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## Modulation of in:out and out:out conformations in [X.X'.X''] Phosphatranes by Lewis Acids

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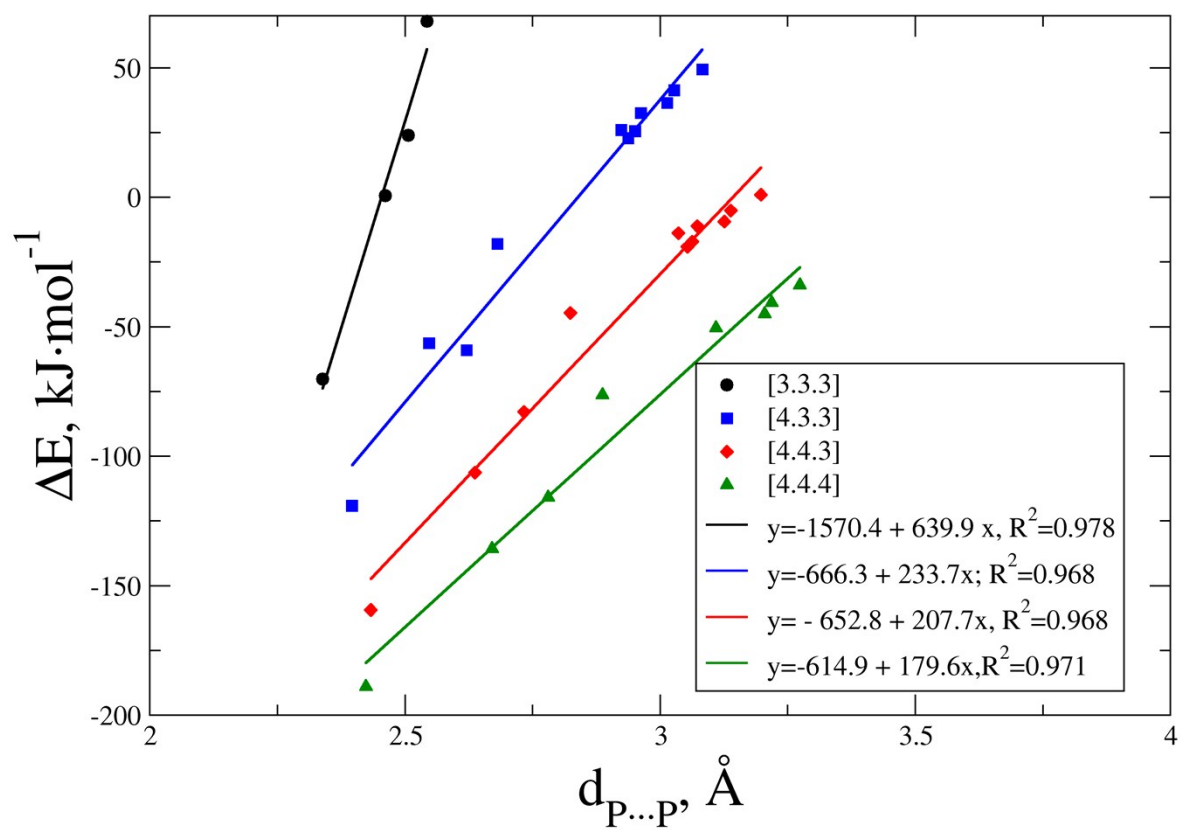
<sup>‡</sup> School of Chemistry, Trinity Biomedical Sciences Institute, Trinity College Dublin, 152–160 Pearse St., Dublin 2, Ireland

<sup>§</sup> Instituto de Química Médica, CSIC, Juan de la Cierva, 3, E-28006 Madrid, Spain

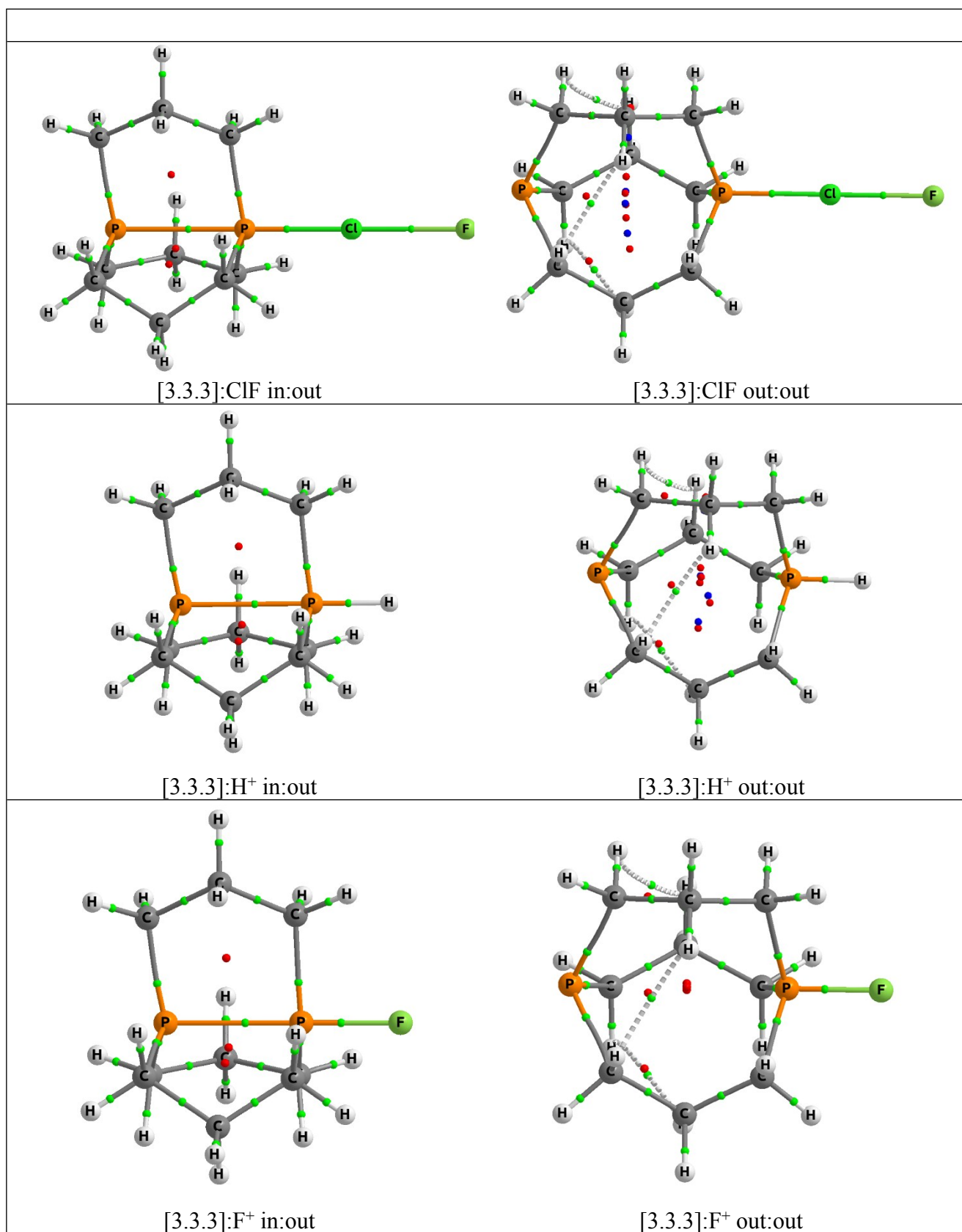
- **Figure S1.** Linear relationships between the P-P distance in the IO structures ( $d_{pp}$ ) and the relative energy ( $\Delta E$ ) between in:out and out:out conformations.
- **Figure S2.** AIM molecular graphs of all complexes studied at MP2/jul-cc-pVDZ computational level.
- **Figure S3.** Exponential relationships between the P-P distance and the Laplacian and H at the BCP in the IO structures.
- **Figure S4.** Electron density shift maps at 0.001 a.u. for the  $[4.4.3]^{OO}$ ,  $[4.4.3]^{OO}:ClF$ ,  $[4.4.4]^{OO}$  and  $[4.4.3]^{OO}:ClF$  complexes. Blue (negative) and yellow (positive) areas correspond to decrease and increase on the electron density upon interaction.
- **Figure S5.** NCI plots of non-covalent interaction for complexes a)  $[3.3.3]^{OO}:ClF$ , b)  $[4.3.3]^{OO}:ClF$ , c)  $[4.4.3]^{OO}:ClF$  and d)  $[4.4.4]^{OO}:ClF$ . Blue and green areas correspond to  $\lambda_2 > 0$  (strongly attractive) and  $\lambda_2 \approx 0$  (weak) respectively, while red areas correspond to  $\lambda_2 < 0$  (repulsive).  $\lambda_2$  is one of the three eigenvalues of the electron density Hessian with  $\lambda_1 \leq \lambda_2 \leq \lambda_3$ .
- **Figure S6.** NCI plots of non-covalent interaction for complexes  $[4.4.4]^{IO}$ ,  $[4.4.4]^{IO}:ClF$  and  $[4.4.4]^{IO}:LiH$ . Blue and green areas correspond to  $\lambda_2 > 0$  (strongly attractive) and  $\lambda_2 \approx 0$  (weak) respectively, while red areas correspond to  $\lambda_2 < 0$  (repulsive).  $\lambda_2$  is one of the three eigenvalues of the electron density Hessian with  $\lambda_1 \leq \lambda_2 \leq \lambda_3$ .
- **Table S1.** Cartesian coordinates of all complexes studied at MP2/jul-cc-pVDZ computational level.
- **Table S2.** P...P distances in Å, pyramidalisation (pyr) in degrees calculated at MP2/jul-cc-pVDZ computational level.

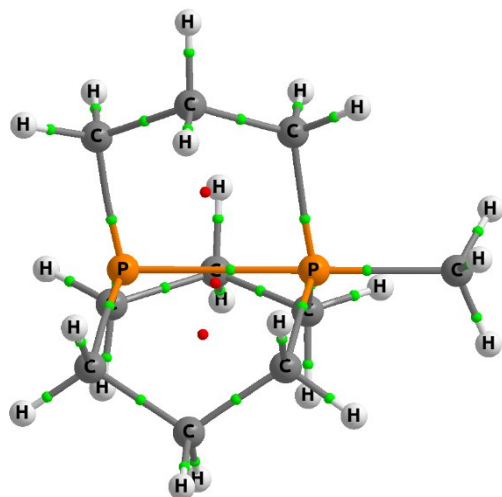
- **Table S3.** Electron density ( $\rho_{\text{BCP}}$ ), Laplacian ( $\nabla^2\rho_{\text{BCP}}$ ) and total electron energy density ( $H_{\text{BCP}}$ ) (au) at the P $\cdots$ P BCP in the in:out systems, at MP2/jul-cc-pVDZ computational level.

**Figure S1.** Linear relationships between the P-P distance in the IO structures ( $d_{pp}$ ) and the relative energy ( $\Delta E$ ) between in:out and out:out conformations.

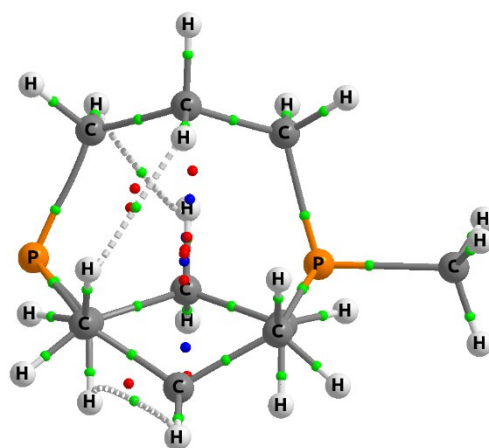


**Figure S2.** AIM molecular graphs of all complexes studied at MP2/jul-cc-pVDZ computational level.



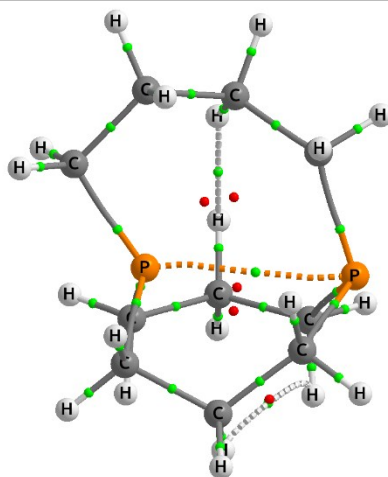


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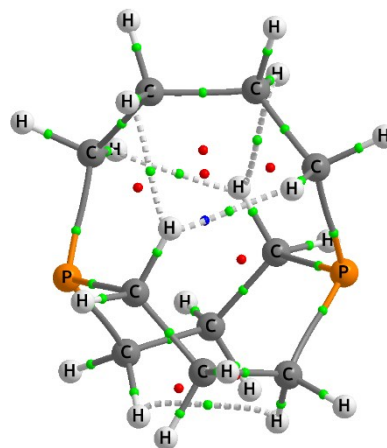


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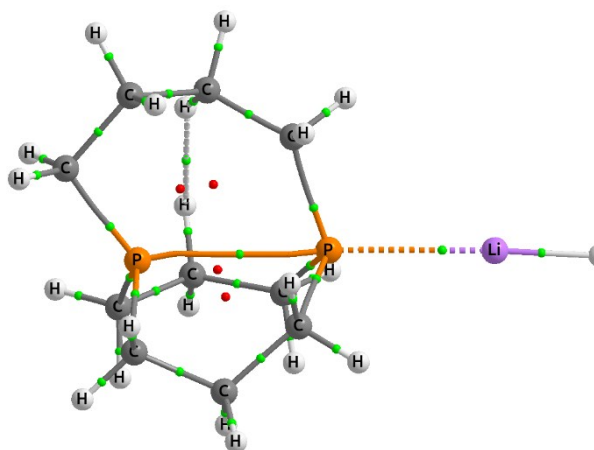
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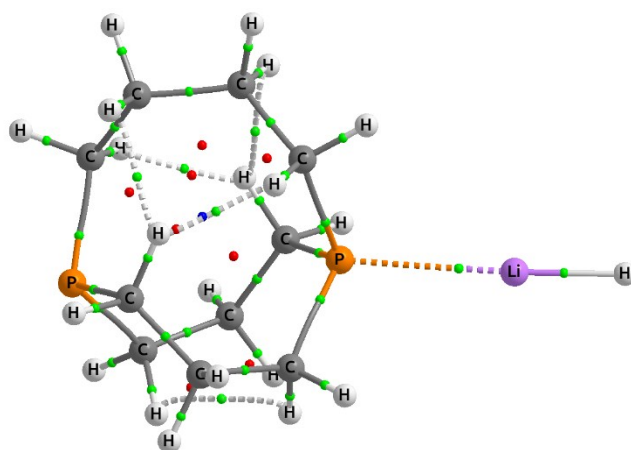
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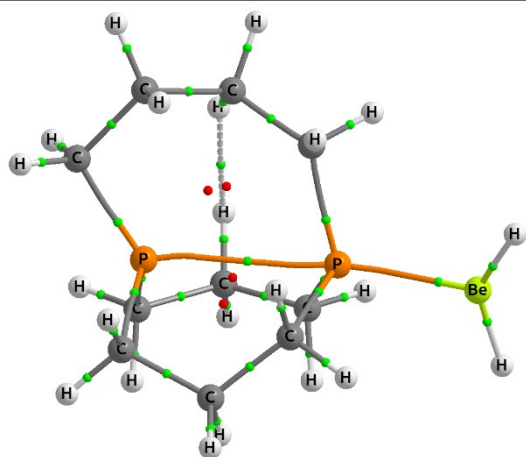
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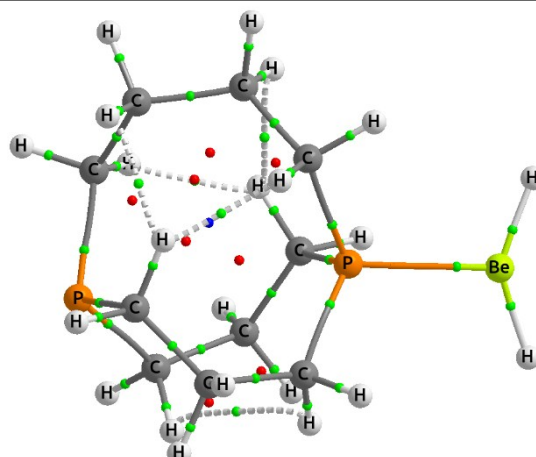
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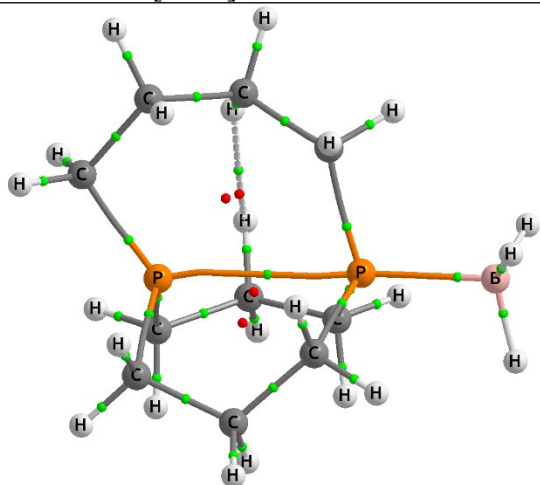
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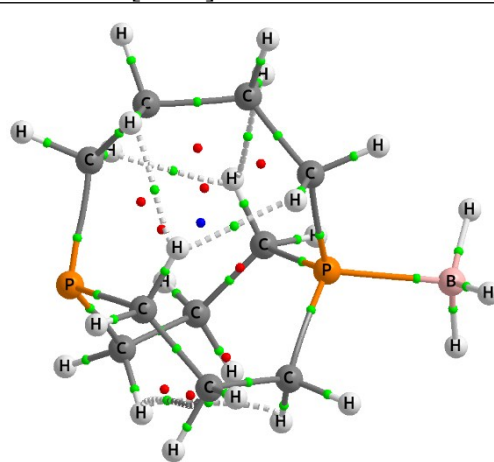
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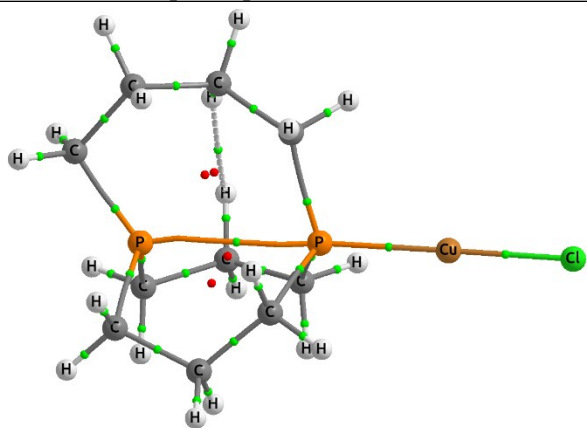
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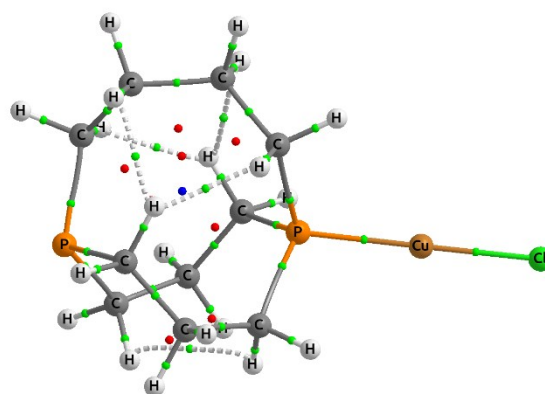
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[4.3.3]: BH<sub>3</sub> out:out



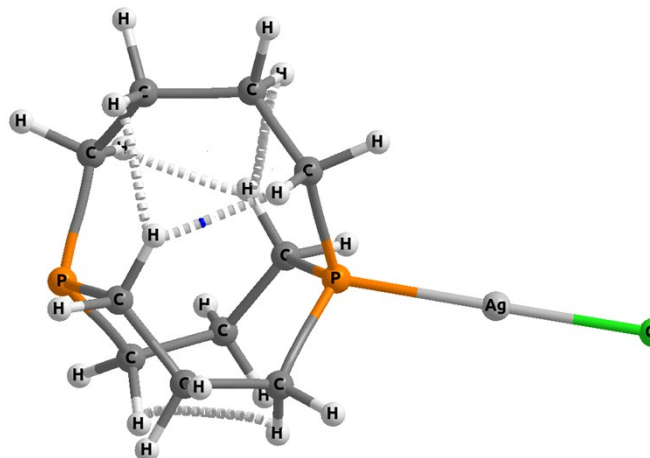
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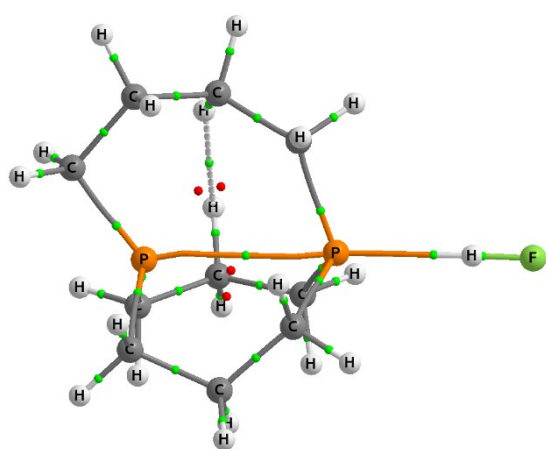
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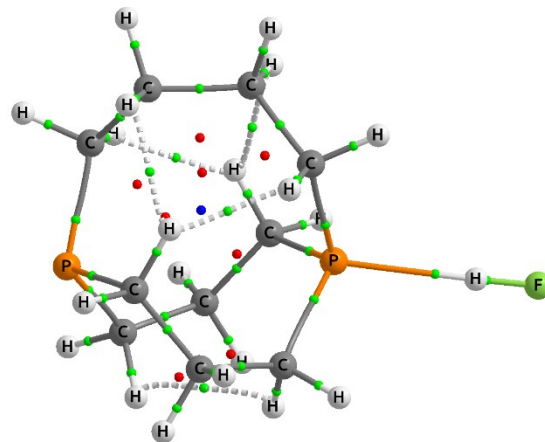
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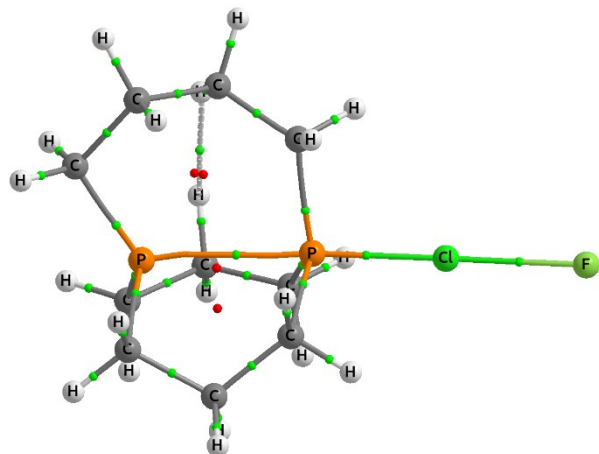
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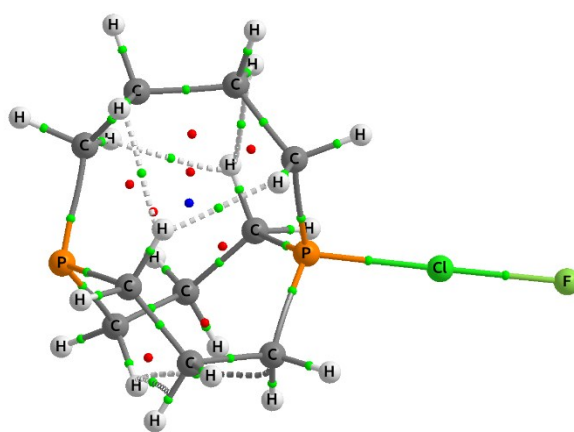
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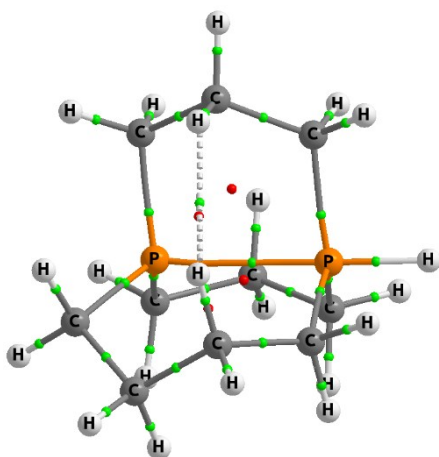
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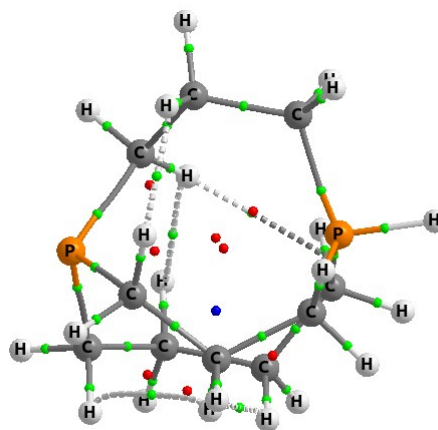
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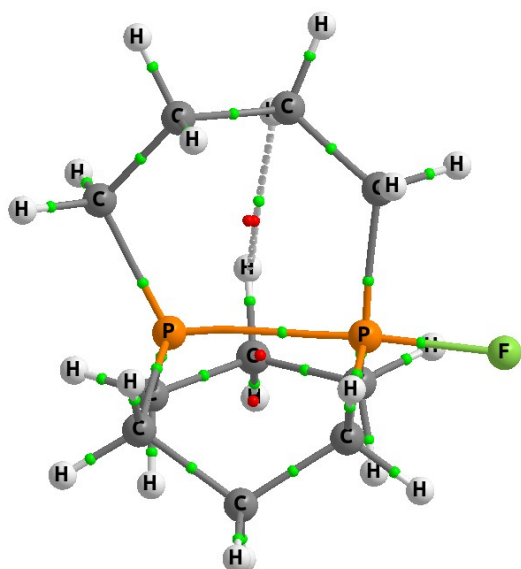
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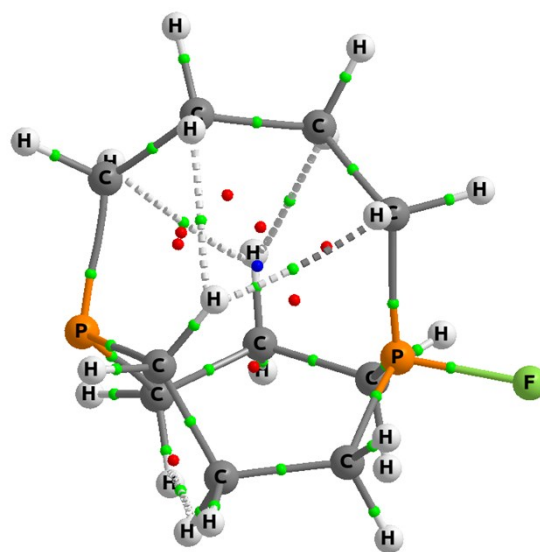
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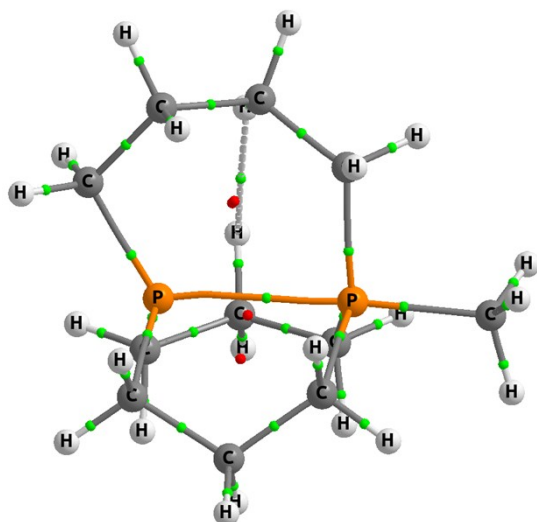
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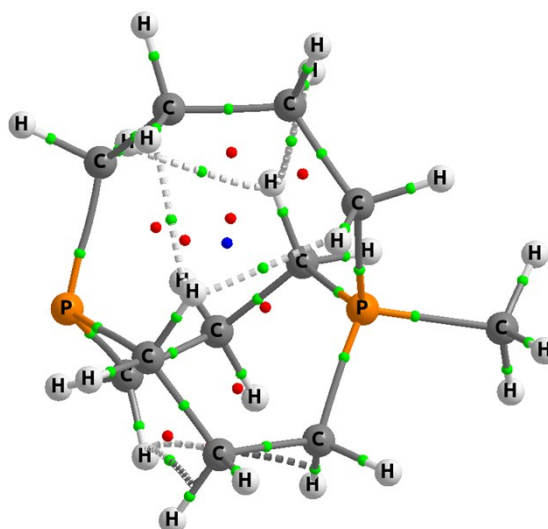
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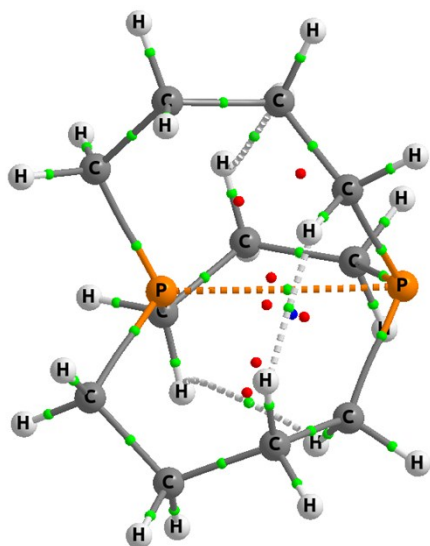


