***Supporting Information:***

# Extended Hypervalent E'---E–E---E' 4c–6e (E, E' = Se, S) Interactions: Structure, Stability, and Reactivity of 1-(8-PhE'$C_{10}H_6$)EE($C_{10}H_6$E'Ph-8')-1'

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Optimized structures given by Cartesian coordinates for **5**, **6**, **13**–**20**, together with the total energies and the method for the calculations. S1-S18

Optimized structures given by Cartesian coordinates for **5**, **6**, **13**–**22**, together with the total energies and the method for the calculations.

The 6-311+G(d) basis sets are employed for S, Se, and B and the 6-311G(d) basis sets for C and H at the B3LYP level.

**5** (**A**)
B3LYP/6-311+G(d) for Se and 6-311G(d) for C and H
Total energy: -5573.8509725 hartrees

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 1.024414 | 0.617625 | -1.264448 |
| 6 | 0 | 0.756882 | 1.869443 | 0.195190 |
| 6 | 0 | 0.001285 | 3.077446 | 0.044218 |
| 6 | 0 | 1.380288 | 1.577349 | 1.391235 |
| 6 | 0 | -0.088631 | 3.961347 | 1.171320 |
| 6 | 0 | 1.291522 | 2.460721 | 2.489867 |
| 6 | 0 | 0.571564 | 3.623173 | 2.381081 |
| 1 | 0 | 1.943800 | 0.656861 | 1.489636 |
| 1 | 0 | 1.793256 | 2.208351 | 3.418350 |
| 1 | 0 | 0.496311 | 4.303978 | 3.224055 |
| 6 | 0 | -0.664830 | 3.449315 | -1.151917 |
| 6 | 0 | -1.380288 | 4.620591 | -1.232319 |
| 6 | 0 | -1.470148 | 5.487147 | -0.121019 |
| 6 | 0 | -0.835451 | 5.162196 | 1.051982 |
| 1 | 0 | -0.597155 | 2.794817 | -2.011786 |
| 1 | 0 | -1.879892 | 4.882657 | -2.159432 |
| 1 | 0 | -2.038756 | 6.408215 | -0.198482 |
| 1 | 0 | -0.896243 | 5.824035 | 1.911076 |
| 34 | 0 | -1.024414 | -0.617625 | -1.264448 |
| 6 | 0 | -0.756882 | -1.869443 | 0.195190 |
| 6 | 0 | -0.001285 | -3.077446 | 0.044218 |
| 6 | 0 | -1.380288 | -1.577349 | 1.391235 |
| 6 | 0 | 0.088631 | -3.961347 | 1.171320 |
| 6 | 0 | -1.291522 | -2.460721 | 2.489867 |
| 6 | 0 | -0.571564 | -3.623173 | 2.381081 |
| 1 | 0 | -1.943800 | -0.656861 | 1.489636 |
| 1 | 0 | -1.793256 | -2.208351 | 3.418350 |
| 1 | 0 | -0.496311 | -4.303978 | 3.224055 |
| 6 | 0 | 0.664830 | -3.449315 | -1.151917 |
| 6 | 0 | 1.380288 | -4.620591 | -1.232319 |
| 6 | 0 | 1.470148 | -5.487147 | -0.121019 |
| 6 | 0 | 0.835451 | -5.162196 | 1.051982 |
| 1 | 0 | 0.597155 | -2.794817 | -2.011786 |
| 1 | 0 | 1.879892 | -4.882657 | -2.159432 |
| 1 | 0 | 2.038756 | -6.408215 | -0.198482 |
| 1 | 0 | 0.896243 | -5.824035 | 1.911076 |

**5** (**B**)
B3LYP/6-311+G(d) for Se and 6-311G(d) for C and H
Total energy: -5573.8464589 hartrees

| | | | | |
|---|---|---|---|---|
| 34 | 0 | -0.580833 | 1.016690 | -1.270294 |
| 1 | 0 | -1.289250 | 3.567904 | -1.590353 |
| 34 | 0 | 0.580833 | -1.016690 | -1.270294 |
| 1 | 0 | 1.289250 | -3.567904 | -1.590353 |
| 6 | 0 | 0.343396 | 2.090774 | 0.086334 |
| 6 | 0 | 0.061754 | 3.493288 | 0.111668 |
| 6 | 0 | 1.203261 | 1.530671 | 0.999606 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.695898 | 4.291095 | 1.122011 |
| 6 | 0 | 1.828114 | 2.331061 | 1.982231 |
| 6 | 0 | 1.578877 | 3.677714 | 2.046987 |
| 1 | 0 | 1.416462 | 0.468412 | 0.969300 |
| 1 | 0 | 2.505402 | 1.862500 | 2.688984 |
| 1 | 0 | 2.054272 | 4.292047 | 2.805515 |
| 6 | 0 | -0.807626 | 4.141875 | -0.805700 |
| 6 | 0 | -1.045819 | 5.493289 | -0.730439 |
| 6 | 0 | -0.425531 | 6.274500 | 0.268842 |
| 6 | 0 | 0.425531 | 5.683445 | 1.169328 |
| 1 | 0 | -1.712174 | 5.963726 | -1.446067 |
| 1 | 0 | -0.621081 | 7.340689 | 0.319428 |
| 1 | 0 | 0.909797 | 6.278732 | 1.937979 |
| 6 | 0 | -0.343396 | -2.090774 | 0.086334 |
| 6 | 0 | -0.061754 | -3.493288 | 0.111668 |
| 6 | 0 | -1.203261 | -1.530671 | 0.999606 |
| 6 | 0 | -0.695898 | -4.291095 | 1.122011 |
| 6 | 0 | -1.828114 | -2.331061 | 1.982231 |
| 6 | 0 | -1.578877 | -3.677714 | 2.046987 |
| 1 | 0 | -1.416462 | -0.468412 | 0.969300 |
| 1 | 0 | -2.505402 | -1.862500 | 2.688984 |
| 1 | 0 | -2.054272 | -4.292047 | 2.805515 |
| 6 | 0 | 0.807626 | -4.141875 | -0.805700 |
| 6 | 0 | 1.045819 | -5.493289 | -0.730439 |
| 6 | 0 | 0.425531 | -6.274500 | 0.268842 |
| 6 | 0 | -0.425531 | -5.683445 | 1.169328 |
| 1 | 0 | 1.712174 | -5.963726 | -1.446067 |
| 1 | 0 | 0.621081 | -7.340689 | 0.319428 |
| 1 | 0 | -0.909797 | -6.278732 | 1.937979 |

**6** (**A**)
B3LYP/6-311+G(d) for S and 6-311G(d) for C and H
Total energy: -1567.1701857 hartrees

| | | | | |
|---|---|---|---|---|
| 16 | 0 | 0.656868 | 0.847321 | -1.425520 |
| 6 | 0 | 0.042178 | 1.864971 | -0.086439 |
| 6 | 0 | -1.083963 | 2.738499 | -0.248151 |
| 6 | 0 | 0.733385 | 1.830896 | 1.108832 |
| 6 | 0 | -1.472523 | 3.552970 | 0.866155 |
| 6 | 0 | 0.346998 | 2.645844 | 2.194794 |
| 6 | 0 | -0.733385 | 3.482887 | 2.075725 |
| 1 | 0 | 1.583203 | 1.165969 | 1.209817 |
| 1 | 0 | 0.908569 | 2.600213 | 3.122091 |
| 1 | 0 | -1.037873 | 4.108618 | 2.909657 |
| 6 | 0 | -1.833760 | 2.839257 | -1.447716 |
| 6 | 0 | -2.908896 | 3.691292 | -1.541508 |
| 6 | 0 | -3.294004 | 4.488829 | -0.441626 |
| 6 | 0 | -2.588092 | 4.420005 | 0.733830 |
| 1 | 0 | -1.542975 | 2.237231 | -2.299274 |
| 1 | 0 | -3.466340 | 3.753134 | -2.470584 |
| 1 | 0 | -4.145230 | 5.156097 | -0.530111 |
| 1 | 0 | -2.874182 | 5.033308 | 1.583350 |
| 16 | 0 | -0.656868 | -0.847321 | -1.425520 |
| 6 | 0 | -0.042178 | -1.864971 | -0.086439 |
| 6 | 0 | 1.083963 | -2.738499 | -0.248151 |
| 6 | 0 | -0.733385 | -1.830896 | 1.108832 |
| 6 | 0 | 1.472523 | -3.552970 | 0.866155 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.346998 | -2.645844 | 2.194794 |
| 6 | 0 | 0.733385 | -3.482887 | 2.075725 |
| 1 | 0 | -1.583203 | -1.165969 | 1.209817 |
| 1 | 0 | -0.908569 | -2.600213 | 3.122091 |
| 1 | 0 | 1.037873 | -4.108618 | 2.909657 |
| 6 | 0 | 1.833760 | -2.839257 | -1.447716 |
| 6 | 0 | 2.908896 | -3.691292 | -1.541508 |
| 6 | 0 | 3.294004 | -4.488829 | -0.441626 |
| 6 | 0 | 2.588092 | -4.420005 | 0.733830 |
| 1 | 0 | 1.542975 | -2.237231 | -2.299274 |
| 1 | 0 | 3.466340 | -3.753134 | -2.470584 |
| 1 | 0 | 4.145230 | -5.156097 | -0.530111 |
| 1 | 0 | 2.874182 | -5.033308 | 1.583350 |

