*Supporting Information*

# Polar Coordinate Representation of $H_b(r_c)$ versus $(\hbar^2/8m)\nabla^2\rho_b(r_c)$ at BCP in AIM Analysis: Classification and Evaluation of Weak to Strong Interactions

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**Table S1.** AIM Parameters for $Cl_3^-$ and $Br_3^-$ Under Variously Fixed $w$ in $r = r_o + wa_o$, Where $r_o$ and $a_o$ Stand for the Optimized Distances and Bohr Radius, Respectively.

| $w^a$ | $\rho_b(\boldsymbol{r}_c)$ ($ea_o^{-3}$) | $\nabla^2\rho_b(\boldsymbol{r}_c)$ ($ea_o^{-5}$) | $G_b(\boldsymbol{r}_c)$ (au) | $V_b(\boldsymbol{r}_c)$ (au) | $k$ | $H_b(\boldsymbol{r}_c)$ (au) | $H_b(\boldsymbol{r}_c)$–$V_b(\boldsymbol{r}_c)/2$ (au) |
|---|---|---|---|---|---|---|---|
| $Cl_3^-$ | | | | | | | |
| –1.2 | 0.3170 | –0.7177 | 0.2053 | –0.5900 | –0.348 | –0.3847 | –0.0897 |
| –1.0 | 0.2557 | –0.3890 | 0.1508 | –0.3988 | –0.378 | –0.2480 | –0.0486 |
| –0.8 | 0.2049 | –0.1700 | 0.1161 | –0.2747 | –0.423 | –0.1586 | –0.0213 |
| –0.6 | 0.1632 | –0.0267 | 0.0925 | –0.1917 | –0.483 | –0.0992 | –0.00334 |
| –0.4 | 0.1299 | 0.0570 | 0.0750 | –0.1358 | –0.552 | –0.0608 | 0.00712 |
| –0.2 | 0.1039 | 0.0950 | 0.0606 | –0.0974 | –0.622 | –0.0368 | 0.0119 |
| –0.1 | 0.0931 | 0.1029 | 0.0543 | –0.0828 | –0.655 | –0.0285 | 0.0129 |
| 0.0 | 0.0836 | 0.1060 | 0.0485 | –0.0705 | –0.688 | –0.0220 | 0.0133 |
| 0.1 | 0.0751 | 0.1059 | 0.0434 | –0.0603 | –0.720 | –0.0169 | 0.0132 |
| 0.2 | 0.0675 | 0.1036 | 0.0387 | –0.0516 | –0.751 | –0.0128 | 0.0130 |
| 0.4 | 0.0544 | 0.0958 | 0.0310 | –0.0381 | –0.814 | –0.00709 | 0.0120 |
| 0.6 | 0.0438 | 0.0865 | 0.0251 | –0.0285 | –0.879 | –0.00346 | 0.0108 |
| 0.8 | 0.0351 | 0.0769 | 0.0204 | –0.0216 | –0.945 | –0.00118 | 0.00961 |
| 1.0 | 0.0281 | 0.0672 | 0.0166 | –0.0164 | –1.012 | $1.90e^{-4}$ | 0.00840 |
| 1.2 | 0.0225 | 0.0578 | 0.0135 | –0.0125 | –1.077 | $9.63e^{-4}$ | 0.00723 |
| 1.4 | 0.0181 | 0.0491 | 0.0109 | –0.00957 | –1.141 | 0.00135 | 0.00613 |
| 1.5 | 0.0162 | 0.0450 | 0.00981 | –0.00837 | –1.172 | 0.00144 | 0.00562 |
| 1.6 | 0.0146 | 0.0411 | 0.00880 | –0.00732 | –1.202 | 0.00148 | 0.00514 |
| 1.7 | 0.0131 | 0.0375 | 0.00789 | –0.00641 | –1.232 | 0.00148 | 0.00469 |
| 1.8 | 0.0118 | 0.0341 | 0.00707 | –0.00561 | –1.260 | 0.00146 | 0.00427 |
| 1.9 | 0.0106 | 0.0310 | 0.00634 | –0.00492 | –1.287 | 0.00141 | 0.00388 |
| 2.0 | 0.00953 | 0.0281 | 0.00568 | –0.00432 | –1.313 | 0.00135 | 0.00351 |
| 2.1 | 0.00858 | 0.0255 | 0.00508 | –0.00380 | –1.337 | 0.00128 | 0.00318 |
| 2.5 | 0.00571 | 0.0170 | 0.00328 | –0.00233 | –1.409 | $9.54e^{-4}$ | 0.00212 |
| 3.0 | 0.00350 | 0.0102 | 0.00194 | –0.00134 | –1.449 | $6.01e^{-4}$ | 0.00127 |
| 3.5 | 0.00219 | 0.00619 | 0.00118 | $-8.03e^{-4}$ | –1.463 | $3.72e^{-4}$ | $7.73e^{-4}$ |
| 4.0 | 0.00139 | 0.00388 | $7.30e^{-4}$ | $-4.89e^{-4}$ | –1.492 | $2.41e^{-4}$ | $4.85e^{-4}$ |
| 5.0 | $5.52e^{-4}$ | 0.00161 | $2.91e^{-4}$ | $-1.80e^{-4}$ | –1.618 | $1.11e^{-4}$ | $2.01e^{-4}$ |
| 6.0 | $2.18e^{-4}$ | $6.56e^{-4}$ | $1.16e^{-4}$ | $-6.74e^{-5}$ | –1.716 | $4.83e^{-5}$ | $8.20e^{-5}$ |
| 7.0 | $8.66e^{-5}$ | $2.55e^{-4}$ | $4.45e^{-5}$ | $-2.51e^{-5}$ | –1.771 | $1.94e^{-5}$ | $3.19e^{-5}$ |
| 8.0 | $3.42e^{-5}$ | $9.80e^{-5}$ | $1.66e^{-5}$ | $-8.70e^{-6}$ | –1.907 | $7.90e^{-6}$ | $1.23e^{-5}$ |
| 9.0 | $1.28e^{-5}$ | $3.72e^{-5}$ | $6.07e^{-6}$ | $-2.84e^{-6}$ | –2.134 | $3.22e^{-6}$ | $4.65e^{-6}$ |
| 10.0 | $4.48e^{-6}$ | $1.36e^{-5}$ | $2.20e^{-6}$ | $-1.01e^{-6}$ | –2.184 | $1.19e^{-6}$ | $1.70e^{-6}$ |