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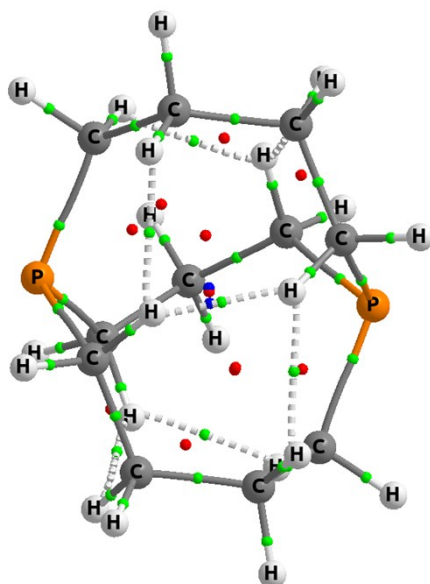


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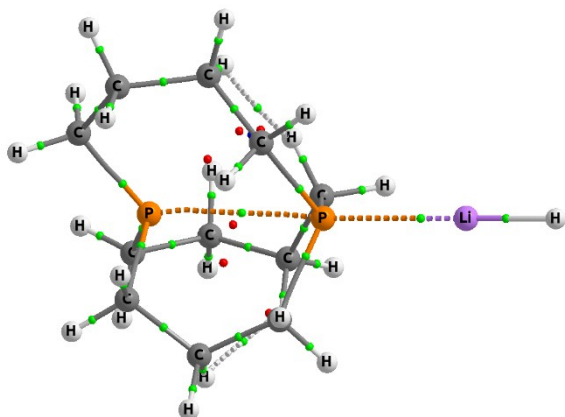
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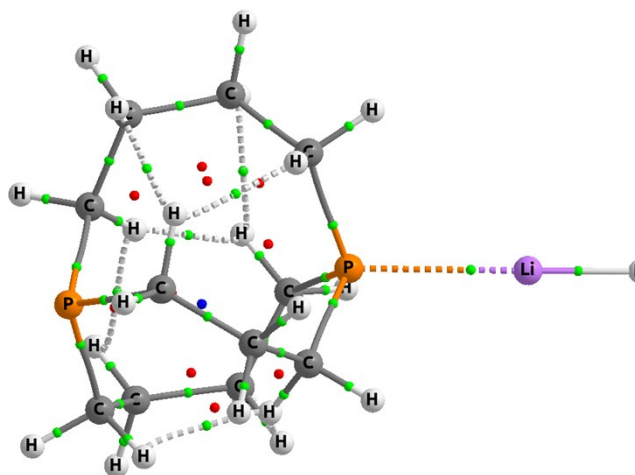
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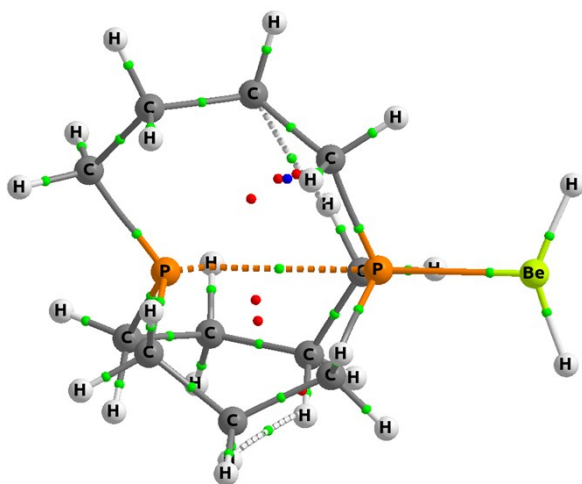
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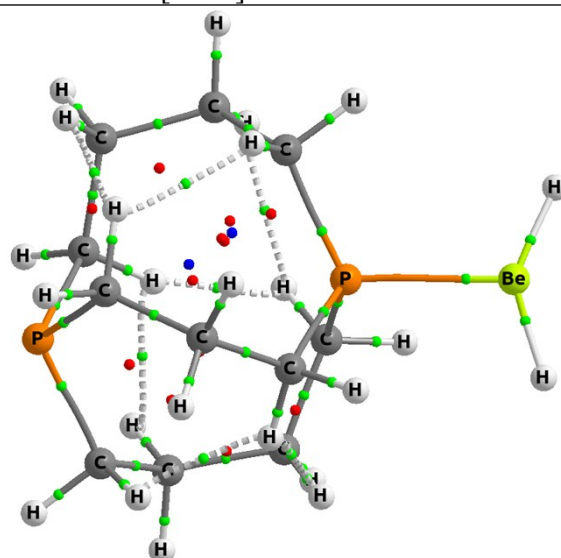
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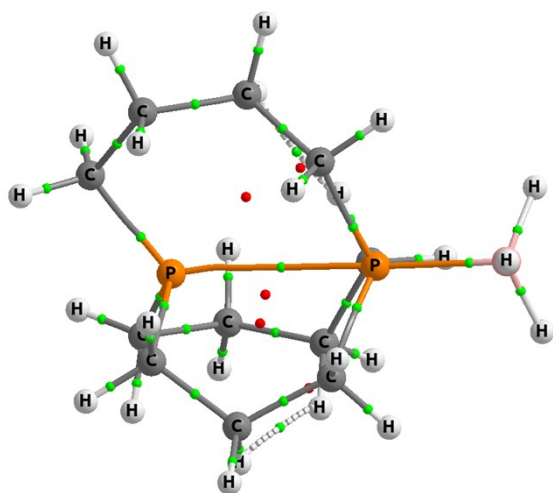
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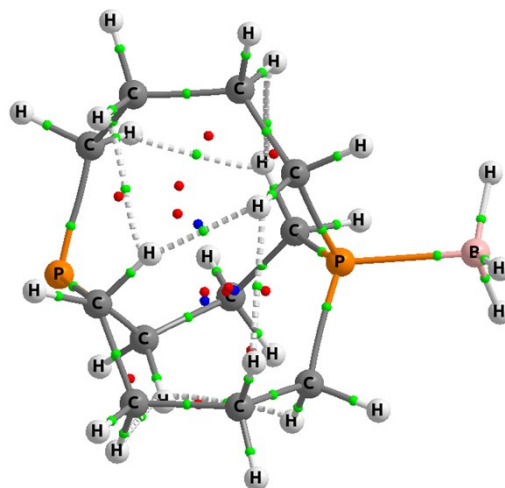
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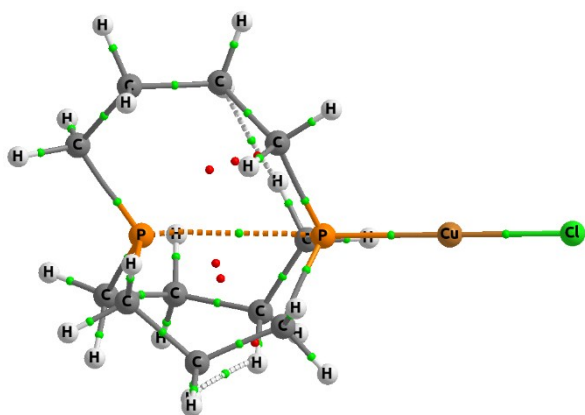
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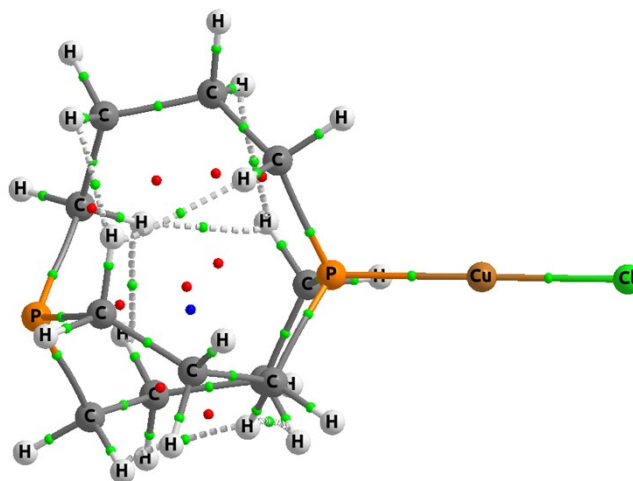
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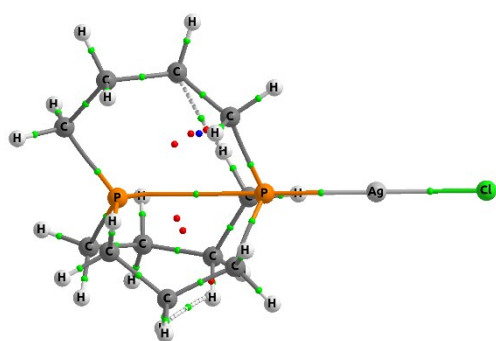
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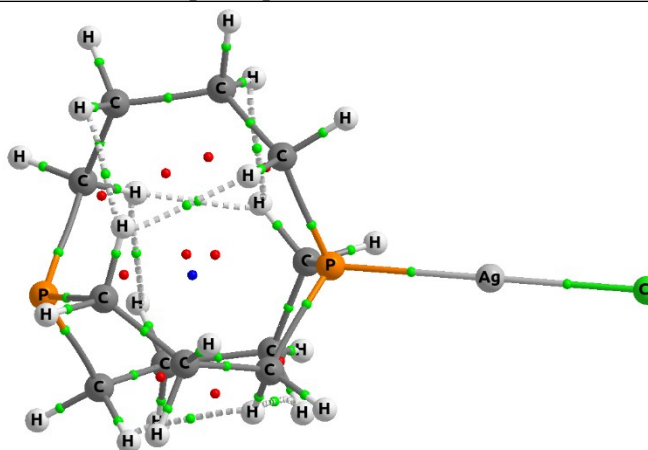
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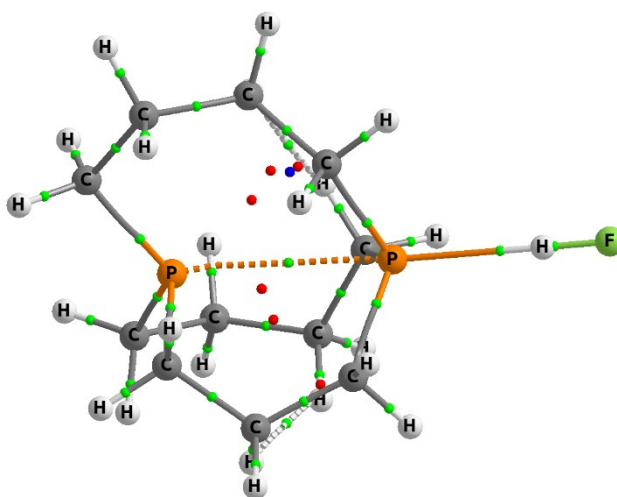
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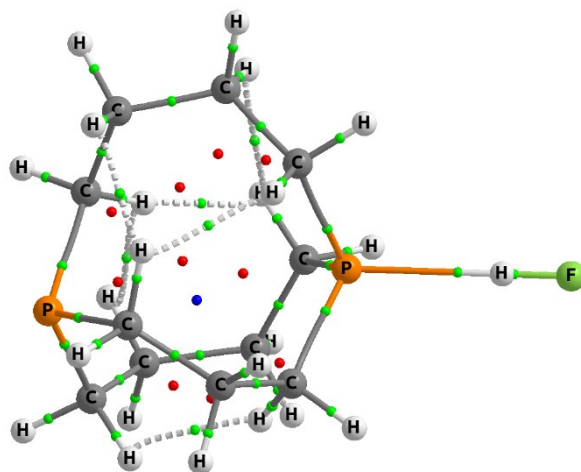
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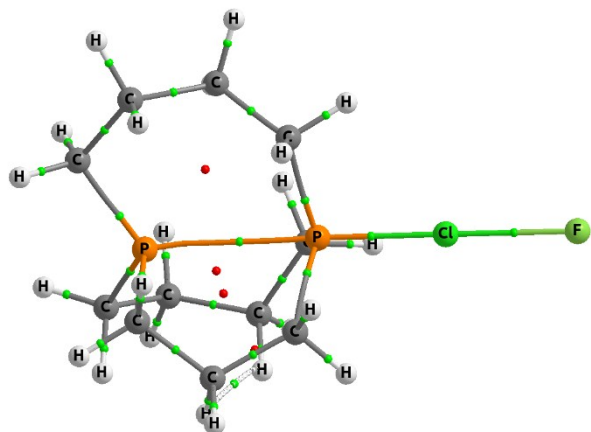
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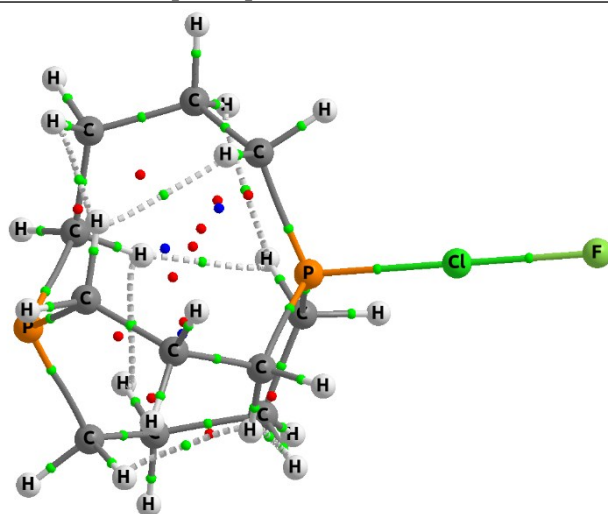
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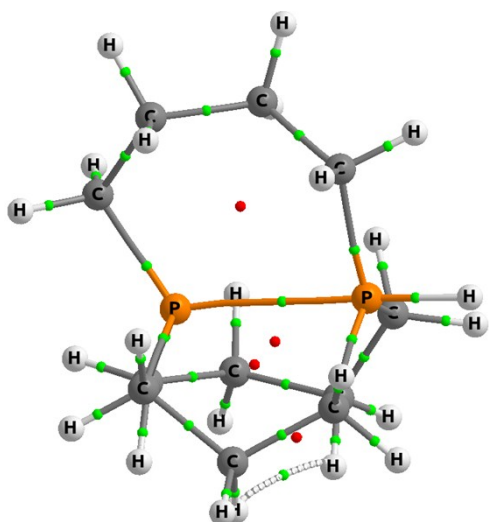
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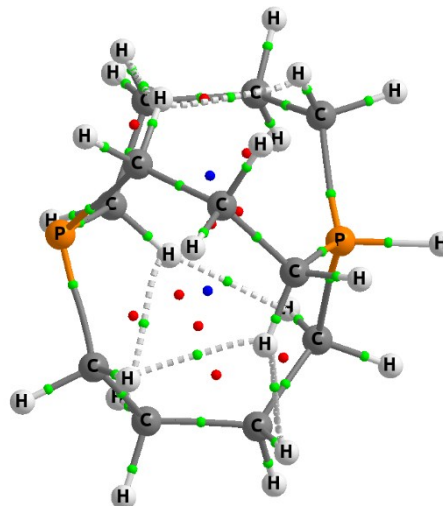
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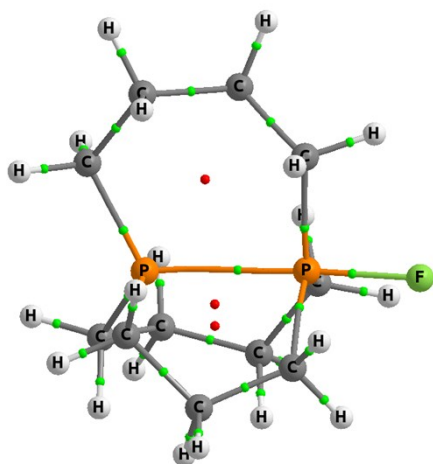
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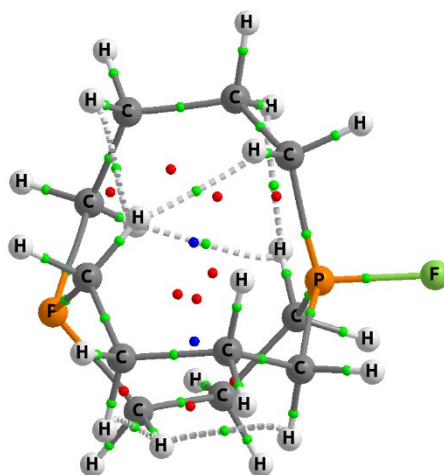
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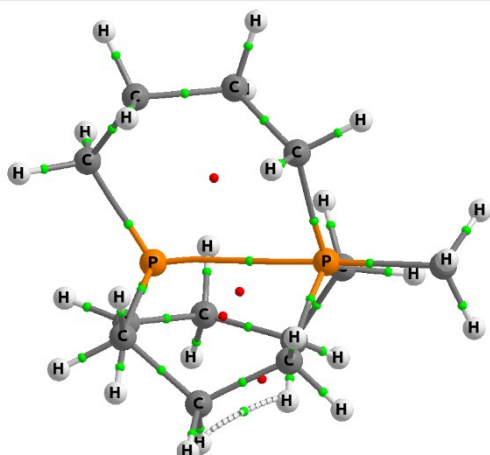
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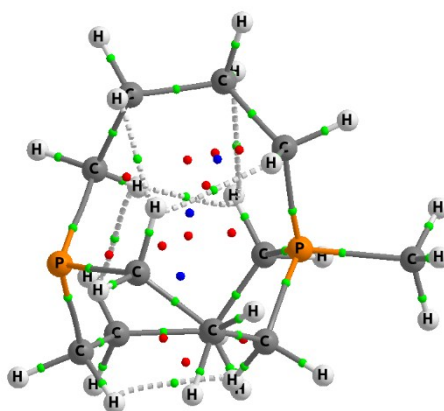
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[4.4.3]: F<sup>+</sup> out:out

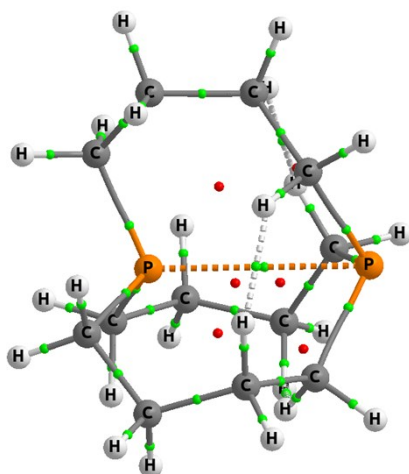


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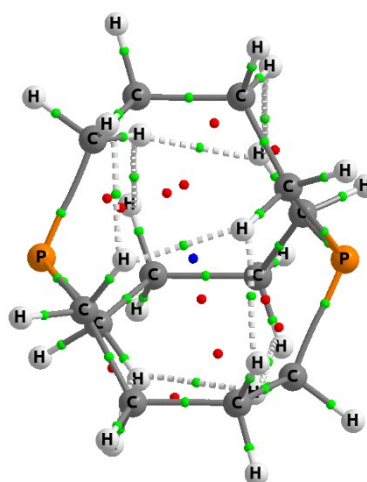


