
| 1 | 0 | -0.187161 | 3.395725 | 0.652153 |
| 1 | 0 | -0.304143 | 3.345467 | 3.111307 |
| 1 | 0 | 0.187161 | -3.395725 | 0.652153 |
| 1 | 0 | 0.304143 | -3.345467 | 3.111307 |
| 34 | 0 | 0.348606 | 1.518813 | -1.494248 |
| 6 | 0 | 1.708794 | 2.954714 | -1.342427 |
| 1 | 0 | 1.261364 | 3.912188 | -1.081798 |
| 1 | 0 | 2.465011 | 2.672724 | -0.612282 |
| 1 | 0 | 2.163980 | 3.029415 | -2.330767 |
| 34 | 0 | -0.348606 | -1.518813 | -1.494248 |
| 6 | 0 | -1.708794 | -2.954714 | -1.342427 |
| 1 | 0 | -1.261364 | -3.912188 | -1.081798 |
| 1 | 0 | -2.465011 | -2.672724 | -0.612282 |
| 1 | 0 | -2.163980 | -3.029415 | -2.330767 |

**5** (G = H: O): **A**; HF=-2902.0303 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.009578 | -0.131231 | -0.086239 |
| 6 | 0 | 2.176356 | 0.690573 | 0.063496 |
| 6 | 0 | -0.256188 | 0.519868 | -0.090930 |
| 6 | 0 | -0.376381 | 1.881575 | 0.006620 |
| 6 | 0 | 0.781691 | 2.681352 | 0.149534 |
| 6 | 0 | 2.024296 | 2.097582 | 0.182310 |
| 1 | 0 | -1.367334 | 2.325152 | -0.032855 |
| 1 | 0 | 0.679137 | 3.758433 | 0.231483 |
| 1 | 0 | 2.914454 | 2.709737 | 0.293037 |
| 6 | 0 | 1.184360 | -1.534055 | -0.225505 |
| 6 | 0 | 2.438639 | -2.097666 | -0.208103 |
| 6 | 0 | 3.585965 | -1.288369 | -0.047576 |
| 6 | 0 | 3.454199 | 0.073117 | 0.082256 |
| 1 | 0 | 0.318954 | -2.174296 | -0.365654 |
| 1 | 0 | 2.549945 | -3.171003 | -0.322581 |
| 1 | 0 | 4.569736 | -1.745737 | -0.033056 |
| 1 | 0 | 4.333643 | 0.699712 | 0.198493 |
| 34 | 0 | -1.958844 | -0.469275 | -0.318495 |
| 6 | 0 | -2.073028 | -1.061276 | 1.574876 |
| 1 | 0 | -2.999532 | -1.625830 | 1.672737 |
| 1 | 0 | -1.211922 | -1.680240 | 1.827474 |
| 1 | 0 | -2.105926 | -0.160753 | 2.185280 |
| 8 | 0 | -3.097173 | 0.753922 | -0.403745 |

**6** (G = F: O): **A**; HF=-3001.3000 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.016518 | 0.020850 | -0.051151 |
| 6 | 0 | 2.173262 | 0.866531 | 0.064201 |
| 6 | 0 | -0.270362 | 0.632321 | -0.071021 |
| 6 | 0 | -0.406584 | 1.995112 | -0.002062 |
| 6 | 0 | 0.732713 | 2.823473 | 0.119008 |
| 6 | 0 | 1.988464 | 2.271452 | 0.151096 |
| 1 | 0 | -1.406998 | 2.417038 | -0.048556 |
| 1 | 0 | 0.605025 | 3.899226 | 0.179883 |
| 1 | 0 | 2.865757 | 2.905124 | 0.237347 |
| 6 | 0 | 1.267343 | -1.368538 | -0.137788 |
| 6 | 0 | 2.516283 | -1.922704 | -0.121472 |
| 6 | 0 | 3.638231 | -1.072970 | -0.008774 |
| 6 | 0 | 3.468708 | 0.286746 | 0.083154 |

| | | | | |
|---|---|---|---|---|
| 9 | 0 | 0.192538 | -2.202202 | -0.243195 |
| 1 | 0 | 2.623879 | -2.998509 | -0.195522 |
| 1 | 0 | 4.632512 | -1.505531 | 0.004376 |
| 1 | 0 | 4.329991 | 0.941303 | 0.169924 |
| 34 | 0 | -2.002100 | -0.335181 | -0.312016 |
| 6 | 0 | -2.125980 | -0.969889 | 1.566191 |
| 1 | 0 | -3.089164 | -1.471056 | 1.655035 |
| 1 | 0 | -1.310415 | -1.657674 | 1.782374 |
| 1 | 0 | -2.094397 | -0.087788 | 2.202868 |
| 8 | 0 | -3.101152 | 0.924941 | -0.342338 |

**7** (G = Cl: O): **A**; HF=-3361.6478 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.681171 | -1.667418 | -0.007765 |
| 6 | 0 | -1.384421 | -1.219088 | -0.089551 |
| 6 | 0 | -1.037839 | 0.163941 | -0.050159 |
| 6 | 0 | -2.150762 | 1.080007 | 0.056783 |
| 6 | 0 | -3.479234 | 0.592319 | 0.140363 |
| 6 | 0 | -3.743858 | -0.752357 | 0.113595 |
| 1 | 0 | -2.878270 | -2.731897 | -0.044817 |
| 6 | 0 | 0.270783 | 0.741309 | -0.113738 |
| 6 | 0 | -1.915420 | 2.479654 | 0.072984 |
| 1 | 0 | -4.288438 | 1.310862 | 0.223234 |
| 1 | 0 | -4.761715 | -1.121048 | 0.177335 |
| 6 | 0 | -0.646377 | 2.984923 | -0.017711 |
| 6 | 0 | 0.450070 | 2.102256 | -0.113462 |
| 1 | 0 | -2.770742 | 3.143645 | 0.151782 |
| 1 | 0 | -0.474438 | 4.056110 | -0.014681 |
| 1 | 0 | 1.465665 | 2.483356 | -0.188321 |
| 17 | 0 | -0.149430 | -2.467636 | -0.280389 |
| 34 | 0 | 2.049905 | -0.206010 | -0.253098 |
| 6 | 0 | 2.162932 | -0.631871 | 1.686187 |
| 1 | 0 | 3.127726 | -1.115136 | 1.836805 |
| 1 | 0 | 2.128523 | 0.320803 | 2.211441 |
| 1 | 0 | 1.348650 | -1.288822 | 1.985628 |
| 8 | 0 | 3.109794 | 1.081779 | -0.378954 |

**8** (G = Br: O): **A**; HF=-5475.5651 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.737107 | -1.253286 | 0.103593 |
| 6 | 0 | -1.423395 | -0.862009 | -0.012479 |
| 6 | 0 | -1.019995 | 0.507682 | -0.032892 |
| 6 | 0 | -2.100522 | 1.468581 | 0.043790 |
| 6 | 0 | -3.445550 | 1.037823 | 0.162686 |
| 6 | 0 | -3.762976 | -0.294348 | 0.199436 |
| 1 | 0 | -2.982635 | -2.307989 | 0.112565 |
| 6 | 0 | 0.306163 | 1.043745 | -0.123675 |
| 6 | 0 | -1.821291 | 2.859274 | -0.005565 |
| 1 | 0 | -4.224462 | 1.791373 | 0.221382 |
| 1 | 0 | -4.793051 | -0.620917 | 0.291287 |
| 6 | 0 | -0.538719 | 3.319673 | -0.128271 |
| 6 | 0 | 0.526515 | 2.397483 | -0.186128 |
| 1 | 0 | -2.655369 | 3.552051 | 0.049664 |
| 1 | 0 | -0.331976 | 4.383592 | -0.176190 |
| 1 | 0 | 1.553616 | 2.742673 | -0.278334 |
| 35 | 0 | -0.165715 | -2.310924 | -0.200847 |
| 34 | 0 | 2.072742 | 0.056331 | -0.205153 |
| 6 | 0 | 2.168277 | -0.260235 | 1.756192 |
| 1 | 0 | 3.113185 | -0.771014 | 1.938838 |
| 1 | 0 | 2.171569 | 0.723960 | 2.220946 |
| 1 | 0 | 1.328798 | -0.864584 | 2.093655 |
| 8 | 0 | 3.154839 | 1.318956 | -0.391134 |