continue

| $w^a$ | $\rho_b(\boldsymbol{r}_c)$ ($ea_o^{-3}$) | $\nabla^2\rho_b(\boldsymbol{r}_c)$ ($ea_o^{-5}$) | $G_b(\boldsymbol{r}_c)$ (au) | $V_b(\boldsymbol{r}_c)$ (au) | $k$ | $H_b(\boldsymbol{r}_c)$ (au) | $H_b(\boldsymbol{r}_c)$–$V_b(\boldsymbol{r}_c)/2$ (au) |
|---|---|---|---|---|---|---|---|
| $Br_3^-$ | | | | | | | |
| –1.2 | 0.2168 | –0.2042 | 0.1426 | –0.3362 | –0.4241 | –0.1937 | –0.0255 |
| –1.0 | 0.1794 | –0.1150 | 0.1058 | –0.2404 | –0.4402 | –0.1346 | –0.0144 |
| –0.8 | 0.1481 | –0.0457 | 0.0817 | –0.1748 | –0.4673 | –0.0931 | –0.00572 |
| –0.6 | 0.1218 | 0.0047 | 0.0650 | –0.1287 | –0.5046 | –0.0638 | $5.93e^{-4}$ |
| –0.4 | 0.1002 | 0.0368 | 0.0523 | –0.0955 | –0.5481 | –0.0431 | 0.00460 |
| –0.2 | 0.0824 | 0.0543 | 0.0423 | –0.0709 | –0.5958 | –0.0287 | 0.00679 |
| –0.1 | 0.0748 | 0.0593 | 0.0380 | –0.0611 | –0.6213 | –0.0231 | 0.00741 |
| 0.0 | 0.0678 | 0.0623 | 0.0341 | –0.0526 | –0.6482 | –0.0185 | 0.00779 |
| 0.1 | 0.0614 | 0.0639 | 0.0306 | –0.0452 | –0.677 | –0.0146 | 0.00799 |
| 0.2 | 0.0556 | 0.0643 | 0.0275 | –0.0389 | –0.707 | –0.0114 | 0.00804 |
| 0.4 | 0.0456 | 0.0625 | 0.0222 | –0.0288 | –0.771 | –0.00659 | 0.00781 |
| 0.6 | 0.0372 | 0.0582 | 0.0180 | –0.0215 | –0.839 | –0.00345 | 0.00728 |
| 0.8 | 0.0304 | 0.0527 | 0.0147 | –0.0162 | –0.908 | –0.00149 | 0.00659 |
| 1.0 | 0.0248 | 0.0467 | 0.0120 | –0.0123 | –0.975 | $-3.12e^{-4}$ | 0.00584 |
| 1.5 | 0.0150 | 0.0324 | 0.00725 | –0.0064 | –1.132 | $8.48e^{-4}$ | 0.00405 |
| 1.6 | 0.0136 | 0.0299 | 0.00655 | –0.0056 | –1.162 | $9.14e^{-4}$ | 0.00373 |
| 1.7 | 0.0123 | 0.0275 | 0.00592 | –0.00497 | –1.191 | $9.50e^{-4}$ | 0.00344 |
| 1.8 | 0.0111 | 0.0252 | 0.00535 | –0.00439 | –1.220 | $9.63e^{-4}$ | 0.00316 |
| 1.9 | 0.0101 | 0.0231 | 0.00483 | –0.00387 | –1.247 | $9.57e^{-4}$ | 0.00289 |
| 2.0 | 0.0091 | 0.0212 | 0.00436 | –0.00342 | –1.274 | $9.37e^{-4}$ | 0.00265 |
| 2.1 | 0.00829 | 0.0194 | 0.00394 | –0.00303 | –1.299 | $9.07e^{-4}$ | 0.00242 |
| 2.5 | 0.00562 | 0.0134 | 0.00262 | –0.00189 | –1.389 | $7.34e^{-4}$ | 0.00168 |
| 3.0 | 0.00349 | 0.00839 | 0.00159 | –0.00108 | –1.472 | $5.09e^{-4}$ | 0.00105 |
| 3.5 | 0.00218 | 0.00526 | $9.76e^{-4}$ | $-6.37e^{-4}$ | –1.532 | $3.39e^{-4}$ | $6.58e^{-4}$ |
| 4.0 | 0.00137 | 0.00334 | $6.08e^{-4}$ | $-3.82e^{-4}$ | –1.591 | $2.26e^{-4}$ | $4.17e^{-4}$ |
| 5.0 | $5.52e^{-4}$ | 0.00138 | $2.44e^{-4}$ | $-1.41e^{-4}$ | –1.725 | $1.02e^{-4}$ | $1.73e^{-4}$ |
| 6.0 | $2.25e^{-4}$ | $5.83e^{-4}$ | $1.00e^{-4}$ | $-5.44e^{-5}$ | –1.839 | $4.57e^{-5}$ | $7.29e^{-5}$ |
| 7.0 | $9.43e^{-5}$ | $2.45e^{-4}$ | $4.14e^{-5}$ | $-2.15e^{-5}$ | –1.924 | $1.99e^{-5}$ | $3.06e^{-5}$ |
| 8.0 | $4.07e^{-5}$ | $1.04e^{-4}$ | $1.73e^{-5}$ | $-8.63e^{-6}$ | –2.005 | $8.63e^{-6}$ | $1.30e^{-5}$ |
| 9.0 | $1.80e^{-5}$ | $4.49e^{-5}$ | $7.44e^{-6}$ | $-3.67e^{-6}$ | –2.027 | $3.77e^{-6}$ | $5.61e^{-6}$ |
| 10.0 | $8.16e^{-6}$ | $2.04e^{-5}$ | $3.40e^{-6}$ | $-1.70e^{-6}$ | –2.004 | $1.70e^{-6}$ | $2.55e^{-6}$ |