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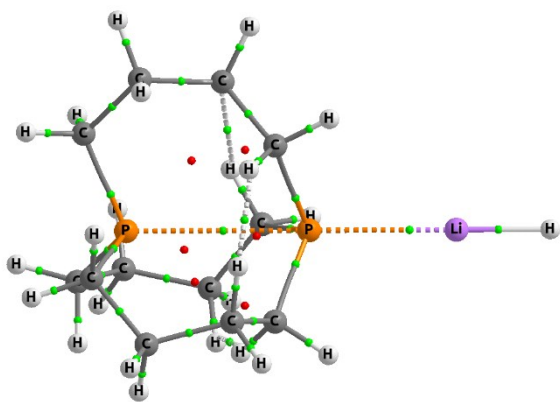
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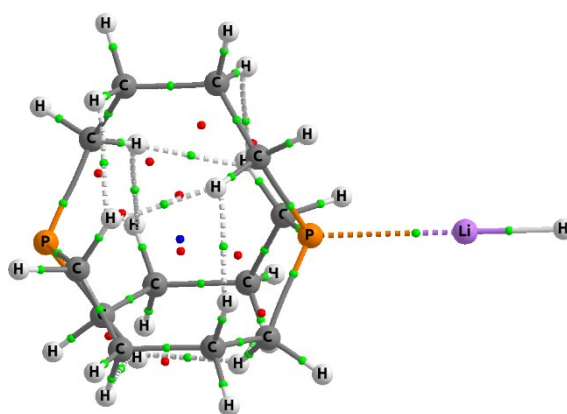
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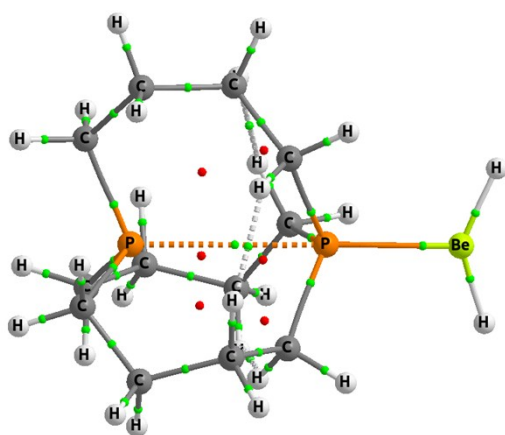
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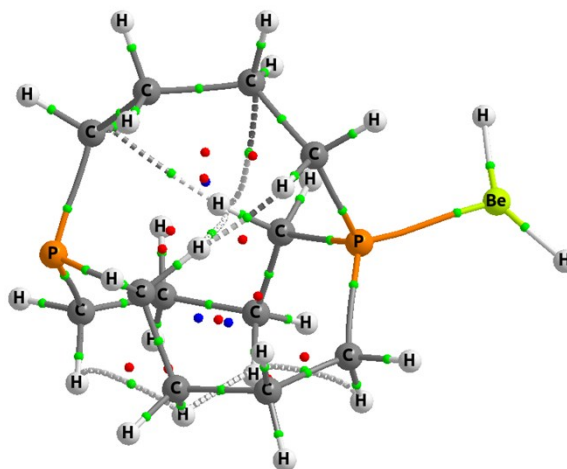
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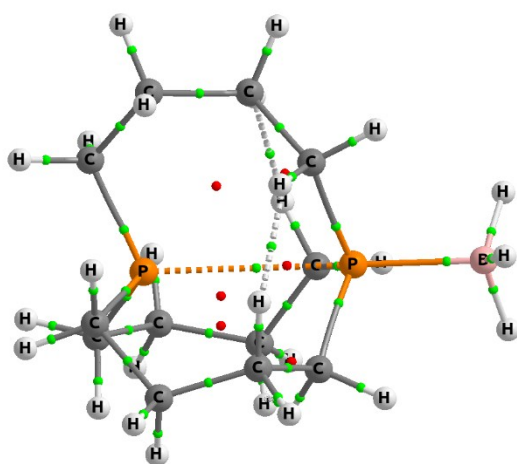
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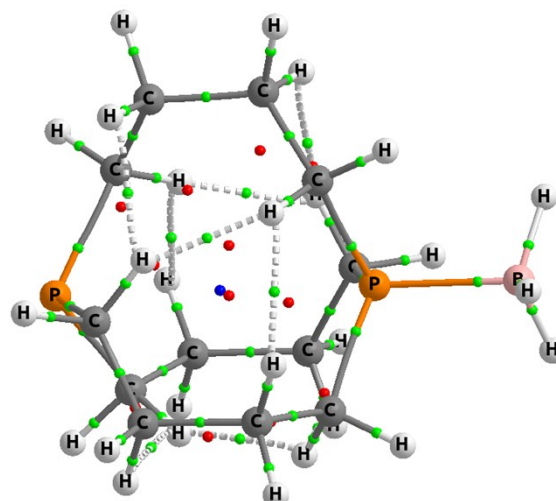
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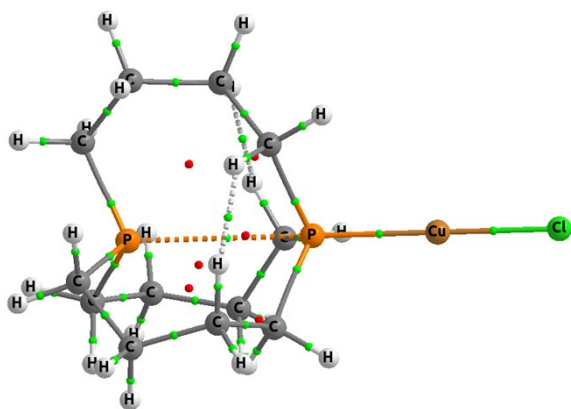
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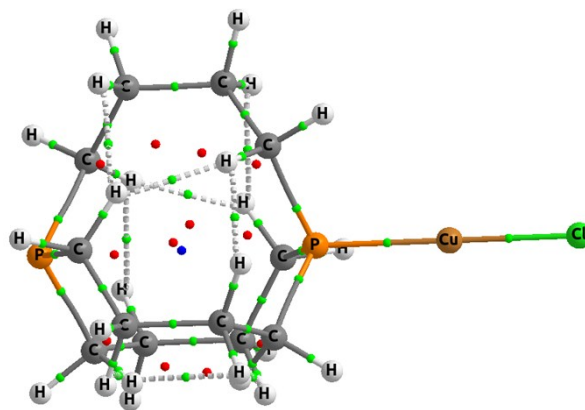
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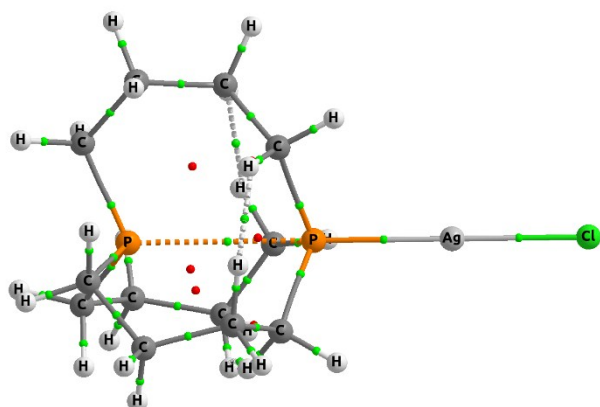
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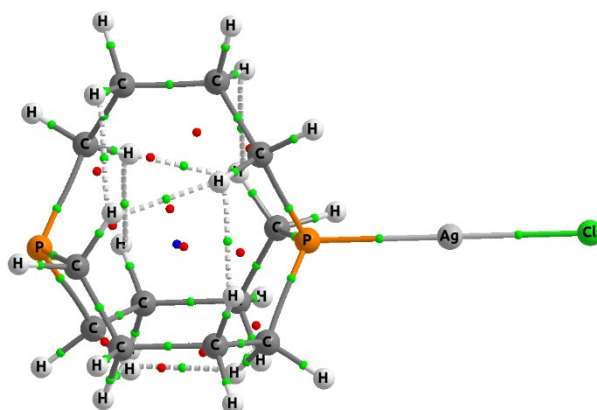
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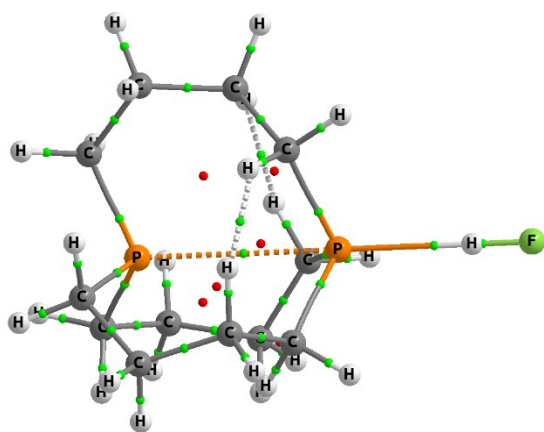
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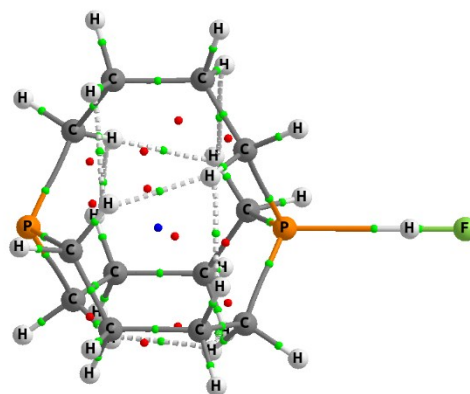
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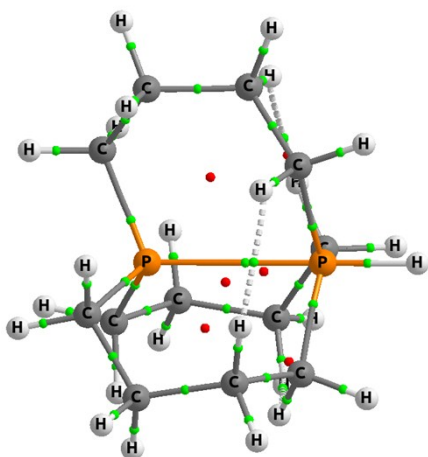
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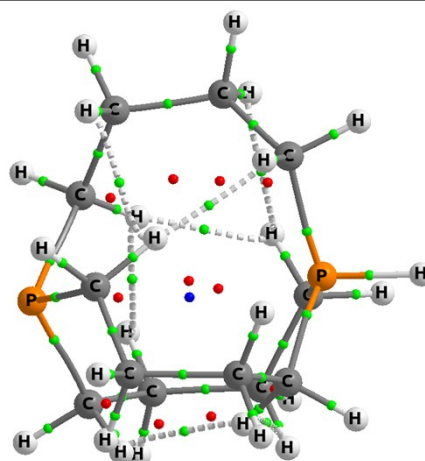
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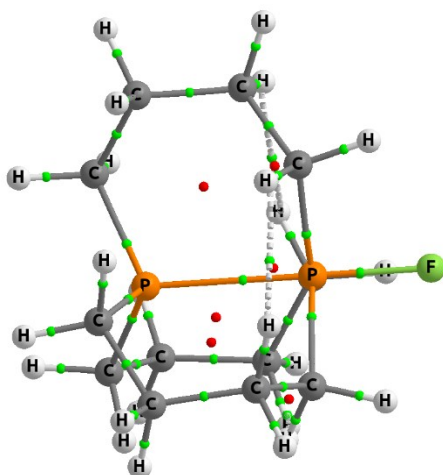
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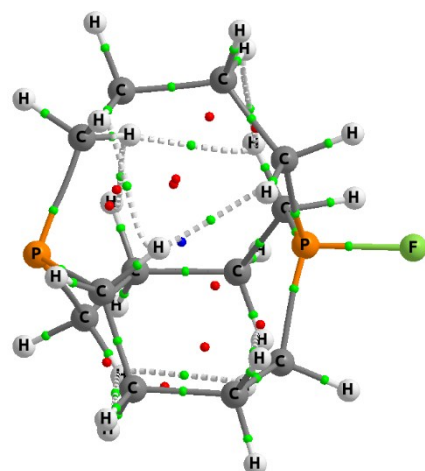
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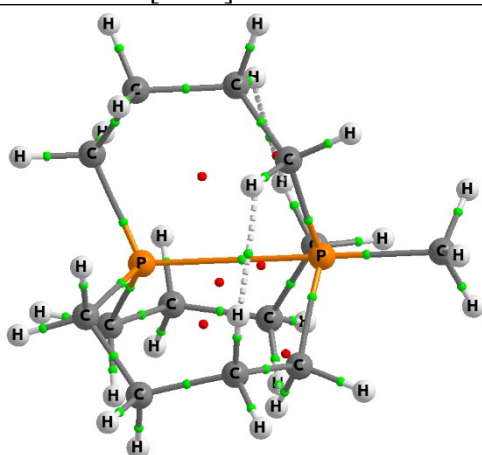
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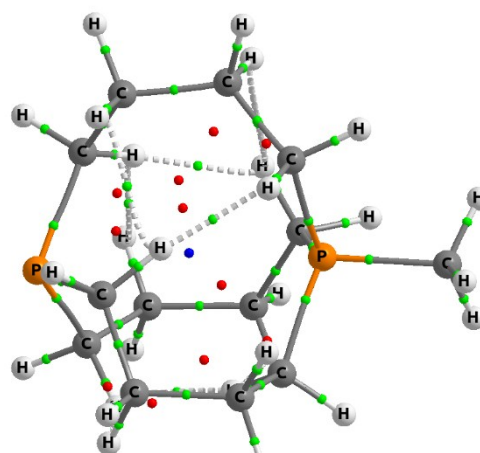
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[4.4.4]:  $\text{F}^+$  out:out

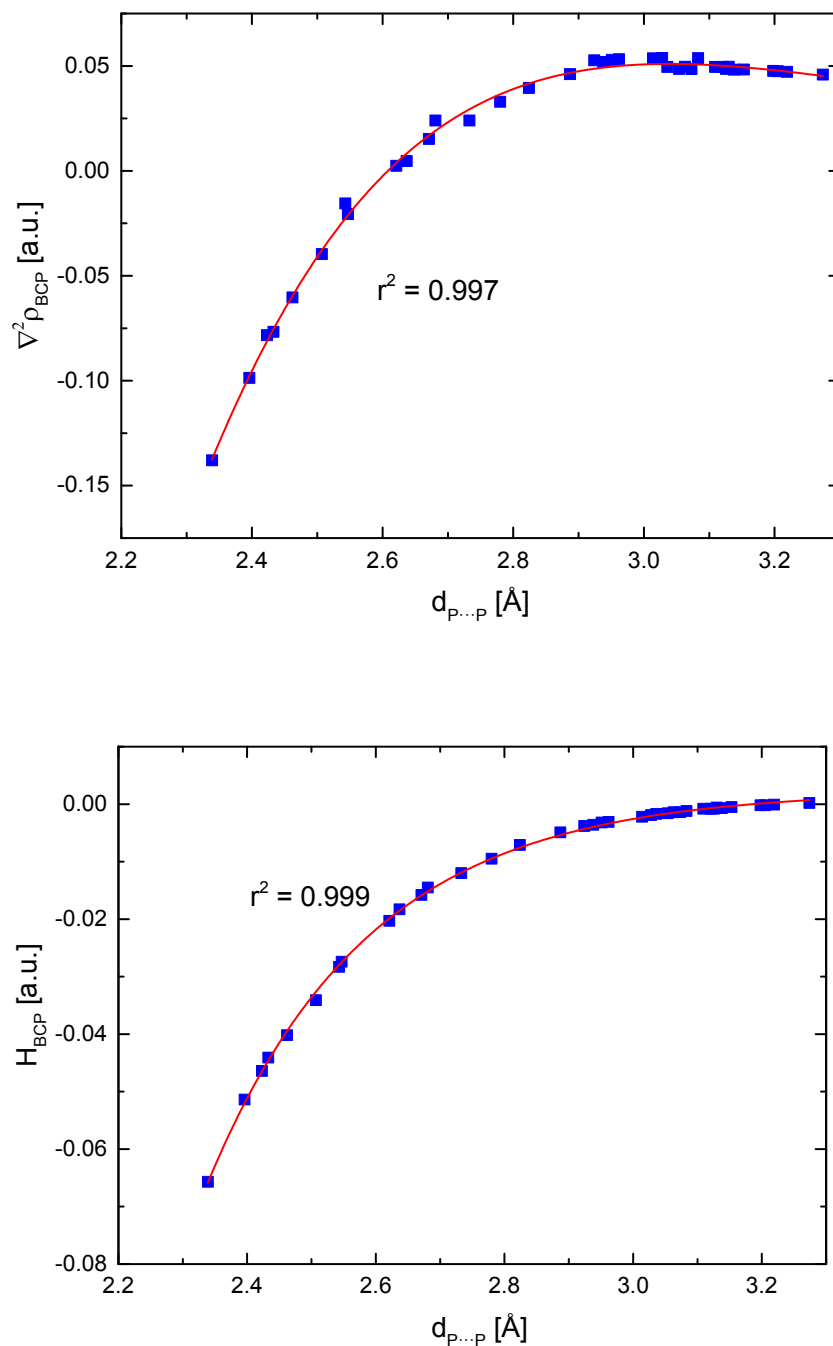


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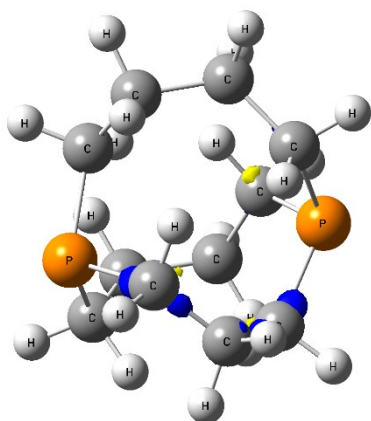


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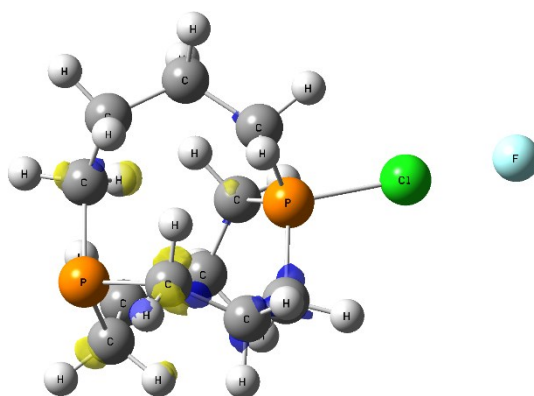
**Figure S3.** Exponential relationships between the P-P distance and the Laplacian and H at the BCP in the IO structures.



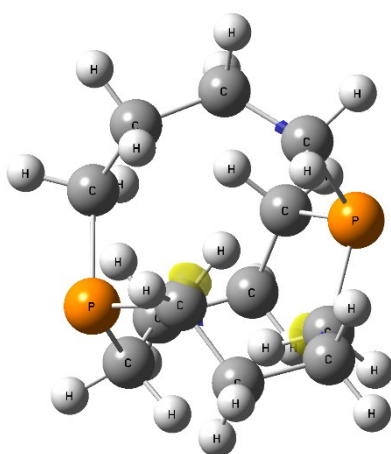
**Figure S4 .** Electron density shift maps at 0.001a.u. for the  $[4.4.3]^{OO}$ ,  $[4.4.3]^{OO}:ClF$ ,  $[4.4.4]^{OO}$  and  $[4.4.3]^{OO}:ClF$  complexes. Blue (negative) and yellow (positive) areas correspond to decrease and increase on the electron density upon interaction.



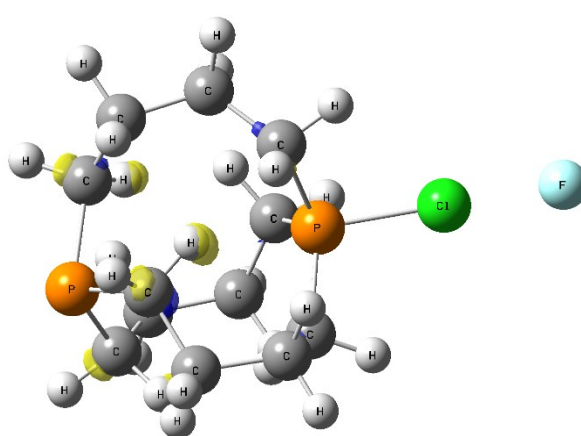
[4.4.3]<sup>00</sup>



[4.4.3]<sup>00</sup>:C1F

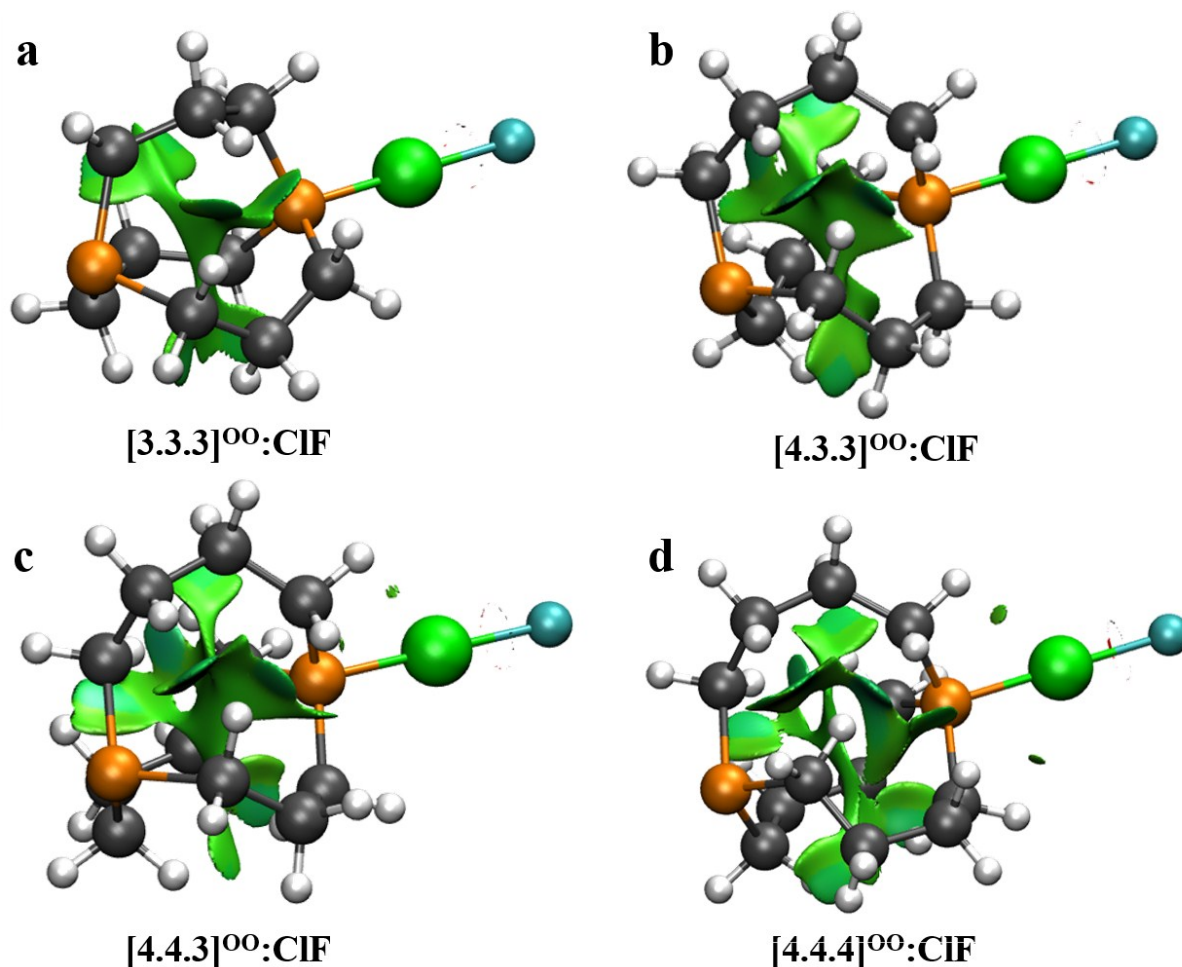


[4.4.4]<sup>00</sup>

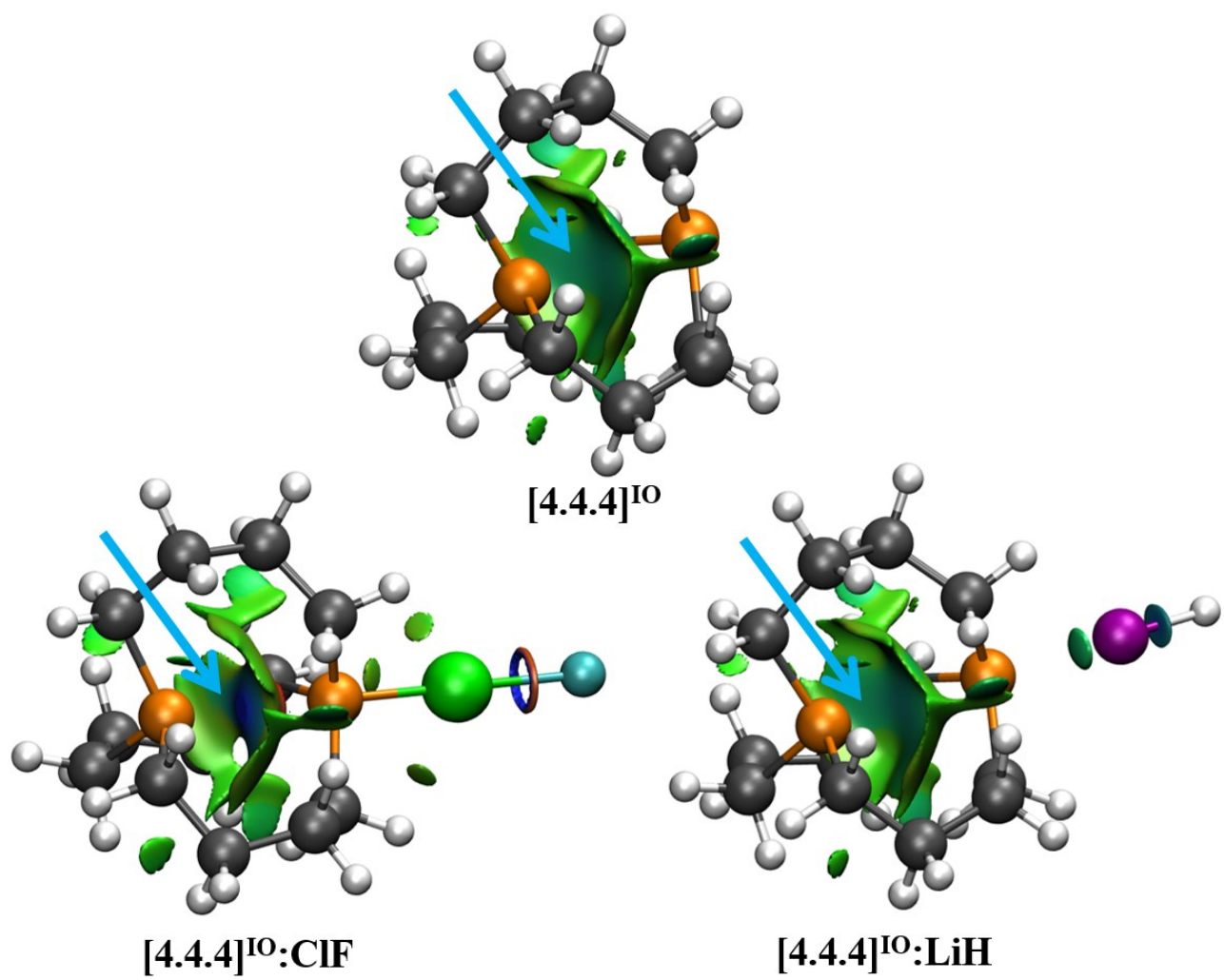


[4.4.4]<sup>00</sup>:C1F

**Figure S5.** NCI plots of non-covalent interaction for complexes a) [3.3.3]<sup>00</sup>:ClF, b) [4.3.3]<sup>00</sup>:ClF, c) [4.4.3]<sup>00</sup>:ClF and d) [4.4.4]<sup>00</sup>:ClF. Blue and green areas correspond to  $\lambda_2 > 0$  (strongly attractive) and  $\lambda_2 \approx 0$  (weak) respectively, while red areas correspond to  $\lambda_2 < 0$  (repulsive).  $\lambda_2$  is one of the three eigenvalues of the electron density Hessian with  $\lambda_1 \leq \lambda_2 \leq \lambda_3$ .



**Figure S6.** NCI plots of non-covalent interaction for complexes [4.4.4]<sup>10</sup>, [4.4.4]<sup>10</sup>:ClF and [4.4.4]<sup>10</sup>:LiH. Blue and green areas correspond to  $\lambda_2 > 0$  (strongly attractive) and  $\lambda_2 \approx 0$  (weak) respectively, while red areas correspond to  $\lambda_2 < 0$  (repulsive).  $\lambda_2$  is one of the three eigenvalues of the electron density Hessian with  $\lambda_1 \leq \lambda_2 \leq \lambda_3$ .