**1** (G = *t*-MeSe: LO): **AA**; HF=-5342.8896 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -1.061309 | 0.587255 | 0.011558 |
| 6 | 0 | -2.183579 | 1.501802 | -0.015865 |
| 6 | 0 | -1.374242 | -0.806056 | 0.169370 |
| 6 | 0 | -3.507808 | 1.018652 | 0.154290 |
| 6 | 0 | 0.238040 | 1.177449 | -0.126159 |
| 6 | 0 | -1.973383 | 2.893528 | -0.210102 |
| 6 | 0 | -2.681684 | -1.228968 | 0.337469 |
| 6 | 0 | -3.759105 | -0.318041 | 0.339597 |
| 6 | 0 | 0.399640 | 2.530023 | -0.326908 |
| 6 | 0 | -0.709579 | 3.402489 | -0.372816 |
| 1 | 0 | -2.879616 | -2.288833 | 0.460325 |
| 1 | 0 | -4.773645 | -0.681679 | 0.474235 |
| 1 | 0 | -4.323170 | 1.737635 | 0.136375 |
| 1 | 0 | 1.414991 | 2.906234 | -0.445966 |
| 1 | 0 | -0.553974 | 4.466292 | -0.528787 |
| 1 | 0 | -2.842695 | 3.546231 | -0.230160 |
| 34 | 0 | -0.044671 | -2.223502 | 0.167875 |
| 6 | 0 | 0.209480 | -2.398234 | -1.784256 |
| 1 | 0 | 0.854347 | -3.267510 | -1.932727 |
| 1 | 0 | -0.755906 | -2.564458 | -2.263380 |
| 1 | 0 | 0.695155 | -1.506331 | -2.184391 |
| 34 | 0 | 2.037675 | 0.265917 | -0.086875 |
| 6 | 0 | 2.133914 | 0.190935 | 1.898666 |
| 1 | 0 | 3.040183 | -0.362851 | 2.153160 |
| 1 | 0 | 2.217746 | 1.230232 | 2.221050 |
| 1 | 0 | 1.252294 | -0.293892 | 2.318092 |
| 8 | 0 | 3.063730 | 1.541477 | -0.422610 |

**1** (G = *c*-MeSe: LO): **AA**; HF=-5342.8869 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.853454 | -0.575059 | -0.298385 |
| 6 | 0 | -1.480491 | -0.441187 | -0.229783 |
| 6 | 0 | -0.872960 | 0.845759 | -0.050097 |
| 6 | 0 | -1.774852 | 1.968515 | 0.094805 |
| 6 | 0 | -3.177794 | 1.773456 | 0.052082 |
| 6 | 0 | -3.713920 | 0.528207 | -0.147334 |
| 1 | 0 | -3.281662 | -1.554877 | -0.478820 |
| 6 | 0 | 0.527134 | 1.154668 | -0.018222 |
| 6 | 0 | -1.266004 | 3.280944 | 0.277833 |
| 1 | 0 | -3.822711 | 2.638972 | 0.169431 |
| 1 | 0 | -4.788216 | 0.385440 | -0.197228 |
| 6 | 0 | 0.081341 | 3.519679 | 0.298810 |
| 6 | 0 | 0.976961 | 2.443257 | 0.132799 |
| 1 | 0 | -1.974463 | 4.096411 | 0.388445 |
| 1 | 0 | 0.466559 | 4.525858 | 0.426880 |
| 1 | 0 | 2.050060 | 2.616323 | 0.096880 |
| 34 | 0 | -0.468305 | -2.099042 | -0.396150 |
| 34 | 0 | 2.089439 | -0.089424 | -0.333879 |
| 6 | 0 | -1.078360 | -2.959361 | 1.277996 |
| 1 | 0 | -2.156723 | -3.102405 | 1.258128 |
| 1 | 0 | -0.582837 | -3.929515 | 1.321310 |
| 1 | 0 | -0.792926 | -2.360303 | 2.141100 |
| 6 | 0 | 2.276646 | -0.648488 | 1.566317 |
| 1 | 0 | 3.087082 | -1.376109 | 1.598669 |
| 1 | 0 | 2.555473 | 0.254080 | 2.107099 |
| 1 | 0 | 1.352821 | -1.077652 | 1.945302 |
| 8 | 0 | 3.362942 | 0.993661 | -0.462145 |

**5** (G = H: $OH^+$): **A**; HF=-2902.4017 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.053261 | -0.169845 | 0.004443 |
| 6 | 0 | 2.190255 | 0.709706 | 0.012008 |
| 6 | 0 | -0.231871 | 0.461074 | 0.007211 |
| 6 | 0 | -0.399770 | 1.833786 | -0.001050 |
| 6 | 0 | 0.730195 | 2.667401 | -0.003939 |
| 6 | 0 | 1.991437 | 2.111677 | 0.007735 |
| 1 | 0 | -1.387821 | 2.278028 | -0.041565 |
| 1 | 0 | 0.600351 | 3.743046 | -0.017789 |
| 1 | 0 | 2.863558 | 2.757515 | 0.009253 |
| 6 | 0 | 1.283218 | -1.569192 | 0.004869 |
| 6 | 0 | 2.563484 | -2.071661 | 0.007555 |
| 6 | 0 | 3.681060 | -1.207847 | 0.015883 |
| 6 | 0 | 3.495646 | 0.151748 | 0.018435 |
| 1 | 0 | 0.453059 | -2.268589 | 0.007383 |
| 1 | 0 | 2.716515 | -3.145147 | 0.004796 |
| 1 | 0 | 4.681947 | -1.623823 | 0.020926 |
| 1 | 0 | 4.347853 | 0.823130 | 0.025742 |
| 34 | 0 | -1.792882 | -0.653953 | -0.048685 |
| 6 | 0 | -2.855644 | 0.050764 | 1.424217 |
| 1 | 0 | -3.826741 | -0.438222 | 1.376139 |
| 1 | 0 | -2.330339 | -0.200876 | 2.345015 |
| 1 | 0 | -2.944460 | 1.127567 | 1.299248 |
| 8 | 0 | -2.815172 | 0.197085 | -1.275369 |
| 1 | 0 | -2.702187 | -0.200544 | -2.155108 |

**6** (G = F: $OH^+$): **A**; HF=-3001.6744 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.023671 | 0.029527 | -0.049217 |
| 6 | 0 | 2.194421 | 0.850867 | 0.055072 |
| 6 | 0 | -0.244089 | 0.676353 | -0.062025 |
| 6 | 0 | -0.373974 | 2.041751 | 0.028082 |
| 6 | 0 | 0.788328 | 2.838076 | 0.136609 |
| 6 | 0 | 2.033324 | 2.257632 | 0.145218 |
| 1 | 0 | -1.350339 | 2.508933 | 0.009772 |
| 1 | 0 | 0.682341 | 3.914163 | 0.208027 |
| 1 | 0 | 2.920322 | 2.877452 | 0.221374 |
| 6 | 0 | 1.229701 | -1.360474 | -0.116616 |
| 6 | 0 | 2.453051 | -1.959615 | -0.102584 |
| 6 | 0 | 3.597885 | -1.134568 | -0.013412 |
| 6 | 0 | 3.471036 | 0.231449 | 0.066621 |
| 9 | 0 | 0.090614 | -2.135244 | -0.192027 |
| 1 | 0 | 2.532758 | -3.038709 | -0.158177 |
| 1 | 0 | 4.578642 | -1.595005 | -0.004333 |
| 1 | 0 | 4.352911 | 0.857823 | 0.142400 |
| 34 | 0 | -1.856955 | -0.397826 | -0.302524 |
| 6 | 0 | -2.258761 | -0.884530 | 1.550743 |
| 1 | 0 | -3.230663 | -1.374847 | 1.545351 |
| 1 | 0 | -1.476133 | -1.563146 | 1.884677 |
| 1 | 0 | -2.272797 | 0.037274 | 2.128595 |
| 8 | 0 | -3.049222 | 0.952675 | -0.326694 |
| 1 | 0 | -3.509881 | 0.979126 | -1.181024 |