[a] $w$ in $r = r_o + wa_o$.

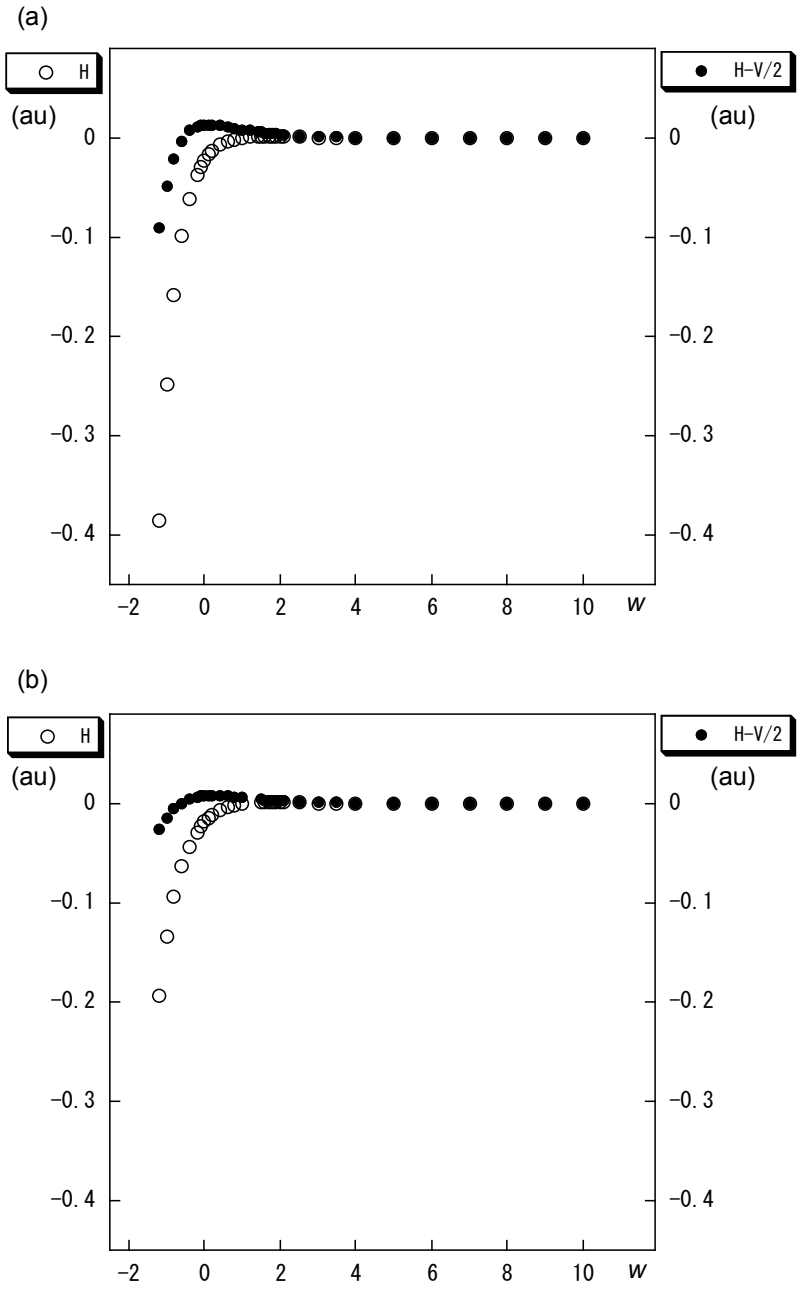


Figure S1. Plots of $H_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ versus $w$ in $r = r_o + wa_o$, where $r_o$ and $a_o$ stand for the optimized X–X distance and the Bohr radius, respectively: (a) For $Cl_3^-$ with $r_o$ = 2.4022 Å and (b) for $Br_3^-$ with $r_o$ = 2.4392 Å.