**Table S1.** Cartesian coordinates of all complexes studied at MP2/jul-cc-pVDZ computational level.

|                | oo       | io       | ts       |
|----------------|----------|----------|----------|
| [3.3.3]        |          |          |          |
| [3.3.3]agcl_oo |          |          |          |
| P              | -0.00007 | -0.00002 | 0.99917  |
| P              | 0.00010  | 0.00002  | -3.04780 |
| C              | 0.17935  | 1.73149  | 0.33547  |
| C              | 0.19690  | 1.71479  | -2.29547 |
| H              | -0.23997 | 2.36017  | 1.13908  |
| H              | 1.26241  | 1.95597  | 0.31622  |
| H              | -0.18691 | 2.37740  | -3.09164 |
| H              | 1.28216  | 1.92633  | -2.24545 |
| C              | -1.58925 | -0.71042 | 0.33535  |
| H              | -1.92407 | -1.38792 | 1.13894  |
| H              | -2.32520 | 0.11528  | 0.31607  |
| C              | -1.58340 | -0.68689 | -2.29559 |
| H              | -1.96532 | -1.35058 | -3.09178 |
| H              | -2.30921 | 0.14722  | -2.24560 |
| C              | 1.38666  | -1.02789 | -2.29544 |
| H              | 1.02715  | -2.07349 | -2.24541 |
| H              | 2.15243  | -1.02687 | -3.09158 |
| C              | 1.40982  | -1.02109 | 0.33549  |
| H              | 1.06276  | -2.07130 | 0.31624  |
| H              | 2.16391  | -0.97223 | 1.13913  |
| C              | -0.49297 | 2.13031  | -0.98707 |
| H              | -1.54571 | 1.79770  | -0.98859 |
| H              | -0.53907 | 3.23514  | -0.98357 |
| C              | 2.09141  | -0.63821 | -0.98702 |
| H              | 3.07128  | -1.15070 | -0.98349 |
| H              | 2.32972  | 0.43979  | -0.98851 |
| C              | -1.59839 | -1.49209 | -0.98718 |
| H              | -2.53216 | -2.08443 | -0.98373 |
| H              | -0.78398 | -2.23748 | -0.98864 |
| Ag             | -0.00014 | -0.00001 | 3.31837  |
| Cl             | -0.00022 | 0.00000  | 5.60566  |
| [3.3.3]beh2_oo |          |          |          |
| P              | 1.73534  | 0.02577  | -0.09335 |
| P              | -2.28451 | -0.02123 | 0.08005  |
| C              | 1.03382  | 1.57841  | -0.83330 |
| C              | -1.58960 | 1.52664  | -0.73774 |
| H              | 1.84832  | 2.30919  | -0.68205 |
| H              | 0.97141  | 1.42015  | -1.92647 |
| H              | -2.39343 | 2.26807  | -0.58109 |
| H              | -1.58038 | 1.33916  | -1.82868 |
| C              | 1.15948  | -0.08436 | 1.67390  |
| H              | 1.99754  | -0.59026 | 2.18753  |
| H              | 1.14002  | 0.94641  | 2.07352  |

|    |          |          |          |
|----|----------|----------|----------|
| C  | -1.46372 | -0.10301 | 1.77316  |
| H  | -2.23154 | -0.60001 | 2.39281  |
| H  | -1.41190 | 0.93381  | 2.15742  |
| C  | -1.56361 | -1.46422 | -0.89183 |
| H  | -1.47699 | -2.31511 | -0.18911 |
| H  | -2.38936 | -1.73780 | -1.57284 |
| C  | 1.05804  | -1.43709 | -1.01691 |
| H  | 1.07711  | -2.29346 | -0.31785 |
| H  | 1.84500  | -1.65472 | -1.76109 |
| C  | -0.27149 | 2.18079  | -0.29486 |
| H  | -0.22955 | 2.24421  | 0.80662  |
| H  | -0.29791 | 3.22956  | -0.64507 |
| C  | -0.29038 | -1.34139 | -1.74362 |
| H  | -0.31086 | -2.17133 | -2.47439 |
| H  | -0.32722 | -0.41956 | -2.35058 |
| C  | -0.13497 | -0.83389 | 2.02141  |
| H  | -0.08539 | -1.05403 | 3.10414  |
| H  | -0.14351 | -1.82004 | 1.52519  |
| Be | 3.94773  | -0.02932 | 0.06542  |
| H  | 4.33319  | -1.34732 | 0.16273  |
| H  | 4.48670  | 1.23101  | 0.15574  |

[3.3.3]bh3\_oo

|   |          |          |          |
|---|----------|----------|----------|
| P | 0.00000  | 0.00000  | 1.66247  |
| P | 0.00000  | 0.00000  | -2.32924 |
| C | 1.72900  | -0.18641 | 1.03527  |
| C | 1.71952  | -0.20397 | -1.58671 |
| H | 2.32789  | 0.23595  | 1.86219  |
| H | 1.95625  | -1.26841 | 1.02287  |
| H | 2.37874  | 0.17242  | -2.38936 |
| H | 1.92051  | -1.29135 | -1.53567 |
| C | -0.70306 | 1.59057  | 1.03527  |
| H | -1.36828 | 1.89803  | 1.86219  |
| H | 0.12035  | 2.32837  | 1.02287  |
| C | -0.68312 | 1.59114  | -1.58671 |
| H | -1.33869 | 1.97384  | -2.38936 |
| H | 0.15809  | 2.30889  | -1.53567 |
| C | -1.03641 | -1.38716 | -1.58671 |
| H | -2.07860 | -1.01754 | -1.53567 |
| H | -1.04005 | -2.14626 | -2.38936 |
| C | -1.02594 | -1.40415 | 1.03527  |
| H | -2.07661 | -1.05996 | 1.02287  |
| H | -0.95960 | -2.13398 | 1.86219  |
| C | 2.15017  | 0.48154  | -0.28013 |
| H | 1.83335  | 1.53936  | -0.28360 |
| H | 3.25569  | 0.50912  | -0.27908 |
| C | -0.65806 | -2.10287 | -0.28013 |
| H | -1.18694 | -3.07407 | -0.27908 |

|                    |          |          |          |                    |          |          |          |                     |          |          |          |
|--------------------|----------|----------|----------|--------------------|----------|----------|----------|---------------------|----------|----------|----------|
| H                  | 0.41645  | -2.35740 | -0.28360 |                    |          |          |          |                     |          |          |          |
| C                  | -1.49211 | 1.62134  | -0.28013 |                    |          |          |          |                     |          |          |          |
| H                  | -2.06875 | 2.56495  | -0.27908 |                    |          |          |          |                     |          |          |          |
| H                  | -2.24980 | 0.81805  | -0.28360 |                    |          |          |          |                     |          |          |          |
| B                  | 0.00000  | 0.00000  | 3.59914  |                    |          |          |          |                     |          |          |          |
| H                  | -1.18765 | 0.00090  | 3.90956  |                    |          |          |          |                     |          |          |          |
| H                  | 0.59304  | -1.02898 | 3.90956  |                    |          |          |          |                     |          |          |          |
| H                  | 0.59461  | 1.02808  | 3.90956  |                    |          |          |          |                     |          |          |          |
| [3.3.3]ch3_plus_oo |          |          |          | [3.3.3]ch3_plus_io |          |          |          | [3.3.3]ch3_plus_ts_ |          |          |          |
| P                  | 0.00000  | 0.00000  | -1.57043 | P                  | 0.00000  | 0.00000  | 1.41394  | P                   | 0.00000  | 0.00000  | 1.52840  |
| P                  | 0.00000  | 0.00000  | 2.28380  | P                  | 0.00000  | 0.00000  | -1.09301 | P                   | 0.00000  | 0.00000  | -1.47130 |
| C                  | 0.54643  | -1.67365 | -1.06694 | C                  | 1.62498  | 0.90463  | 1.16964  | C                   | 0.16309  | 1.81673  | 1.20674  |
| C                  | 0.57669  | -1.64022 | 1.54873  | C                  | 1.54572  | 0.93679  | -1.40121 | C                   | -0.03914 | 1.84000  | -1.33588 |
| H                  | 0.22021  | -2.32135 | -1.90128 | H                  | 1.78525  | 1.52119  | 2.07026  | H                   | -0.18968 | 2.30444  | 2.13196  |
| H                  | 1.65173  | -1.67562 | -1.07885 | H                  | 2.40090  | 0.11320  | 1.18227  | H                   | 1.24837  | 2.01964  | 1.12987  |
| H                  | 0.35321  | -2.35802 | 2.35710  | H                  | 1.51709  | 1.56772  | -2.30370 | H                   | -0.60400 | 2.25408  | -2.18689 |
| H                  | 1.68160  | -1.60504 | 1.49880  | H                  | 2.35854  | 0.19812  | -1.52223 | H                   | 1.01445  | 2.14858  | -1.47572 |
| C                  | -1.72263 | 0.36360  | -1.06694 | C                  | -1.59592 | 0.95496  | 1.16964  | C                   | -1.65488 | -0.76713 | 1.20674  |
| H                  | -2.12045 | 0.96997  | -1.90128 | H                  | -2.21001 | 0.78548  | 2.07026  | H                   | -1.90087 | -1.31649 | 2.13196  |
| H                  | -2.27699 | -0.59263 | -1.07885 | H                  | -1.29849 | 2.02264  | 1.18227  | H                   | -2.37325 | 0.07130  | 1.12987  |
| C                  | -1.70882 | 0.32068  | 1.54873  | C                  | -1.58414 | 0.87024  | -1.40121 | C                   | -1.57392 | -0.95390 | -1.33588 |
| H                  | -2.21871 | 0.87312  | 2.35710  | H                  | -2.11623 | 0.52998  | -2.30370 | H                   | -1.65009 | -1.65012 | -2.18689 |
| H                  | -2.23081 | -0.65379 | 1.49880  | H                  | -1.35084 | 1.94349  | -1.52223 | H                   | -2.36795 | -0.19575 | -1.47572 |
| C                  | 1.13213  | 1.31954  | 1.54873  | C                  | 0.03842  | -1.80702 | -1.40121 | C                   | 1.61306  | -0.88611 | -1.33588 |
| H                  | 0.54921  | 2.25883  | 1.49880  | H                  | -1.00769 | -2.14161 | -1.52223 | H                   | 1.35350  | -1.95283 | -1.47572 |
| H                  | 1.86550  | 1.48490  | 2.35710  | H                  | 0.59914  | -2.09770 | -2.30370 | H                   | 2.25409  | -0.60396 | -2.18689 |
| C                  | 1.17621  | 1.31004  | -1.06694 | C                  | -0.02906 | -1.85959 | 1.16964  | C                   | 1.49179  | -1.04960 | 1.20674  |
| H                  | 0.62526  | 2.26825  | -1.07885 | H                  | -1.10241 | -2.13584 | 1.18227  | H                   | 1.12488  | -2.09095 | 1.12987  |
| H                  | 1.90025  | 1.35138  | -1.90128 | H                  | 0.42476  | -2.30667 | 2.07026  | H                   | 2.09055  | -0.98795 | 2.13196  |
| C                  | -0.00291 | -2.23170 | 0.25598  | C                  | 1.74244  | 1.76194  | -0.10484 | C                   | -0.58607 | 2.37021  | -0.00606 |
| H                  | -1.10504 | -2.16945 | 0.26007  | H                  | 0.99779  | 2.57861  | -0.06942 | H                   | -1.66404 | 2.14433  | 0.07963  |
| H                  | 0.22967  | -3.31110 | 0.24444  | H                  | 2.73354  | 2.24594  | -0.11900 | H                   | -0.50035 | 3.47138  | 0.00932  |
| C                  | 1.93417  | 1.11333  | 0.25598  | C                  | 0.65466  | -2.38996 | -0.10484 | C                   | 2.34570  | -0.67755 | -0.00606 |
| H                  | 2.75267  | 1.85445  | 0.24444  | H                  | 0.57827  | -3.49028 | -0.11900 | H                   | 3.25648  | -1.30237 | 0.00932  |
| H                  | 2.43132  | 0.12773  | 0.26007  | H                  | 1.73425  | -2.15342 | -0.06942 | H                   | 2.68906  | 0.36894  | 0.07963  |
| C                  | -1.93126 | 1.11837  | 0.25598  | C                  | -2.39710 | 0.62803  | -0.10484 | C                   | -1.75963 | -1.69266 | -0.00606 |
| H                  | -2.98233 | 1.45665  | 0.24444  | H                  | -3.31181 | 1.24435  | -0.11900 | H                   | -2.75613 | -2.16901 | 0.00932  |
| H                  | -1.32628 | 2.04172  | 0.26007  | H                  | -2.73204 | -0.42520 | -0.06942 | H                   | -1.02502 | -2.51327 | 0.07963  |
| C                  | 0.00000  | 0.00000  | -3.39368 | C                  | 0.00000  | 0.00000  | 3.29034  | C                   | 0.00000  | 0.00000  | 3.37899  |
| H                  | -0.78905 | -0.67493 | -3.76189 | H                  | -0.13851 | 1.02532  | 3.67400  | H                   | -0.91876 | 0.48066  | 3.75381  |
| H                  | -0.18998 | 1.02080  | -3.76189 | H                  | -0.81869 | -0.63262 | 3.67400  | H                   | 0.04312  | -1.03600 | 3.75381  |
| H                  | 0.97903  | -0.34587 | -3.76189 | H                  | 0.95721  | -0.39270 | 3.67400  | H                   | 0.87565  | 0.55534  | 3.75381  |
| [3.3.3]clf_oo      |          |          |          | [3.3.3]clf_io      |          |          |          | [3.3.3]clf_ts_      |          |          |          |
| P                  | 0.00000  | 0.00000  | -1.57812 | P                  | 0.00000  | 0.00000  | 1.34640  | P                   | 0.00000  | 0.00000  | 1.54708  |
| P                  | 0.00000  | 0.00000  | 2.33482  | P                  | 0.00000  | 0.00000  | -1.19685 | P                   | 0.00000  | 0.00000  | -1.38160 |
| C                  | 0.01086  | 1.75124  | -1.01955 | C                  | 1.84639  | -0.16394 | 1.05736  | C                   | 0.15745  | 1.81548  | 1.18740  |

|                |          |          |          |    |          |          |          |    |          |          |          |
|----------------|----------|----------|----------|----|----------|----------|----------|----|----------|----------|----------|
| C              | -0.02467 | 1.73561  | 1.59811  | C  | 1.80464  | -0.08811 | -1.51369 | C  | -0.03733 | 1.83886  | -1.36021 |
| H              | 0.51424  | 2.26985  | -1.85565 | H  | 2.31238  | 0.24923  | 1.96709  | H  | -0.19244 | 2.29524  | 2.11733  |
| H              | -1.03753 | 2.10162  | -1.02831 | H  | 2.03772  | -1.25540 | 1.07227  | H  | 1.24423  | 2.01493  | 1.11817  |
| H              | 0.41075  | 2.34949  | 2.40641  | H  | 2.13759  | 0.44828  | -2.41704 | H  | -0.60064 | 2.23520  | -2.22119 |
| H              | -1.08538 | 2.04665  | 1.54152  | H  | 2.06188  | -1.15664 | -1.63031 | H  | 1.01818  | 2.14264  | -1.49588 |
| C              | 1.51118  | -0.88503 | -1.01955 | C  | -0.78122 | 1.68099  | 1.05736  | C  | -1.65098 | -0.77138 | 1.18740  |
| H              | 1.70863  | -1.58027 | -1.85565 | H  | -1.37202 | 1.87796  | 1.96709  | H  | -1.89152 | -1.31427 | 2.11733  |
| H              | 2.33882  | -0.15228 | -1.02831 | H  | 0.06835  | 2.39242  | 1.07227  | H  | -2.36709 | 0.07007  | 1.11817  |
| C              | 1.51542  | -0.84644 | 1.59811  | C  | -0.82601 | 1.60692  | -1.51369 | C  | -1.57384 | -0.95176 | -1.36021 |
| H              | 1.82934  | -1.53046 | 2.40641  | H  | -1.45701 | 1.62707  | -2.41704 | H  | -1.63542 | -1.63777 | -2.22119 |
| H              | 2.31514  | -0.08336 | 1.54152  | H  | -0.02927 | 2.36396  | -1.63031 | H  | -2.36467 | -0.18955 | -1.49588 |
| C              | -1.49075 | -0.88917 | 1.59811  | C  | -0.97863 | -1.51881 | -1.51369 | C  | 1.61117  | -0.88710 | -1.36021 |
| H              | -1.22976 | -1.96329 | 1.54152  | H  | -2.03262 | -1.20733 | -1.63031 | H  | 1.34649  | -1.95309 | -1.49588 |
| H              | -2.24009 | -0.81902 | 2.40641  | H  | -0.68058 | -2.07535 | -2.41704 | H  | 2.23606  | -0.59743 | -2.22119 |
| C              | -1.52205 | -0.86621 | -1.01955 | C  | -1.06517 | -1.51705 | 1.05736  | C  | 1.49353  | -1.04410 | 1.18740  |
| H              | -1.30129 | -1.94934 | -1.02831 | H  | -2.10607 | -1.13702 | 1.07227  | H  | 1.12286  | -2.08500 | 1.11817  |
| H              | -2.22286 | -0.68958 | -1.85565 | H  | -0.94035 | -2.12719 | 1.96709  | H  | 2.08395  | -0.98096 | 2.11733  |
| C              | 0.71124  | 2.10225  | 0.30036  | C  | 2.42620  | 0.48219  | -0.21395 | C  | -0.58420 | 2.37509  | -0.02883 |
| H              | 1.73251  | 1.68269  | 0.30640  | H  | 2.26199  | 1.57542  | -0.17767 | H  | -1.66280 | 2.14791  | 0.05198  |
| H              | 0.84660  | 3.19931  | 0.29565  | H  | 3.51996  | 0.33300  | -0.22510 | H  | -0.49963 | 3.47721  | -0.01490 |
| C              | -2.17622 | -0.43517 | 0.30036  | C  | -0.79551 | -2.34224 | -0.21395 | C  | 2.34899  | -0.68161 | -0.02883 |
| H              | -3.19399 | -0.86648 | 0.29565  | H  | -1.47159 | -3.21487 | -0.22510 | H  | 3.26117  | -1.30591 | -0.01490 |
| H              | -2.32351 | 0.65905  | 0.30640  | H  | 0.23336  | -2.74665 | -0.17767 | H  | 2.69154  | 0.36607  | 0.05198  |
| C              | 1.46498  | -1.66708 | 0.30036  | C  | -1.63068 | 1.86005  | -0.21395 | C  | -1.76479 | -1.69348 | -0.02883 |
| H              | 2.34739  | -2.33283 | 0.29565  | H  | -2.04836 | 2.88187  | -0.22510 | H  | -2.76154 | -2.17130 | -0.01490 |
| H              | 0.59100  | -2.34174 | 0.30640  | H  | -2.49535 | 1.17123  | -0.17767 | H  | -1.02874 | -2.51398 | 0.05198  |
| Cl             | 0.00000  | 0.00000  | -3.69699 | Cl | 0.00000  | 0.00000  | 3.44899  | Cl | 0.00000  | 0.00000  | 3.65710  |
| F              | 0.00000  | 0.00000  | -5.71508 | F  | 0.00000  | 0.00000  | 5.70777  | F  | 0.00000  | 0.00000  | 5.79555  |
| [3.3.3]cucl_oo |          |          |          |    |          |          |          |    |          |          |          |
| P              | 0.00014  | -0.00084 | 1.02292  |    |          |          |          |    |          |          |          |
| P              | -0.00024 | 0.00122  | -3.02847 |    |          |          |          |    |          |          |          |
| C              | 0.20129  | 1.72663  | 0.35551  |    |          |          |          |    |          |          |          |
| C              | 0.21363  | 1.71354  | -2.27538 |    |          |          |          |    |          |          |          |
| H              | -0.20816 | 2.36012  | 1.16044  |    |          |          |          |    |          |          |          |
| H              | 1.28652  | 1.93912  | 0.33316  |    |          |          |          |    |          |          |          |
| H              | -0.16550 | 2.38029  | -3.07039 |    |          |          |          |    |          |          |          |
| H              | 1.30102  | 1.91432  | -2.22733 |    |          |          |          |    |          |          |          |
| C              | -1.59628 | -0.68973 | 0.35442  |    |          |          |          |    |          |          |          |
| H              | -1.94050 | -1.36169 | 1.15870  |    |          |          |          |    |          |          |          |
| H              | -2.32285 | 0.14393  | 0.33249  |    |          |          |          |    |          |          |          |
| C              | -1.59030 | -0.67042 | -2.27646 |    |          |          |          |    |          |          |          |
| H              | -1.97783 | -1.33154 | -3.07212 |    |          |          |          |    |          |          |          |
| H              | -2.30795 | 0.17081  | -2.22801 |    |          |          |          |    |          |          |          |
| C              | 1.37619  | -1.04069 | -2.27696 |    |          |          |          |    |          |          |          |
| H              | 1.00639  | -2.08282 | -2.22940 |    |          |          |          |    |          |          |          |
| H              | 2.14271  | -1.04519 | -3.07243 |    |          |          |          |    |          |          |          |
| C              | 1.39519  | -1.03831 | 0.35392  |    |          |          |          |    |          |          |          |

|                  |          |          |          |                  |          |          |          |                   |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|----------|-------------------|----------|----------|----------|
| H                | 1.03659  | -2.08438 | 0.33109  |                  |          |          |          |                   |          |          |          |
| H                | 2.14901  | -1.00101 | 1.15843  |                  |          |          |          |                   |          |          |          |
| C                | -0.46945 | 2.13426  | -0.96491 |                  |          |          |          |                   |          |          |          |
| H                | -1.52543 | 1.81218  | -0.96566 |                  |          |          |          |                   |          |          |          |
| H                | -0.50450 | 3.23950  | -0.96073 |                  |          |          |          |                   |          |          |          |
| C                | 2.08283  | -0.66038 | -0.96664 |                  |          |          |          |                   |          |          |          |
| H                | 3.05751  | -1.18265 | -0.96335 |                  |          |          |          |                   |          |          |          |
| H                | 2.33191  | 0.41517  | -0.96680 |                  |          |          |          |                   |          |          |          |
| C                | -1.61354 | -1.47337 | -0.96662 |                  |          |          |          |                   |          |          |          |
| H                | -2.55318 | -2.05633 | -0.96320 |                  |          |          |          |                   |          |          |          |
| H                | -0.80662 | -2.22685 | -0.96771 |                  |          |          |          |                   |          |          |          |
| Cl               | 0.00080  | -0.00284 | 5.20795  |                  |          |          |          |                   |          |          |          |
| Cu               | 0.00061  | -0.00204 | 3.14519  |                  |          |          |          |                   |          |          |          |
| [3.3.3]f_plus_oo |          |          |          | [3.3.3]f_plus_io |          |          |          | [3.3.3]f_plus_ts_ |          |          |          |
| P                | 0.00000  | 0.00000  | -1.43553 | P                | 0.00000  | 0.00000  | 1.27739  | P                 | 0.00000  | 0.00000  | 1.46471  |
| P                | 0.00000  | 0.00000  | 2.29240  | P                | 0.00000  | 0.00000  | -1.06127 | P                 | 0.00000  | 0.00000  | -1.66747 |
| C                | 0.02065  | 1.76247  | -1.02837 | C                | 1.60176  | 0.94124  | 1.18142  | C                 | 0.10105  | 1.80600  | 1.22727  |
| C                | -0.02525 | 1.74881  | 1.57721  | C                | 1.56340  | 0.90486  | -1.37820 | C                 | 0.05218  | 1.82951  | -1.31266 |
| H                | 0.55817  | 2.21013  | -1.88527 | H                | 1.65894  | 1.56550  | 2.08666  | H                 | -0.35481 | 2.21040  | 2.14847  |
| H                | -1.01959 | 2.13099  | -1.06718 | H                | 2.40070  | 0.17946  | 1.26400  | H                 | 1.17356  | 2.07302  | 1.24659  |
| H                | 0.40822  | 2.34968  | 2.39529  | H                | 1.53649  | 1.50100  | -2.30368 | H                 | -0.41025 | 2.32127  | -2.18399 |
| H                | -1.08547 | 2.06143  | 1.52585  | H                | 2.36675  | 0.15237  | -1.47182 | H                 | 1.12735  | 2.08971  | -1.34688 |
| C                | 1.51602  | -0.89912 | -1.02837 | C                | -1.61602 | 0.91655  | 1.18142  | C                 | -1.61457 | -0.81549 | 1.22727  |
| H                | 1.63494  | -1.58846 | -1.88527 | H                | -2.18523 | 0.65393  | 2.08666  | H                 | -1.73686 | -1.41247 | 2.14847  |
| H                | 2.35528  | -0.18250 | -1.06718 | H                | -1.35576 | 1.98934  | 1.26400  | H                 | -2.38206 | -0.02018 | 1.24659  |
| C                | 1.52714  | -0.85254 | 1.57721  | C                | -1.56533 | 0.90151  | -1.37820 | C                 | -1.61049 | -0.86957 | -1.31266 |
| H                | 1.83077  | -1.52837 | 2.39529  | H                | -2.06815 | 0.58014  | -2.30368 | H                 | -1.80515 | -1.51592 | -2.18399 |
| H                | 2.32799  | -0.09067 | 1.52585  | H                | -1.31534 | 1.97348  | -1.47182 | H                 | -2.37342 | -0.06855 | -1.34688 |
| C                | -1.50189 | -0.89628 | 1.57721  | C                | 0.00193  | -1.80637 | -1.37820 | C                 | 1.55831  | -0.95995 | -1.31266 |
| H                | -1.24251 | -1.97076 | 1.52585  | H                | -1.05142 | -2.12585 | -1.47182 | H                 | 1.24607  | -2.02117 | -1.34688 |
| H                | -2.23899 | -0.82131 | 2.39529  | H                | 0.53166  | -2.08114 | -2.30368 | H                 | 2.21540  | -0.80534 | -2.18399 |
| C                | -1.53667 | -0.86335 | -1.02837 | C                | 0.01426  | -1.85778 | 1.18142  | C                 | 1.51352  | -0.99051 | 1.22727  |
| H                | -1.33569 | -1.94848 | -1.06718 | H                | -1.04494 | -2.16880 | 1.26400  | H                 | 1.20851  | -2.05284 | 1.24659  |
| H                | -2.19312 | -0.62167 | -1.88527 | H                | 0.52630  | -2.21943 | 2.08666  | H                 | 2.09167  | -0.79793 | 2.14847  |
| C                | 0.71612  | 2.14018  | 0.29167  | C                | 1.75753  | 1.77036  | -0.10661 | C                 | -0.59144 | 2.34241  | -0.02294 |
| H                | 1.74683  | 1.74538  | 0.29907  | H                | 1.02587  | 2.59886  | -0.10724 | H                 | -1.66638 | 2.09057  | -0.00140 |
| H                | 0.82029  | 3.23873  | 0.27200  | H                | 2.75614  | 2.23679  | -0.12761 | H                 | -0.53405 | 3.44484  | -0.00211 |
| C                | -2.21151 | -0.44991 | 0.29167  | C                | 0.65441  | -2.40724 | -0.10661 | C                 | 2.32431  | -0.65900 | -0.02294 |
| H                | -3.21497 | -0.90897 | 0.27200  | H                | 0.55905  | -3.50528 | -0.12761 | H                 | 3.25035  | -1.25992 | -0.00211 |
| H                | -2.38496 | 0.64011  | 0.29907  | H                | 1.73774  | -2.18786 | -0.10724 | H                 | 2.64367  | 0.39784  | -0.00140 |
| C                | 1.49539  | -1.69027 | 0.29167  | C                | -2.41194 | 0.63688  | -0.10661 | C                 | -1.73287 | -1.68341 | -0.02294 |
| H                | 2.39468  | -2.32976 | 0.27200  | H                | -3.31519 | 1.26849  | -0.12761 | H                 | -2.71630 | -2.18492 | -0.00211 |
| H                | 0.63813  | -2.38549 | 0.29907  | H                | -2.76361 | -0.41100 | -0.10724 | H                 | -0.97730 | -2.48841 | -0.00140 |
| F                | 0.00000  | 0.00000  | -3.05528 | F                | 0.00000  | 0.00000  | 2.98884  | F                 | 0.00000  | 0.00000  | 3.11705  |
| [3.3.3]hf_oo     |          |          |          |                  |          |          |          |                   |          |          |          |
| P                | 0.00000  | 0.00000  | 1.02711  |                  |          |          |          |                   |          |          |          |