**7** (G = Cl: $OH^+$): **A**; HF=-3362.0250 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.620390 | -1.734907 | -0.025834 |
| 6 | 0 | -1.345619 | -1.230898 | -0.070059 |
| 6 | 0 | -1.055389 | 0.157240 | -0.044046 |
| 6 | 0 | -2.192790 | 1.038562 | 0.043932 |
| 6 | 0 | -3.504021 | 0.500615 | 0.082263 |
| 6 | 0 | -3.717316 | -0.853533 | 0.047345 |
| 1 | 0 | -2.779767 | -2.806144 | -0.048052 |
| 6 | 0 | 0.230286 | 0.781894 | -0.076752 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -1.993508 | 2.441673 | 0.097412 |
| 1 | 0 | -4.341897 | 1.186257 | 0.144427 |
| 1 | 0 | -4.722041 | -1.258079 | 0.078657 |
| 6 | 0 | -0.736738 | 2.987791 | 0.072732 |
| 6 | 0 | 0.391568 | 2.147551 | -0.017816 |
| 1 | 0 | -2.866021 | 3.083018 | 0.161768 |
| 1 | 0 | -0.595394 | 4.061151 | 0.117646 |
| 1 | 0 | 1.380905 | 2.584792 | -0.047555 |
| 17 | 0 | -0.020176 | -2.404115 | -0.170633 |
| 34 | 0 | 1.892510 | -0.255522 | -0.271424 |
| 6 | 0 | 2.353875 | -0.547749 | 1.613910 |
| 1 | 0 | 3.320370 | -1.048298 | 1.628505 |
| 1 | 0 | 2.406802 | 0.438066 | 2.071649 |
| 1 | 0 | 1.578853 | -1.163368 | 2.063195 |
| 8 | 0 | 3.038590 | 1.147799 | -0.388814 |
| 1 | 0 | 3.447356 | 1.168496 | -1.269050 |

**8** (G = Br: $OH^+$): **A**; HF=-5475.9442 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.646149 | -1.446751 | 0.021893 |
| 6 | 0 | -1.370022 | -0.943618 | -0.029957 |
| 6 | 0 | -1.078229 | 0.445918 | -0.033547 |
| 6 | 0 | -2.221798 | 1.324956 | 0.035999 |
| 6 | 0 | -3.532443 | 0.786675 | 0.081928 |
| 6 | 0 | -3.745452 | -0.567129 | 0.073652 |
| 1 | 0 | -2.810893 | -2.517210 | 0.023525 |
| 6 | 0 | 0.202342 | 1.083471 | -0.076651 |
| 6 | 0 | -2.034582 | 2.730306 | 0.065993 |
| 1 | 0 | -4.370308 | 1.473554 | 0.129142 |
| 1 | 0 | -4.749448 | -0.973117 | 0.111044 |
| 6 | 0 | -0.783184 | 3.286215 | 0.035167 |
| 6 | 0 | 0.349796 | 2.451686 | -0.039809 |
| 1 | 0 | -2.913270 | 3.364312 | 0.118033 |
| 1 | 0 | -0.649344 | 4.361107 | 0.063109 |
| 1 | 0 | 1.335478 | 2.896331 | -0.076132 |
| 35 | 0 | 0.053281 | -2.245810 | -0.104375 |
| 34 | 0 | 1.893085 | 0.077783 | -0.252860 |
| 6 | 0 | 2.377041 | -0.125857 | 1.640302 |
| 1 | 0 | 3.336292 | -0.639562 | 1.668869 |
| 1 | 0 | 2.453611 | 0.883555 | 2.039440 |
| 1 | 0 | 1.599895 | -0.701726 | 2.135116 |
| 8 | 0 | 3.005089 | 1.515502 | -0.413589 |
| 1 | 0 | 3.393629 | 1.532226 | -1.302892 |

**1** (G = *t*-MeSe: $LOH^+$): **AA**; HF=-5343.2854 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.436245 | -1.631897 | 0.342540 |
| 6 | 0 | -1.235263 | -0.975224 | 0.178300 |
| 6 | 0 | -1.169556 | 0.436815 | 0.003131 |
| 6 | 0 | -2.419135 | 1.151873 | -0.017976 |
| 6 | 0 | -3.636969 | 0.440311 | 0.132581 |
| 6 | 0 | -3.651677 | -0.918807 | 0.319142 |
| 1 | 0 | -2.450370 | -2.705277 | 0.495276 |
| 6 | 0 | 0.015235 | 1.221029 | -0.138158 |
| 6 | 0 | -2.425515 | 2.561068 | -0.178115 |
| 1 | 0 | -4.566499 | 0.999359 | 0.111728 |
| 1 | 0 | -4.587736 | -1.450032 | 0.446355 |
| 6 | 0 | -1.257570 | 3.265490 | -0.309984 |
| 6 | 0 | -0.019950 | 2.589575 | -0.276688 |
| 1 | 0 | -3.380294 | 3.076080 | -0.193580 |
| 1 | 0 | -1.268338 | 4.342679 | -0.428295 |
| 1 | 0 | 0.901969 | 3.148643 | -0.364151 |

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 0.386413 | -2.027505 | 0.196692 |
| 34 | 0 | 1.814193 | 0.398277 | -0.128121 |
| 6 | 0 | 0.521423 | -2.469882 | -1.727717 |
| 1 | 0 | 0.535091 | -1.561202 | -2.326490 |
| 1 | 0 | 1.447909 | -3.028270 | -1.856155 |
| 1 | 0 | -0.328821 | -3.092761 | -1.995291 |
| 6 | 0 | 2.189377 | 0.384401 | 1.806554 |
| 1 | 0 | 3.052240 | -0.260306 | 1.963909 |
| 1 | 0 | 2.419405 | 1.417222 | 2.055912 |
| 1 | 0 | 1.318224 | 0.020596 | 2.343365 |
| 8 | 0 | 2.749546 | 2.017820 | -0.283638 |
| 1 | 0 | 3.245317 | 2.015953 | -1.116542 |

**1** (G = *c*-MeSe: $LOH^+$): **AA**; HF=-5343.2821 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.579855 | -1.380060 | -0.413730 |
| 6 | 0 | -1.317895 | -0.844698 | -0.267518 |
| 6 | 0 | -1.120307 | 0.549344 | -0.051353 |
| 6 | 0 | -2.297933 | 1.364956 | 0.093047 |
| 6 | 0 | -3.580335 | 0.776149 | -0.048741 |
| 6 | 0 | -3.723584 | -0.562319 | -0.313565 |
| 1 | 0 | -2.700365 | -2.441428 | -0.600630 |
| 6 | 0 | 0.134383 | 1.225011 | 0.043404 |
| 6 | 0 | -2.169738 | 2.747702 | 0.382665 |
| 1 | 0 | -4.454370 | 1.410270 | 0.055326 |
| 1 | 0 | -4.707514 | -1.000806 | -0.433225 |
| 6 | 0 | -0.938335 | 3.335652 | 0.514756 |
| 6 | 0 | 0.229949 | 2.569569 | 0.320959 |
| 1 | 0 | -3.072666 | 3.337959 | 0.498465 |
| 1 | 0 | -0.848059 | 4.391369 | 0.742249 |
| 1 | 0 | 1.199122 | 3.049828 | 0.361073 |
| 34 | 0 | 0.192620 | -2.058934 | -0.296770 |
| 34 | 0 | 1.821757 | 0.318259 | -0.421747 |
| 6 | 0 | 0.046383 | -2.743414 | 1.556846 |
| 1 | 0 | -0.848763 | -3.358535 | 1.620061 |
| 1 | 0 | 0.928355 | -3.355292 | 1.742374 |
| 1 | 0 | -0.012196 | -1.919720 | 2.265070 |
| 6 | 0 | 2.618807 | -0.006651 | 1.345489 |
| 1 | 0 | 3.549610 | -0.545447 | 1.177739 |
| 1 | 0 | 2.812399 | 0.979524 | 1.760388 |
| 1 | 0 | 1.931170 | -0.577346 | 1.960349 |
| 8 | 0 | 2.859092 | 1.869838 | -0.529278 |
| 1 | 0 | 3.052489 | 2.066410 | -1.458980 |