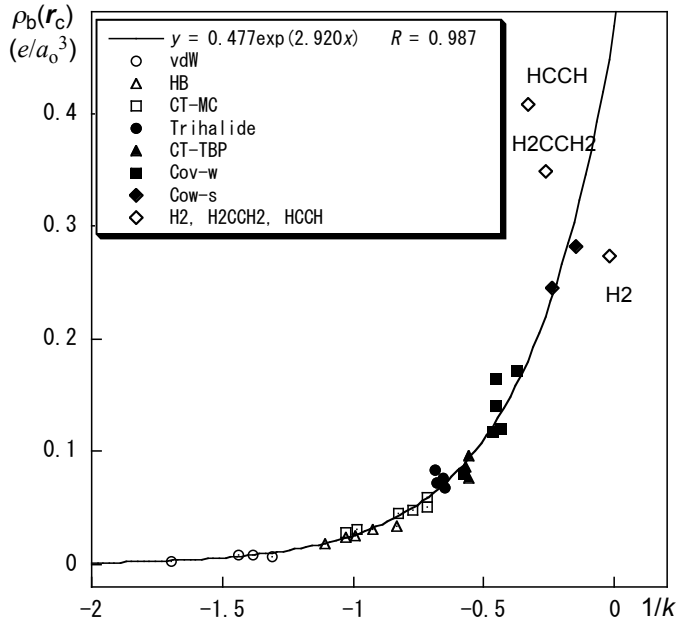


Figure S2. Plot of $\rho_b(\boldsymbol{r}_c)$ versus $1/k$ for the species in Scheme 2.

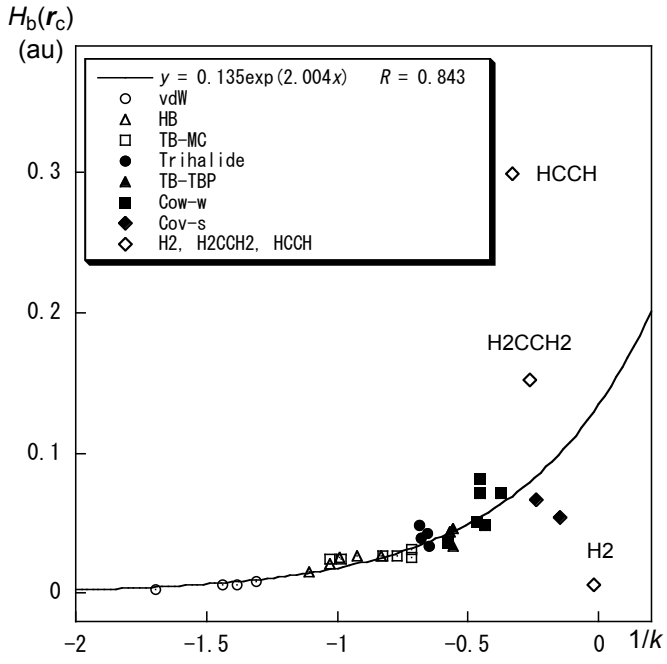


Figure S3. Plot of $H_b(\boldsymbol{r}_c)$ versus $1/k$ for the species in Scheme 2.

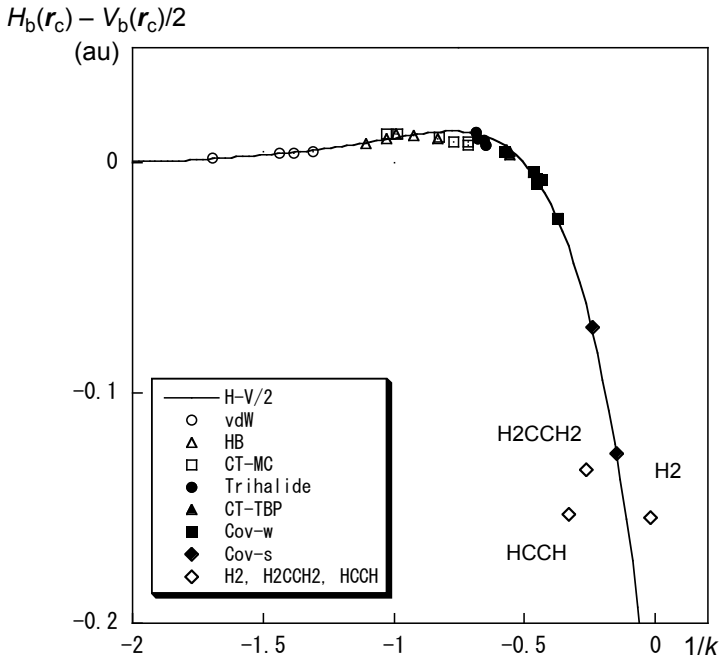


Figure S4. Plot of $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ versus $1/k$ for the species in Scheme 2.

Optimized structures given by Cartesian coordinates for examined molecules and adducts, together with the total energies.
The MP2 level of the Gaussian 03 program.
The 6-311+G(3d,2p) basis sets for C and H and the 6-311+G(3df) basis sets for atoms other than C and H.
The 6-311++G(3df,3pd) basis sets are applied to C and H when hydrocarbons are calculated.