|                  |          |          |          |                  |          |          |                   |   |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|-------------------|---|----------|----------|----------|
| P                | 0.00000  | 0.00000  | -3.06361 |                  |          |          |                   |   |          |          |          |
| C                | -1.73120 | 0.00842  | 0.31869  |                  |          |          |                   |   |          |          |          |
| C                | -1.72504 | 0.01759  | -2.31151 |                  |          |          |                   |   |          |          |          |
| H                | -2.33282 | -0.45975 | 1.11829  |                  |          |          |                   |   |          |          |          |
| H                | -2.06177 | 1.06392  | 0.28551  |                  |          |          |                   |   |          |          |          |
| H                | -2.34450 | -0.43479 | -3.10675 |                  |          |          |                   |   |          |          |          |
| H                | -2.04688 | 1.07573  | -2.26410 |                  |          |          |                   |   |          |          |          |
| C                | 0.85830  | -1.50347 | 0.31869  |                  |          |          |                   |   |          |          |          |
| H                | 1.56456  | -1.79041 | 1.11829  |                  |          |          |                   |   |          |          |          |
| H                | 0.10950  | -2.31751 | 0.28551  |                  |          |          |                   |   |          |          |          |
| C                | 0.84728  | -1.50272 | -2.31151 |                  |          |          |                   |   |          |          |          |
| H                | 1.54878  | -1.81300 | -3.10675 |                  |          |          |                   |   |          |          |          |
| H                | 0.09184  | -2.31051 | -2.26410 |                  |          |          |                   |   |          |          |          |
| C                | 0.87775  | 1.48513  | -2.31151 |                  |          |          |                   |   |          |          |          |
| H                | 1.95505  | 1.23479  | -2.26410 |                  |          |          |                   |   |          |          |          |
| H                | 0.79571  | 2.24778  | -3.10675 |                  |          |          |                   |   |          |          |          |
| C                | 0.87289  | 1.49505  | 0.31869  |                  |          |          |                   |   |          |          |          |
| H                | 1.95227  | 1.25359  | 0.28551  |                  |          |          |                   |   |          |          |          |
| H                | 0.76826  | 2.25015  | 1.11829  |                  |          |          |                   |   |          |          |          |
| C                | -2.06514 | -0.70663 | -0.99941 |                  |          |          |                   |   |          |          |          |
| H                | -1.62399 | -1.71885 | -1.00041 |                  |          |          |                   |   |          |          |          |
| H                | -3.15973 | -0.86809 | -0.99897 |                  |          |          |                   |   |          |          |          |
| C                | 0.42061  | 2.14177  | -0.99941 |                  |          |          |                   |   |          |          |          |
| H                | 0.82808  | 3.17045  | -0.99897 |                  |          |          |                   |   |          |          |          |
| H                | -0.67657 | 2.26584  | -1.00041 |                  |          |          |                   |   |          |          |          |
| C                | 1.64452  | -1.43515 | -0.99941 |                  |          |          |                   |   |          |          |          |
| H                | 2.33165  | -2.30236 | -0.99897 |                  |          |          |                   |   |          |          |          |
| H                | 2.30056  | -0.54699 | -1.00041 |                  |          |          |                   |   |          |          |          |
| H                | 0.00000  | 0.00000  | 3.20803  |                  |          |          |                   |   |          |          |          |
| F                | 0.00000  | 0.00000  | 4.16184  |                  |          |          |                   |   |          |          |          |
| [3.3.3]h_plus_oo |          |          |          | [3.3.3]h_plus_io |          |          | [3.3.3]h_plus_ts_ |   |          |          |          |
| P                | 0.00000  | 0.00000  | -1.50400 | P                | 0.00000  | 0.00000  | 1.27004           | P | 0.00000  | 0.00000  | 1.31957  |
| P                | 0.00000  | 0.00000  | 2.30474  | P                | 0.00000  | 0.00000  | -1.19151          | P | 0.00000  | 0.00000  | -1.68847 |
| C                | 0.02082  | 1.77132  | -1.04067 | C                | 1.85730  | -0.13501 | 1.08361           | C | 1.82092  | -0.19837 | 1.05769  |
| C                | -0.02894 | 1.74136  | 1.57366  | C                | 1.80608  | -0.11841 | -1.48980          | C | 1.83968  | -0.07109 | -1.48844 |
| H                | 0.54849  | 2.26325  | -1.87712 | H                | 2.29558  | 0.33511  | 1.98034           | H | 2.28457  | 0.19418  | 1.97858  |
| H                | -1.02368 | 2.13067  | -1.06409 | H                | 2.08291  | -1.21797 | 1.14530           | H | 2.01416  | -1.28752 | 1.03370  |
| H                | 0.40633  | 2.34880  | 2.38605  | H                | 2.14194  | 0.39579  | -2.40413          | H | 2.29822  | 0.43509  | -2.35327 |
| H                | -1.08858 | 2.05596  | 1.52130  | H                | 2.05066  | -1.19151 | -1.58770          | H | 2.08477  | -1.14586 | -1.58745 |
| C                | 1.52360  | -0.90369 | -1.04067 | C                | -0.81173 | 1.67597  | 1.08361           | C | -0.73867 | 1.67615  | 1.05769  |
| H                | 1.68579  | -1.60664 | -1.87712 | H                | -1.43801 | 1.82047  | 1.98034           | H | -1.31045 | 1.88140  | 1.97858  |
| H                | 2.35705  | -0.17880 | -1.06409 | H                | 0.01334  | 2.41283  | 1.14530           | H | 0.10794  | 2.38807  | 1.03370  |
| C                | 1.52253  | -0.84562 | 1.57366  | C                | -0.80049 | 1.62331  | -1.48980          | C | -0.85828 | 1.62875  | -1.48844 |
| H                | 1.83096  | -1.52630 | 2.38605  | H                | -1.41373 | 1.65708  | -2.40413          | H | -1.52591 | 1.77277  | -2.35327 |
| H                | 2.32480  | -0.08524 | 1.52130  | H                | 0.00655  | 2.37168  | -1.58770          | H | -0.05004 | 2.37839  | -1.58745 |
| C                | -1.49359 | -0.89575 | 1.57366  | C                | -1.00558 | -1.50490 | -1.48980          | C | -0.98140 | -1.55766 | -1.48844 |
| H                | -1.23622 | -1.97071 | 1.52130  | H                | -2.05721 | -1.18016 | -1.58770          | H | -2.03473 | -1.23253 | -1.58745 |

|               |          |          |          |   |          |          |          |   |          |          |          |
|---------------|----------|----------|----------|---|----------|----------|----------|---|----------|----------|----------|
| H             | -2.23729 | -0.82251 | 2.38605  | H | -0.72821 | -2.05287 | -2.40413 | H | -0.77231 | -2.20786 | -2.35327 |
| C             | -1.54442 | -0.86763 | -1.04067 | C | -1.04557 | -1.54097 | 1.08361  | C | -1.08226 | -1.47778 | 1.05769  |
| H             | -1.33337 | -1.95187 | -1.06409 | H | -2.09625 | -1.19486 | 1.14530  | H | -2.12210 | -1.10056 | 1.03370  |
| H             | -2.23428 | -0.65662 | -1.87712 | H | -0.85757 | -2.15559 | 1.98034  | H | -0.97412 | -2.07558 | 1.97858  |
| C             | 0.71274  | 2.12562  | 0.28577  | C | 2.43736  | 0.47692  | -0.20577 | C | 2.39303  | 0.49433  | -0.17765 |
| H             | 1.74011  | 1.72175  | 0.29262  | H | 2.28563  | 1.57206  | -0.19417 | H | 2.20714  | 1.58188  | -0.12284 |
| H             | 0.82881  | 3.22355  | 0.27507  | H | 3.52807  | 0.31492  | -0.22103 | H | 3.49014  | 0.36865  | -0.16452 |
| C             | -2.19721 | -0.44556 | 0.28577  | C | -0.80565 | -2.34928 | -0.20577 | C | -0.76841 | -2.31958 | -0.17765 |
| H             | -3.20608 | -0.89400 | 0.27507  | H | -1.49130 | -3.21286 | -0.22103 | H | -1.42581 | -3.20687 | -0.16452 |
| H             | -2.36113 | 0.64611  | 0.29262  | H | 0.21863  | -2.76544 | -0.19417 | H | 0.26638  | -2.70238 | -0.12284 |
| C             | 1.48447  | -1.68006 | 0.28577  | C | -1.63171 | 1.87235  | -0.20577 | C | -1.62461 | 1.82526  | -0.17765 |
| H             | 2.37727  | -2.32955 | 0.27507  | H | -2.03677 | 2.89793  | -0.22103 | H | -2.06433 | 2.83822  | -0.16452 |
| H             | 0.62102  | -2.36786 | 0.29262  | H | -2.50426 | 1.19338  | -0.19417 | H | -2.47352 | 1.12050  | -0.12284 |
| H             | 0.00000  | 0.00000  | -2.91613 | H | 0.00000  | 0.00000  | 2.72646  | H | 0.00000  | 0.00000  | 2.74803  |
| [3.3.3]lih_oo |          |          |          |   |          |          |          |   |          |          |          |
| P             | 0.00000  | 0.00000  | -1.83368 |   |          |          |          |   |          |          |          |
| P             | 0.00000  | 0.00000  | 2.25018  |   |          |          |          |   |          |          |          |
| C             | -0.57076 | 1.63777  | -1.13325 |   |          |          |          |   |          |          |          |
| C             | -0.57506 | 1.62621  | 1.49707  |   |          |          |          |   |          |          |          |
| H             | -0.32419 | 2.36131  | -1.93058 |   |          |          |          |   |          |          |          |
| H             | -1.67618 | 1.60591  | -1.09823 |   |          |          |          |   |          |          |          |
| H             | -0.34541 | 2.35906  | 2.29125  |   |          |          |          |   |          |          |          |
| H             | -1.68043 | 1.59048  | 1.45118  |   |          |          |          |   |          |          |          |
| C             | 1.70373  | -0.32459 | -1.13325 |   |          |          |          |   |          |          |          |
| H             | 2.20704  | -0.89990 | -1.93058 |   |          |          |          |   |          |          |          |
| H             | 2.22884  | 0.64866  | -1.09823 |   |          |          |          |   |          |          |          |
| C             | 1.69587  | -0.31509 | 1.49707  |   |          |          |          |   |          |          |          |
| H             | 2.21571  | -0.88040 | 2.29125  |   |          |          |          |   |          |          |          |
| H             | 2.21761  | 0.66006  | 1.45118  |   |          |          |          |   |          |          |          |
| C             | -1.12081 | -1.31113 | 1.49707  |   |          |          |          |   |          |          |          |
| H             | -0.53718 | -2.25054 | 1.45118  |   |          |          |          |   |          |          |          |
| H             | -1.87030 | -1.47866 | 2.29125  |   |          |          |          |   |          |          |          |
| C             | -1.13297 | -1.31318 | -1.13325 |   |          |          |          |   |          |          |          |
| H             | -0.55267 | -2.25457 | -1.09823 |   |          |          |          |   |          |          |          |
| H             | -1.88286 | -1.46141 | -1.93058 |   |          |          |          |   |          |          |          |
| C             | 0.00000  | 2.18239  | 0.18519  |   |          |          |          |   |          |          |          |
| H             | 1.10042  | 2.09314  | 0.18479  |   |          |          |          |   |          |          |          |
| H             | -0.20201 | 3.26992  | 0.18289  |   |          |          |          |   |          |          |          |
| C             | -1.89001 | -1.09120 | 0.18519  |   |          |          |          |   |          |          |          |
| H             | -2.73082 | -1.80991 | 0.18289  |   |          |          |          |   |          |          |          |
| H             | -2.36293 | -0.09358 | 0.18479  |   |          |          |          |   |          |          |          |
| C             | 1.89001  | -1.09120 | 0.18519  |   |          |          |          |   |          |          |          |
| H             | 2.93284  | -1.46001 | 0.18289  |   |          |          |          |   |          |          |          |
| H             | 1.26251  | -1.99956 | 0.18479  |   |          |          |          |   |          |          |          |
| Li            | 0.00000  | 0.00000  | -4.43375 |   |          |          |          |   |          |          |          |
| H             | 0.00000  | 0.00000  | -6.07258 |   |          |          |          |   |          |          |          |

|                |          |          |          |                |                            |
|----------------|----------|----------|----------|----------------|----------------------------|
| [3.3.3]oo      |          |          |          |                |                            |
| P              | 0.00000  | 0.00000  | 2.09603  |                |                            |
| P              | 0.00000  | 0.00000  | -2.04687 |                |                            |
| C              | 1.71012  | -0.20810 | 1.34133  |                |                            |
| C              | 1.71032  | -0.20861 | -1.29204 |                |                            |
| H              | 2.37767  | 0.17733  | 2.13321  |                |                            |
| H              | 1.91434  | -1.29530 | 1.29749  |                |                            |
| H              | 2.37784  | 0.17648  | -2.08406 |                |                            |
| H              | 1.91449  | -1.29571 | -1.24739 |                |                            |
| C              | -0.67485 | 1.58506  | 1.34133  |                |                            |
| H              | -1.34241 | 1.97046  | 2.13321  |                |                            |
| H              | 0.16459  | 2.30551  | 1.29749  |                |                            |
| C              | -0.67450 | 1.58549  | -1.29204 |                |                            |
| H              | -1.34176 | 1.97103  | -2.08406 |                |                            |
| H              | 0.16487  | 2.30585  | -1.24739 |                |                            |
| C              | -1.03582 | -1.37688 | -1.29204 |                |                            |
| H              | -2.07936 | -1.01014 | -1.24739 |                |                            |
| H              | -1.03609 | -2.14751 | -2.08406 |                |                            |
| C              | -1.03528 | -1.37696 | 1.34133  |                |                            |
| H              | -2.07893 | -1.01022 | 1.29749  |                |                            |
| H              | -1.03526 | -2.14779 | 2.13321  |                |                            |
| C              | 2.12114  | 0.46979  | 0.02453  |                |                            |
| H              | 1.79017  | 1.52319  | 0.02450  |                |                            |
| H              | 3.22718  | 0.51481  | 0.02477  |                |                            |
| C              | -0.65372 | -2.07186 | 0.02453  |                |                            |
| H              | -1.16775 | -3.05223 | 0.02477  |                |                            |
| H              | 0.42404  | -2.31193 | 0.02450  |                |                            |
| C              | -1.46742 | 1.60207  | 0.02453  |                |                            |
| H              | -2.05943 | 2.53742  | 0.02477  |                |                            |
| H              | -2.21421 | 0.78874  | 0.02450  |                |                            |
| [4.3.3]        |          |          |          |                |                            |
| [4.3.3]agcl_oo |          |          |          | [4.3.3]agcl_io |                            |
| P              | 1.71271  | 0.03091  | -0.01492 | P              | -1.54502 0.36151 -0.09821  |
| P              | -2.16861 | -0.62973 | 0.05456  | P              | 1.24327 -0.56072 -0.03008  |
| C              | 1.21203  | -1.40208 | 1.07354  | C              | -1.26400 -0.95021 -1.43806 |
| C              | -1.18550 | -0.42592 | 1.65018  | C              | 1.09924 -1.98706 -1.18598  |
| H              | 2.09417  | -1.55765 | 1.71624  | H              | -0.84647 -0.38548 -2.29504 |
| H              | 1.22616  | -2.25244 | 0.36841  | H              | -2.28519 -1.25030 -1.73110 |
| H              | -0.80763 | 0.59942  | 1.72226  | H              | 1.42488 -1.65463 -2.18831  |
| H              | -1.93726 | -0.52093 | 2.45385  | H              | 1.66659 -2.89489 -0.91510  |
| C              | 1.16840  | 1.67531  | 0.72495  | C              | -0.57038 1.94426 -0.43613  |
| H              | 2.09894  | 2.26417  | 0.77387  | H              | -1.26608 2.72128 -0.06568  |
| H              | 0.87010  | 1.50690  | 1.77351  | H              | -0.62655 2.02164 -1.54103  |
| C              | -2.08138 | 1.11295  | -0.70804 | C              | 2.72026 0.53103 -0.23916   |
| H              | -1.73471 | 1.04155  | -1.75371 | H              | 3.18406 0.69697 0.74996    |
| H              | -3.14531 | 1.39919  | -0.78440 | H              | 3.49389 0.12702 -0.91391   |
| C              | -1.13479 | -1.80024 | -1.00433 | C              | 1.12524 -1.26473 1.68154   |
| H              | -1.89084 | -2.30736 | -1.62879 | H              | 2.07940 -1.23631 2.23627   |
|                |          |          |          | [4.3.3]agcl_ts |                            |
|                |          |          |          | P              | -0.11579 0.08107 0.02457   |
|                |          |          |          | P              | 3.17606 -0.53770 0.01379   |
|                |          |          |          | C              | 0.51102 -0.80987 -1.51063  |
|                |          |          |          | C              | 2.76972 -1.92627 -1.12117  |
|                |          |          |          | H              | 1.14888 -0.10830 -2.07457  |
|                |          |          |          | H              | -0.39831 -0.98349 -2.10917 |
|                |          |          |          | H              | 3.21771 -1.62875 -2.08831  |
|                |          |          |          | H              | 3.27525 -2.85660 -0.80880  |
|                |          |          |          | C              | 0.40689 1.87213 -0.05221   |
|                |          |          |          | H              | -0.20394 2.34147 0.74284   |
|                |          |          |          | H              | -0.04622 2.22216 -1.00031  |
|                |          |          |          | C              | 3.88674 1.01865 -0.66944   |
|                |          |          |          | H              | 4.53014 1.43871 0.12619    |
|                |          |          |          | H              | 4.55868 0.75979 -1.50709   |
|                |          |          |          | C              | 2.99094 -0.81605 1.82175   |
|                |          |          |          | H              | 3.86653 -0.41216 2.36028   |

|                |          |          |          |                |          |          |          |                |          |          |          |
|----------------|----------|----------|----------|----------------|----------|----------|----------|----------------|----------|----------|----------|
| H              | -0.82186 | -2.57254 | -0.27919 | H              | 0.81530  | -2.32303 | 1.60513  | H              | 3.02698  | -1.91548 | 1.94625  |
| C              | 0.80085  | -0.10505 | -1.63538 | C              | -1.31427 | -0.36415 | 1.62881  | C              | 0.41304  | -0.69788 | 1.64990  |
| H              | 0.12257  | 0.75010  | -1.71047 | H              | -2.02835 | 0.21289  | 2.24194  | H              | -0.46049 | -0.50378 | 2.29622  |
| H              | 1.56785  | 0.03698  | -2.41445 | H              | -1.75883 | -1.37605 | 1.53982  | H              | 0.41007  | -1.79176 | 1.47778  |
| C              | -1.38979 | 2.27676  | 0.04749  | C              | 2.09982  | 1.84932  | -0.76906 | C              | 2.83156  | 2.05900  | -1.09054 |
| C              | 0.13465  | 2.53777  | -0.04188 | C              | 0.86212  | 2.32245  | 0.04555  | C              | 1.85197  | 2.40674  | 0.05245  |
| C              | -0.05606 | -1.41507 | 1.96511  | C              | -0.43008 | -2.23160 | -1.18988 | C              | 1.25475  | -2.14015 | -1.30390 |
| C              | 0.03878  | -1.40185 | -1.93463 | C              | 0.03376  | -0.43294 | 2.38371  | C              | 1.68091  | -0.26841 | 2.40751  |
| H              | -0.45394 | -2.44567 | 1.98181  | H              | -0.73778 | -2.69576 | -0.23433 | H              | 0.83985  | -2.69297 | -0.44280 |
| H              | 0.74920  | -2.24675 | -1.99248 | H              | -0.17733 | -0.85271 | 3.38490  | H              | 1.58144  | -0.63636 | 3.44701  |
| H              | 0.27235  | 3.55870  | 0.35967  | H              | 0.87006  | 3.42846  | 0.02750  | H              | 1.74598  | 3.50594  | 0.10108  |
| H              | -1.69288 | 2.25858  | 1.10999  | H              | 1.80738  | 1.71534  | -1.82714 | H              | 2.28097  | 1.69630  | -1.97561 |
| H              | 0.26303  | -1.21100 | 3.00228  | H              | -0.69050 | -2.96244 | -1.97622 | H              | 1.08645  | -2.78567 | -2.18508 |
| H              | -1.85045 | 3.19769  | -0.35613 | H              | 2.86496  | 2.64702  | -0.75553 | H              | 3.36074  | 2.97474  | -1.41442 |
| H              | 0.43510  | 2.61514  | -1.10219 | H              | 0.99309  | 2.05096  | 1.10855  | H              | 2.30031  | 2.11084  | 1.01534  |
| H              | -0.35731 | -1.28730 | -2.95905 | H              | 0.40635  | 0.59204  | 2.55373  | H              | 1.72086  | 0.83106  | 2.47723  |
| Ag             | 4.00826  | -0.06151 | -0.33385 | Cl             | -6.00795 | 1.54987  | -0.42505 | Ag             | -2.44349 | 0.03185  | -0.01992 |
| Cl             | 6.27121  | -0.14327 | -0.65707 | Ag             | -3.79198 | 0.96819  | -0.26448 | Cl             | -4.73453 | -0.02357 | -0.06622 |
| [4.3.3]beh2_oo |          |          |          | [4.3.3]beh2_io |          |          |          | [4.3.3]beh2_ts |          |          |          |
| P              | 1.66636  | 0.02870  | 0.09383  | P              | -1.60061 | 0.43689  | -0.17425 | P              | -0.94363 | 1.54797  | -0.36778 |
| P              | -2.19993 | -0.61470 | 0.02016  | P              | 1.18454  | -0.55330 | 0.02135  | P              | 0.42598  | -1.40796 | 0.33835  |
| C              | 1.13705  | -1.42077 | 1.13601  | C              | -1.30313 | -0.93385 | -1.44644 | C              | -1.20275 | 0.25523  | -1.71015 |
| C              | -1.26683 | -0.44366 | 1.64993  | C              | 1.02315  | -2.02666 | -1.07320 | C              | -0.79851 | -2.11449 | -0.83719 |
| H              | 2.00207  | -1.58558 | 1.80184  | H              | -0.84261 | -0.42140 | -2.31320 | H              | -0.23257 | 0.08100  | -2.20684 |
| H              | 1.18344  | -2.25819 | 0.41767  | H              | -2.32139 | -1.22934 | -1.76516 | H              | -1.85648 | 0.75950  | -2.44621 |
| H              | -0.87510 | 0.57455  | 1.74693  | H              | 1.38795  | -1.75071 | -2.07928 | H              | -0.18819 | -2.44518 | -1.69927 |
| H              | -2.04595 | -0.53862 | 2.42723  | H              | 1.54972  | -2.94145 | -0.74755 | H              | -1.28375 | -3.01634 | -0.42436 |
| C              | 1.11288  | 1.66937  | 0.81703  | C              | -0.56885 | 1.96606  | -0.55291 | C              | 0.82221  | 2.13797  | -0.39488 |
| H              | 2.05553  | 2.24191  | 0.87157  | H              | -1.25880 | 2.78300  | -0.26273 | H              | 0.77906  | 3.06156  | 0.21565  |
| H              | 0.79181  | 1.51525  | 1.86104  | H              | -0.57654 | 1.98579  | -1.66132 | H              | 0.93720  | 2.50153  | -1.43493 |
| C              | -2.06499 | 1.12804  | -0.73244 | C              | 2.69250  | 0.49737  | -0.18375 | C              | 2.18074  | -1.22290 | -0.18887 |
| H              | -1.64706 | 1.05682  | -1.75135 | H              | 3.13043  | 0.69164  | 0.81218  | H              | 2.79462  | -1.32378 | 0.72570  |
| H              | -3.12095 | 1.41631  | -0.87835 | H              | 3.47895  | 0.05813  | -0.82089 | H              | 2.45055  | -2.07263 | -0.84105 |
| C              | -1.14119 | -1.77542 | -1.02199 | C              | 0.98331  | -1.17407 | 1.75820  | C              | -0.11561 | -1.09725 | 2.06829  |
| H              | -1.87983 | -2.27795 | -1.67088 | H              | 1.91527  | -1.13641 | 2.34940  | H              | 0.64692  | -1.46100 | 2.77981  |
| H              | -0.84184 | -2.55510 | -0.29938 | H              | 0.65773  | -2.22983 | 1.71766  | H              | -1.00768 | -1.73742 | 2.21009  |
| C              | 0.85012  | -0.09977 | -1.57817 | C              | -1.43654 | -0.23333 | 1.57628  | C              | -1.46207 | 0.98745  | 1.34122  |
| H              | 0.22999  | 0.79180  | -1.71767 | H              | -2.16917 | 0.36887  | 2.14430  | H              | -1.87910 | 1.91438  | 1.77626  |
| H              | 1.67458  | -0.00901 | -2.30962 | H              | -1.89704 | -1.23869 | 1.50494  | H              | -2.33824 | 0.32844  | 1.19033  |
| C              | -1.41556 | 2.28451  | 0.06894  | C              | 2.11070  | 1.80678  | -0.77998 | C              | 2.46974  | 0.12914  | -0.86852 |
| C              | 0.10937  | 2.54767  | 0.03151  | C              | 0.85214  | 2.33296  | -0.02862 | C              | 2.07301  | 1.33288  | 0.01620  |
| C              | -0.16022 | -1.45355 | 1.98237  | C              | -0.51409 | -2.22529 | -1.11418 | C              | -1.84179 | -1.08566 | -1.31223 |
| C              | 0.05264  | -1.36598 | -1.92105 | C              | -0.12000 | -0.29524 | 2.38347  | C              | -0.47851 | 0.37012  | 2.34924  |
| H              | -0.56875 | -2.47996 | 1.95671  | H              | -0.86360 | -2.63572 | -0.14863 | H              | -2.61106 | -0.93314 | -0.53515 |
| H              | 0.74512  | -2.22433 | -1.99042 | H              | -0.37236 | -0.67198 | 3.39242  | H              | -0.94822 | 0.42632  | 3.35033  |
| H              | 0.23778  | 3.56438  | 0.44694  | H              | 0.88968  | 3.43743  | -0.08127 | H              | 2.90448  | 2.06138  | 0.00954  |
| H              | -1.75473 | 2.24529  | 1.12009  | H              | 1.85178  | 1.63759  | -1.84175 | H              | 1.94526  | 0.17486  | -1.83880 |