**5** (G = H: OH•OH): **A**; HF=-2978.4664 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -1.110376 | -0.100827 | -0.043787 |
| 6 | 0 | -2.332643 | 0.659042 | 0.013690 |
| 6 | 0 | 0.107717 | 0.643641 | -0.160257 |
| 6 | 0 | 0.101280 | 2.016402 | -0.255544 |
| 6 | 0 | -1.110789 | 2.738004 | -0.237089 |
| 6 | 0 | -2.299823 | 2.071924 | -0.095892 |
| 1 | 0 | 1.037587 | 2.555605 | -0.294409 |
| 1 | 0 | -1.085980 | 3.819769 | -0.314615 |
| 1 | 0 | -3.237199 | 2.619067 | -0.058556 |
| 6 | 0 | -1.211791 | -1.517052 | 0.042935 |
| 6 | 0 | -2.429529 | -2.134423 | 0.207112 |
| 6 | 0 | -3.622917 | -1.384497 | 0.286079 |
| 6 | 0 | -3.569594 | -0.017642 | 0.182249 |
| 1 | 0 | -0.324910 | -2.115725 | -0.087309 |
| 1 | 0 | -2.472230 | -3.217622 | 0.262368 |
| 1 | 0 | -4.574910 | -1.888723 | 0.417000 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -4.478976 | 0.574405 | 0.228796 |
| 34 | 0 | 1.931748 | -0.125958 | -0.250509 |
| 6 | 0 | 2.019609 | -1.332330 | 1.288076 |
| 1 | 0 | 3.076163 | -1.414723 | 1.533117 |
| 1 | 0 | 1.489537 | -0.852201 | 2.105400 |
| 1 | 0 | 1.604782 | -2.293154 | 1.004328 |
| 8 | 0 | 1.389971 | -1.730215 | -1.290579 |
| 1 | 0 | 1.448851 | -1.524740 | -2.232956 |
| 8 | 0 | 2.513203 | 1.298212 | 1.025935 |
| 1 | 0 | 3.365598 | 1.623197 | 0.705863 |

**6** (G = F: OH•OH): **A**; HF=-3077.7265 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.110186 | 0.033723 | -0.090468 |
| 6 | 0 | 2.329455 | 0.795926 | 0.019196 |
| 6 | 0 | -0.127541 | 0.754615 | -0.063033 |
| 6 | 0 | -0.130786 | 2.131101 | -0.038773 |
| 6 | 0 | 1.070752 | 2.868540 | 0.013522 |
| 6 | 0 | 2.270198 | 2.211956 | 0.076088 |
| 1 | 0 | -1.076108 | 2.656043 | -0.065497 |
| 1 | 0 | 1.029122 | 3.952346 | 0.031050 |
| 1 | 0 | 3.200310 | 2.765830 | 0.156863 |
| 6 | 0 | 1.285085 | -1.361545 | -0.273860 |
| 6 | 0 | 2.503381 | -1.985825 | -0.241671 |
| 6 | 0 | 3.674103 | -1.226305 | -0.053553 |
| 6 | 0 | 3.586718 | 0.138425 | 0.052133 |
| 9 | 0 | 0.216245 | -2.125036 | -0.574062 |
| 1 | 0 | 2.541628 | -3.058706 | -0.390082 |
| 1 | 0 | 4.637376 | -1.723751 | -0.025833 |
| 1 | 0 | 4.482765 | 0.742426 | 0.151664 |
| 34 | 0 | -1.928485 | 0.040224 | 0.340125 |
| 6 | 0 | -2.401771 | -1.468604 | -0.809967 |
| 1 | 0 | -3.482797 | -1.396299 | -0.912511 |
| 1 | 0 | -1.932068 | -1.323678 | -1.777278 |
| 1 | 0 | -2.093534 | -2.380119 | -0.313125 |
| 8 | 0 | -1.161838 | -1.270744 | 1.600050 |
| 1 | 0 | -1.135113 | -0.851993 | 2.471040 |
| 8 | 0 | -2.604964 | 1.199238 | -1.151525 |
| 1 | 0 | -3.433560 | 1.595627 | -0.849878 |

**7** (G = Cl: OH•OH): **A**; HF=-3438.0676 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.125045 | 0.176354 | -0.105695 |
| 6 | 0 | 2.281784 | 1.028351 | 0.046920 |
| 6 | 0 | -0.149353 | 0.838604 | -0.203655 |
| 6 | 0 | -0.211914 | 2.202264 | -0.390452 |
| 6 | 0 | 0.947988 | 3.005372 | -0.385037 |
| 6 | 0 | 2.156988 | 2.434985 | -0.099187 |
| 1 | 0 | -1.184667 | 2.657591 | -0.517517 |
| 1 | 0 | 0.856992 | 4.074615 | -0.543142 |
| 1 | 0 | 3.049939 | 3.044503 | -0.000590 |
| 6 | 0 | 1.410963 | -1.217987 | -0.211647 |
| 6 | 0 | 2.662033 | -1.732498 | 0.043334 |
| 6 | 0 | 3.740958 | -0.885468 | 0.353232 |
| 6 | 0 | 3.560319 | 0.472111 | 0.305339 |
| 1 | 0 | 2.817979 | -2.800545 | -0.048006 |
| 1 | 0 | 4.716552 | -1.311959 | 0.559801 |
| 1 | 0 | 4.398016 | 1.147742 | 0.445531 |
| 17 | 0 | 0.259052 | -2.346545 | -0.894698 |
| 34 | 0 | -1.901376 | 0.163067 | 0.486302 |
| 6 | 0 | -2.675713 | -1.319472 | -0.531312 |
| 1 | 0 | -3.749153 | -1.172580 | -0.429005 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -2.389339 | -1.211060 | -1.572131 |
| 1 | 0 | -2.343626 | -2.247032 | -0.081724 |
| 8 | 0 | -1.015492 | -1.185321 | 1.612114 |
| 1 | 0 | -0.785643 | -0.761017 | 2.450004 |
| 8 | 0 | -2.819553 | 1.329903 | -0.874702 |
| 1 | 0 | -3.558375 | 1.754360 | -0.417971 |

**8** (G = Br: OH•OH): **A**; HF=-5551.9834 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.057601 | 0.540541 | -0.041184 |
| 6 | 0 | 2.125871 | 1.511148 | 0.029662 |
| 6 | 0 | -0.265817 | 1.067812 | -0.255142 |
| 6 | 0 | -0.436478 | 2.373311 | -0.659861 |
| 6 | 0 | 0.651502 | 3.267233 | -0.755721 |
| 6 | 0 | 1.888014 | 2.862600 | -0.336145 |
| 1 | 0 | -1.441944 | 2.715443 | -0.866425 |
| 1 | 0 | 0.477915 | 4.285477 | -1.086768 |
| 1 | 0 | 2.718871 | 3.560427 | -0.298056 |
| 6 | 0 | 1.475285 | -0.822822 | 0.039915 |
| 6 | 0 | 2.750000 | -1.175799 | 0.422541 |
| 6 | 0 | 3.726649 | -0.193873 | 0.672747 |
| 6 | 0 | 3.431242 | 1.120534 | 0.422564 |
| 1 | 0 | 3.017104 | -2.224140 | 0.473315 |
| 1 | 0 | 4.721400 | -0.493657 | 0.984371 |
| 1 | 0 | 4.197495 | 1.885318 | 0.499910 |
| 35 | 0 | 0.427856 | -2.261066 | -0.668859 |
| 34 | 0 | -1.950554 | 0.364595 | 0.575511 |
| 6 | 0 | -2.679930 | -1.238785 | -0.279016 |
| 1 | 0 | -3.754473 | -1.142353 | -0.138720 |
| 1 | 0 | -2.444397 | -1.202963 | -1.337625 |
| 1 | 0 | -2.273727 | -2.104876 | 0.228072 |
| 8 | 0 | -0.956824 | -0.832721 | 1.775104 |
| 1 | 0 | -0.711962 | -0.326076 | 2.561387 |
| 8 | 0 | -3.017925 | 1.343929 | -0.823701 |
| 1 | 0 | -3.708043 | 1.827412 | -0.350161 |