**6** (**B**)
B3LYP/6-311+G(d) for S and 6-311G(d) for C and H
Total energy: -1567.1662638 hartrees

| | | | | |
|---|---|---|---|---|
| 16 | 0 | -0.396181 | 0.959042 | -1.452315 |
| 1 | 0 | -1.063440 | 3.434415 | -1.844611 |
| 16 | 0 | 0.396181 | -0.959042 | -1.452315 |
| 1 | 0 | 1.063440 | -3.434415 | -1.844611 |
| 6 | 0 | 0.532487 | 1.883201 | -0.203167 |
| 6 | 0 | 0.324264 | 3.300659 | -0.176376 |
| 6 | 0 | 1.381348 | 1.283950 | 0.696988 |
| 6 | 0 | 1.020676 | 4.067351 | 0.815124 |
| 6 | 0 | 2.066099 | 2.055219 | 1.662035 |
| 6 | 0 | 1.890346 | 3.413111 | 1.724848 |
| 1 | 0 | 1.536691 | 0.212457 | 0.667537 |
| 1 | 0 | 2.732076 | 1.554471 | 2.357199 |
| 1 | 0 | 2.413263 | 4.004941 | 2.469725 |
| 6 | 0 | -0.532487 | 3.987330 | -1.077819 |
| 6 | 0 | -0.698587 | 5.349842 | -1.003655 |
| 6 | 0 | -0.015682 | 6.102260 | -0.023657 |
| 6 | 0 | 0.823927 | 5.471906 | 0.860890 |
| 1 | 0 | -1.357564 | 5.850669 | -1.705337 |
| 1 | 0 | -0.154780 | 7.177343 | 0.025664 |
| 1 | 0 | 1.355128 | 6.044431 | 1.615607 |
| 6 | 0 | -0.532487 | -1.883201 | -0.203167 |
| 6 | 0 | -0.324264 | -3.300659 | -0.176376 |
| 6 | 0 | -1.381348 | -1.283950 | 0.696988 |
| 6 | 0 | -1.020676 | -4.067351 | 0.815124 |
| 6 | 0 | -2.066099 | -2.055219 | 1.662035 |
| 6 | 0 | -1.890346 | -3.413111 | 1.724848 |
| 1 | 0 | -1.536691 | -0.212457 | 0.667537 |
| 1 | 0 | -2.732076 | -1.554471 | 2.357199 |
| 1 | 0 | -2.413263 | -4.004941 | 2.469725 |
| 6 | 0 | 0.532487 | -3.987330 | -1.077819 |
| 6 | 0 | 0.698587 | -5.349842 | -1.003655 |
| 6 | 0 | 0.015682 | -6.102260 | -0.023657 |
| 6 | 0 | -0.823927 | -5.471906 | 0.860890 |
| 1 | 0 | 1.357564 | -5.850669 | -1.705337 |
| 1 | 0 | 0.154780 | -7.177343 | 0.025664 |
| 1 | 0 | -1.355128 | -6.044431 | 1.615607 |

**13** (**AA**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H

Total energy: -6448.8860604 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.423825 | 3.610864 | -0.494424 |
| 6 | 0 | -1.093784 | 2.916447 | 0.579423 |
| 6 | 0 | -1.426662 | 3.715536 | 1.740438 |
| 6 | 0 | -1.054318 | 5.081231 | 1.820042 |
| 6 | 0 | -0.373827 | 5.687141 | 0.800896 |
| 6 | 0 | -0.074007 | 4.942870 | -0.353388 |
| 6 | 0 | -1.461689 | 1.522671 | 0.646240 |
| 6 | 0 | -2.136457 | 1.027921 | 1.749738 |
| 6 | 0 | -2.497320 | 1.838457 | 2.841372 |
| 6 | 0 | -2.131929 | 3.155372 | 2.836471 |
| 1 | 0 | -1.320762 | 5.635112 | 2.715155 |
| 1 | 0 | -0.079800 | 6.729513 | 0.864794 |
| 1 | 0 | 0.440421 | 5.424333 | -1.176629 |
| 1 | 0 | -2.378494 | -0.027942 | 1.778058 |
| 1 | 0 | -3.033481 | 1.407942 | 3.680570 |
| 1 | 0 | -2.369061 | 3.799594 | 3.677718 |
| 16 | 0 | 0.074007 | 2.912432 | -2.081967 |
| 34 | 0 | -1.182068 | 0.130760 | -0.696521 |
| 6 | 0 | 0.423825 | -3.610864 | -0.494424 |
| 6 | 0 | 1.093784 | -2.916447 | 0.579423 |
| 6 | 0 | 1.426662 | -3.715536 | 1.740438 |
| 6 | 0 | 1.054318 | -5.081231 | 1.820042 |
| 6 | 0 | 0.373827 | -5.687141 | 0.800896 |
| 6 | 0 | 0.074007 | -4.942870 | -0.353388 |
| 6 | 0 | 1.461689 | -1.522671 | 0.646240 |
| 6 | 0 | 2.136457 | -1.027921 | 1.749738 |
| 6 | 0 | 2.497320 | -1.838457 | 2.841372 |
| 6 | 0 | 2.131929 | -3.155372 | 2.836471 |
| 1 | 0 | 1.320762 | -5.635112 | 2.715155 |
| 1 | 0 | 0.079800 | -6.729513 | 0.864794 |
| 1 | 0 | -0.440421 | -5.424333 | -1.176629 |
| 1 | 0 | 2.378494 | 0.027942 | 1.778058 |
| 1 | 0 | 3.033481 | -1.407942 | 3.680570 |
| 1 | 0 | 2.369061 | -3.799594 | 3.677718 |
| 16 | 0 | -0.074007 | -2.912432 | -2.081967 |
| 34 | 0 | 1.182068 | -0.130760 | -0.696521 |
| 6 | 0 | -1.511078 | 2.905036 | -2.993279 |
| 1 | 0 | -2.193714 | 2.158902 | -2.586213 |
| 1 | 0 | -1.968101 | 3.894509 | -2.978462 |
| 1 | 0 | -1.267709 | 2.638413 | -4.022988 |
| 6 | 0 | 1.511078 | -2.905036 | -2.993279 |
| 1 | 0 | 2.193714 | -2.158902 | -2.586213 |
| 1 | 0 | 1.968101 | -3.894509 | -2.978462 |
| 1 | 0 | 1.267709 | -2.638413 | -4.022988 |