HeHF; MP2 = -103.2264577 a.u

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 0.000000 | -0.000000 | -0.313374 |
| 9 | 0 | 0.000000 | 0.000000 | 0.603446 |
| 2 | 0 | -0.000000 | -0.000000 | -2.558821 |

NeHF; MP2 = -229.1262449 a.u

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 0.000000 | 0.000000 | -0.686500 |
| 9 | 0 | 0.000000 | 0.000000 | -1.603336 |
| 10 | 0 | 0.000000 | -0.000000 | 1.511653 |

ArHF; MP2 = -627.3457567 a.u

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 0.000000 | 0.000000 | -1.321248 |
| 9 | 0 | 0.000000 | 0.000000 | -2.239031 |
| 18 | 0 | 0.000000 | 0.000000 | 1.192918 |

KrHF; MP2 = -2852.4747779 a.u

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 0.000000 | 0.000000 | -1.888239 |
| 9 | 0 | 0.000000 | 0.000000 | -2.806467 |
| 36 | 0 | 0.000000 | 0.000000 | 0.754068 |

NNHF; MP2 = -209.6952455 a.u

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 0.000000 | 0.000000 | -0.866346 |
| 1 | 0 | 0.000000 | 0.000000 | 1.162948 |
| 7 | 0 | 0.000000 | 0.000000 | -1.978524 |
| 9 | 0 | 0.000000 | 0.000000 | 2.083460 |

HFHF; MP2 = -200.6735338 a.u

| | | | | |
|---|---|---|---|---|
| 9 | 0 | -1.301251 | -0.090019 | -0.000015 |
| 1 | 0 | 0.518298 | -0.081339 | 0.000312 |
| 1 | 0 | -1.728900 | 0.724273 | 0.000024 |
| 9 | 0 | 1.435763 | 0.018582 | -0.000023 |

HCNHF; MP2 = -193.6003383 a.u

| | | | | |
|---|---|---|---|---|
| 7 | 0 | 0.000000 | 0.000000 | -0.725403 |
| 6 | 0 | 0.000000 | 0.000000 | -1.887377 |
| 1 | 0 | 0.000000 | 0.000000 | -2.953345 |
| 1 | 0 | 0.000000 | 0.000000 | 1.098422 |
| 9 | 0 | 0.000000 | 0.000000 | 2.028556 |

$H_2OHOH$; MP2 = -152.6570271 a.u

| | | | | |
|---|---|---|---|---|
| 8 | 0 | 0.000439 | -1.386583 | 0.000000 |
| 1 | 0 | 0.488262 | -1.714488 | 0.758756 |
| 1 | 0 | 0.488262 | -1.714488 | -0.758756 |
| 1 | 0 | -0.078554 | 0.554494 | -0.000000 |
| 8 | 0 | 0.000439 | 1.517165 | -0.000000 |
| 1 | 0 | -0.904990 | 1.829832 | -0.000000 |

$Me_2OHOH$; MP2 = -231.062976 a.u

| | | | | |
|---|---|---|---|---|
| 8 | 0 | 0.700291 | -0.122840 | 0.000000 |
| 6 | 0 | 0.700291 | 0.677861 | 1.167428 |
| 1 | 0 | 0.699653 | 0.005798 | 2.019487 |
| 1 | 0 | -0.190143 | 1.310480 | 1.204015 |
| 1 | 0 | 1.591468 | 1.308929 | 1.200650 |
| 6 | 0 | 0.700291 | 0.677861 | -1.167428 |
| 1 | 0 | 0.699653 | 0.005798 | -2.019487 |
| 1 | 0 | 1.591468 | 1.308929 | -1.200650 |
| 1 | 0 | -0.190143 | 1.310480 | -1.204015 |
| 1 | 0 | -0.962702 | -0.964050 | 0.000000 |
| 8 | 0 | -1.911162 | -1.164561 | 0.000000 |
| 1 | 0 | -1.955786 | -2.121493 | 0.000000 |

$Me_2OCl_2$ (MC); MP2 = -1074.0612133 a.u

| | | | | |
|---|---|---|---|---|
| 8 | 0 | 1.836163 | 0.565961 | 0.000000 |
| 6 | 0 | 1.836163 | 1.363317 | 1.170043 |
| 1 | 0 | 1.816125 | 0.688454 | 2.018663 |
| 1 | 0 | 0.955545 | 2.009251 | 1.198146 |
| 1 | 0 | 2.734606 | 1.982188 | 1.215143 |
| 6 | 0 | 1.836163 | 1.363317 | -1.170043 |
| 1 | 0 | 1.816125 | 0.688454 | -2.018663 |
| 1 | 0 | 0.955545 | 2.009251 | -1.198146 |
| 1 | 0 | 2.734606 | 1.982188 | -1.215143 |
| 17 | 0 | -0.472398 | -0.520087 | 0.000000 |
| 17 | 0 | -2.335591 | -1.259164 | 0.000000 |