**1** (G = *t*-MeSe: LOH•OH): **A**; HF=-5419.3063 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.950288 | 0.843180 | -0.046850 |
| 6 | 0 | 1.868105 | 1.954240 | 0.072072 |
| 6 | 0 | 1.537976 | -0.463879 | -0.026733 |
| 6 | 0 | 3.207398 | 1.733289 | 0.477721 |
| 6 | 0 | -0.435107 | 1.198265 | -0.240979 |
| 6 | 0 | 1.451970 | 3.271837 | -0.258068 |
| 6 | 0 | 2.856703 | -0.629778 | 0.352409 |
| 6 | 0 | 3.680377 | 0.461671 | 0.680103 |
| 6 | 0 | -0.783791 | 2.480129 | -0.604274 |
| 6 | 0 | 0.173152 | 3.516331 | -0.673569 |
| 1 | 0 | 3.291282 | -1.623020 | 0.329714 |
| 1 | 0 | 4.705322 | 0.292058 | 0.993254 |
| 1 | 0 | 3.859596 | 2.592901 | 0.597958 |
| 1 | 0 | -1.826632 | 2.691638 | -0.799203 |
| 1 | 0 | -0.137629 | 4.509980 | -0.978241 |
| 1 | 0 | 2.180379 | 4.074711 | -0.195130 |
| 34 | 0 | 0.697603 | -1.981318 | -0.893658 |
| 6 | 0 | 0.735853 | -3.289809 | 0.583304 |
| 1 | 0 | 1.760689 | -3.537350 | 0.854864 |
| 1 | 0 | 0.190559 | -2.860185 | 1.419802 |
| 1 | 0 | 0.238903 | -4.186577 | 0.210254 |
| 34 | 0 | -2.015109 | 0.258468 | 0.571080 |
| 6 | 0 | -2.574261 | -1.389748 | -0.325907 |
| 1 | 0 | -3.645461 | -1.433595 | -0.136266 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -2.043188 | -2.221880 | 0.117135 |
| 1 | 0 | -2.388940 | -1.282140 | -1.388681 |
| 8 | 0 | -0.879997 | -0.863087 | 1.740284 |
| 1 | 0 | -0.657560 | -0.336248 | 2.519702 |
| 8 | 0 | -3.220778 | 1.142360 | -0.771150 |
| 1 | 0 | -3.937923 | 1.548063 | -0.265949 |

**1** (G = *c*-MeSe: LOH•OH): **A**; HF=-5419.3102 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.655638 | 0.993124 | -0.063839 |
| 6 | 0 | -1.278566 | 2.298089 | -0.054157 |
| 6 | 0 | -1.525564 | -0.115649 | -0.343850 |
| 6 | 0 | -2.591555 | 2.473935 | -0.562551 |
| 6 | 0 | 0.750383 | 0.977934 | 0.266540 |
| 6 | 0 | -0.609518 | 3.413870 | 0.514514 |
| 6 | 0 | -2.788615 | 0.108788 | -0.858793 |
| 6 | 0 | -3.315912 | 1.404990 | -1.017973 |
| 6 | 0 | 1.345744 | 2.073354 | 0.850104 |
| 6 | 0 | 0.645966 | 3.283796 | 1.039546 |
| 1 | 0 | -3.411511 | -0.745620 | -1.099426 |
| 1 | 0 | -4.310519 | 1.538671 | -1.430673 |
| 1 | 0 | -3.011966 | 3.474907 | -0.569934 |
| 1 | 0 | 2.395075 | 2.008211 | 1.111098 |
| 1 | 0 | 1.142964 | 4.119334 | 1.520881 |
| 1 | 0 | -1.127951 | 4.367711 | 0.540260 |
| 34 | 0 | -1.205522 | -1.947533 | 0.240414 |
| 6 | 0 | -2.569005 | -1.930547 | 1.685893 |
| 1 | 0 | -2.348697 | -1.150036 | 2.412862 |
| 1 | 0 | -3.573002 | -1.799479 | 1.284923 |
| 1 | 0 | -2.502629 | -2.905333 | 2.172658 |
| 34 | 0 | 2.113994 | -0.265712 | -0.553095 |
| 6 | 0 | 2.353763 | -1.785511 | 0.651759 |
| 1 | 0 | 3.152172 | -2.379231 | 0.210008 |
| 1 | 0 | 1.421652 | -2.333943 | 0.701183 |
| 1 | 0 | 2.668133 | -1.377603 | 1.607220 |
| 8 | 0 | 0.785168 | -1.369217 | -1.509848 |
| 1 | 0 | 0.646884 | -0.986770 | -2.386782 |
| 8 | 0 | 3.616478 | 0.525916 | 0.513151 |
| 1 | 0 | 4.189257 | 0.988872 | -0.112708 |

**5** (G = H: OH•OH): **B**; HF=-2978.4683 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.102447 | -0.349320 | 0.000000 |
| 6 | 0 | 2.424319 | 0.210588 | 0.000000 |
| 6 | 0 | 0.000000 | 0.555238 | 0.000000 |
| 6 | 0 | 2.585745 | 1.619272 | 0.000000 |
| 6 | 0 | 0.977096 | -1.765507 | 0.000000 |
| 6 | 0 | 3.544359 | -0.661865 | 0.000000 |
| 6 | 0 | 0.187684 | 1.913629 | 0.000000 |
| 6 | 0 | 1.494279 | 2.450825 | 0.000000 |
| 6 | 0 | 2.084105 | -2.580141 | 0.000000 |
| 6 | 0 | 3.383569 | -2.025353 | 0.000000 |
| 1 | 0 | 3.590597 | 2.030457 | 0.000000 |
| 1 | 0 | -0.007553 | -2.221023 | 0.000000 |
| 1 | 0 | 4.539675 | -0.227393 | 0.000000 |
| 1 | 0 | -0.655373 | 2.592830 | 0.000000 |
| 1 | 0 | 1.623847 | 3.527990 | 0.000000 |
| 1 | 0 | 1.959053 | -3.658033 | 0.000000 |
| 1 | 0 | 4.249538 | -2.679033 | 0.000000 |
| 34 | 0 | -1.804960 | -0.201310 | 0.000000 |
| 6 | 0 | -2.966628 | 1.357608 | 0.000000 |
| 1 | 0 | -2.781049 | 1.910932 | 0.915053 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -2.781049 | 1.910932 | -0.915053 |
| 1 | 0 | -3.979642 | 0.959779 | 0.000000 |
| 8 | 0 | -1.885792 | -0.002233 | 1.979896 |
| 1 | 0 | -1.559299 | -0.808502 | 2.401482 |
| 8 | 0 | -1.885792 | -0.002233 | -1.979896 |
| 1 | 0 | -1.559299 | -0.808502 | -2.401482 |