**13** (**AB**)

B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H

Total energy: -6448.8882934 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.428636 | 3.695458 | -0.519117 |
| 6 | 0 | -0.885304 | 2.945580 | 0.632594 |
| 6 | 0 | -0.962048 | 3.663171 | 1.885293 |
| 6 | 0 | -0.536813 | 5.011168 | 1.986037 |
| 6 | 0 | -0.047104 | 5.661930 | 0.889326 |
| 6 | 0 | -0.005938 | 5.004488 | -0.351921 |
| 6 | 0 | -1.273049 | 1.558805 | 0.678010 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -1.762737 | 0.994191 | 1.843723 |
| 6 | 0 | -1.887312 | 1.732100 | 3.034084 |
| 6 | 0 | -1.472564 | 3.034946 | 3.050604 |
| 1 | 0 | -0.605375 | 5.508715 | 2.948116 |
| 1 | 0 | 0.295925 | 6.689346 | 0.957233 |
| 1 | 0 | 0.362891 | 5.565675 | -1.197671 |
| 1 | 0 | -2.037700 | -0.053496 | 1.839084 |
| 1 | 0 | -2.281783 | 1.257852 | 3.926632 |
| 1 | 0 | -1.525731 | 3.620083 | 3.963764 |
| 16 | 0 | -0.453117 | 3.001489 | -2.176960 |
| 34 | 0 | -1.162369 | 0.271763 | -0.781018 |
| 6 | 0 | 0.428636 | -3.695458 | -0.519117 |
| 6 | 0 | 0.885304 | -2.945580 | 0.632594 |
| 6 | 0 | 0.962048 | -3.663171 | 1.885293 |
| 6 | 0 | 0.536813 | -5.011168 | 1.986037 |
| 6 | 0 | 0.047104 | -5.661930 | 0.889326 |
| 6 | 0 | 0.005938 | -5.004488 | -0.351921 |
| 6 | 0 | 1.273049 | -1.558805 | 0.678010 |
| 6 | 0 | 1.762737 | -0.994191 | 1.843723 |
| 6 | 0 | 1.887312 | -1.732100 | 3.034084 |
| 6 | 0 | 1.472564 | -3.034946 | 3.050604 |
| 1 | 0 | 0.605375 | -5.508715 | 2.948116 |
| 1 | 0 | -0.295925 | -6.689346 | 0.957233 |
| 1 | 0 | -0.362891 | -5.565675 | -1.197671 |
| 1 | 0 | 2.037700 | 0.053496 | 1.839084 |
| 1 | 0 | 2.281783 | -1.257852 | 3.926632 |
| 1 | 0 | 1.525731 | -3.620083 | 3.963764 |
| 16 | 0 | 0.453117 | -3.001489 | -2.176960 |
| 34 | 0 | 1.162369 | -0.271763 | -0.781018 |
| 6 | 0 | 0.005938 | 4.422233 | -3.230830 |
| 1 | 0 | -0.686507 | 5.258403 | -3.124418 |
| 1 | 0 | 1.032352 | 4.753462 | -3.067028 |
| 1 | 0 | -0.071196 | 4.031862 | -4.246539 |
| 6 | 0 | -0.005938 | -4.422233 | -3.230830 |
| 1 | 0 | 0.686507 | -5.258403 | -3.124418 |
| 1 | 0 | -1.032352 | -4.753462 | -3.067028 |
| 1 | 0 | 0.071196 | -4.031862 | -4.246539 |

**13** (**BA**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -6448.8984744 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.219629 | 4.420760 | -0.299705 |
| 6 | 0 | 0.605053 | 3.479864 | 0.404914 |
| 6 | 0 | 1.527332 | 4.036660 | 1.368112 |
| 6 | 0 | 1.642596 | 5.442275 | 1.520127 |
| 6 | 0 | 0.880772 | 6.304936 | 0.779006 |
| 6 | 0 | -0.062494 | 5.782022 | -0.125105 |
| 6 | 0 | 0.602462 | 2.047167 | 0.248897 |
| 6 | 0 | 1.393219 | 1.270927 | 1.070730 |
| 6 | 0 | 2.248582 | 1.831554 | 2.037868 |
| 6 | 0 | 2.330733 | 3.190273 | 2.171279 |
| 1 | 0 | 2.358340 | 5.821955 | 2.243122 |
| 1 | 0 | 0.983713 | 7.378957 | 0.892973 |
| 1 | 0 | -0.694129 | 6.455912 | -0.692790 |
| 1 | 0 | 1.386484 | 0.194790 | 0.953220 |
| 1 | 0 | 2.850575 | 1.174418 | 2.657427 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -3.006328 | -3.641814 | 2.891071 |
| 16 | 0 | -1.527332 | 3.926888 | -1.430819 |
| 34 | 0 | -0.441235 | 1.130111 | -1.159336 |
| 6 | 0 | 0.219629 | -4.420760 | -0.299705 |
| 6 | 0 | -0.605053 | -3.479864 | 0.404914 |
| 6 | 0 | -1.527332 | -4.036660 | 1.368112 |
| 6 | 0 | -1.642596 | -5.442275 | 1.520127 |
| 6 | 0 | -0.880772 | -6.304936 | 0.779006 |
| 6 | 0 | 0.062494 | -5.782022 | -0.125105 |
| 6 | 0 | -0.602462 | -2.047167 | 0.248897 |
| 6 | 0 | -1.393219 | -1.270927 | 1.070730 |
| 6 | 0 | -2.248582 | -1.831554 | 2.037868 |
| 6 | 0 | -2.330733 | -3.190273 | 2.171279 |
| 1 | 0 | -2.358340 | -5.821955 | 2.243122 |
| 1 | 0 | -0.983713 | -7.378957 | 0.892973 |
| 1 | 0 | 0.694129 | -6.455912 | -0.692790 |
| 1 | 0 | -1.386484 | -0.194790 | 0.953220 |
| 1 | 0 | -2.850575 | -1.174418 | 2.657427 |
| 1 | 0 | -3.006328 | -3.641814 | 2.891071 |
| 16 | 0 | 1.527332 | -3.926888 | -1.430819 |
| 34 | 0 | 0.441235 | -1.130111 | -1.159336 |
| 6 | 0 | -2.920633 | 3.706861 | -0.258584 |
| 1 | 0 | -2.706852 | 2.910014 | 0.453295 |
| 1 | 0 | -3.130552 | 4.639154 | 0.265926 |
| 1 | 0 | -3.787163 | 3.426109 | -0.858948 |
| 6 | 0 | 2.920633 | -3.706861 | -0.258584 |
| 1 | 0 | 2.706852 | -2.910014 | 0.453295 |
| 1 | 0 | 3.130552 | -4.639154 | 0.265926 |
| 1 | 0 | 3.787163 | -3.426109 | -0.858948 |

**14** (**AA**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -6448.86878 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.288583 | 3.524599 | -0.271000 |
| 6 | 0 | -0.897930 | 2.814523 | 0.825681 |
| 6 | 0 | -1.169225 | 3.591501 | 2.016859 |
| 6 | 0 | -0.784561 | 4.953080 | 2.104376 |
| 6 | 0 | -0.155699 | 5.573973 | 1.061600 |
| 6 | 0 | 0.071411 | 4.853083 | -0.125011 |
| 6 | 0 | -1.267620 | 1.419256 | 0.888640 |
| 6 | 0 | -1.900337 | 0.908011 | 2.009840 |
| 6 | 0 | -2.204004 | 1.699689 | 3.131383 |
| 6 | 0 | -1.826375 | 3.013504 | 3.133802 |
| 1 | 0 | -1.001302 | 5.491477 | 3.022072 |
| 1 | 0 | 0.146347 | 6.613960 | 1.128108 |
| 1 | 0 | 0.529202 | 5.358697 | -0.966681 |
| 1 | 0 | -2.153077 | -0.145520 | 2.019132 |
| 1 | 0 | -2.707128 | 1.258972 | 3.985530 |
| 1 | 0 | -2.019629 | 3.643269 | 3.997038 |
| 34 | 0 | 0.155699 | 2.836747 | -2.046945 |
| 16 | 0 | -1.046316 | 0.185225 | -0.402332 |
| 6 | 0 | 0.288583 | -3.524599 | -0.271000 |
| 6 | 0 | 0.897930 | -2.814523 | 0.825681 |
| 6 | 0 | 1.169225 | -3.591501 | 2.016859 |
| 6 | 0 | 0.784561 | -4.953080 | 2.104376 |
| 6 | 0 | 0.155699 | -5.573973 | 1.061600 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.071411 | -4.853083 | -0.125011 |
| 6 | 0 | 1.267620 | -1.419256 | 0.888640 |
| 6 | 0 | 1.900337 | -0.908011 | 2.009840 |
| 6 | 0 | 2.204004 | -1.699689 | 3.131383 |
| 6 | 0 | 1.826375 | -3.013504 | 3.133802 |
| 1 | 0 | 1.001302 | -5.491477 | 3.022072 |
| 1 | 0 | -0.146347 | -6.613960 | 1.128108 |
| 1 | 0 | -0.529202 | -5.358697 | -0.966681 |
| 1 | 0 | 2.153077 | 0.145520 | 2.019132 |
| 1 | 0 | 2.707128 | -1.258972 | 3.985530 |
| 1 | 0 | 2.019629 | -3.643269 | 3.997038 |
| 34 | 0 | -0.155699 | -2.836747 | -2.046945 |
| 16 | 0 | 1.046316 | -0.185225 | -0.402332 |
| 6 | 0 | 1.655720 | -2.709988 | -2.814913 |
| 1 | 0 | 2.197611 | -1.883259 | -2.359547 |
| 1 | 0 | 2.185075 | -3.651507 | -2.680327 |
| 1 | 0 | 1.517163 | -2.517442 | -3.879411 |
| 6 | 0 | -1.655720 | 2.709988 | -2.814913 |
| 1 | 0 | -2.197611 | 1.883259 | -2.359547 |
| 1 | 0 | -2.185075 | 3.651507 | -2.680327 |
| 1 | 0 | -1.517163 | 2.517442 | -3.879411 |