$Me_2OBr_2$ (MC); MP2 = -5300.1230866 a.u

| | | | | |
|---|---|---|---|---|
| 8 | 0 | 0.466479 | 2.608457 | 0.000000 |
| 6 | 0 | -0.176463 | 3.081076 | 1.172389 |
| 1 | 0 | 0.360911 | 2.671026 | 2.020233 |
| 1 | 0 | -1.216196 | 2.748414 | 1.203686 |
| 1 | 0 | -0.146554 | 4.171434 | 1.211061 |
| 6 | 0 | -0.176463 | 3.081076 | -1.172389 |
| 1 | 0 | 0.360911 | 2.671026 | -2.020233 |
| 1 | 0 | -1.216196 | 2.748414 | -1.203686 |
| 1 | 0 | -0.146554 | 4.171434 | -1.211061 |
| 35 | 0 | 0.187589 | 0.032175 | 0.000000 |
| 35 | 0 | -0.176463 | -2.232813 | 0.000000 |

$Me_2SCl_2$ (MC); MP2 = -1396.6733142 a.u

| | | | | |
|---|---|---|---|---|
| 16 | 0 | 1.831602 | -0.228556 | 0.000000 |
| 6 | 0 | 1.831602 | 0.940154 | 1.368636 |
| 1 | 0 | 1.766846 | 0.363875 | 2.286694 |
| 1 | 0 | 0.966256 | 1.593865 | 1.292442 |
| 1 | 0 | 2.749888 | 1.521506 | 1.369011 |
| 6 | 0 | 1.831602 | 0.940154 | -1.368636 |
| 1 | 0 | 1.766846 | 0.363875 | -2.286694 |
| 1 | 0 | 2.749888 | 1.521506 | -1.369011 |
| 1 | 0 | 0.966256 | 1.593865 | -1.292442 |
| 17 | 0 | -0.792450 | -0.446466 | 0.000000 |
| 17 | 0 | -2.869363 | -0.411384 | 0.000000 |

$Me_2SBr_2$ (MC); MP2 = -5622.7372659 a.u

| | | | | |
|---|---|---|---|---|
| 16 | 0 | 0.740176 | 2.485612 | 0.000000 |
| 6 | 0 | -0.370313 | 2.844216 | 1.370730 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 0.156466 | 2.594953 | 2.286950 |
| 1 | 0 | -1.263036 | 2.229360 | 1.289123 |
| 1 | 0 | -0.630408 | 3.899487 | 1.374833 |
| 6 | 0 | -0.370313 | 2.844216 | -1.370730 |
| 1 | 0 | 0.156466 | 2.594953 | -2.286950 |
| 1 | 0 | -0.630408 | 3.899487 | -1.374833 |
| 1 | 0 | -1.263036 | 2.229360 | -1.289123 |
| 35 | 0 | 0.258167 | -0.163220 | 0.000000 |
| 35 | 0 | -0.370313 | -2.446722 | 0.000000 |

$Me_2SeCl_2$ (MC); MP2 = -3399.0874544 a.u

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 1.440904 | -0.261642 | 0.000000 |
| 6 | 0 | 1.440904 | 1.025919 | 1.443396 |
| 1 | 0 | 1.337540 | 0.469329 | 2.369288 |
| 1 | 0 | 0.588674 | 1.685449 | 1.311265 |
| 1 | 0 | 2.374593 | 1.579326 | 1.440773 |
| 6 | 0 | 1.440904 | 1.025919 | -1.443396 |
| 1 | 0 | 1.337540 | 0.469329 | -2.369288 |
| 1 | 0 | 2.374593 | 1.579326 | -1.440773 |
| 1 | 0 | 0.588674 | 1.685449 | -1.311265 |
| 17 | 0 | -1.126639 | -0.374165 | 0.000000 |
| 17 | 0 | -3.278254 | -0.266035 | 0.000000 |

$Me_2SeBr_2$ (MC); MP2 = -7625.1512354 a.u

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 2.250839 | -0.124642 | 0.000000 |
| 6 | 0 | 2.250839 | 1.165056 | 1.444146 |
| 1 | 0 | 2.152712 | 0.608634 | 2.370776 |
| 1 | 0 | 1.398260 | 1.825160 | 1.317605 |
| 1 | 0 | 3.184031 | 1.719395 | 1.437572 |
| 6 | 0 | 2.250839 | 1.165056 | -1.444146 |
| 1 | 0 | 2.152712 | 0.608634 | -2.370776 |
| 1 | 0 | 3.184031 | 1.719395 | -1.437572 |
| 1 | 0 | 1.398260 | 1.825160 | -1.317605 |
| 35 | 0 | -0.472361 | -0.296734 | 0.000000 |
| 35 | 0 | -2.870741 | -0.218958 | 0.000000 |

$Cl_3^-$; MP2 = -1379.1646832 a.u

| | | | | |
|---|---|---|---|---|
| 17 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 17 | 0 | 0.000000 | 0.000000 | 2.295600 |
| 17 | 0 | 0.000000 | 0.000000 | -2.295600 |

$BrCl_2^-$; MP2 = -3492.2070891 a.u

| | | | | |
|---|---|---|---|---|
| 35 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 17 | 0 | 0.000000 | 0.000000 | 2.402152 |
| 17 | 0 | 0.000000 | 0.000000 | -2.402152 |

$Br_3^-$; MP2 = -7718.2617316 a.u

| | | | | |
|---|---|---|---|---|
| 35 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 35 | 0 | 0.000000 | 0.000000 | 2.547353 |
| 35 | 0 | 0.000000 | 0.000000 | -2.547353 |