|                    |          |          |          |                    |          |          |          |                    |          |          |          |
|--------------------|----------|----------|----------|--------------------|----------|----------|----------|--------------------|----------|----------|----------|
| H                  | 0.11999  | -1.28036 | 3.03644  | H                  | -0.76880 | -2.98622 | -1.87362 | H                  | -2.37679 | -1.49922 | -2.18681 |
| H                  | -1.86736 | 3.20979  | -0.33470 | H                  | 2.88907  | 2.59221  | -0.77005 | H                  | 3.55048  | 0.17905  | -1.10026 |
| H                  | 0.44255  | 2.63367  | -1.01833 | H                  | 0.93921  | 2.09262  | 1.04635  | H                  | 1.98383  | 0.99660  | 1.06302  |
| H                  | -0.32530 | -1.21538 | -2.94806 | H                  | 0.26768  | 0.72828  | 2.52767  | H                  | 0.43563  | 0.98439  | 2.40665  |
| Be                 | 3.80036  | -0.05579 | -0.46425 | H                  | -4.50196 | -0.06237 | 0.15436  | H                  | -3.61794 | 2.69874  | -0.69116 |
| H                  | 4.22933  | -1.35949 | -0.54700 | H                  | -3.94260 | 1.75917  | -1.56548 | H                  | -1.77176 | 4.03646  | -1.88497 |
| H                  | 4.22686  | 1.21375  | -0.78219 | Be                 | -3.73322 | 0.82661  | -0.57272 | Be                 | -2.34842 | 3.08399  | -1.07605 |
| [4.3.3]bh3_oo      |          |          |          | [4.3.3]bh3_io      |          |          |          | [4.3.3]bh3_ts      |          |          |          |
| P                  | 1.72724  | 0.04951  | 0.00527  | P                  | -1.61619 | 0.40982  | -0.14200 | P                  | -1.03636 | 1.47198  | -0.41755 |
| P                  | -2.10394 | -0.64910 | 0.00978  | P                  | 1.14009  | -0.54992 | 0.03247  | P                  | 0.43440  | -1.40531 | 0.33919  |
| C                  | 1.26559  | -1.38585 | 1.08408  | C                  | -1.35370 | -0.93774 | -1.42863 | C                  | -1.24142 | 0.18233  | -1.75393 |
| C                  | -1.15132 | -0.45363 | 1.62703  | C                  | 0.98681  | -2.00453 | -1.08788 | C                  | -0.73425 | -2.16162 | -0.86269 |
| H                  | 2.14999  | -1.48098 | 1.73793  | H                  | -0.91850 | -0.41987 | -2.30534 | H                  | -0.26874 | 0.05043  | -2.25928 |
| H                  | 1.33350  | -2.24396 | 0.39227  | H                  | -2.38550 | -1.21723 | -1.70823 | H                  | -1.92046 | 0.67996  | -2.46810 |
| H                  | -0.78107 | 0.57349  | 1.71815  | H                  | 1.34315  | -1.70358 | -2.08999 | H                  | -0.08965 | -2.45942 | -1.71186 |
| H                  | -1.91816 | -0.56360 | 2.41441  | H                  | 1.52934  | -2.91661 | -0.78218 | H                  | -1.18188 | -3.08795 | -0.46190 |
| C                  | 1.17538  | 1.68336  | 0.72120  | C                  | -0.63358 | 1.96004  | -0.53193 | C                  | 0.68916  | 2.15348  | -0.41515 |
| H                  | 2.12287  | 2.25005  | 0.75603  | H                  | -1.34248 | 2.75231  | -0.22445 | H                  | 0.57513  | 3.07139  | 0.19363  |
| H                  | 0.87696  | 1.53719  | 1.77275  | H                  | -0.65009 | 1.98058  | -1.64006 | H                  | 0.80275  | 2.51811  | -1.45508 |
| C                  | -1.99263 | 1.08018  | -0.77628 | C                  | 2.63180  | 0.52065  | -0.18449 | C                  | 2.18600  | -1.13499 | -0.16376 |
| H                  | -1.56329 | 0.99577  | -1.78908 | H                  | 3.06809  | 0.72326  | 0.81051  | H                  | 2.78853  | -1.20056 | 0.76155  |
| H                  | -3.05196 | 1.34743  | -0.93610 | H                  | 3.42265  | 0.08674  | -0.81997 | H                  | 2.50432  | -1.97789 | -0.80287 |
| C                  | -1.04388 | -1.80957 | -1.03106 | C                  | 0.96834  | -1.18731 | 1.76529  | C                  | -0.15598 | -1.09363 | 2.05352  |
| H                  | -1.78379 | -2.35021 | -1.64713 | H                  | 1.90773  | -1.15131 | 2.34441  | H                  | 0.60472  | -1.42291 | 2.78353  |
| H                  | -0.69795 | -2.56198 | -0.30081 | H                  | 0.64364  | -2.24315 | 1.72011  | H                  | -1.02536 | -1.76715 | 2.18181  |
| C                  | 0.92830  | -0.12466 | -1.65650 | C                  | -1.44949 | -0.25672 | 1.60347  | C                  | -1.57003 | 0.92461  | 1.28280  |
| H                  | 0.33109  | 0.77573  | -1.83863 | H                  | -2.18676 | 0.35173  | 2.15787  | H                  | -2.01946 | 1.85315  | 1.67910  |
| H                  | 1.77973  | -0.07627 | -2.35799 | H                  | -1.90096 | -1.26651 | 1.53352  | H                  | -2.41730 | 0.22883  | 1.13226  |
| C                  | -1.36541 | 2.26007  | 0.00750  | C                  | 2.03755  | 1.82233  | -0.78363 | C                  | 2.42747  | 0.22126  | -0.85164 |
| C                  | 0.15329  | 2.54806  | -0.05241 | C                  | 0.78451  | 2.34703  | -0.02339 | C                  | 1.97097  | 1.41481  | 0.01697  |
| C                  | -0.02028 | -1.44208 | 1.94653  | C                  | -0.54773 | -2.22340 | -1.12532 | C                  | -1.81737 | -1.18608 | -1.35926 |
| C                  | 0.10887  | -1.38485 | -1.97474 | C                  | -0.13163 | -0.31361 | 2.40569  | C                  | -0.58176 | 0.36059  | 2.31446  |
| H                  | -0.41230 | -2.47477 | 1.92697  | H                  | -0.88518 | -2.65598 | -0.16492 | H                  | -2.60503 | -1.06895 | -0.59427 |
| H                  | 0.79658  | -2.24364 | -2.07843 | H                  | -0.37373 | -0.69368 | 3.41578  | H                  | -1.06931 | 0.40724  | 3.30743  |
| H                  | 0.27373  | 3.56890  | 0.35502  | H                  | 0.81279  | 3.45114  | -0.08420 | H                  | 2.76857  | 2.17993  | 0.01020  |
| H                  | -1.69162 | 2.22414  | 1.06291  | H                  | 1.76910  | 1.64526  | -1.84188 | H                  | 1.91339  | 0.23761  | -1.82859 |
| H                  | 0.26957  | -1.26253 | 2.99672  | H                  | -0.79535 | -2.97471 | -1.89658 | H                  | -2.31779 | -1.63014 | -2.23952 |
| H                  | -1.84047 | 3.17161  | -0.40041 | H                  | 2.81310  | 2.61042  | -0.78647 | H                  | 3.50819  | 0.31233  | -1.07031 |
| H                  | 0.46871  | 2.63030  | -1.10812 | H                  | 0.88349  | 2.11486  | 1.05263  | H                  | 1.88736  | 1.08560  | 1.06666  |
| H                  | -0.31153 | -1.22768 | -2.98410 | H                  | 0.25404  | 0.71107  | 2.54817  | H                  | 0.30588  | 1.01180  | 2.37998  |
| H                  | 3.92489  | -1.05222 | -0.66306 | H                  | -4.11209 | -0.10736 | -0.06441 | H                  | -2.06039 | 3.80245  | -0.04201 |
| H                  | 3.86154  | 0.97752  | -0.98238 | H                  | -3.66950 | 1.82268  | 0.49387  | H                  | -1.87772 | 3.27121  | -2.02849 |
| H                  | 4.09614  | 0.24751  | 0.92739  | H                  | -3.61199 | 1.27746  | -1.48879 | H                  | -3.33867 | 2.42205  | -0.87066 |
| B                  | 3.65402  | 0.05257  | -0.20064 | B                  | -3.48299 | 0.91960  | -0.31845 | B                  | -2.21928 | 2.93537  | -0.89681 |
| [4.3.3]ch3_plus_oo |          |          |          | [4.3.3]ch3_plus_io |          |          |          | [4.3.3]ch3_plus_ts |          |          |          |
| P                  | 1.53717  | 0.02473  | 0.00684  | P                  | -1.30445 | 0.31517  | -0.07767 | P                  | -0.94998 | 1.34509  | -0.39068 |

|               |          |          |          |               |          |          |          |               |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| P             | -2.16352 | -0.60806 | 0.07914  | P             | 1.15635  | -0.57928 | 0.03446  | P             | 0.43247  | -1.51299 | 0.38719  |
| C             | 1.21155  | -1.39834 | 1.12360  | C             | -1.33737 | -0.96049 | -1.44720 | C             | -1.22780 | 0.16968  | -1.79199 |
| C             | -1.18257 | -0.44238 | 1.69172  | C             | 1.03367  | -1.91500 | -1.22080 | C             | -0.79103 | -2.15154 | -0.84120 |
| H             | 2.09973  | -1.41103 | 1.78041  | H             | -1.02179 | -0.40655 | -2.35319 | H             | -0.26073 | 0.02174  | -2.30062 |
| H             | 1.31891  | -2.27563 | 0.45993  | H             | -2.39570 | -1.23628 | -1.59086 | H             | -1.89392 | 0.70837  | -2.48784 |
| H             | -0.79873 | 0.57854  | 1.81423  | H             | 1.37255  | -1.50459 | -2.18916 | H             | -0.14808 | -2.51070 | -1.66734 |
| H             | -1.94489 | -0.55722 | 2.48131  | H             | 1.63936  | -2.80658 | -0.99011 | H             | -1.27699 | -3.04701 | -0.41833 |
| C             | 1.14731  | 1.69344  | 0.70263  | C             | -0.58227 | 1.98489  | -0.47551 | C             | 0.68688  | 2.18424  | -0.35886 |
| H             | 2.11994  | 2.21719  | 0.68366  | H             | -1.32495 | 2.70698  | -0.09022 | H             | 0.51631  | 3.05015  | 0.31035  |
| H             | 0.88795  | 1.57191  | 1.76676  | H             | -0.65694 | 2.04037  | -1.58009 | H             | 0.78152  | 2.60257  | -1.38015 |
| C             | -2.04189 | 1.12012  | -0.71068 | C             | 2.60079  | 0.54525  | -0.17345 | C             | 2.12928  | -1.08500 | -0.21792 |
| H             | -1.64310 | 1.03762  | -1.73679 | H             | 3.01280  | 0.74724  | 0.83125  | H             | 2.77533  | -1.19063 | 0.67361  |
| H             | -3.10211 | 1.39326  | -0.84684 | H             | 3.40012  | 0.09073  | -0.78208 | H             | 2.41646  | -1.91013 | -0.89386 |
| C             | -1.14563 | -1.79368 | -0.98361 | C             | 1.04595  | -1.31552 | 1.72207  | C             | -0.15930 | -1.04780 | 2.07339  |
| H             | -1.91218 | -2.33129 | -1.56732 | H             | 2.01516  | -1.33581 | 2.24658  | H             | 0.62329  | -1.34042 | 2.79470  |
| H             | -0.77822 | -2.55061 | -0.26884 | H             | 0.68758  | -2.35636 | 1.63026  | H             | -1.00806 | -1.73592 | 2.25092  |
| C             | 0.82713  | -0.15228 | -1.67620 | C             | -1.31882 | -0.31882 | 1.68136  | C             | -1.60453 | 0.91421  | 1.28104  |
| H             | 0.26208  | 0.76856  | -1.86344 | H             | -2.01995 | 0.34381  | 2.21815  | H             | -2.05786 | 1.85839  | 1.63291  |
| H             | 1.69358  | -0.13036 | -2.36035 | H             | -1.82059 | -1.30434 | 1.60402  | H             | -2.43525 | 0.19949  | 1.13476  |
| C             | -1.39459 | 2.29567  | 0.06036  | C             | 2.04471  | 1.84641  | -0.79171 | C             | 2.38062  | 0.27838  | -0.87650 |
| C             | 0.12015  | 2.57314  | -0.05193 | C             | 0.83058  | 2.41228  | -0.01494 | C             | 1.98525  | 1.46022  | 0.02876  |
| C             | -0.07952 | -1.46896 | 1.98246  | C             | -0.47869 | -2.22874 | -1.27280 | C             | -1.84154 | -1.17888 | -1.39762 |
| C             | -0.03401 | -1.39154 | -1.98147 | C             | 0.00540  | -0.44202 | 2.45616  | C             | -0.60407 | 0.39899  | 2.32094  |
| H             | -0.48733 | -2.49018 | 1.90417  | H             | -0.78736 | -2.76505 | -0.35669 | H             | -2.66653 | -1.03805 | -0.67766 |
| H             | 0.62481  | -2.26341 | -2.14016 | H             | -0.21694 | -0.86666 | 3.45003  | H             | -1.09654 | 0.45261  | 3.30886  |
| H             | 0.27859  | 3.58679  | 0.35650  | H             | 0.84331  | 3.51139  | -0.11583 | H             | 2.77167  | 2.23280  | -0.00608 |
| H             | -1.68607 | 2.26057  | 1.12511  | H             | 1.76423  | 1.67314  | -1.84714 | H             | 1.85947  | 0.33895  | -1.84820 |
| H             | 0.21750  | -1.35013 | 3.03751  | H             | -0.69331 | -2.91003 | -2.11303 | H             | -2.30103 | -1.62457 | -2.29726 |
| H             | -1.87340 | 3.21128  | -0.32971 | H             | 2.84846  | 2.60178  | -0.80617 | H             | 3.45796  | 0.34115  | -1.11030 |
| H             | 0.40992  | 2.65049  | -1.11510 | H             | 0.95360  | 2.21655  | 1.06670  | H             | 1.93864  | 1.12534  | 1.07822  |
| H             | -0.49278 | -1.19092 | -2.96419 | H             | 0.42365  | 0.56461  | 2.63274  | H             | 0.26613  | 1.07383  | 2.37488  |
| C             | 3.34950  | -0.00979 | -0.20852 | C             | -3.10734 | 0.80704  | -0.17116 | C             | -2.04877 | 2.74550  | -0.86088 |
| H             | 3.64441  | 0.77362  | -0.92482 | H             | -3.33596 | 1.61310  | 0.54460  | H             | -1.96006 | 3.56692  | -0.13288 |
| H             | 3.84291  | 0.17335  | 0.75909  | H             | -3.34970 | 1.15909  | -1.18872 | H             | -1.77707 | 3.11263  | -1.86361 |
| H             | 3.65659  | -0.99416 | -0.59728 | H             | -3.74683 | -0.06221 | 0.05684  | H             | -3.09351 | 2.39239  | -0.88141 |
| [4.3.3]clf_oo |          |          |          | [4.3.3]clf_io |          |          |          | [4.3.3]clf_ts |          |          |          |
| P             | 1.58734  | 0.01706  | -0.01238 | P             | -1.32760 | 0.31005  | -0.09619 | P             | -0.97189 | 1.36494  | -0.39862 |
| P             | -2.16652 | -0.61027 | 0.08906  | P             | 1.19749  | -0.58240 | 0.03115  | P             | 0.43328  | -1.46376 | 0.36643  |
| C             | 1.22155  | -1.38878 | 1.12367  | C             | -1.27911 | -0.97593 | -1.45658 | C             | -1.23114 | 0.15734  | -1.78253 |
| C             | -1.17981 | -0.44406 | 1.69389  | C             | 1.09007  | -1.93954 | -1.20451 | C             | -0.75361 | -2.16771 | -0.85559 |
| H             | 2.10736  | -1.37759 | 1.78349  | H             | -0.94770 | -0.41852 | -2.35464 | H             | -0.26577 | 0.02438  | -2.30112 |
| H             | 1.35856  | -2.27522 | 0.47834  | H             | -2.33740 | -1.24187 | -1.61494 | H             | -1.91218 | 0.69408  | -2.46474 |
| H             | -0.78437 | 0.57353  | 1.79811  | H             | 1.43307  | -1.54021 | -2.17631 | H             | -0.10103 | -2.49376 | -1.68815 |
| H             | -1.93627 | -0.54882 | 2.49126  | H             | 1.69139  | -2.83168 | -0.96113 | H             | -1.21525 | -3.08117 | -0.44294 |
| C             | 1.15233  | 1.67842  | 0.69321  | C             | -0.55775 | 1.96972  | -0.45561 | C             | 0.69097  | 2.16041  | -0.38100 |
| H             | 2.12449  | 2.20305  | 0.67341  | H             | -1.30014 | 2.67227  | -0.03549 | H             | 0.52145  | 3.04636  | 0.26097  |
| H             | 0.89936  | 1.54982  | 1.75887  | H             | -0.66470 | 2.05872  | -1.55488 | H             | 0.77701  | 2.56253  | -1.40917 |

|                |          |          |          |                |          |          |          |                |          |          |          |
|----------------|----------|----------|----------|----------------|----------|----------|----------|----------------|----------|----------|----------|
| C              | -2.02971 | 1.10790  | -0.71584 | C              | 2.65124  | 0.53245  | -0.18339 | C              | 2.15841  | -1.10414 | -0.18596 |
| H              | -1.59362 | 1.00945  | -1.72443 | H              | 3.06810  | 0.74359  | 0.81771  | H              | 2.78022  | -1.18852 | 0.72507  |
| H              | -3.08478 | 1.38304  | -0.88674 | H              | 3.45108  | 0.08516  | -0.79768 | H              | 2.46338  | -1.93943 | -0.84155 |
| C              | -1.14409 | -1.79021 | -0.97041 | C              | 1.08693  | -1.31097 | 1.72490  | C              | -0.15846 | -1.07890 | 2.06839  |
| H              | -1.90237 | -2.36833 | -1.52689 | H              | 2.05126  | -1.31719 | 2.26014  | H              | 0.61259  | -1.39507 | 2.79275  |
| H              | -0.72381 | -2.51477 | -0.25238 | H              | 0.74108  | -2.35639 | 1.63346  | H              | -1.01895 | -1.75978 | 2.21554  |
| C              | 0.83769  | -0.15564 | -1.68660 | C              | -1.29487 | -0.34153 | 1.65588  | C              | -1.58367 | 0.90853  | 1.28746  |
| H              | 0.32360  | 0.79170  | -1.89191 | H              | -2.01387 | 0.31241  | 2.17940  | H              | -2.02157 | 1.86123  | 1.63591  |
| H              | 1.71197  | -0.18457 | -2.36021 | H              | -1.79273 | -1.32792 | 1.57236  | H              | -2.43345 | 0.21551  | 1.14347  |
| C              | -1.39181 | 2.28539  | 0.06094  | C              | 2.07487  | 1.82739  | -0.80113 | C              | 2.40959  | 0.25321  | -0.86106 |
| C              | 0.12354  | 2.56284  | -0.04675 | C              | 0.86334  | 2.38541  | -0.01140 | C              | 1.99049  | 1.44540  | 0.02199  |
| C              | -0.07445 | -1.47270 | 1.97241  | C              | -0.42488 | -2.24332 | -1.26139 | C              | -1.82257 | -1.20043 | -1.38929 |
| C              | -0.07561 | -1.35520 | -1.99808 | C              | 0.02471  | -0.44893 | 2.44174  | C              | -0.59251 | 0.37097  | 2.32474  |
| H              | -0.48663 | -2.49301 | 1.88714  | H              | -0.73995 | -2.76488 | -0.33864 | H              | -2.63269 | -1.07066 | -0.65073 |
| H              | 0.55499  | -2.23480 | -2.21754 | H              | -0.20225 | -0.87072 | 3.43690  | H              | -1.08169 | 0.42229  | 3.31565  |
| H              | 0.27715  | 3.57753  | 0.36349  | H              | 0.87826  | 3.48621  | -0.10327 | H              | 2.77739  | 2.21909  | -0.01556 |
| H              | -1.68676 | 2.24337  | 1.12503  | H              | 1.77795  | 1.64034  | -1.84996 | H              | 1.89137  | 0.29320  | -1.83517 |
| H              | 0.21429  | -1.36250 | 3.03159  | H              | -0.64014 | -2.93736 | -2.09205 | H              | -2.29741 | -1.64890 | -2.28046 |
| H              | -1.87521 | 3.20012  | -0.32786 | H              | 2.87077  | 2.59186  | -0.83537 | H              | 3.48941  | 0.32178  | -1.08728 |
| H              | 0.40869  | 2.64541  | -1.11077 | H              | 0.99928  | 2.18149  | 1.06749  | H              | 1.94005  | 1.12097  | 1.07553  |
| H              | -0.57923 | -1.11241 | -2.95031 | H              | 0.43067  | 0.56327  | 2.61729  | H              | 0.28775  | 1.03282  | 2.38258  |
| Cl             | 3.69740  | -0.02001 | -0.26555 | Cl             | -3.35261 | 0.85300  | -0.22225 | F              | -3.47036 | 4.57022  | -1.44694 |
| F              | 5.69916  | -0.03294 | -0.51471 | F              | -5.48730 | 1.40385  | -0.32804 | Cl             | -2.22979 | 2.97853  | -0.92592 |
| [4.3.3]cucl_oo |          |          |          | [4.3.3]cucl_io |          |          |          | [4.3.3]cucl_ts |          |          |          |
| P              | 1.73453  | 0.02696  | -0.01901 | P              | -1.57238 | 0.37255  | -0.09937 | P              | -0.48554 | 0.08888  | 0.02054  |
| P              | -2.15296 | -0.62755 | 0.05468  | P              | 1.22753  | -0.55706 | -0.03357 | P              | 2.81067  | -0.54131 | 0.01787  |
| C              | 1.22814  | -1.40518 | 1.06751  | C              | -1.28266 | -0.93964 | -1.43714 | C              | 0.14687  | -0.80522 | -1.51053 |
| C              | -1.16836 | -0.42534 | 1.64948  | C              | 1.07672  | -1.98734 | -1.18404 | C              | 2.40482  | -1.92586 | -1.12194 |
| H              | 2.11172  | -1.56684 | 1.70662  | H              | -0.85743 | -0.37799 | -2.29214 | H              | 0.78535  | -0.10452 | -2.07486 |
| H              | 1.23386  | -2.25517 | 0.36227  | H              | -2.30252 | -1.23719 | -1.73768 | H              | -0.76192 | -0.97856 | -2.11024 |
| H              | -0.79306 | 0.60085  | 1.72194  | H              | 1.40192  | -1.65997 | -2.18821 | H              | 2.85179  | -1.62355 | -2.08813 |
| H              | -1.91924 | -0.52258 | 2.45375  | H              | 1.63972  | -2.89738 | -0.91133 | H              | 2.90949  | -2.85860 | -0.81515 |
| C              | 1.18652  | 1.66866  | 0.72376  | C              | -0.58466 | 1.94625  | -0.44443 | C              | 0.05502  | 1.87506  | -0.05751 |
| H              | 2.11857  | 2.25497  | 0.77522  | H              | -1.27895 | 2.73109  | -0.08882 | H              | -0.55660 | 2.35154  | 0.73246  |
| H              | 0.88612  | 1.50000  | 1.77153  | H              | -0.62938 | 2.01305  | -1.55038 | H              | -0.39005 | 2.22632  | -1.00886 |
| C              | -2.06161 | 1.11377  | -0.71048 | C              | 2.70666  | 0.53211  | -0.24295 | C              | 3.53658  | 1.01035  | -0.65947 |
| H              | -1.71271 | 1.03971  | -1.75515 | H              | 3.17305  | 0.69464  | 0.74557  | H              | 4.17661  | 1.42738  | 0.14046  |
| H              | -3.12488 | 1.40188  | -0.78929 | H              | 3.47857  | 0.12981  | -0.92074 | H              | 4.21227  | 0.74967  | -1.49354 |
| C              | -1.12243 | -1.80007 | -1.00453 | C              | 1.10973  | -1.25606 | 1.68033  | C              | 2.62008  | -0.82283 | 1.82477  |
| H              | -1.87973 | -2.30595 | -1.62857 | H              | 2.06371  | -1.22537 | 2.23538  | H              | 3.49576  | -0.42464 | 2.36746  |
| H              | -0.81036 | -2.57266 | -0.27931 | H              | 0.80052  | -2.31486 | 1.60726  | H              | 2.64948  | -1.92268 | 1.94758  |
| C              | 0.81921  | -0.10958 | -1.63755 | C              | -1.33058 | -0.35822 | 1.62468  | C              | 0.04340  | -0.69446 | 1.64394  |
| H              | 0.14577  | 0.74896  | -1.71660 | H              | -2.04725 | 0.21234  | 2.24080  | H              | -0.83126 | -0.50112 | 2.28904  |
| H              | 1.58819  | 0.02631  | -2.41580 | H              | -1.76935 | -1.37238 | 1.53436  | H              | 0.03985  | -1.78802 | 1.47066  |
| C              | -1.36882 | 2.27735  | 0.04427  | C              | 2.08638  | 1.85286  | -0.76774 | C              | 2.48637  | 2.05394  | -1.08514 |
| C              | 0.15634  | 2.53465  | -0.04343 | C              | 0.84570  | 2.32343  | 0.04476  | C              | 1.50213  | 2.40277  | 0.05381  |
| C              | -0.03625 | -1.41227 | 1.96369  | C              | -0.45438 | -2.22415 | -1.18478 | C              | 0.88921  | -2.13640 | -1.30380 |