**14** (**AB**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -6448.8768181 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.449747 | 3.560325 | -0.314504 |
| 6 | 0 | -0.791459 | 2.837201 | 0.885006 |
| 6 | 0 | -0.789306 | 3.576462 | 2.124693 |
| 6 | 0 | -0.374530 | 4.930481 | 2.161634 |
| 6 | 0 | 0.025814 | 5.558044 | 1.014434 |
| 6 | 0 | -0.025814 | 4.873828 | -0.213468 |
| 6 | 0 | -1.141695 | 1.444291 | 0.980413 |
| 6 | 0 | -1.551473 | 0.890098 | 2.181455 |
| 6 | 0 | -1.610883 | 1.650137 | 3.362944 |
| 6 | 0 | -1.211782 | 2.959019 | 3.331066 |
| 1 | 0 | -0.377709 | 5.452338 | 3.113274 |
| 1 | 0 | 0.364353 | 6.589035 | 1.033261 |
| 1 | 0 | 0.268473 | 5.418122 | -1.099300 |
| 1 | 0 | -1.812962 | -0.160880 | 2.204216 |
| 1 | 0 | -1.942573 | 1.189316 | 4.287324 |
| 1 | 0 | -1.213360 | 3.557196 | 4.237400 |
| 34 | 0 | -0.653770 | 2.803355 | -2.100171 |
| 16 | 0 | -1.038595 | 0.284464 | -0.378523 |
| 6 | 0 | 0.449747 | -3.560325 | -0.314504 |
| 6 | 0 | 0.791459 | -2.837201 | 0.885006 |
| 6 | 0 | 0.789306 | -3.576462 | 2.124693 |
| 6 | 0 | 0.374530 | -4.930481 | 2.161634 |
| 6 | 0 | -0.025814 | -5.558044 | 1.014434 |
| 6 | 0 | 0.025814 | -4.873828 | -0.213468 |
| 6 | 0 | 1.141695 | -1.444291 | 0.980413 |
| 6 | 0 | 1.551473 | -0.890098 | 2.181455 |
| 6 | 0 | 1.610883 | -1.650137 | 3.362944 |
| 6 | 0 | 1.211782 | -2.959019 | 3.331066 |
| 1 | 0 | 0.377709 | -5.452338 | 3.113274 |
| 1 | 0 | -0.364353 | -6.589035 | 1.033261 |
| 1 | 0 | -0.268473 | -5.418122 | -1.099300 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 1.812962 | 0.160880 | 2.204216 |
| 1 | 0 | 1.942573 | -1.189316 | 4.287324 |
| 1 | 0 | 1.213360 | -3.557196 | 4.237400 |
| 34 | 0 | 0.653770 | -2.803355 | -2.100171 |
| 16 | 0 | 1.038595 | -0.284464 | -0.378523 |
| 6 | 0 | 0.424121 | -4.439977 | -3.188571 |
| 1 | 0 | 1.132181 | -5.216203 | -2.900578 |
| 1 | 0 | -0.598023 | -4.815896 | -3.158949 |
| 1 | 0 | 0.647443 | -4.112796 | -4.205065 |
| 6 | 0 | -0.424121 | 4.439977 | -3.188571 |
| 1 | 0 | -1.132181 | 5.216203 | -2.900578 |
| 1 | 0 | 0.598023 | 4.815896 | -3.158949 |
| 1 | 0 | -0.647443 | 4.112796 | -4.205065 |

**14** (**BA**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -6448.8728693 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 4.255791 | -0.018969 | -0.259117 |
| 6 | 0 | 3.282120 | -0.775206 | 0.478915 |
| 6 | 0 | 3.807404 | -1.697915 | 1.461594 |
| 6 | 0 | 5.207102 | -1.870325 | 1.612239 |
| 6 | 0 | 6.097918 | -1.166875 | 0.849259 |
| 6 | 0 | 5.609610 | -0.230249 | -0.080578 |
| 6 | 0 | 1.843539 | -0.713182 | 0.348442 |
| 6 | 0 | 1.049080 | -1.460703 | 1.196047 |
| 6 | 0 | 1.585453 | -2.320928 | 2.169808 |
| 6 | 0 | 2.940464 | -2.450636 | 2.291353 |
| 1 | 0 | 5.557164 | -2.583071 | 2.352715 |
| 1 | 0 | 7.167347 | -1.309799 | 0.963152 |
| 1 | 0 | 6.310409 | 0.352684 | -0.666477 |
| 1 | 0 | -0.026236 | -1.407727 | 1.095738 |
| 1 | 0 | 0.912018 | -2.884785 | 2.807169 |
| 1 | 0 | 3.374972 | -3.126050 | 3.021438 |
| 34 | 0 | 3.835771 | 1.371340 | -1.555313 |
| 16 | 0 | 1.039328 | 0.296310 | -0.938836 |
| 6 | 0 | -4.255807 | 0.018674 | -0.258967 |
| 6 | 0 | -3.282252 | 0.775189 | 0.478937 |
| 6 | 0 | -3.807674 | 1.697775 | 1.461661 |
| 6 | 0 | -5.207402 | 1.869748 | 1.612526 |
| 6 | 0 | -6.098119 | 1.166004 | 0.849703 |
| 6 | 0 | -5.609663 | 0.229540 | -0.080219 |
| 6 | 0 | -1.843668 | 0.713572 | 0.348286 |
| 6 | 0 | -1.049320 | 1.461432 | 1.195694 |
| 6 | 0 | -1.585812 | 2.321569 | 2.169466 |
| 6 | 0 | -2.940845 | 2.450828 | 2.291235 |
| 1 | 0 | -5.557570 | 2.582403 | 2.353040 |
| 1 | 0 | -7.167574 | 1.308594 | 0.963763 |
| 1 | 0 | -6.310373 | -0.353590 | -0.666029 |
| 1 | 0 | 0.025998 | 1.408779 | 1.095219 |
| 1 | 0 | -0.912457 | 2.885698 | 2.806669 |
| 1 | 0 | -3.375455 | 3.126142 | 3.021352 |
| 34 | 0 | -3.835582 | -1.371353 | -1.555400 |
| 16 | 0 | -1.039316 | -0.295905 | -0.938923 |
| 6 | 0 | 3.618060 | 2.882859 | -0.299367 |
| 1 | 0 | 2.734824 | 2.732838 | 0.318429 |
| 1 | 0 | 4.510190 | 2.987208 | 0.315458 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -3.487264 | -3.773431 | -0.914543 |
| 6 | 0 | -3.617252 | -2.883004 | -0.299725 |
| 1 | 0 | -2.733955 | -2.732834 | 0.317948 |
| 1 | 0 | -4.509257 | -2.987695 | 0.315224 |
| 1 | 0 | -3.486307 | -3.773444 | -0.915059 |