**6** (G = F: OH•OH): **B**; HF=-3077.7354 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.121081 | -0.237968 | 0.000000 |
| 6 | 0 | 2.442268 | 0.335374 | 0.000000 |
| 6 | 0 | 0.000000 | 0.647932 | 0.000000 |
| 6 | 0 | 2.586563 | 1.745129 | 0.000000 |
| 6 | 0 | 1.075319 | -1.655367 | 0.000000 |
| 6 | 0 | 3.585047 | -0.506811 | 0.000000 |
| 6 | 0 | 0.189457 | 2.007441 | 0.000000 |
| 6 | 0 | 1.486769 | 2.562113 | 0.000000 |
| 6 | 0 | 2.179286 | -2.460732 | 0.000000 |
| 6 | 0 | 3.461326 | -1.872806 | 0.000000 |
| 1 | 0 | 3.587260 | 2.165235 | 0.000000 |
| 9 | 0 | -0.142711 | -2.267077 | 0.000000 |
| 1 | 0 | 4.566828 | -0.044621 | 0.000000 |
| 1 | 0 | -0.656265 | 2.681391 | 0.000000 |
| 1 | 0 | 1.601468 | 3.640867 | 0.000000 |
| 1 | 0 | 2.047395 | -3.536402 | 0.000000 |
| 1 | 0 | 4.340032 | -2.508175 | 0.000000 |
| 34 | 0 | -1.843137 | -0.042598 | 0.000000 |
| 6 | 0 | -2.915919 | 1.580270 | 0.000000 |
| 1 | 0 | -2.710462 | 2.126905 | 0.915050 |
| 1 | 0 | -2.710462 | 2.126905 | -0.915050 |
| 1 | 0 | -3.947041 | 1.230204 | 0.000000 |
| 8 | 0 | -1.873824 | 0.157711 | 1.982677 |
| 1 | 0 | -1.726845 | -0.710548 | 2.381399 |
| 8 | 0 | -1.873824 | 0.157711 | -1.982677 |
| 1 | 0 | -1.726845 | -0.710548 | -2.381399 |

**7** (G = Cl: OH•OH): **B**; HF=-3438.0811 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.422032 | -2.201206 | 0.000000 |
| 6 | 0 | -1.233720 | -1.509213 | 0.000000 |
| 6 | 0 | -1.162754 | -0.079929 | 0.000000 |
| 6 | 0 | -2.447699 | 0.588891 | 0.000000 |
| 6 | 0 | -3.657003 | -0.151296 | 0.000000 |
| 6 | 0 | -3.651991 | -1.519986 | 0.000000 |
| 1 | 0 | -2.399808 | -3.284068 | 0.000000 |
| 6 | 0 | 0.000000 | 0.763163 | 0.000000 |
| 6 | 0 | -2.519196 | 2.003982 | 0.000000 |
| 1 | 0 | -4.593449 | 0.397114 | 0.000000 |
| 1 | 0 | -4.578207 | -2.083914 | 0.000000 |
| 6 | 0 | -1.383005 | 2.764041 | 0.000000 |
| 6 | 0 | -0.125556 | 2.131860 | 0.000000 |
| 1 | 0 | -3.499139 | 2.470341 | 0.000000 |
| 1 | 0 | -1.436429 | 3.847401 | 0.000000 |
| 1 | 0 | 0.753630 | 2.759746 | 0.000000 |
| 17 | 0 | 0.205373 | -2.536574 | 0.000000 |
| 34 | 0 | 1.857744 | 0.080324 | 0.000000 |
| 6 | 0 | 2.938779 | 1.700695 | 0.000000 |
| 1 | 0 | 3.965385 | 1.336828 | 0.000000 |
| 1 | 0 | 2.741516 | 2.249023 | 0.915689 |
| 1 | 0 | 2.741516 | 2.249023 | -0.915689 |
| 8 | 0 | 1.890330 | 0.289720 | 1.981603 |
| 1 | 0 | 1.695058 | -0.566150 | 2.386685 |

| | | | | |
|---|---|---|---|---|
| 8 | 0 | 1.890330 | 0.289720 | -1.981603 |
| 1 | 0 | 1.695058 | -0.566150 | -2.386685 |

**8** (G = Br: OH•OH): **B**; HF=-5551.9983 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -2.551323 | -1.792779 | 0.000000 |
| 6 | 0 | -1.330078 | -1.157655 | 0.000000 |
| 6 | 0 | -1.193364 | 0.268741 | 0.000000 |
| 6 | 0 | -2.451025 | 0.992360 | 0.000000 |
| 6 | 0 | -3.692754 | 0.308502 | 0.000000 |
| 6 | 0 | -3.750369 | -1.057898 | 0.000000 |
| 1 | 0 | -2.586619 | -2.874755 | 0.000000 |
| 6 | 0 | 0.000000 | 1.070318 | 0.000000 |
| 6 | 0 | -2.468064 | 2.409036 | 0.000000 |
| 1 | 0 | -4.602730 | 0.899793 | 0.000000 |
| 1 | 0 | -4.700613 | -1.580439 | 0.000000 |
| 6 | 0 | -1.304532 | 3.125193 | 0.000000 |
| 6 | 0 | -0.074174 | 2.443265 | 0.000000 |
| 1 | 0 | -3.429881 | 2.911784 | 0.000000 |
| 1 | 0 | -1.315597 | 4.209766 | 0.000000 |
| 1 | 0 | 0.827680 | 3.037824 | 0.000000 |
| 35 | 0 | 0.158171 | -2.388872 | 0.000000 |
| 34 | 0 | 1.837087 | 0.332497 | 0.000000 |
| 6 | 0 | 2.969526 | 1.918820 | 0.000000 |
| 1 | 0 | 3.983421 | 1.520805 | 0.000000 |
| 1 | 0 | 2.791157 | 2.473417 | 0.915767 |
| 1 | 0 | 2.791157 | 2.473417 | -0.915767 |
| 8 | 0 | 1.877247 | 0.542110 | 1.981501 |
| 1 | 0 | 1.643034 | -0.303590 | 2.387399 |
| 8 | 0 | 1.877247 | 0.542110 | -1.981501 |
| 1 | 0 | 1.643034 | -0.303590 | -2.387399 |

**1** (G = *t*-MeSe: LOH•OH): **B**; HF=-5419.3207 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.000000 | 1.272162 | 0.000000 |
| 6 | 0 | -0.209430 | 2.705547 | 0.000000 |
| 6 | 0 | 1.376334 | 0.827879 | 0.000000 |
| 6 | 0 | 0.885642 | 3.605759 | 0.000000 |
| 6 | 0 | -1.196285 | 0.475902 | 0.000000 |
| 6 | 0 | -1.517763 | 3.250173 | 0.000000 |
| 6 | 0 | 2.403252 | 1.752091 | 0.000000 |
| 6 | 0 | 2.169515 | 3.139492 | 0.000000 |
| 6 | 0 | -2.447132 | 1.047354 | 0.000000 |
| 6 | 0 | -2.620492 | 2.442125 | 0.000000 |
| 1 | 0 | 3.432329 | 1.422780 | 0.000000 |
| 1 | 0 | 3.012803 | 3.822281 | 0.000000 |
| 1 | 0 | 0.679335 | 4.671157 | 0.000000 |
| 1 | 0 | -3.331709 | 0.426356 | 0.000000 |
| 1 | 0 | -3.621509 | 2.859972 | 0.000000 |
| 1 | 0 | -1.623118 | 4.330523 | 0.000000 |
| 34 | 0 | 1.883492 | -1.058640 | 0.000000 |
| 6 | 0 | 3.849388 | -0.937587 | 0.000000 |
| 1 | 0 | 4.177149 | -1.977526 | 0.000000 |
| 1 | 0 | 4.218539 | -0.446215 | 0.898644 |
| 1 | 0 | 4.218539 | -0.446215 | -0.898644 |
| 34 | 0 | -1.172463 | -1.493933 | 0.000000 |
| 6 | 0 | -3.049544 | -2.015635 | 0.000000 |
| 1 | 0 | -3.026871 | -3.104183 | 0.000000 |
| 1 | 0 | -3.504099 | -1.652506 | -0.916007 |
| 1 | 0 | -3.504099 | -1.652506 | 0.916007 |
| 8 | 0 | -1.384609 | -1.489937 | -1.977485 |
| 1 | 0 | -0.504716 | -1.509510 | -2.378441 |

| | | | | |
|---|---|---|---|---|
| 8 | 0 | -1.384609 | -1.489937 | 1.977485 |
| 1 | 0 | -0.504716 | -1.509510 | 2.378441 |