|                  |          |          |          |                  |          |          |          |                  |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|----------|------------------|----------|----------|----------|
| C                | 0.05130  | -1.40344 | -1.93561 | C                | 0.01703  | -0.42355 | 2.38007  | C                | 1.31004  | -0.26941 | 2.40593  |
| H                | -0.43430 | -2.44272 | 1.98761  | H                | -0.76207 | -2.68337 | -0.22683 | H                | 0.47434  | -2.68814 | -0.44210 |
| H                | 0.75876  | -2.25062 | -1.99467 | H                | -0.19335 | -0.84175 | 3.38218  | H                | 1.20643  | -0.63651 | 3.44538  |
| H                | 0.29554  | 3.55544  | 0.35799  | H                | 0.85544  | 3.42953  | 0.03018  | H                | 1.40125  | 3.50242  | 0.10393  |
| H                | -1.67328 | 2.26092  | 1.10647  | H                | 1.79633  | 1.72313  | -1.82702 | H                | 1.93910  | 1.69233  | -1.97272 |
| H                | 0.28624  | -1.20268 | 2.99879  | H                | -0.71844 | -2.95762 | -1.96752 | H                | 0.71994  | -2.78270 | -2.18432 |
| H                | -1.82735 | 3.19867  | -0.36099 | H                | 2.85127  | 2.65082  | -0.74926 | H                | 3.01888  | 2.96887  | -1.40620 |
| H                | 0.45763  | 2.61119  | -1.10354 | H                | 0.97371  | 2.04859  | 1.10718  | H                | 1.94561  | 2.10358  | 1.01795  |
| H                | -0.34641 | -1.28772 | -2.95933 | H                | 0.38894  | 0.60190  | 2.54853  | H                | 1.35483  | 0.82988  | 2.47541  |
| Cl               | 5.87589  | -0.10743 | -0.61127 | Cu               | -3.63114 | 0.92551  | -0.24831 | Cu               | -2.61696 | 0.04543  | -0.02718 |
| Cu               | 3.83545  | -0.04672 | -0.31367 | Cl               | -5.62943 | 1.44353  | -0.39110 | Cl               | -4.68196 | -0.01186 | -0.07779 |
| [4.3.3]f_plus_oo |          |          |          | [4.3.3]f_plus_io |          |          |          | [4.3.3]f_plus_ts |          |          |          |
| P                | 1.56961  | -0.01248 | 0.14695  | P                | -1.09214 | 0.24344  | -0.07757 | P                | -0.85925 | 1.24559  | -0.37534 |
| P                | -2.18119 | -0.74502 | 0.16025  | P                | 1.13895  | -0.62001 | 0.05704  | P                | 0.46905  | -1.66642 | 0.44804  |
| C                | 1.35342  | -1.14624 | 1.55176  | C                | -1.33258 | -1.01621 | -1.42920 | C                | -1.19915 | 0.14723  | -1.79473 |
| C                | -1.13502 | -0.58932 | 1.73216  | C                | 1.05698  | -1.88557 | -1.26597 | C                | -0.76726 | -2.17002 | -0.84899 |
| H                | 1.75355  | -0.55696 | 2.39890  | H                | -1.13777 | -0.46688 | -2.37023 | H                | -0.25892 | 0.01009  | -2.35410 |
| H                | 2.07771  | -1.95837 | 1.35686  | H                | -2.40208 | -1.27508 | -1.41919 | H                | -1.88687 | 0.74234  | -2.42101 |
| H                | -0.69865 | 0.41361  | 1.87184  | H                | 1.38480  | -1.41032 | -2.20813 | H                | -0.10829 | -2.51204 | -1.67040 |
| H                | -1.87930 | -0.69674 | 2.53838  | H                | 1.71017  | -2.74990 | -1.06540 | H                | -1.26363 | -3.07689 | -0.46387 |
| C                | 1.05843  | 1.72075  | 0.39098  | C                | -0.55575 | 1.96591  | -0.48981 | C                | 0.71420  | 2.15906  | -0.33688 |
| H                | 2.00078  | 2.24104  | 0.13176  | H                | -1.34499 | 2.60278  | -0.05723 | H                | 0.49592  | 3.00115  | 0.34752  |
| H                | 0.91568  | 1.86912  | 1.47563  | H                | -0.68026 | 2.03608  | -1.58747 | H                | 0.77419  | 2.59247  | -1.35380 |
| C                | -2.41018 | 1.03986  | -0.40408 | C                | 2.54436  | 0.55430  | -0.09689 | C                | 2.12423  | -1.09059 | -0.19199 |
| H                | -2.42180 | 1.02655  | -1.51044 | H                | 2.88706  | 0.78362  | 0.92774  | H                | 2.77784  | -1.18533 | 0.69599  |
| H                | -3.44913 | 1.27493  | -0.11372 | H                | 3.38026  | 0.07418  | -0.63327 | H                | 2.42719  | -1.91407 | -0.86404 |
| C                | -1.14021 | -1.51995 | -1.21726 | C                | 1.01741  | -1.37465 | 1.72965  | C                | -0.18260 | -1.05796 | 2.08002  |
| H                | -1.94187 | -1.86735 | -1.89381 | H                | 1.99992  | -1.44393 | 2.22350  | H                | 0.57100  | -1.36161 | 2.82751  |
| H                | -0.69491 | -2.45451 | -0.82684 | H                | 0.60996  | -2.39551 | 1.62441  | H                | -1.05267 | -1.72184 | 2.24895  |
| C                | 1.30238  | -0.68276 | -1.51248 | C                | -1.27823 | -0.27777 | 1.69773  | C                | -1.58062 | 0.91191  | 1.26382  |
| H                | 1.95173  | -0.05545 | -2.15231 | H                | -1.94098 | 0.47641  | 2.15254  | H                | -1.98446 | 1.90074  | 1.54890  |
| H                | 1.75980  | -1.68954 | -1.48135 | H                | -1.85864 | -1.21914 | 1.65435  | H                | -2.43913 | 0.22961  | 1.13726  |
| C                | -1.53555 | 2.20277  | 0.10509  | C                | 2.04639  | 1.83769  | -0.79046 | C                | 2.38528  | 0.26177  | -0.86534 |
| C                | -0.09528 | 2.35434  | -0.42599 | C                | 0.83773  | 2.47142  | -0.07080 | C                | 2.03469  | 1.46540  | 0.02526  |
| C                | -0.05343 | -1.67477 | 1.88025  | C                | -0.43951 | -2.26439 | -1.33388 | C                | -1.81404 | -1.19722 | -1.40485 |
| C                | -0.12796 | -0.74564 | -2.07181 | C                | 0.02718  | -0.46072 | 2.48758  | C                | -0.59274 | 0.39952  | 2.31318  |
| H                | -0.27947 | -2.55687 | 1.26057  | H                | -0.71898 | -2.86025 | -0.44642 | H                | -2.64195 | -1.05492 | -0.68951 |
| H                | -0.03422 | -1.24851 | -3.04985 | H                | -0.20081 | -0.88996 | 3.47701  | H                | -1.08283 | 0.47564  | 3.30007  |
| H                | 0.13952  | 3.43176  | -0.41032 | H                | 0.83632  | 3.55476  | -0.27768 | H                | 2.81061  | 2.24234  | -0.06786 |
| H                | -1.52662 | 2.22659  | 1.20972  | H                | 1.79292  | 1.63078  | -1.84669 | H                | 1.86214  | 0.32676  | -1.83593 |
| H                | -0.01233 | -2.04036 | 2.91844  | H                | -0.62280 | -2.90832 | -2.20924 | H                | -2.26920 | -1.64147 | -2.30695 |
| H                | -2.06706 | 3.12371  | -0.19207 | H                | 2.88075  | 2.55790  | -0.80867 | H                | 3.46162  | 0.29287  | -1.10802 |
| H                | -0.02645 | 2.06244  | -1.48665 | H                | 0.96594  | 2.38074  | 1.02460  | H                | 2.03403  | 1.16070  | 1.08508  |
| H                | -0.49753 | 0.26646  | -2.29026 | H                | 0.49498  | 0.52314  | 2.67122  | H                | 0.29204  | 1.05584  | 2.35805  |
| F                | 3.18664  | 0.12391  | 0.17315  | F                | -2.74370 | 0.70064  | -0.17014 | F                | -1.82067 | 2.50829  | -0.80762 |
| [4.3.3]hf_oo     |          |          |          | [4.3.3]hf_io     |          |          |          | [4.3.3]hf_ts     |          |          |          |

|                  |          |          |          |                  |          |          |          |                  |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|----------|------------------|----------|----------|----------|
| P                | 1.76243  | 0.01887  | -0.01798 | P                | -1.63110 | 0.39006  | -0.10905 | P                | -1.76079 | 0.17408  | -0.12628 |
| P                | -2.17302 | -0.62490 | 0.06235  | P                | 1.24757  | -0.54685 | -0.06921 | P                | 1.53102  | -0.58127 | 0.11132  |
| C                | 1.20529  | -1.40972 | 1.05977  | C                | -1.28579 | -0.94691 | -1.41994 | C                | -1.01921 | -0.76655 | -1.58938 |
| C                | -1.18480 | -0.42195 | 1.65306  | C                | 1.08407  | -2.00140 | -1.18807 | C                | 1.17949  | -1.95780 | -1.05346 |
| H                | 2.08477  | -1.60760 | 1.69725  | H                | -0.86362 | -0.39419 | -2.28255 | H                | -0.32386 | -0.09370 | -2.12081 |
| H                | 1.18599  | -2.25398 | 0.34769  | H                | -2.30033 | -1.26367 | -1.72722 | H                | -1.88484 | -0.92872 | -2.25640 |
| H                | -0.80566 | 0.60293  | 1.71707  | H                | 1.39576  | -1.69684 | -2.20357 | H                | 1.69501  | -1.66750 | -1.98874 |
| H                | -1.93364 | -0.51399 | 2.46024  | H                | 1.64247  | -2.91227 | -0.90602 | H                | 1.63296  | -2.90742 | -0.71821 |
| C                | 1.17213  | 1.65578  | 0.72420  | C                | -0.56887 | 1.92481  | -0.45726 | C                | -1.08178 | 1.92104  | -0.17880 |
| H                | 2.09756  | 2.25574  | 0.78301  | H                | -1.25682 | 2.73925  | -0.15383 | H                | -1.72951 | 2.45312  | 0.54585  |
| H                | 0.86977  | 1.48932  | 1.77220  | H                | -0.56852 | 1.96093  | -1.56595 | H                | -1.41983 | 2.28451  | -1.16998 |
| C                | -2.07327 | 1.11090  | -0.71170 | C                | 2.73931  | 0.53303  | -0.25355 | C                | 2.40929  | 0.91927  | -0.49293 |
| H                | -1.70876 | 1.02924  | -1.75026 | H                | 3.21687  | 0.66397  | 0.73457  | H                | 2.99373  | 1.31037  | 0.36083  |
| H                | -3.13465 | 1.40181  | -0.80552 | H                | 3.50343  | 0.15149  | -0.95212 | H                | 3.14158  | 0.62838  | -1.26713 |
| C                | -1.14714 | -1.79656 | -0.99929 | C                | 1.11651  | -1.23544 | 1.65090  | C                | 1.21439  | -0.87068 | 1.89872  |
| H                | -1.90534 | -2.29982 | -1.62489 | H                | 2.06951  | -1.19684 | 2.20830  | H                | 2.06480  | -0.51329 | 2.50664  |
| H                | -0.83572 | -2.57087 | -0.27569 | H                | 0.81736  | -2.29757 | 1.58129  | H                | 1.18517  | -1.97129 | 2.01548  |
| C                | 0.81601  | -0.11733 | -1.62753 | C                | -1.33480 | -0.35041 | 1.60716  | C                | -1.33864 | -0.62311 | 1.52918  |
| H                | 0.15645  | 0.75154  | -1.71762 | H                | -2.04530 | 0.20817  | 2.24398  | H                | -2.24344 | -0.40057 | 2.12463  |
| H                | 1.57949  | -0.00053 | -2.41727 | H                | -1.76672 | -1.36847 | 1.52331  | H                | -1.37463 | -1.71684 | 1.35649  |
| C                | -1.38317 | 2.27386  | 0.04564  | C                | 2.11648  | 1.87152  | -0.73458 | C                | 1.43743  | 2.00178  | -1.00347 |
| C                | 0.14293  | 2.52728  | -0.03837 | C                | 0.85356  | 2.30646  | 0.06771  | C                | 0.37526  | 2.38694  | 0.05246  |
| C                | -0.05149 | -1.40734 | 1.96744  | C                | -0.45030 | -2.22901 | -1.16247 | C                | -0.32896 | -2.11819 | -1.32947 |
| C                | 0.02655  | -1.39836 | -1.93004 | C                | 0.01839  | -0.41498 | 2.35564  | C                | -0.11031 | -0.26035 | 2.38516  |
| H                | -0.45209 | -2.43703 | 2.00833  | H                | -0.74232 | -2.67360 | -0.19268 | H                | -0.81102 | -2.64983 | -0.48984 |
| H                | 0.72257  | -2.25495 | -1.99770 | H                | -0.18198 | -0.84236 | 3.35657  | H                | -0.30204 | -0.62389 | 3.41385  |
| H                | 0.28167  | 3.54894  | 0.36244  | H                | 0.85666  | 3.41314  | 0.07970  | H                | 0.32160  | 3.49061  | 0.10266  |
| H                | -1.69109 | 2.25746  | 1.10693  | H                | 1.84619  | 1.78001  | -1.80307 | H                | 0.95066  | 1.65270  | -1.93059 |
| H                | 0.27807  | -1.18571 | 2.99839  | H                | -0.72413 | -2.97680 | -1.92895 | H                | -0.46154 | -2.76960 | -2.21321 |
| H                | -1.83950 | 3.19603  | -0.36097 | H                | 2.87480  | 2.67442  | -0.67161 | H                | 2.02537  | 2.89697  | -1.28253 |
| H                | 0.44135  | 2.60387  | -1.09963 | H                | 0.96896  | 2.00794  | 1.12476  | H                | 0.72511  | 2.06435  | 1.04718  |
| H                | -0.37556 | -1.27441 | -2.95168 | H                | 0.38485  | 0.61098  | 2.53142  | H                | -0.01906 | 0.83572  | 2.46257  |
| H                | 3.91433  | -0.02659 | -0.32092 | H                | -3.70701 | 0.93880  | -0.24463 | F                | -4.85962 | 0.24685  | -0.40861 |
| F                | 4.85777  | -0.02515 | -0.46563 | F                | -4.64036 | 1.16575  | -0.29373 | H                | -3.90384 | 0.23376  | -0.32071 |
| [4.3.3]h_plus_oo |          |          |          | [4.3.3]h_plus_io |          |          |          | [4.3.3]h_plus_ts |          |          |          |
| P                | -1.78872 | 0.53991  | 0.00276  | P                | -1.21313 | 0.28086  | -0.09284 | P                | -0.88446 | 1.28148  | -0.38689 |
| P                | 1.64672  | -1.27723 | -0.01380 | P                | 1.17330  | -0.59893 | 0.04371  | P                | 0.44933  | -1.56952 | 0.40742  |
| C                | -2.04185 | -0.95983 | -1.03104 | C                | -1.32378 | -1.00631 | -1.44390 | C                | -1.20193 | 0.14492  | -1.81026 |
| C                | 0.45371  | -1.22069 | -1.47932 | C                | 1.06805  | -1.90908 | -1.23860 | C                | -0.78034 | -2.16884 | -0.84186 |
| H                | -2.35778 | -0.53536 | -2.00332 | H                | -1.07648 | -0.46240 | -2.37673 | H                | -0.24451 | -0.00826 | -2.33528 |
| H                | -2.93325 | -1.44735 | -0.59494 | H                | -2.38900 | -1.28695 | -1.50649 | H                | -1.87258 | 0.70773  | -2.48142 |
| H                | 0.27109  | -0.19864 | -1.84999 | H                | 1.40001  | -1.46990 | -2.19677 | H                | -0.13204 | -2.53605 | -1.66042 |
| H                | 1.01139  | -1.72810 | -2.28383 | H                | 1.69526  | -2.78984 | -1.02487 | H                | -1.27513 | -3.06024 | -0.42062 |
| C                | -0.83747 | 1.92579  | -0.76533 | C                | -0.56750 | 1.97999  | -0.47263 | C                | 0.72611  | 2.16936  | -0.35263 |
| H                | -1.52369 | 2.77933  | -0.61813 | H                | -1.32824 | 2.65594  | -0.03863 | H                | 0.53219  | 3.02761  | 0.31927  |
| H                | -0.82095 | 1.73321  | -1.85297 | H                | -0.67847 | 2.07091  | -1.57131 | H                | 0.81457  | 2.59041  | -1.37245 |
| C                | 2.41645  | 0.44463  | -0.02299 | C                | 2.60056  | 0.54830  | -0.14822 | C                | 2.13706  | -1.09925 | -0.20499 |

|               |          |          |          |               |          |          |          |               |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| H             | 2.58239  | 0.72884  | 1.03347  | H             | 2.98881  | 0.76584  | 0.86264  | H             | 2.78212  | -1.20698 | 0.68726  |
| H             | 3.42803  | 0.28031  | -0.43380 | H             | 3.41536  | 0.08883  | -0.73240 | H             | 2.42659  | -1.92447 | -0.88018 |
| C             | 0.64643  | -1.29906 | 1.59044  | C             | 1.03928  | -1.34146 | 1.72573  | C             | -0.16231 | -1.05984 | 2.07893  |
| H             | 1.41858  | -1.65725 | 2.29556  | H             | 2.00659  | -1.38400 | 2.25227  | H             | 0.61161  | -1.35857 | 2.80702  |
| H             | -0.07344 | -2.13721 | 1.53380  | H             | 0.66183  | -2.37438 | 1.62301  | H             | -1.01796 | -1.74081 | 2.25154  |
| C             | -1.43847 | 0.25329  | 1.77684  | C             | -1.30569 | -0.29800 | 1.67940  | C             | -1.58287 | 0.91421  | 1.28119  |
| H             | -1.80527 | 1.16796  | 2.27840  | H             | -1.98081 | 0.41935  | 2.17801  | H             | -2.00390 | 1.88320  | 1.60347  |
| H             | -2.12609 | -0.56383 | 2.06663  | H             | -1.85283 | -1.25985 | 1.62788  | H             | -2.43402 | 0.22288  | 1.14313  |
| C             | 1.80987  | 1.62823  | -0.80384 | C             | 2.05297  | 1.83757  | -0.79689 | C             | 2.40189  | 0.26013  | -0.86535 |
| C             | 0.56104  | 2.34683  | -0.24927 | C             | 0.84390  | 2.42668  | -0.03205 | C             | 2.02563  | 1.45074  | 0.03564  |
| C             | -0.88203 | -1.94515 | -1.23214 | C             | -0.43699 | -2.25653 | -1.29604 | C             | -1.82275 | -1.19718 | -1.41188 |
| C             | -0.00332 | -0.06147 | 2.22328  | C             | 0.01206  | -0.45050 | 2.46034  | C             | -0.59448 | 0.38970  | 2.32550  |
| H             | -0.81828 | -2.63404 | -0.37484 | H             | -0.73057 | -2.81512 | -0.38857 | H             | -2.65353 | -1.04852 | -0.70038 |
| H             | -0.07209 | -0.22442 | 3.31341  | H             | -0.21740 | -0.87449 | 3.45244  | H             | -1.09206 | 0.44585  | 3.31039  |
| H             | 0.64058  | 3.40174  | -0.56277 | H             | 0.85410  | 3.52250  | -0.16199 | H             | 2.81392  | 2.22030  | -0.01266 |
| H             | 1.63938  | 1.35002  | -1.85942 | H             | 1.77481  | 1.64426  | -1.84946 | H             | 1.88256  | 0.32653  | -1.83768 |
| H             | -1.14985 | -2.57063 | -2.09882 | H             | -0.63386 | -2.92900 | -2.14730 | H             | -2.27460 | -1.64757 | -2.31279 |
| H             | 2.60536  | 2.39314  | -0.84072 | H             | 2.86382  | 2.58467  | -0.82453 | H             | 3.47980  | 0.30559  | -1.09981 |
| H             | 0.57438  | 2.37736  | 0.85223  | H             | 0.97265  | 2.25925  | 1.05393  | H             | 1.98554  | 1.12429  | 1.08823  |
| H             | 0.63961  | 0.82107  | 2.09573  | H             | 0.45068  | 0.54701  | 2.64011  | H             | 0.28176  | 1.05637  | 2.38535  |
| H             | -3.10626 | 1.04821  | 0.03012  | H             | -2.60783 | 0.67155  | -0.17593 | H             | -1.71481 | 2.37712  | -0.75124 |
| [4.3.3]lih_oo |          |          |          | [4.3.3]lih_io |          |          |          | [4.3.3]lih_ts |          |          |          |
| P             | 1.68291  | 0.01640  | -0.00221 | P             | -1.58290 | 0.38051  | -0.10643 | P             | -1.05285 | 1.49858  | -0.39634 |
| P             | -2.24651 | -0.62225 | 0.06202  | P             | 1.28086  | -0.55764 | -0.06273 | P             | 0.46274  | -1.44079 | 0.31466  |
| C             | 1.12778  | -1.41352 | 1.07421  | C             | -1.24899 | -0.95419 | -1.42219 | C             | -1.18223 | 0.16168  | -1.72652 |
| C             | -1.26439 | -0.42012 | 1.65743  | C             | 1.11798  | -2.00877 | -1.18577 | C             | -0.73228 | -2.19889 | -0.85726 |
| H             | 2.00298  | -1.61778 | 1.71539  | H             | -0.82344 | -0.40003 | -2.28205 | H             | -0.17831 | 0.00526  | -2.15680 |
| H             | 1.10444  | -2.25636 | 0.36056  | H             | -2.26198 | -1.27143 | -1.73416 | H             | -1.80118 | 0.62705  | -2.51440 |
| H             | -0.89021 | 0.60640  | 1.72653  | H             | 1.43144  | -1.70230 | -2.20006 | H             | -0.11164 | -2.52084 | -1.71500 |
| H             | -2.01633 | -0.51609 | 2.46105  | H             | 1.67618  | -2.91957 | -0.90443 | H             | -1.19535 | -3.10914 | -0.43746 |
| C             | 1.10116  | 1.65595  | 0.73977  | C             | -0.53100 | 1.92113  | -0.45744 | C             | 0.71532  | 2.12296  | -0.38913 |
| H             | 2.02483  | 2.25715  | 0.80796  | H             | -1.21706 | 2.73725  | -0.15386 | H             | 0.65102  | 3.03780  | 0.23281  |
| H             | 0.79092  | 1.48460  | 1.78436  | H             | -0.53140 | 1.95532  | -1.56623 | H             | 0.84897  | 2.49822  | -1.42364 |
| C             | -2.14229 | 1.11487  | -0.70961 | C             | 2.77071  | 0.52311  | -0.24934 | C             | 2.21234  | -1.19451 | -0.20249 |
| H             | -1.78210 | 1.03482  | -1.74995 | H             | 3.24755  | 0.65570  | 0.73875  | H             | 2.82707  | -1.28377 | 0.71261  |
| H             | -3.20324 | 1.40793  | -0.80040 | H             | 3.53458  | 0.13782  | -0.94584 | H             | 2.51481  | -2.02553 | -0.86426 |
| C             | -1.21791 | -1.79665 | -0.99496 | C             | 1.14983  | -1.24737 | 1.65633  | C             | -0.08949 | -1.16393 | 2.04595  |
| H             | -1.97436 | -2.29645 | -1.62513 | H             | 2.10254  | -1.21077 | 2.21383  | H             | 0.68792  | -1.49613 | 2.75685  |
| H             | -0.91371 | -2.57344 | -0.27093 | H             | 0.84828  | -2.30868 | 1.58673  | H             | -0.95404 | -1.84072 | 2.18774  |
| C             | 0.74470  | -0.11763 | -1.61607 | C             | -1.29920 | -0.35822 | 1.61285  | C             | -1.51977 | 0.86879  | 1.31800  |
| H             | 0.07933  | 0.74723  | -1.69661 | H             | -2.00809 | 0.20051  | 2.25122  | H             | -1.98112 | 1.76143  | 1.77933  |
| H             | 1.50309  | 0.00985  | -2.40878 | H             | -1.73176 | -1.37589 | 1.52698  | H             | -2.35862 | 0.16207  | 1.16307  |
| C             | -1.45022 | 2.27654  | 0.04797  | C             | 2.15162  | 1.86109  | -0.73474 | C             | 2.45228  | 0.17713  | -0.86348 |
| C             | 0.07666  | 2.52704  | -0.03038 | C             | 0.89109  | 2.30111  | 0.06709  | C             | 1.98900  | 1.35159  | 0.02881  |
| C             | -0.13099 | -1.40309 | 1.97863  | C             | -0.41566 | -2.23708 | -1.16286 | C             | -1.79793 | -1.19715 | -1.34475 |
| C             | -0.03853 | -1.40214 | -1.91997 | C             | 0.05418  | -0.42390 | 2.36067  | C             | -0.51240 | 0.28678  | 2.32738  |
| H             | -0.52993 | -2.43294 | 2.02282  | H             | -0.71093 | -2.68258 | -0.19463 | H             | -2.57979 | -1.07276 | -0.57470 |