**15** (**AA**)
B3LYP/6-311+G(d) for Se and 6-311G(d) for C and H
Total energy: -10455.547313 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.316822 | 3.649503 | -0.179197 |
| 6 | 0 | -0.989713 | 2.952419 | 0.889664 |
| 6 | 0 | -1.291993 | 3.741594 | 2.067503 |
| 6 | 0 | -0.892928 | 5.098545 | 2.163111 |
| 6 | 0 | -0.215817 | 5.706853 | 1.143956 |
| 6 | 0 | 0.055574 | 4.973660 | -0.025272 |
| 6 | 0 | -1.393622 | 1.567437 | 0.942766 |
| 6 | 0 | -2.065233 | 1.072589 | 2.048341 |
| 6 | 0 | -2.390397 | 1.873821 | 3.157516 |
| 6 | 0 | -1.994768 | 3.181695 | 3.165237 |
| 1 | 0 | -1.137652 | 5.643402 | 3.069902 |
| 1 | 0 | 0.096701 | 6.743238 | 1.217298 |
| 1 | 0 | 0.564453 | 5.464522 | -0.845948 |
| 1 | 0 | -2.334996 | 0.023295 | 2.062804 |
| 1 | 0 | -2.925054 | 1.443665 | 3.997839 |
| 1 | 0 | -2.206160 | 3.819800 | 4.017973 |
| 34 | 0 | 0.215817 | 2.945380 | -1.923905 |
| 34 | 0 | -1.174368 | 0.188157 | -0.423668 |
| 6 | 0 | 0.316822 | -3.649503 | -0.179197 |
| 6 | 0 | 0.989713 | -2.952419 | 0.889664 |
| 6 | 0 | 1.291993 | -3.741594 | 2.067503 |
| 6 | 0 | 0.892928 | -5.098545 | 2.163111 |
| 6 | 0 | 0.215817 | -5.706853 | 1.143956 |
| 6 | 0 | -0.055574 | -4.973660 | -0.025272 |
| 6 | 0 | 1.393622 | -1.567437 | 0.942766 |
| 6 | 0 | 2.065233 | -1.072589 | 2.048341 |
| 6 | 0 | 2.390397 | -1.873821 | 3.157516 |
| 6 | 0 | 1.994768 | -3.181695 | 3.165237 |
| 1 | 0 | 1.137652 | -5.643402 | 3.069902 |
| 1 | 0 | -0.096701 | -6.743238 | 1.217298 |
| 1 | 0 | -0.564453 | -5.464522 | -0.845948 |
| 1 | 0 | 2.334996 | -0.023295 | 2.062804 |
| 1 | 0 | 2.925054 | -1.443665 | 3.997839 |
| 1 | 0 | 2.206160 | -3.819800 | 4.017973 |
| 34 | 0 | -0.215817 | -2.945380 | -1.923905 |
| 34 | 0 | 1.174368 | -0.188157 | -0.423668 |
| 6 | 0 | 1.539304 | -2.934809 | -2.822742 |
| 1 | 0 | 2.019872 | -3.904520 | -2.707460 |
| 1 | 0 | 1.336399 | -2.749591 | -3.878100 |
| 1 | 0 | 2.161429 | -2.136163 | -2.422096 |
| 6 | 0 | -1.539304 | 2.934809 | -2.822742 |
| 1 | 0 | -2.019872 | 3.904520 | -2.707460 |
| 1 | 0 | -1.336399 | 2.749591 | -3.878100 |
| 1 | 0 | -2.161429 | 2.136163 | -2.422096 |

**15** (**AB**)
B3LYP/6-311+G(d) for Se and 6-311G(d) for C and H

Total energy: -10455.5557621 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -3.780432 | -0.265352 | -0.163398 |
| 6 | 0 | -3.102312 | 0.948276 | 0.215945 |
| 6 | 0 | -3.786103 | 2.192242 | -0.051214 |
| 6 | 0 | -5.016528 | 2.207763 | -0.753976 |
| 6 | 0 | -5.577775 | 1.038290 | -1.186993 |
| 6 | 0 | -4.962451 | -0.188523 | -0.878052 |
| 6 | 0 | -1.811437 | 1.058581 | 0.839198 |
| 6 | 0 | -1.323007 | 2.282438 | 1.261229 |
| 6 | 0 | -2.045281 | 3.473606 | 1.062001 |
| 6 | 0 | -3.238172 | 3.423721 | 0.392784 |
| 1 | 0 | -5.496064 | 3.162534 | -0.945288 |
| 1 | 0 | -6.507060 | 1.040676 | -1.747587 |
| 1 | 0 | -5.454847 | -1.092931 | -1.207150 |
| 1 | 0 | -0.348986 | 2.323469 | 1.733164 |
| 1 | 0 | -1.638415 | 4.417276 | 1.409869 |
| 1 | 0 | -3.794747 | 4.333679 | 0.189138 |
| 34 | 0 | -3.179596 | -2.039099 | 0.388137 |
| 34 | 0 | -0.559577 | -0.410007 | 1.062325 |
| 6 | 0 | 3.780441 | -0.265338 | 0.163381 |
| 6 | 0 | 3.102304 | 0.948284 | -0.215953 |
| 6 | 0 | 3.786086 | 2.192257 | 0.051201 |
| 6 | 0 | 5.016518 | 2.207789 | 0.753951 |
| 6 | 0 | 5.577780 | 1.038321 | 1.186962 |
| 6 | 0 | 4.962465 | -0.188499 | 0.878025 |
| 6 | 0 | 1.811421 | 1.058578 | -0.839191 |
| 6 | 0 | 1.322975 | 2.282431 | -1.261216 |
| 6 | 0 | 2.045242 | 3.473605 | -1.061996 |
| 6 | 0 | 3.238140 | 3.423730 | -0.392791 |
| 1 | 0 | 5.496046 | 3.162564 | 0.945261 |
| 1 | 0 | 6.507070 | 1.040715 | 1.747548 |
| 1 | 0 | 5.454874 | -1.092902 | 1.207115 |
| 1 | 0 | 0.348949 | 2.323453 | -1.733138 |
| 1 | 0 | 1.638363 | 4.417272 | -1.409858 |
| 1 | 0 | 3.794708 | 4.333694 | -0.189150 |
| 34 | 0 | 3.179624 | -2.039091 | -0.388158 |
| 34 | 0 | 0.559568 | -0.410018 | -1.062299 |
| 6 | 0 | 4.879523 | -3.034444 | -0.160057 |
| 1 | 0 | 5.120409 | -3.209609 | 0.887774 |
| 1 | 0 | 4.693528 | -3.995168 | -0.642209 |
| 1 | 0 | 5.700747 | -2.530190 | -0.667597 |
| 6 | 0 | -4.879501 | -3.034458 | 0.160107 |
| 1 | 0 | -5.120434 | -3.209615 | -0.887715 |
| 1 | 0 | -4.693480 | -3.995185 | 0.642243 |
| 1 | 0 | -5.700704 | -2.530211 | 0.667689 |

**15** (**BA**)

B3LYP/6-311+G(d) for Se and 6-311G(d) for C and H

Total energy: -10455.5599887 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.011054 | 4.453464 | -0.107015 |
| 6 | 0 | 0.768107 | 3.462829 | 0.604156 |
| 6 | 0 | 1.711449 | 3.966179 | 1.578892 |
| 6 | 0 | 1.904918 | 5.362368 | 1.737538 |
| 6 | 0 | 1.202436 | 6.269355 | 0.991921 |
| 6 | 0 | 0.241335 | 5.802854 | 0.075129 |
| 6 | 0 | 0.687170 | 2.031375 | 0.450750 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.429021 | 1.213715 | 1.279028 |
| 6 | 0 | 2.305640 | 1.725172 | 2.253380 |
| 6 | 0 | 2.459416 | 3.077096 | 2.389218 |
| 1 | 0 | 2.633244 | 5.697465 | 2.469871 |
| 1 | 0 | 1.363332 | 7.335570 | 1.111658 |
| 1 | 0 | -0.343975 | 6.516702 | -0.492736 |
| 1 | 0 | 1.364920 | 0.139738 | 1.161366 |
| 1 | 0 | 2.865622 | 1.035545 | 2.876929 |
| 1 | 0 | 3.150865 | 3.491520 | 3.116158 |
| 34 | 0 | -1.429021 | 4.038443 | -1.345215 |
| 34 | 0 | -0.396950 | 1.157658 | -0.954371 |
| 6 | 0 | -0.011054 | -4.453464 | -0.107015 |
| 6 | 0 | -0.768107 | -3.462829 | 0.604156 |
| 6 | 0 | -1.711449 | -3.966179 | 1.578892 |
| 6 | 0 | -1.904918 | -5.362368 | 1.737538 |
| 6 | 0 | -1.202436 | -6.269355 | 0.991921 |
| 6 | 0 | -0.241335 | -5.802854 | 0.075129 |
| 6 | 0 | -0.687170 | -2.031375 | 0.450750 |
| 6 | 0 | -1.429021 | -1.213715 | 1.279028 |
| 6 | 0 | -2.305640 | -1.725172 | 2.253380 |
| 6 | 0 | -2.459416 | -3.077096 | 2.389218 |
| 1 | 0 | -2.633244 | -5.697465 | 2.469871 |
| 1 | 0 | -1.363332 | -7.335570 | 1.111658 |
| 1 | 0 | 0.343975 | -6.516702 | -0.492736 |
| 1 | 0 | -1.364920 | -0.139738 | 1.161366 |
| 1 | 0 | -2.865622 | -1.035545 | 2.876929 |
| 1 | 0 | -3.150865 | -3.491520 | 3.116158 |
| 34 | 0 | 1.429021 | -4.038443 | -1.345215 |
| 34 | 0 | 0.396950 | -1.157658 | -0.954371 |
| 6 | 0 | -2.893353 | 3.877315 | -0.025526 |
| 1 | 0 | -2.700581 | 3.039550 | 0.641470 |
| 1 | 0 | -2.991514 | 4.805918 | 0.533700 |
| 1 | 0 | -3.802436 | 3.690140 | -0.597311 |
| 6 | 0 | 2.893353 | -3.877315 | -0.025526 |
| 1 | 0 | 2.700581 | -3.039550 | 0.641470 |
| 1 | 0 | 2.991514 | -4.805918 | 0.533700 |
| 1 | 0 | 3.802436 | -3.690140 | -0.597311 |