$ClBr_2^-$; MP2 = -5605.2225539 a.u

| | | | | |
|---|---|---|---|---|
| 17 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 35 | 0 | 0.000000 | 0.000000 | 2.439200 |
| 35 | 0 | 0.000000 | 0.000000 | -2.439200 |

$Me_2SCl_2$ (TB); MP2 = -1396.699423 a.u

| | | | | |
|---|---|---|---|---|
| 16 | 0 | 0.000000 | 0.000000 | 0.286988 |
| 6 | 0 | 0.000000 | 1.389238 | -0.869455 |
| 1 | 0 | 0.000000 | 2.290531 | -0.264242 |
| 1 | 0 | -0.902913 | 1.329056 | -1.464774 |
| 1 | 0 | 0.902913 | 1.329056 | -1.464774 |
| 6 | 0 | 0.000000 | -1.389238 | -0.869455 |
| 1 | 0 | 0.000000 | -2.290531 | -0.264242 |
| 1 | 0 | 0.902913 | -1.329056 | -1.464774 |
| 1 | 0 | -0.902913 | -1.329056 | -1.464774 |
| 17 | 0 | -2.263787 | 0.000000 | 0.359683 |
| 17 | 0 | 2.263787 | 0.000000 | 0.359683 |

$Me_2SBr_2$ (TB); MP2 = -5622.743386 a.u

| | | | | |
|---|---|---|---|---|
| 16 | 0 | 0.000000 | 0.000000 | 0.131287 |
| 6 | 0 | 0.000000 | 1.387365 | -1.032253 |
| 1 | 0 | 0.000000 | 2.290372 | -0.429272 |
| 1 | 0 | -0.902584 | 1.326018 | -1.628638 |
| 1 | 0 | 0.902584 | 1.326018 | -1.628638 |
| 6 | 0 | 0.000000 | -1.387365 | -1.032253 |
| 1 | 0 | 0.000000 | -2.290372 | -0.429272 |
| 1 | 0 | 0.902584 | -1.326018 | -1.628638 |
| 1 | 0 | -0.902584 | -1.326018 | -1.628638 |
| 35 | 0 | -2.435730 | 0.000000 | 0.252279 |
| 35 | 0 | 2.435730 | 0.000000 | 0.252279 |

$Me_2SeCl_2$ (TB); MP2 = -3399.1299736 a.u

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 0.000000 | 0.000000 | 0.289297 |
| 6 | 0 | 0.000000 | 1.459017 | -0.983328 |
| 1 | 0 | 0.000000 | 2.375814 | -0.402556 |
| 1 | 0 | -0.906086 | 1.372268 | -1.570571 |
| 1 | 0 | 0.906086 | 1.372268 | -1.570571 |
| 6 | 0 | 0.000000 | -1.459017 | -0.983328 |
| 1 | 0 | 0.000000 | -2.375814 | -0.402556 |
| 1 | 0 | 0.906086 | -1.372268 | -1.570571 |
| 1 | 0 | -0.906086 | -1.372268 | -1.570571 |
| 17 | 0 | -2.354614 | 0.000000 | 0.266213 |
| 17 | 0 | 2.354614 | 0.000000 | 0.266213 |

$Me_2SeBr_2$ (TB); MP2 = -7625.1728957 a.u

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 0.000000 | 0.000000 | 0.191694 |
| 6 | 0 | 0.000000 | 1.458821 | -1.087394 |
| 1 | 0 | 0.000000 | 2.375801 | -0.506634 |
| 1 | 0 | -0.905721 | 1.371903 | -1.675556 |
| 1 | 0 | 0.905721 | 1.371903 | -1.675556 |
| 6 | 0 | 0.000000 | -1.458821 | -1.087394 |
| 1 | 0 | 0.000000 | -2.375801 | -0.506634 |
| 1 | 0 | 0.905721 | -1.371903 | -1.675556 |
| 1 | 0 | -0.905721 | -1.371903 | -1.675556 |
| 35 | 0 | -2.519541 | 0.000000 | 0.203523 |
| 35 | 0 | 2.519541 | 0.000000 | 0.203523 |

$Cl_2$; MP2 = -919.3581145 a.u

| | | | | |
|---|---|---|---|---|
| 17 | 0 | 0.000000 | 0.000000 | 0.992258 |
| 17 | 0 | 0.000000 | 0.000000 | -0.992258 |

$Br_2$; MP2 = -5145.4191746 a.u

| | | | | |
|---|---|---|---|---|
| 35 | 0 | 0.000000 | 0.000000 | 1.134504 |

| | | | | |
|---|---|---|---|---|
| 35 | 0 | 0.000000 | 0.000000 | -1.134504 |

$Me_2SCl^+$; MP2 = -936.7244983 a.u

| | | | | |
|---|---|---|---|---|
| 16 | 0 | 0.574516 | 0.308485 | 0.000000 |
| 6 | 0 | -0.239891 | 1.087658 | 1.388179 |
| 1 | 0 | 0.105102 | 0.582084 | 2.285281 |
| 1 | 0 | -1.316358 | 1.009887 | 1.269493 |
| 1 | 0 | 0.093549 | 2.124488 | 1.387913 |
| 6 | 0 | -0.239891 | 1.087658 | -1.388179 |
| 1 | 0 | 0.105102 | 0.582084 | -2.285281 |
| 1 | 0 | 0.093549 | 2.124488 | -1.387913 |
| 1 | 0 | -1.316358 | 1.009887 | -1.269493 |
| 17 | 0 | -0.239891 | -1.495327 | -0.000000 |