**1** (G = *c*-MeSe: LOH•OH): **B**; HF=-5419.3207 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.608589 | 1.116748 | -0.000001 |
| 6 | 0 | -1.112037 | 2.475170 | -0.000002 |
| 6 | 0 | -1.603597 | 0.066998 | -0.000004 |
| 6 | 0 | -2.504557 | 2.740468 | -0.000006 |
| 6 | 0 | 0.822813 | 0.991271 | 0.000004 |
| 6 | 0 | -0.224854 | 3.580232 | 0.000001 |
| 6 | 0 | -2.947699 | 0.386445 | -0.000008 |
| 6 | 0 | -3.407813 | 1.715888 | -0.000009 |
| 6 | 0 | 1.646828 | 2.092284 | 0.000007 |
| 6 | 0 | 1.130219 | 3.399487 | 0.000005 |
| 1 | 0 | -3.692720 | -0.395761 | -0.000010 |
| 1 | 0 | -4.475221 | 1.910671 | -0.000012 |
| 1 | 0 | -2.833944 | 3.774498 | -0.000007 |
| 1 | 0 | 2.720979 | 1.972246 | 0.000011 |
| 1 | 0 | 1.808480 | 4.246038 | 0.000007 |
| 1 | 0 | -0.649897 | 4.579004 | 0.000000 |
| 34 | 0 | -1.147022 | -1.832437 | -0.000004 |
| 6 | 0 | -2.932682 | -2.665619 | -0.000004 |
| 1 | 0 | -2.723458 | -3.735708 | -0.000023 |
| 1 | 0 | -3.491728 | -2.410355 | -0.898668 |
| 1 | 0 | -3.491715 | -2.410384 | 0.898676 |
| 34 | 0 | 1.745388 | -0.749616 | 0.000007 |
| 6 | 0 | 3.642316 | -0.306334 | -0.000010 |
| 1 | 0 | 4.145730 | -1.271737 | -0.000010 |
| 1 | 0 | 3.865696 | 0.230854 | 0.916055 |
| 1 | 0 | 3.865681 | 0.230847 | -0.916081 |
| 8 | 0 | 1.929477 | -0.644944 | 1.977284 |
| 1 | 0 | 1.167111 | -1.084672 | 2.378313 |
| 8 | 0 | 1.929449 | -0.644965 | -1.977274 |
| 1 | 0 | 1.167078 | -1.084700 | -2.378287 |

**5** (G = H: OH•OH): **C**; HF=-2978.4686 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -1.153350 | -0.099414 | 0.052869 |
| 6 | 0 | -2.318413 | 0.729382 | -0.073305 |
| 6 | 0 | 0.119860 | 0.540012 | 0.015803 |
| 6 | 0 | 0.236260 | 1.901680 | -0.102834 |
| 6 | 0 | -0.918602 | 2.705274 | -0.230423 |
| 6 | 0 | -2.165114 | 2.131148 | -0.223601 |
| 1 | 0 | 1.209105 | 2.376265 | -0.081482 |
| 1 | 0 | -0.808173 | 3.779778 | -0.332028 |
| 1 | 0 | -3.054084 | 2.746468 | -0.323856 |
| 6 | 0 | -1.344119 | -1.496504 | 0.232396 |
| 6 | 0 | -2.603322 | -2.045540 | 0.271407 |
| 6 | 0 | -3.747754 | -1.228860 | 0.128828 |
| 6 | 0 | -3.603378 | 0.126264 | -0.036809 |
| 1 | 0 | -0.485484 | -2.147366 | 0.357173 |
| 1 | 0 | -2.720261 | -3.114907 | 0.413990 |
| 1 | 0 | -4.736306 | -1.675112 | 0.156224 |
| 1 | 0 | -4.477633 | 0.762447 | -0.138596 |
| 34 | 0 | 1.734696 | -0.563347 | 0.147472 |
| 6 | 0 | 3.099050 | 0.533213 | -0.706091 |
| 1 | 0 | 3.945348 | -0.130658 | -0.869452 |
| 1 | 0 | 2.700459 | 0.865926 | -1.659448 |
| 1 | 0 | 3.357753 | 1.332952 | -0.020280 |
| 8 | 0 | 2.273793 | 0.399807 | 1.801360 |
| 1 | 0 | 1.861626 | -0.016391 | 2.570564 |

| | | | | |
|---|---|---|---|---|
| 8 | 0 | 1.439520 | -1.199200 | -1.718038 |
| 1 | 0 | 0.914776 | -2.010383 | -1.722876 |

**6** (G = F: OH•OH): **C**; HF=-3077.7371 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -1.143086 | 0.056544 | -0.062050 |
| 6 | 0 | -2.268456 | 0.941176 | 0.091119 |
| 6 | 0 | 0.165045 | 0.628256 | -0.069744 |
| 6 | 0 | -2.043130 | 2.337128 | 0.195429 |
| 6 | 0 | -1.463674 | -1.314568 | -0.222475 |
| 6 | 0 | -3.587382 | 0.416730 | 0.121993 |
| 6 | 0 | 0.333933 | 1.989747 | -0.008764 |
| 6 | 0 | -0.774596 | 2.852161 | 0.129305 |
| 6 | 0 | -2.735786 | -1.812611 | -0.196869 |
| 6 | 0 | -3.819223 | -0.928849 | -0.009502 |
| 1 | 0 | -2.899352 | 2.993446 | 0.315200 |
| 9 | 0 | -0.451825 | -2.198775 | -0.452593 |
| 1 | 0 | -4.415260 | 1.107082 | 0.247195 |
| 1 | 0 | 1.326366 | 2.413560 | -0.083961 |
| 1 | 0 | -0.610351 | 3.922845 | 0.188627 |
| 1 | 0 | -2.888748 | -2.877014 | -0.331681 |
| 1 | 0 | -4.829868 | -1.321004 | 0.014588 |
| 34 | 0 | 1.797195 | -0.477879 | -0.122933 |
| 6 | 0 | 3.035510 | 0.577249 | 0.952352 |
| 1 | 0 | 3.409623 | 1.388848 | 0.337413 |
| 1 | 0 | 2.507365 | 0.898476 | 1.845069 |
| 1 | 0 | 3.834649 | -0.108572 | 1.226641 |
| 8 | 0 | 2.485360 | 0.626944 | -1.637307 |
| 1 | 0 | 2.179423 | 0.250494 | -2.473577 |
| 8 | 0 | 1.290370 | -1.246110 | 1.632700 |
| 1 | 0 | 0.947168 | -2.135726 | 1.479645 |