**16** (**AA**)
B3LYP/6-311+G(d) for S and 6-311G(d) for C and H
Total energy: -2442.207074 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.374630 | 3.475719 | 0.628931 |
| 6 | 0 | 0.991389 | 2.741532 | -0.448990 |
| 6 | 0 | 1.281293 | 3.492846 | -1.650368 |
| 6 | 0 | 0.887574 | 4.849071 | -1.774943 |
| 6 | 0 | 0.235422 | 5.488439 | -0.757074 |
| 6 | 0 | 0.002339 | 4.796419 | 0.444454 |
| 6 | 0 | 1.347793 | 1.342513 | -0.477522 |
| 6 | 0 | 2.007893 | 0.808826 | -1.572090 |
| 6 | 0 | 2.347233 | 1.580423 | -2.697452 |
| 6 | 0 | 1.966082 | 2.892905 | -2.738722 |
| 1 | 0 | 1.115543 | 5.368575 | -2.700690 |
| 1 | 0 | -0.075057 | 6.523468 | -0.854041 |
| 1 | 0 | -0.467202 | 5.313941 | 1.272725 |
| 1 | 0 | 2.247784 | -0.247850 | -1.560084 |
| 1 | 0 | 2.871555 | 1.122675 | -3.529573 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -2.176278 | 3.503009 | -3.611965 |
| 16 | 0 | -0.002339 | 2.850833 | 2.278029 |
| 16 | 0 | 1.054113 | 0.123999 | 0.813952 |
| 6 | 0 | -0.374630 | -3.475719 | 0.628931 |
| 6 | 0 | -0.991389 | -2.741532 | -0.448990 |
| 6 | 0 | -1.281293 | -3.492846 | -1.650368 |
| 6 | 0 | -0.887574 | -4.849071 | -1.774943 |
| 6 | 0 | -0.235422 | -5.488439 | -0.757074 |
| 6 | 0 | -0.002339 | -4.796419 | 0.444454 |
| 6 | 0 | -1.347793 | -1.342513 | -0.477522 |
| 6 | 0 | -2.007893 | -0.808826 | -1.572090 |
| 6 | 0 | -2.347233 | -1.580423 | -2.697452 |
| 6 | 0 | -1.966082 | -2.892905 | -2.738722 |
| 1 | 0 | -1.115543 | -5.368575 | -2.700690 |
| 1 | 0 | 0.075057 | -6.523468 | -0.854041 |
| 1 | 0 | 0.467202 | -5.313941 | 1.272725 |
| 1 | 0 | -2.247784 | 0.247850 | -1.560084 |
| 1 | 0 | -2.871555 | -1.122675 | -3.529573 |
| 1 | 0 | -2.176278 | -3.503009 | -3.611965 |
| 16 | 0 | 0.002339 | -2.850833 | 2.278029 |
| 16 | 0 | -1.054113 | -0.123999 | 0.813952 |
| 6 | 0 | -1.662597 | -2.768686 | 3.028369 |
| 1 | 0 | -2.265979 | -1.992310 | 2.558860 |
| 1 | 0 | -2.163211 | -3.735224 | 2.968607 |
| 1 | 0 | -1.507889 | -2.509447 | 4.076916 |
| 6 | 0 | 1.662597 | 2.768686 | 3.028369 |
| 1 | 0 | 2.265979 | 1.992310 | 2.558860 |
| 1 | 0 | 2.163211 | 3.735224 | 2.968607 |
| 1 | 0 | 1.507889 | 2.509447 | 4.076916 |

**16** (**AB**)
B3LYP/6-311+G(d) for S and 6-311G(d) for C and H
Total energy: -2442.2097899 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 3.582059 | 0.688707 | -0.086553 |
| 6 | 0 | 2.922914 | -0.492860 | 0.427630 |
| 6 | 0 | 3.676403 | -1.724327 | 0.407191 |
| 6 | 0 | 4.972499 | -1.779936 | -0.162741 |
| 6 | 0 | 5.534549 | -0.656462 | -0.700400 |
| 6 | 0 | 4.842786 | 0.565856 | -0.649417 |
| 6 | 0 | 1.587974 | -0.578521 | 0.964081 |
| 6 | 0 | 1.110872 | -1.762668 | 1.501532 |
| 6 | 0 | 1.887396 | -2.933933 | 1.525569 |
| 6 | 0 | 3.136082 | -2.911252 | 0.967261 |
| 1 | 0 | 5.502391 | -2.727014 | -0.163762 |
| 1 | 0 | 6.520732 | -0.688506 | -1.152370 |
| 1 | 0 | 5.338673 | 1.432978 | -1.060048 |
| 1 | 0 | 0.102345 | -1.778819 | 1.896355 |
| 1 | 0 | 1.484433 | -3.843116 | 1.959151 |
| 1 | 0 | 3.745734 | -3.809483 | 0.943690 |
| 16 | 0 | 2.842813 | 2.320979 | 0.044368 |
| 16 | 0 | 0.397595 | 0.762985 | 0.995122 |
| 6 | 0 | -3.582080 | 0.688695 | 0.086524 |
| 6 | 0 | -2.922910 | -0.492868 | -0.427638 |
| 6 | 0 | -3.676385 | -1.724343 | -0.407206 |
| 6 | 0 | -4.972491 | -1.779964 | 0.162704 |
| 6 | 0 | -5.534565 | -0.656493 | 0.700345 |

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -4.842815 | 0.565832 | 0.649367 |
| 6 | 0 | -1.587958 | -0.578518 | -0.964060 |
| 6 | 0 | -1.110833 | -1.762662 | -1.501496 |
| 6 | 0 | -1.887344 | -2.933935 | -1.525543 |
| 6 | 0 | -3.136041 | -2.911266 | -0.967259 |
| 1 | 0 | -5.502372 | -2.727048 | 0.163721 |
| 1 | 0 | -6.520755 | -0.688546 | 1.152298 |
| 1 | 0 | -5.338720 | 1.432952 | 1.059981 |
| 1 | 0 | -0.102297 | -1.778805 | -1.896297 |
| 1 | 0 | -1.484363 | -3.843117 | -1.959112 |
| 1 | 0 | -3.745683 | -3.809503 | -0.943694 |
| 16 | 0 | -2.842856 | 2.320976 | -0.044401 |
| 16 | 0 | -0.397590 | 0.762999 | -0.995078 |
| 6 | 0 | -4.159117 | 3.423261 | 0.577836 |
| 1 | 0 | -5.075831 | 3.348959 | -0.008879 |
| 1 | 0 | -4.370857 | 3.269848 | 1.637029 |
| 1 | 0 | -3.745337 | 4.424750 | 0.451992 |
| 6 | 0 | 4.159095 | 3.423290 | -0.577780 |
| 1 | 0 | 5.075821 | 3.348894 | 0.008903 |
| 1 | 0 | 4.370802 | 3.269986 | -1.636995 |
| 1 | 0 | 3.745350 | 4.424778 | -0.451814 |