$Me_2SBr^+$; MP2 = -3049.7488791 a.u

| | | | | |
|---|---|---|---|---|
| 16 | 0 | 0.651132 | 0.788460 | 0.000000 |
| 6 | 0 | -0.181174 | 1.556726 | 1.389772 |
| 1 | 0 | 0.175774 | 1.063065 | 2.288634 |
| 1 | 0 | -1.255878 | 1.455022 | 1.275060 |
| 1 | 0 | 0.128639 | 2.600776 | 1.384143 |
| 6 | 0 | -0.181174 | 1.556726 | -1.389772 |
| 1 | 0 | 0.175774 | 1.063065 | -2.288634 |
| 1 | 0 | 0.128639 | 2.600776 | -1.384143 |
| 1 | 0 | -1.255878 | 1.455022 | -1.275060 |
| 35 | 0 | -0.181174 | -1.186680 | -0.000000 |

$Me_2SeCl^+$; MP2 = -2939.1449271 a.u

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 0.492822 | 0.237709 | 0.000000 |
| 6 | 0 | -0.453485 | 1.058712 | 1.461838 |
| 1 | 0 | -0.137261 | 0.552606 | 2.368423 |
| 1 | 0 | -1.518759 | 0.950691 | 1.286596 |
| 1 | 0 | -0.146434 | 2.102622 | 1.475411 |
| 6 | 0 | -0.453485 | 1.058712 | -1.461838 |
| 1 | 0 | -0.137261 | 0.552606 | -2.368423 |
| 1 | 0 | -0.146434 | 2.102622 | -1.475411 |
| 1 | 0 | -1.518759 | 0.950691 | -1.286596 |
| 17 | 0 | -0.453485 | -1.646970 | 0.000000 |

$Me_2SeBr^+$; MP2 = -5052.1699673 a.u

| | | | | |
|---|---|---|---|---|
| 34 | 0 | 0.597964 | 0.646958 | 0.000000 |
| 6 | 0 | -0.366603 | 1.454914 | 1.462771 |
| 1 | 0 | -0.039356 | 0.958596 | 2.370715 |
| 1 | 0 | -1.429690 | 1.324296 | 1.290512 |
| 1 | 0 | -0.081187 | 2.504820 | 1.471568 |
| 6 | 0 | -0.366603 | 1.454914 | -1.462771 |
| 1 | 0 | -0.039356 | 0.958596 | -2.370715 |
| 1 | 0 | -0.081187 | 2.504820 | -1.471568 |
| 1 | 0 | -1.429690 | 1.324296 | -1.290512 |
| 35 | 0 | -0.366603 | -1.400884 | 0.000000 |

$H_2$; MP2 = -1.1649453 a.u

| | | | | |
|---|---|---|---|---|
| 1 | 0 | 0.000000 | 0.000000 | 0.368299 |
| 1 | 0 | 0.000000 | 0.000000 | -0.368299 |

$CH_4$; MP2 = -40.4119815 a.u

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 1 | 0 | 0.626656 | 0.626656 | 0.626656 |

| | | | | |
|---|---|---|---|---|
| 1 | 0 | -0.626656 | -0.626656 | 0.626656 |
| 1 | 0 | 0.626656 | -0.626656 | -0.626656 |
| 1 | 0 | -0.626656 | 0.626656 | -0.626656 |

$C_2H_6$; MP2 = -79.6307609 a.u

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.000000 | 0.000000 | 0.761814 |
| 6 | 0 | -0.000000 | -0.000000 | -0.761814 |
| 1 | 0 | 0.000000 | 1.014950 | 1.155067 |
| 1 | 0 | -0.878972 | -0.507475 | 1.155067 |
| 1 | 0 | 0.878972 | -0.507475 | 1.155067 |
| 1 | 0 | -0.000000 | -1.014950 | -1.155067 |
| 1 | 0 | -0.878972 | 0.507475 | -1.155067 |
| 1 | 0 | 0.878972 | 0.507475 | -1.155067 |

$C_2H_4$; MP2 = -78.4000171 a.u

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.000000 | 0.000000 | 0.667426 |
| 6 | 0 | 0.000000 | 0.000000 | -0.667426 |
| 1 | 0 | 0.000000 | 0.935424 | 1.207493 |
| 1 | 0 | 0.000000 | -0.935424 | 1.207493 |
| 1 | 0 | 0.000000 | 0.935424 | -1.207493 |
| 1 | 0 | 0.000000 | -0.935424 | -1.207493 |

$C_2H_2$; MP2 = -77.1597093 a.u

| | | | | |
|---|---|---|---|---|
| 6 | 0 | 0.000000 | 0.000000 | 0.605371 |
| 6 | 0 | 0.000000 | 0.000000 | -0.605371 |
| 1 | 0 | 0.000000 | 0.000000 | 1.667060 |
| 1 | 0 | 0.000000 | 0.000000 | -1.667060 |