**7** (G = Cl: OH•OH): **C**; HF=-3438.0833 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 2.881018 | -1.510043 | 0.035755 |
| 6 | 0 | 1.568953 | -1.141013 | -0.139847 |
| 6 | 0 | 1.130722 | 0.216392 | -0.073168 |
| 6 | 0 | 2.184654 | 1.194827 | 0.066620 |
| 6 | 0 | 3.530592 | 0.787530 | 0.249655 |
| 6 | 0 | 3.874089 | -0.538266 | 0.260400 |
| 1 | 0 | 3.149251 | -2.557570 | -0.028291 |
| 6 | 0 | -0.206095 | 0.721923 | -0.174565 |
| 6 | 0 | 1.883211 | 2.579029 | -0.001316 |
| 1 | 0 | 4.288540 | 1.554725 | 0.371212 |
| 1 | 0 | 4.903463 | -0.847580 | 0.403988 |
| 6 | 0 | 0.602798 | 3.011026 | -0.216961 |
| 6 | 0 | -0.444061 | 2.070471 | -0.294103 |
| 1 | 0 | 2.697318 | 3.289342 | 0.103002 |
| 1 | 0 | 0.378963 | 4.068919 | -0.302912 |
| 1 | 0 | -1.455740 | 2.418324 | -0.453269 |
| 17 | 0 | 0.473843 | -2.456184 | -0.587122 |
| 34 | 0 | -1.838459 | -0.388823 | 0.009620 |
| 6 | 0 | -2.996395 | 0.792219 | 1.048053 |
| 1 | 0 | -3.761998 | 0.142558 | 1.467904 |
| 1 | 0 | -3.429036 | 1.522108 | 0.372317 |
| 1 | 0 | -2.401746 | 1.221599 | 1.848493 |
| 8 | 0 | -1.199304 | -0.937462 | 1.806174 |
| 1 | 0 | -0.863577 | -1.841650 | 1.753422 |
| 8 | 0 | -2.641871 | 0.539638 | -1.564843 |
| 1 | 0 | -2.380687 | 0.082361 | -2.375652 |

**8** (G = Br: OH•OH): **C**; HF=-5552.0007 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 2.949837 | -0.869874 | 0.288855 |
| 6 | 0 | 1.614091 | -0.675945 | 0.027497 |
| 6 | 0 | 1.021494 | 0.621656 | -0.045791 |
| 6 | 0 | 1.953004 | 1.724975 | 0.021568 |
| 6 | 0 | 3.325176 | 1.497665 | 0.297054 |
| 6 | 0 | 3.813520 | 0.228932 | 0.460908 |
| 1 | 0 | 3.346109 | -1.876830 | 0.330557 |
| 6 | 0 | -0.358815 | 0.962830 | -0.223247 |
| 6 | 0 | 1.505203 | 3.050459 | -0.213298 |
| 1 | 0 | 3.985811 | 2.356113 | 0.364447 |
| 1 | 0 | 4.862175 | 0.056511 | 0.676913 |
| 6 | 0 | 0.197097 | 3.307565 | -0.521303 |
| 6 | 0 | -0.737912 | 2.252720 | -0.509117 |
| 1 | 0 | 2.231430 | 3.855670 | -0.162918 |
| 1 | 0 | -0.136490 | 4.316431 | -0.739305 |
| 1 | 0 | -1.776858 | 2.462174 | -0.725554 |
| 35 | 0 | 0.650217 | -2.287574 | -0.422789 |
| 34 | 0 | -1.869679 | -0.276211 | 0.125942 |
| 6 | 0 | -3.110378 | 0.905776 | 1.065318 |
| 1 | 0 | -3.812403 | 0.241692 | 1.566110 |
| 1 | 0 | -3.613063 | 1.523426 | 0.328905 |
| 1 | 0 | -2.541915 | 1.463455 | 1.803087 |
| 8 | 0 | -1.142494 | -0.561384 | 1.949234 |
| 1 | 0 | -0.734863 | -1.436443 | 1.987089 |
| 8 | 0 | -2.796680 | 0.385964 | -1.515368 |
| 1 | 0 | -2.518940 | -0.143137 | -2.275359 |

**1** (G = *t*-MeSe: LOH•OH): **C**; HF=-5419.3241 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.698909 | 0.997114 | -0.017092 |
| 6 | 0 | 1.289615 | 2.315145 | 0.000052 |
| 6 | 0 | 1.589652 | -0.100097 | -0.256100 |
| 6 | 0 | 2.654930 | 2.494751 | -0.343486 |
| 6 | 0 | -0.709274 | 0.940743 | 0.244469 |
| 6 | 0 | 0.522323 | 3.443327 | 0.386441 |
| 6 | 0 | 2.903971 | 0.125406 | -0.605383 |
| 6 | 0 | 3.444326 | 1.425672 | -0.670299 |
| 6 | 0 | -1.408356 | 2.048873 | 0.663168 |
| 6 | 0 | -0.789996 | 3.311705 | 0.752884 |
| 1 | 0 | 3.545503 | -0.721806 | -0.820838 |
| 1 | 0 | 4.483095 | 1.564872 | -0.951060 |
| 1 | 0 | 3.059859 | 3.502088 | -0.338088 |
| 1 | 0 | -2.451531 | 1.945466 | 0.930390 |
| 1 | 0 | -1.368300 | 4.169667 | 1.078827 |
| 1 | 0 | 1.005522 | 4.415616 | 0.399738 |
| 34 | 0 | 1.101724 | -1.960669 | 0.034996 |
| 6 | 0 | 2.283706 | -2.285051 | 1.591882 |
| 1 | 0 | 3.331010 | -2.185840 | 1.312617 |
| 1 | 0 | 2.040296 | -1.597762 | 2.400070 |
| 1 | 0 | 2.090153 | -3.309678 | 1.912023 |
| 34 | 0 | -1.855799 | -0.636584 | -0.118308 |
| 6 | 0 | -3.309335 | 0.236167 | -1.109669 |
| 1 | 0 | -3.848881 | -0.566260 | -1.611986 |
| 1 | 0 | -2.854927 | 0.896172 | -1.841707 |
| 1 | 0 | -3.955111 | 0.741755 | -0.398402 |
| 8 | 0 | -0.876639 | -0.737979 | -1.865102 |
| 1 | 0 | -0.952256 | -1.642193 | -2.199228 |
| 8 | 0 | -2.984084 | -0.249338 | 1.478049 |
| 1 | 0 | -2.622920 | -0.729497 | 2.235463 |

**1** (G = *c*-MeSe: LOH•OH): **C**; HF=-5419.3214 a.u.

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.946110 | 0.854497 | -0.049997 |
| 6 | 0 | -1.788100 | 2.024107 | 0.065570 |
| 6 | 0 | -1.619595 | -0.411451 | -0.100219 |
| 6 | 0 | -3.182053 | 1.885411 | 0.284705 |
| 6 | 0 | 0.461394 | 1.106631 | -0.156466 |
| 6 | 0 | -1.238591 | 3.324987 | -0.062713 |
| 6 | 0 | -2.984245 | -0.492434 | 0.090006 |
| 6 | 0 | -3.771128 | 0.650119 | 0.330994 |
| 6 | 0 | 0.947103 | 2.379850 | -0.333277 |
| 6 | 0 | 0.095559 | 3.502212 | -0.307648 |
| 1 | 0 | -3.468959 | -1.459492 | 0.015716 |
| 1 | 0 | -4.838573 | 0.546844 | 0.494967 |
| 1 | 0 | -3.777335 | 2.786372 | 0.397461 |
| 1 | 0 | 2.004634 | 2.537275 | -0.492157 |
| 1 | 0 | 0.512250 | 4.494124 | -0.446045 |
| 1 | 0 | -1.905554 | 4.177939 | 0.016841 |
| 34 | 0 | -0.759062 | -2.065780 | -0.655995 |
| 6 | 0 | -0.716260 | -2.982074 | 1.095341 |
| 1 | 0 | -0.269455 | -2.303313 | 1.817564 |
| 1 | 0 | -1.724544 | -3.265971 | 1.390521 |
| 1 | 0 | -0.104442 | -3.875799 | 0.968365 |
| 34 | 0 | 1.855239 | -0.272588 | 0.091294 |
| 6 | 0 | 3.341929 | 0.811701 | 0.788255 |
| 1 | 0 | 4.025807 | 0.095159 | 1.244140 |
| 1 | 0 | 2.949218 | 1.483807 | 1.544910 |
| 1 | 0 | 3.827913 | 1.312934 | -0.043669 |
| 8 | 0 | 1.123025 | -0.343084 | 1.971946 |
| 1 | 0 | 1.615948 | -1.020329 | 2.457009 |
| 8 | 0 | 2.637624 | 0.151322 | -1.682243 |
| 1 | 0 | 2.198475 | -0.392284 | -2.350716 |