**16** (**BA**)
B3LYP/6-311+G(d) for S and 6-311G(d) for C and H
Total energy: -2442.2114308 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 2.866487 | 3.119235 | -0.526641 |
| 6 | 0 | 2.775044 | 1.892963 | 0.217634 |
| 6 | 0 | 3.804713 | 1.668058 | 1.206112 |
| 6 | 0 | 4.867416 | 2.594819 | 1.360109 |
| 6 | 0 | 4.944788 | 3.724806 | 0.592255 |
| 6 | 0 | 3.930054 | 3.983372 | -0.346735 |
| 6 | 0 | 1.765708 | 0.868240 | 0.079027 |
| 6 | 0 | 1.782521 | -0.223025 | 0.924956 |
| 6 | 0 | 2.775044 | -0.400557 | 1.905084 |
| 6 | 0 | 3.777682 | 0.519543 | 2.034977 |
| 1 | 0 | 5.627481 | 2.381530 | 2.105573 |
| 1 | 0 | 5.766883 | 4.423221 | 0.707987 |
| 1 | 0 | 3.969242 | 4.886716 | -0.944657 |
| 1 | 0 | 1.022436 | -0.984913 | 0.819309 |
| 1 | 0 | 2.739557 | -1.279043 | 2.541220 |
| 1 | 0 | 4.565176 | 0.389103 | 2.770390 |
| 16 | 0 | 1.647220 | 3.647162 | -1.739017 |
| 16 | 0 | 0.485736 | 0.956811 | -1.217437 |
| 6 | 0 | -2.866487 | -3.119235 | -0.526641 |
| 6 | 0 | -2.775044 | -1.892963 | 0.217634 |
| 6 | 0 | -3.804713 | -1.668058 | 1.206112 |
| 6 | 0 | -4.867416 | -2.594819 | 1.360109 |
| 6 | 0 | -4.944788 | -3.724806 | 0.592255 |
| 6 | 0 | -3.930054 | -3.983372 | -0.346735 |
| 6 | 0 | -1.765708 | -0.868240 | 0.079027 |
| 6 | 0 | -1.782521 | 0.223025 | 0.924956 |
| 6 | 0 | -2.775044 | 0.400557 | 1.905084 |
| 6 | 0 | -3.777682 | -0.519543 | 2.034977 |
| 1 | 0 | -5.627481 | -2.381530 | 2.105573 |
| 1 | 0 | -5.766883 | -4.423221 | 0.707987 |
| 1 | 0 | -3.969242 | -4.886716 | -0.944657 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -1.022436 | 0.984913 | 0.819309 |
| 1 | 0 | -2.739557 | 1.279043 | 2.541220 |
| 1 | 0 | -4.565176 | -0.389103 | 2.770390 |
| 16 | 0 | -1.647220 | -3.647162 | -1.739017 |
| 16 | 0 | -0.485736 | -0.956811 | -1.217437 |
| 6 | 0 | 0.445180 | 4.515419 | -0.661554 |
| 1 | 0 | -0.020269 | 3.824601 | 0.041109 |
| 1 | 0 | 0.926455 | 5.333902 | -0.126125 |
| 1 | 0 | -0.322683 | 4.919090 | -1.322880 |
| 6 | 0 | -0.445180 | -4.515419 | -0.661554 |
| 1 | 0 | 0.020269 | -3.824601 | 0.041109 |
| 1 | 0 | -0.926455 | -5.333902 | -0.126125 |
| 1 | 0 | 0.322683 | -4.919090 | -1.322880 |

**17** (**A**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -3224.4944097 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.727058 | -1.273137 | -0.183695 |
| 6 | 0 | -0.722368 | 0.162934 | -0.033730 |
| 6 | 0 | -2.036819 | 0.784071 | 0.030630 |
| 6 | 0 | -3.211085 | 0.028860 | -0.230005 |
| 6 | 0 | -3.150980 | -1.311979 | -0.496738 |
| 6 | 0 | -1.906576 | -1.962052 | -0.428649 |
| 6 | 0 | 0.442287 | 1.038359 | 0.045083 |
| 6 | 0 | 0.211423 | 2.369417 | 0.423208 |
| 6 | 0 | -1.061771 | 2.922420 | 0.578634 |
| 6 | 0 | -2.180517 | 2.156116 | 0.343228 |
| 1 | 0 | -4.167300 | 0.546953 | -0.205410 |
| 1 | 0 | -4.052552 | -1.884325 | -0.700702 |
| 1 | 0 | -1.861577 | -3.041662 | -0.520150 |
| 1 | 0 | 1.082258 | 3.005110 | 0.535045 |
| 1 | 0 | -1.159316 | 3.973060 | 0.845839 |
| 1 | 0 | -3.180048 | 2.580344 | 0.396316 |
| 16 | 0 | 0.688095 | -2.378481 | -0.047147 |
| 34 | 0 | 2.242820 | 0.635159 | -0.458637 |
| 6 | 0 | 1.301834 | -2.037916 | 1.638224 |
| 1 | 0 | 1.785245 | -1.061190 | 1.664049 |
| 1 | 0 | 0.493558 | -2.108193 | 2.368876 |
| 1 | 0 | 2.044136 | -2.812337 | 1.846990 |

**17** (**B**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -3224.498018 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 1.267592 | -0.047194 | -0.119903 |
| 6 | 0 | 0.053917 | 0.728803 | -0.006698 |
| 6 | 0 | 0.203220 | 2.170354 | -0.001241 |
| 6 | 0 | 1.472691 | 2.767012 | -0.230254 |
| 6 | 0 | 2.578365 | 1.991657 | -0.443286 |
| 6 | 0 | 2.475181 | 0.590425 | -0.374711 |
| 6 | 0 | -1.286574 | 0.183434 | 0.092960 |
| 6 | 0 | -2.333782 | 1.072068 | 0.370550 |
| 6 | 0 | -2.156176 | 2.455030 | 0.447147 |
| 6 | 0 | -0.912824 | 3.008260 | 0.232371 |
| 1 | 0 | 1.540481 | 3.852376 | -0.239582 |
| 1 | 0 | 3.546492 | 2.444730 | -0.645189 |
| 1 | 0 | 3.375964 | 0.010625 | -0.519158 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -3.328120 | 0.652956 | 0.478646 |
| 1 | 0 | -3.014535 | 3.094777 | 0.644867 |
| 1 | 0 | -0.765032 | 4.085331 | 0.241555 |
| 16 | 0 | 1.296663 | -1.828818 | 0.170283 |
| 34 | 0 | -1.737036 | -1.631297 | -0.245747 |
| 6 | 0 | 3.082688 | -2.073614 | 0.616855 |
| 1 | 0 | 3.414263 | -1.378061 | 1.391050 |
| 1 | 0 | 3.762317 | -2.023816 | -0.238227 |
| 1 | 0 | 3.115006 | -3.091139 | 1.014174 |

**18** (**A**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -3224.4910717 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.357530 | 0.857196 | 0.003454 |
| 6 | 0 | 0.855598 | 0.082379 | 0.023556 |
| 6 | 0 | 2.089977 | 0.849928 | 0.071820 |
| 6 | 0 | 2.054397 | 2.260328 | 0.247993 |
| 6 | 0 | 0.871749 | 2.942534 | 0.324024 |
| 6 | 0 | -0.335330 | 2.234278 | 0.166744 |
| 6 | 0 | 0.959254 | -1.378192 | 0.002274 |
| 6 | 0 | 2.246197 | -1.913367 | -0.206623 |
| 6 | 0 | 3.408924 | -1.146386 | -0.238158 |
| 6 | 0 | 3.348573 | 0.219810 | -0.058380 |
| 1 | 0 | 3.002982 | 2.789315 | 0.314190 |
| 1 | 0 | 0.854499 | 4.020715 | 0.464431 |
| 1 | 0 | -1.272772 | 2.777176 | 0.138184 |
| 1 | 0 | 2.315719 | -2.993560 | -0.277040 |
| 1 | 0 | 4.370458 | -1.640742 | -0.367262 |
| 1 | 0 | 4.248873 | 0.827823 | -0.020655 |
| 34 | 0 | -2.130961 | 0.224409 | -0.545127 |
| 16 | 0 | -0.334988 | -2.502390 | 0.300468 |
| 6 | 0 | -2.901987 | -0.345442 | 1.177226 |
| 1 | 0 | -2.333733 | -1.206935 | 1.524416 |
| 1 | 0 | -2.872537 | 0.475907 | 1.893366 |
| 1 | 0 | -3.939937 | -0.619753 | 0.973611 |

**18** (**B**)
B3LYP/6-311+G(d) for S and Se and 6-311G(d) for C and H
Total energy: -3224.5032743 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.451118 | 0.681897 | -0.000773 |
| 6 | 0 | -0.891048 | 0.157437 | -0.000218 |
| 6 | 0 | -1.977532 | 1.115316 | 0.000162 |
| 6 | 0 | -1.704074 | 2.508922 | -0.000626 |
| 6 | 0 | -0.414246 | 2.965277 | -0.001765 |
| 6 | 0 | 0.657522 | 2.054914 | -0.001815 |
| 6 | 0 | -1.224756 | -1.256802 | -0.000133 |
| 6 | 0 | -2.583114 | -1.611453 | 0.001213 |
| 6 | 0 | -3.611728 | -0.668368 | 0.001919 |
| 6 | 0 | -3.324521 | 0.679118 | 0.001270 |
| 1 | 0 | -2.542257 | 3.202026 | -0.000417 |
| 1 | 0 | -0.203273 | 4.032689 | -0.002565 |
| 1 | 0 | 1.658382 | 2.459429 | -0.002666 |
| 1 | 0 | -2.820679 | -2.670092 | 0.001479 |
| 1 | 0 | -4.646556 | -1.007147 | 0.002836 |
| 1 | 0 | -4.115915 | 1.424501 | 0.001585 |
| 34 | 0 | 2.024965 | -0.480398 | 0.000165 |

| | | | | |
|---|---|---|---|---|
| 16 | 0 | -0.022870 | -2.516218 | -0.001871 |
| 6 | 0 | 3.449905 | 0.968533 | 0.002981 |
| 1 | 0 | 3.418045 | 1.593158 | 0.898509 |
| 1 | 0 | 3.422349 | 1.592682 | -0.893051 |
| 1 | 0 | 4.381854 | 0.397030 | 0.005330 |

**19** (**A**)
B3LYP/6-311+G(d) for Se and 6-311G(d) for C and H
Total energy: -5227.8258031 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.041489 | 1.267044 | -0.193498 |
| 6 | 0 | 0.955239 | 0.164255 | -0.036002 |
| 6 | 0 | 2.361852 | 0.531037 | 0.040450 |
| 6 | 0 | 2.779750 | 1.861988 | -0.224780 |
| 6 | 0 | 1.874814 | 2.850670 | -0.501001 |
| 6 | 0 | 0.501861 | 2.552062 | -0.435579 |
| 6 | 0 | 0.624621 | -1.254439 | 0.043173 |
| 6 | 0 | 1.648115 | -2.124718 | 0.444812 |
| 6 | 0 | 2.977679 | -1.730589 | 0.615944 |
| 6 | 0 | 3.347935 | -0.427629 | 0.372640 |
| 1 | 0 | 3.845434 | 2.078406 | -0.194995 |
| 1 | 0 | 2.199873 | 3.867404 | -0.707365 |
| 1 | 0 | -0.220177 | 3.356289 | -0.523470 |
| 1 | 0 | 1.386527 | -3.170475 | 0.559021 |
| 1 | 0 | 3.722853 | -2.471663 | 0.899150 |
| 1 | 0 | 4.386371 | -0.111824 | 0.434584 |
| 34 | 0 | -1.903436 | 1.231867 | -0.031707 |
| 34 | 0 | -1.003821 | -2.093866 | -0.498279 |
| 6 | 0 | -2.108661 | 0.446628 | 1.763197 |
| 1 | 0 | -1.880153 | -0.616532 | 1.704397 |
| 1 | 0 | -1.466396 | 0.963494 | 2.475734 |
| 1 | 0 | -3.155759 | 0.594992 | 2.036332 |

**19** (**B**)
B3LYP/6-311+G(d) for Se and 6-311G(d) for C and H
Total energy: -5227.8374357 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.447963 | 1.006976 | -0.132286 |
| 6 | 0 | 0.892902 | 0.490981 | -0.015483 |
| 6 | 0 | 1.969251 | 1.460517 | 0.011644 |
| 6 | 0 | 1.697145 | 2.842466 | -0.170854 |
| 6 | 0 | 0.415729 | 3.279172 | -0.369147 |
| 6 | 0 | -0.651844 | 2.363228 | -0.340913 |
| 6 | 0 | 1.243245 | -0.911359 | 0.065908 |
| 6 | 0 | 2.580526 | -1.248705 | 0.296687 |
| 6 | 0 | 3.596934 | -0.292248 | 0.377965 |
| 6 | 0 | 3.307146 | 1.043695 | 0.215769 |
| 1 | 0 | 2.530672 | 3.540927 | -0.160065 |
| 1 | 0 | 0.207001 | 4.333976 | -0.534140 |
| 1 | 0 | -1.651624 | 2.748334 | -0.481118 |
| 1 | 0 | 2.827479 | -2.301471 | 0.380770 |
| 1 | 0 | 4.622826 | -0.614564 | 0.546751 |
| 1 | 0 | 4.090616 | 1.797087 | 0.241677 |
| 34 | 0 | -2.033162 | -0.115906 | 0.096099 |
| 34 | 0 | -0.000655 | -2.320407 | -0.213422 |
| 6 | 0 | -3.365351 | 1.379330 | 0.457707 |
| 1 | 0 | -3.024143 | 2.044545 | 1.252830 |
| 1 | 0 | -3.621832 | 1.957098 | -0.433338 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -4.257557 | 0.844419 | 0.793624 |

**20** (**A**)
B3LYP/6-311+G(d) for S and 6-311G(d) for C and H
Total energy: -1221.1588952 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | -0.613884 | 1.051989 | -0.194093 |
| 6 | 0 | 0.428975 | 0.059997 | -0.090825 |
| 6 | 0 | 1.777274 | 0.586526 | 0.060161 |
| 6 | 0 | 2.029186 | 1.979576 | -0.061748 |
| 6 | 0 | 1.014630 | 2.872841 | -0.273148 |
| 6 | 0 | -0.309573 | 2.403026 | -0.298033 |
| 6 | 0 | 0.267747 | -1.396854 | -0.142716 |
| 6 | 0 | 1.401543 | -2.165042 | 0.191555 |
| 6 | 0 | 2.666919 | -1.627470 | 0.418738 |
| 6 | 0 | 2.873317 | -0.268582 | 0.319342 |
| 1 | 0 | 3.058564 | 2.321104 | 0.023915 |
| 1 | 0 | 1.215404 | 3.937207 | -0.369240 |
| 1 | 0 | -1.128288 | 3.111523 | -0.357430 |
| 1 | 0 | 1.267287 | -3.241138 | 0.207379 |
| 1 | 0 | 3.498285 | -2.294626 | 0.641194 |
| 1 | 0 | 3.862743 | 0.165645 | 0.438089 |
| 16 | 0 | -2.395462 | 0.769036 | -0.189782 |
| 16 | 0 | -1.145563 | -2.271018 | -0.673720 |
| 6 | 0 | -2.676306 | -0.052099 | 1.416003 |
| 1 | 0 | -2.283567 | -1.068337 | 1.379787 |
| 1 | 0 | -2.232361 | 0.522607 | 2.231367 |
| 1 | 0 | -3.760629 | -0.085721 | 1.549550 |

**20** (**B**)
B3LYP/6-311+G(d) for S and 6-311G(d) for C and H
Total energy: -1221.1633272 hartrees

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.921371 | 0.451144 | -0.117629 |
| 6 | 0 | -0.487489 | 0.147742 | -0.038580 |
| 6 | 0 | -1.399139 | 1.271890 | 0.012710 |
| 6 | 0 | -0.910848 | 2.600273 | -0.120079 |
| 6 | 0 | 0.425368 | 2.838537 | -0.285860 |
| 6 | 0 | 1.337942 | 1.768197 | -0.273975 |
| 6 | 0 | -1.047223 | -1.196315 | -0.015808 |
| 6 | 0 | -2.430594 | -1.314833 | 0.212186 |
| 6 | 0 | -3.281131 | -0.215329 | 0.317536 |
| 6 | 0 | -2.787086 | 1.066647 | 0.195224 |
| 1 | 0 | -1.625487 | 3.419753 | -0.094012 |
| 1 | 0 | 0.798296 | 3.852945 | -0.411018 |
| 1 | 0 | 2.387137 | 2.000097 | -0.388120 |
| 1 | 0 | -2.836968 | -2.319420 | 0.263453 |
| 1 | 0 | -4.346689 | -0.377778 | 0.473217 |
| 1 | 0 | -3.443923 | 1.931855 | 0.238443 |
| 16 | 0 | 2.182646 | -0.828131 | 0.070037 |
| 16 | 0 | -0.117324 | -2.632985 | -0.320457 |
| 6 | 0 | 3.667868 | 0.206031 | 0.480521 |
| 1 | 0 | 4.071582 | 0.758625 | -0.372633 |
| 1 | 0 | 3.480460 | 0.894800 | 1.307666 |
| 1 | 0 | 4.416204 | -0.526911 | 0.792243 |