|                |          |          |          |                |          |          |          |                |          |          |          |
|----------------|----------|----------|----------|----------------|----------|----------|----------|----------------|----------|----------|----------|
| H              | 0.65872  | -2.25801 | -1.98328 | H              | -0.14969 | -0.84991 | 3.36115  | H              | -0.98852 | 0.32267  | 3.32661  |
| H              | 0.21649  | 3.54775  | 0.37165  | H              | 0.89422  | 3.40755  | 0.07545  | H              | 2.79132  | 2.11240  | 0.04583  |
| H              | -1.76194 | 2.26342  | 1.10807  | H              | 1.88150  | 1.76819  | -1.80309 | H              | 1.94370  | 0.21094  | -1.84249 |
| H              | 0.19743  | -1.17675 | 3.00869  | H              | -0.69011 | -2.98230 | -1.93123 | H              | -2.31069 | -1.62183 | -2.22734 |
| H              | -1.90161 | 3.19948  | -0.36183 | H              | 2.91146  | 2.66216  | -0.67337 | H              | 3.53344  | 0.27806  | -1.07582 |
| H              | 0.38134  | 2.60358  | -1.08977 | H              | 1.00466  | 2.00576  | 1.12507  | H              | 1.89642  | 0.99843  | 1.06907  |
| H              | -0.43385 | -1.27859 | -2.94395 | H              | 0.42161  | 0.60164  | 2.53606  | H              | 0.37418  | 0.93897  | 2.38991  |
| H              | 5.87182  | -0.00971 | -0.59454 | H              | -5.69482 | 1.39693  | -0.33395 | H              | -3.64428 | 4.70162  | -1.38250 |
| Li             | 4.25208  | -0.05036 | -0.34807 | Li             | -4.08776 | 1.04645  | -0.28129 | Li             | -2.62284 | 3.47139  | -1.00561 |
| [4.3.3]oo      |          |          |          | [4.3.3]io      |          |          |          | [4.3.3]ioTS    |          |          |          |
| P              | 1.84048  | 0.05682  | 0.08364  | P              | -1.74526 | 0.41688  | -0.20178 | P              | -1.20617 | 1.53375  | -0.43525 |
| P              | -2.13469 | -0.66504 | -0.03310 | P              | 1.18214  | -0.53694 | -0.04519 | P              | 0.49752  | -1.34881 | 0.29218  |
| C              | 1.20589  | -1.37976 | 1.12442  | C              | -1.31336 | -1.00580 | -1.41261 | C              | -1.18338 | 0.16204  | -1.75374 |
| C              | -1.23399 | -0.43878 | 1.60407  | C              | 1.04286  | -2.06796 | -1.06097 | C              | -0.62463 | -2.18247 | -0.89873 |
| H              | 2.05089  | -1.59385 | 1.80271  | H              | -0.85139 | -0.50274 | -2.28557 | H              | -0.15647 | 0.06047  | -2.14613 |
| H              | 1.21401  | -2.21903 | 0.40617  | H              | -2.31202 | -1.34301 | -1.75060 | H              | -1.79711 | 0.58787  | -2.56836 |
| H              | -0.88984 | 0.59694  | 1.68281  | H              | 1.38009  | -1.84050 | -2.08833 | H              | 0.02757  | -2.46270 | -1.74778 |
| H              | -2.01901 | -0.55237 | 2.37363  | H              | 1.58426  | -2.96157 | -0.69990 | H              | -1.04365 | -3.11984 | -0.49103 |
| C              | 1.13118  | 1.66792  | 0.80678  | C              | -0.59519 | 1.89443  | -0.59467 | C              | 0.55782  | 2.19962  | -0.37917 |
| H              | 2.02827  | 2.29972  | 0.93529  | H              | -1.27900 | 2.74652  | -0.40491 | H              | 0.44648  | 3.11348  | 0.23834  |
| H              | 0.76660  | 1.47981  | 1.83143  | H              | -0.52286 | 1.83870  | -1.70049 | H              | 0.70093  | 2.58283  | -1.41013 |
| C              | -2.03257 | 1.07366  | -0.80014 | C              | 2.69806  | 0.51363  | -0.21766 | C              | 2.24925  | -1.03214 | -0.17374 |
| H              | -1.62113 | 0.99905  | -1.82161 | H              | 3.15970  | 0.66203  | 0.77568  | H              | 2.84464  | -1.09277 | 0.75653  |
| H              | -3.09377 | 1.34704  | -0.94006 | H              | 3.46907  | 0.10447  | -0.89287 | H              | 2.61216  | -1.84082 | -0.83316 |
| C              | -1.03137 | -1.81400 | -1.03928 | C              | 0.99477  | -1.12573 | 1.70839  | C              | -0.09515 | -1.13936 | 2.01882  |
| H              | -1.74426 | -2.32895 | -1.70753 | H              | 1.93332  | -1.05395 | 2.28744  | H              | 0.68843  | -1.43330 | 2.74035  |
| H              | -0.74760 | -2.58349 | -0.29924 | H              | 0.70066  | -2.19148 | 1.68949  | H              | -0.92236 | -1.86561 | 2.13810  |
| C              | 0.92476  | -0.08899 | -1.55435 | C              | -1.45658 | -0.24898 | 1.55679  | C              | -1.62461 | 0.81662  | 1.27047  |
| H              | 0.23903  | 0.75745  | -1.65785 | H              | -2.18024 | 0.33198  | 2.15826  | H              | -2.15406 | 1.66684  | 1.73982  |
| H              | 1.70322  | 0.06076  | -2.32436 | H              | -1.88275 | -1.27243 | 1.51270  | H              | -2.41415 | 0.05906  | 1.09302  |
| C              | -1.39715 | 2.24795  | -0.01254 | C              | 2.10369  | 1.84830  | -0.74620 | C              | 2.42549  | 0.35767  | -0.81966 |
| C              | 0.12833  | 2.52419  | -0.00819 | C              | 0.80291  | 2.30243  | -0.01623 | C              | 1.86430  | 1.49514  | 0.06647  |
| C              | -0.08714 | -1.38697 | 1.97964  | C              | -0.49552 | -2.27751 | -1.05490 | C              | -1.73340 | -1.23256 | -1.39819 |
| C              | 0.18567  | -1.38882 | -1.90025 | C              | -0.12273 | -0.27642 | 2.34258  | C              | -0.60772 | 0.28310  | 2.29986  |
| H              | -0.46471 | -2.42564 | 2.02927  | H              | -0.81157 | -2.65567 | -0.06455 | H              | -2.53225 | -1.15816 | -0.63873 |
| H              | 0.90404  | -2.22975 | -1.92509 | H              | -0.34683 | -0.65872 | 3.35721  | H              | -1.10277 | 0.28167  | 3.29146  |
| H              | 0.22284  | 3.54777  | 0.40182  | H              | 0.80567  | 3.40928  | -0.04214 | H              | 2.62432  | 2.29831  | 0.11384  |
| H              | -1.76482 | 2.23168  | 1.02973  | H              | 1.88359  | 1.74090  | -1.82471 | H              | 1.94061  | 0.36690  | -1.81113 |
| H              | 0.19384  | -1.13480 | 3.01852  | H              | -0.75869 | -3.07314 | -1.77629 | H              | -2.20825 | -1.68082 | -2.29122 |
| H              | -1.84263 | 3.16237  | -0.44856 | H              | 2.86150  | 2.65000  | -0.65940 | H              | 3.50445  | 0.52596  | -1.00226 |
| H              | 0.48353  | 2.61066  | -1.05133 | H              | 0.87410  | 2.04194  | 1.05440  | H              | 1.76491  | 1.12521  | 1.10049  |
| H              | -0.16134 | -1.27794 | -2.94382 | H              | 0.23750  | 0.75707  | 2.48245  | H              | 0.24024  | 0.98268  | 2.38550  |
| [4.4.3]        |          |          |          |                |          |          |          |                |          |          |          |
| [4.4.3]agcl_oo |          |          |          | [4.4.3]agcl_io |          |          |          | [4.4.3]agcl_ts |          |          |          |
| P              | 0.16454  | 0.09269  | 2.10151  | P              | -0.03951 | 0.17716  | 2.11678  | P              | 0.52954  | -1.85541 | -0.51871 |
| P              | 0.07723  | 0.02796  | -2.04225 | P              | -0.24997 | -0.16146 | -0.91065 | P              | -0.40592 | 1.40202  | 0.70010  |
| C              | 0.79848  | -1.62902 | 1.67307  | C              | 0.36726  | -1.64374 | 1.76230  | C              | 2.14333  | -0.97190 | -0.12771 |

|                |          |          |          |                |          |          |          |                |          |          |          |
|----------------|----------|----------|----------|----------------|----------|----------|----------|----------------|----------|----------|----------|
| C              | -0.89930 | -1.44313 | -1.35245 | C              | -0.24207 | -1.82040 | -1.72156 | C              | 0.95447  | 2.28830  | -0.19479 |
| H              | 0.95446  | -2.08348 | 2.66505  | H              | 0.29540  | -2.09679 | 2.76558  | H              | 2.91492  | -1.74183 | -0.28800 |
| H              | 1.80905  | -1.50864 | 1.24695  | H              | 1.45014  | -1.62889 | 1.52970  | H              | 2.14250  | -0.76580 | 0.95524  |
| H              | -1.71076 | -1.10649 | -0.69364 | H              | -1.29150 | -2.06496 | -1.96900 | H              | 0.61285  | 2.35636  | -1.24618 |
| H              | -1.40136 | -1.85128 | -2.24661 | H              | 0.35244  | -1.88750 | -2.64979 | H              | 1.04338  | 3.32316  | 0.17700  |
| C              | -1.64786 | 0.17702  | 1.61913  | C              | -1.78204 | 0.64145  | 1.57938  | C              | -0.47682 | -0.79857 | -1.67598 |
| H              | -2.18086 | 0.08168  | 2.57862  | H              | -2.30048 | 0.86928  | 2.52713  | H              | -0.34195 | -1.24556 | -2.67616 |
| H              | -1.91521 | -0.71432 | 1.03601  | H              | -2.23625 | -0.28258 | 1.18139  | H              | -0.02251 | 0.20080  | -1.69605 |
| C              | -0.92639 | 1.55593  | -1.51165 | C              | -1.33073 | 1.05210  | -1.81580 | C              | -2.12674 | 1.50970  | 0.02376  |
| H              | -0.22075 | 2.31549  | -1.13203 | H              | -0.72299 | 1.93583  | -2.08343 | H              | -2.74909 | 1.08764  | 0.83576  |
| H              | -1.26420 | 1.95438  | -2.48461 | H              | -1.73480 | 0.63500  | -2.75482 | H              | -2.41993 | 2.57136  | -0.05171 |
| C              | 1.68740  | 0.01350  | -1.05586 | C              | 1.46832  | 0.50651  | -1.07676 | C              | -0.15319 | 0.32342  | 2.18235  |
| H              | 2.46880  | 0.06859  | -1.83430 | H              | 1.72049  | 0.84087  | -2.09962 | H              | -0.50346 | 0.83220  | 3.09641  |
| H              | 1.77996  | -0.99845 | -0.63971 | H              | 2.17642  | -0.29626 | -0.79862 | H              | 0.93588  | 0.18595  | 2.30163  |
| C              | 1.05305  | 1.40844  | 1.11345  | C              | 1.32585  | 1.26869  | 1.40720  | C              | -0.27064 | -2.11162 | 1.15192  |
| H              | 0.25964  | 2.05997  | 0.72623  | H              | 1.25924  | 2.18871  | 2.01516  | H              | -1.01977 | -2.90697 | 0.99191  |
| H              | 1.58423  | 2.00825  | 1.86988  | H              | 2.22291  | 0.74177  | 1.78930  | H              | 0.55802  | -2.60999 | 1.69342  |
| C              | -2.20113 | 1.46311  | -0.63668 | C              | -2.46329 | 1.46018  | -0.84459 | C              | -2.44894 | 0.78284  | -1.29850 |
| C              | -2.14112 | 1.45725  | 0.90733  | C              | -1.99464 | 1.82786  | 0.58784  | C              | -1.98728 | -0.68300 | -1.34342 |
| C              | -0.11613 | -2.59336 | -0.67978 | C              | 0.26734  | -2.79185 | -0.62954 | C              | 2.34763  | 1.63704  | -0.15514 |
| C              | -0.06459 | -2.62630 | 0.86311  | C              | -0.38325 | -2.56885 | 0.76285  | C              | 2.53424  | 0.30529  | -0.90766 |
| C              | 2.05784  | 1.06137  | 0.00460  | C              | 1.55083  | 1.66531  | -0.06976 | C              | -0.88866 | -1.02225 | 2.05089  |
| H              | 0.90421  | -2.68177 | -1.09402 | H              | 1.36536  | -2.70294 | -0.53309 | H              | 2.67741  | 1.51280  | 0.89348  |
| H              | -1.09792 | -2.61592 | 1.25487  | H              | -1.43083 | -2.23906 | 0.63247  | H              | 2.03172  | 0.35486  | -1.88981 |
| H              | 3.00453  | 0.73206  | 0.47180  | H              | 2.54635  | 2.14290  | -0.12258 | H              | -0.97170 | -1.46599 | 3.06176  |
| H              | -3.18387 | 1.60572  | 1.24009  | H              | -2.77536 | 2.47007  | 1.03014  | H              | -2.56317 | -1.22421 | -2.11172 |
| H              | -2.81052 | 0.60224  | -0.96716 | H              | -3.19811 | 0.63699  | -0.76929 | H              | -2.00119 | 1.32800  | -2.14991 |
| H              | -0.61786 | -3.53438 | -0.96831 | H              | 0.07497  | -3.82891 | -0.95593 | H              | 3.04168  | 2.37587  | -0.59644 |
| H              | 0.32866  | -3.62386 | 1.13233  | H              | -0.44202 | -3.55334 | 1.26033  | H              | 3.60972  | 0.21735  | -1.13820 |
| H              | -2.80455 | 2.35188  | -0.89934 | H              | -3.00833 | 2.32255  | -1.26975 | H              | -3.54416 | 0.83429  | -1.44398 |
| H              | -1.60243 | 2.34882  | 1.27496  | H              | -1.09378 | 2.46455  | 0.53487  | H              | -2.23386 | -1.16967 | -0.38427 |
| H              | 2.30118  | 2.01492  | -0.49939 | H              | 0.82903  | 2.44846  | -0.35939 | H              | -1.92681 | -0.82579 | 1.73477  |
| Cl             | 0.65483  | 0.94788  | 6.60385  | Cl             | 0.35717  | 0.74210  | 6.69061  | Cl             | 1.28542  | -6.02514 | -2.33754 |
| Ag             | 0.41707  | 0.52189  | 4.36904  | Ag             | 0.16114  | 0.45908  | 4.42214  | Ag             | 0.90996  | -3.95554 | -1.43027 |
| [4.4.3]beh2_oo |          |          |          | [4.4.3]beh2_io |          |          |          | [4.4.3]beh2_ts |          |          |          |
| P              | 1.80079  | -0.00228 | 0.20695  | P              | 0.11928  | 0.19692  | 2.07458  | P              | 0.52010  | -1.85006 | -0.48119 |
| P              | -2.31221 | 0.11010  | 0.31363  | P              | -0.28991 | -0.17458 | -0.94818 | P              | -0.41869 | 1.41402  | 0.68829  |
| C              | 1.39787  | 1.82572  | 0.03605  | C              | 0.45477  | -1.63515 | 1.75633  | C              | 2.14786  | -0.97284 | -0.14434 |
| C              | -1.51715 | 0.88733  | -1.20812 | C              | -0.28366 | -1.84470 | -1.73661 | C              | 0.94027  | 2.30043  | -0.20529 |
| H              | 2.40954  | 2.26110  | -0.04135 | H              | 0.33212  | -2.05210 | 2.77232  | H              | 2.90905  | -1.74187 | -0.36734 |
| H              | 1.00371  | 2.15911  | 1.01177  | H              | 1.54272  | -1.67872 | 1.55146  | H              | 2.20762  | -0.79748 | 0.94292  |
| H              | -0.72476 | 0.23881  | -1.59327 | H              | -1.33599 | -2.12574 | -1.92557 | H              | 0.60583  | 2.36275  | -1.25913 |
| H              | -2.31973 | 0.86744  | -1.96625 | H              | 0.26843  | -1.91920 | -2.69043 | H              | 1.02955  | 3.33715  | 0.16184  |
| C              | 1.33972  | -0.96881 | -1.34228 | C              | -1.64485 | 0.67948  | 1.63680  | C              | -0.49372 | -0.83623 | -1.66503 |
| H              | 2.31996  | -1.28825 | -1.74197 | H              | -2.10199 | 0.93789  | 2.61139  | H              | -0.36203 | -1.33168 | -2.64379 |
| H              | 0.92230  | -0.29389 | -2.10593 | H              | -2.13844 | -0.24720 | 1.29646  | H              | -0.03370 | 0.15849  | -1.73965 |
| C              | -1.87485 | -1.72518 | 0.06337  | C              | -1.42260 | 1.03050  | -1.80075 | C              | -2.13994 | 1.51371  | 0.01499  |

|               |          |          |          |               |          |          |          |               |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| H             | -1.46394 | -2.12858 | 1.00522  | H             | -0.83158 | 1.90712  | -2.12423 | H             | -2.76160 | 1.09432  | 0.82888  |
| H             | -2.86720 | -2.19972 | -0.03531 | H             | -1.89571 | 0.60203  | -2.70175 | H             | -2.43785 | 2.57357  | -0.06906 |
| C             | -1.28056 | 0.76281  | 1.75439  | C             | 1.41526  | 0.50096  | -1.21216 | C             | -0.15080 | 0.35613  | 2.18230  |
| H             | -2.03314 | 0.99154  | 2.52974  | H             | 1.60286  | 0.83457  | -2.24937 | H             | -0.47934 | 0.87795  | 3.09703  |
| H             | -0.92189 | 1.74810  | 1.41992  | H             | 2.13797  | -0.30378 | -0.98056 | H             | 0.93971  | 0.21010  | 2.27920  |
| C             | 0.87051  | -0.79136 | 1.61604  | C             | 1.44902  | 1.25548  | 1.27401  | C             | -0.27027 | -2.08330 | 1.19079  |
| H             | 0.40840  | -1.69459 | 1.20175  | H             | 1.44014  | 2.16750  | 1.89815  | H             | -1.00993 | -2.89069 | 1.03984  |
| H             | 1.66616  | -1.15500 | 2.28933  | H             | 2.36516  | 0.70983  | 1.57883  | H             | 0.56162  | -2.57371 | 1.73451  |
| C             | -1.06006 | -2.19719 | -1.17108 | C             | -2.48197 | 1.45741  | -0.75632 | C             | -2.45476 | 0.77525  | -1.30207 |
| C             | 0.48831  | -2.25211 | -1.18266 | C             | -1.91687 | 1.84669  | 0.63628  | C             | -2.00161 | -0.69413 | -1.32973 |
| C             | -0.96568 | 2.32297  | -1.07502 | C             | 0.30785  | -2.77322 | -0.64648 | C             | 2.33025  | 1.64316  | -0.15282 |
| C             | 0.57007  | 2.40402  | -1.13271 | C             | -0.30525 | -2.56115 | 0.76592  | C             | 2.51918  | 0.31589  | -0.91309 |
| C             | -0.14898 | -0.01079 | 2.45583  | C             | 1.57111  | 1.65797  | -0.21184 | C             | -0.89224 | -0.98915 | 2.07747  |
| H             | -1.33732 | 2.83177  | -0.16760 | H             | 1.40312  | -2.62987 | -0.59113 | H             | 2.64736  | 1.51238  | 0.89902  |
| H             | 0.91573  | 1.95676  | -2.08306 | H             | -1.35929 | -2.24088 | 0.66644  | H             | 2.00808  | 0.36520  | -1.89060 |
| H             | 0.38778  | 0.70655  | 3.10458  | H             | 2.56155  | 2.13298  | -0.33734 | H             | -0.97206 | -1.41472 | 3.09635  |
| H             | 0.74266  | -2.87243 | -2.06171 | H             | -2.66453 | 2.50186  | 1.11547  | H             | -2.58648 | -1.23708 | -2.09061 |
| H             | -1.40647 | -1.65645 | -2.06988 | H             | -3.21089 | 0.63701  | -0.61817 | H             | -1.99650 | 1.30977  | -2.15473 |
| H             | -1.34605 | 2.92538  | -1.91810 | H             | 0.15572  | -3.82339 | -0.95221 | H             | 3.03260  | 2.38173  | -0.58166 |
| H             | 0.84645  | 3.47252  | -1.19633 | H             | -0.34067 | -3.54897 | 1.25990  | H             | 3.59323  | 0.23735  | -1.15454 |
| H             | -1.37143 | -3.24538 | -1.33789 | H             | -3.05405 | 2.31519  | -1.15522 | H             | -3.54872 | 0.83156  | -1.45744 |
| H             | 0.85249  | -2.83628 | -0.31903 | H             | -1.01952 | 2.47776  | 0.51346  | H             | -2.25275 | -1.16672 | -0.36436 |
| H             | -0.59893 | -0.74476 | 3.14938  | H             | 0.83302  | 2.44369  | -0.44861 | H             | -1.93146 | -0.79614 | 1.76201  |
| Be            | 3.95728  | -0.45900 | 0.29538  | H             | -0.32034 | -0.46064 | 4.97122  | H             | 1.67052  | -3.43536 | -2.61659 |
| H             | 4.73370  | 0.53447  | -0.25040 | H             | 0.43936  | 1.94696  | 4.47053  | H             | 1.12822  | -4.84762 | -0.52910 |
| H             | 4.06790  | -1.75773 | 0.74580  | Be            | 0.13311  | 0.61999  | 4.24422  | Be            | 1.18435  | -3.75855 | -1.36476 |
| [4.4.3]bh3_oo |          |          |          | [4.4.3]bh3_io |          |          |          | [4.4.3]bh3_ts |          |          |          |
| P             | 0.11372  | 0.05668  | 2.04842  | P             | -0.03091 | 0.17635  | 2.09815  | P             | 0.52216  | -1.83757 | -0.50370 |
| P             | 0.11145  | -0.00728 | -2.03953 | P             | -0.24596 | -0.15843 | -0.91153 | P             | -0.40464 | 1.37437  | 0.69436  |
| C             | 0.76596  | -1.64991 | 1.64446  | C             | 0.35986  | -1.63604 | 1.77152  | C             | 2.15399  | -1.00089 | -0.16302 |
| C             | -0.87180 | -1.37473 | -1.19326 | C             | -0.22900 | -1.82123 | -1.71536 | C             | 0.94789  | 2.25640  | -0.21484 |
| H             | 0.92988  | -2.04983 | 2.66071  | H             | 0.26132  | -2.05793 | 2.78790  | H             | 2.87768  | -1.79839 | -0.40624 |
| H             | 1.77321  | -1.51528 | 1.21454  | H             | 1.44608  | -1.64571 | 1.55777  | H             | 2.23302  | -0.83862 | 0.92511  |
| H             | -1.46517 | -0.96201 | -0.37221 | H             | -1.27692 | -2.06767 | -1.96776 | H             | 0.61088  | 2.30477  | -1.26860 |
| H             | -1.59855 | -1.69247 | -1.96147 | H             | 0.37125  | -1.89418 | -2.63974 | H             | 1.02870  | 3.29757  | 0.14140  |
| C             | -1.70901 | 0.24395  | 1.67729  | C             | -1.76236 | 0.67466  | 1.60416  | C             | -0.49190 | -0.84762 | -1.69466 |
| H             | -2.12736 | 0.36781  | 2.69183  | H             | -2.21740 | 0.94552  | 2.57409  | H             | -0.36498 | -1.38181 | -2.65343 |
| H             | -2.13163 | -0.69863 | 1.29529  | H             | -2.26764 | -0.24547 | 1.26136  | H             | -0.03129 | 0.14377  | -1.80523 |
| C             | -0.90275 | 1.53094  | -1.56273 | C             | -1.33432 | 1.04864  | -1.81491 | C             | -2.12791 | 1.48438  | 0.02868  |
| H             | -0.22145 | 2.29965  | -1.15884 | H             | -0.73372 | 1.93836  | -2.07930 | H             | -2.74692 | 1.04982  | 0.83652  |
| H             | -1.22432 | 1.92550  | -2.54267 | H             | -1.73819 | 0.63274  | -2.75482 | H             | -2.42608 | 2.54567  | -0.03493 |
| C             | 1.73389  | 0.05768  | -1.07641 | C             | 1.47025  | 0.51894  | -1.07411 | C             | -0.13875 | 0.29926  | 2.17723  |
| H             | 2.49692  | 0.20091  | -1.86201 | H             | 1.71935  | 0.86071  | -2.09547 | H             | -0.46266 | 0.81534  | 3.09677  |
| H             | 1.89387  | -0.97244 | -0.72290 | H             | 2.18016  | -0.28493 | -0.80328 | H             | 0.95076  | 0.14429  | 2.27086  |
| C             | 1.01405  | 1.38533  | 1.11739  | C             | 1.33860  | 1.25433  | 1.41302  | C             | -0.27206 | -2.11717 | 1.15067  |
| H             | 0.24260  | 2.05151  | 0.71334  | H             | 1.27604  | 2.15899  | 2.04494  | H             | -1.01248 | -2.91593 | 0.96346  |
| H             | 1.51005  | 1.95454  | 1.92304  | H             | 2.23101  | 0.71132  | 1.78179  | H             | 0.55748  | -2.62100 | 1.68465  |

|                    |          |          |          |                    |          |          |          |                    |          |          |          |
|--------------------|----------|----------|----------|--------------------|----------|----------|----------|--------------------|----------|----------|----------|
| C                  | -2.19485 | 1.40493  | -0.71146 | C                  | -2.46667 | 1.44218  | -0.83745 | C                  | -2.44603 | 0.77128  | -1.30079 |
| C                  | -2.17394 | 1.45685  | 0.83618  | C                  | -1.99798 | 1.83442  | 0.58899  | C                  | -1.99944 | -0.69863 | -1.36010 |
| C                  | -0.09304 | -2.60361 | -0.67646 | C                  | 0.27366  | -2.78838 | -0.61490 | C                  | 2.34410  | 1.61290  | -0.15873 |
| C                  | -0.04796 | -2.69957 | 0.85872  | C                  | -0.38529 | -2.56399 | 0.77413  | C                  | 2.54839  | 0.28778  | -0.91719 |
| C                  | 2.06200  | 1.06541  | 0.04152  | C                  | 1.55647  | 1.67057  | -0.05667 | C                  | -0.88996 | -1.03949 | 2.05729  |
| H                  | 0.93091  | -2.65366 | -1.08806 | H                  | 1.37083  | -2.69606 | -0.51131 | H                  | 2.65972  | 1.48478  | 0.89395  |
| H                  | -1.08348 | -2.72583 | 1.24566  | H                  | -1.43107 | -2.23066 | 0.63622  | H                  | 2.06040  | 0.34120  | -1.90674 |
| H                  | 2.98640  | 0.71500  | 0.53687  | H                  | 2.55043  | 2.15067  | -0.11641 | H                  | -0.96956 | -1.47883 | 3.07014  |
| H                  | -3.22675 | 1.62184  | 1.13050  | H                  | -2.78935 | 2.47009  | 1.02252  | H                  | -2.58296 | -1.22042 | -2.13616 |
| H                  | -2.76702 | 0.51688  | -1.03446 | H                  | -3.18264 | 0.60342  | -0.74986 | H                  | -1.98770 | 1.32115  | -2.14372 |
| H                  | -0.59419 | -3.51764 | -1.03926 | H                  | 0.08654  | -3.82650 | -0.94178 | H                  | 3.03995  | 2.35840  | -0.58610 |
| H                  | 0.38809  | -3.68063 | 1.12207  | H                  | -0.44945 | -3.54892 | 1.27034  | H                  | 3.62830  | 0.20820  | -1.13161 |
| H                  | -2.82264 | 2.26592  | -1.00779 | H                  | -3.03334 | 2.28862  | -1.26708 | H                  | -3.54003 | 0.83450  | -1.45358 |
| H                  | -1.64676 | 2.36738  | 1.17279  | H                  | -1.10914 | 2.48712  | 0.52424  | H                  | -2.25746 | -1.19575 | -0.40885 |
| H                  | 2.33147  | 2.03204  | -0.42206 | H                  | 0.83046  | 2.45375  | -0.33648 | H                  | -1.92843 | -0.83636 | 1.74616  |
| B                  | 0.37479  | 0.35913  | 3.94469  | B                  | 0.11380  | 0.38886  | 4.02392  | H                  | 1.49752  | -3.33454 | -2.28933 |
| H                  | -0.03020 | 1.50436  | 4.12866  | H                  | 1.24524  | 0.01336  | 4.32291  | H                  | 1.51176  | -4.20087 | -0.42702 |
| H                  | -0.30593 | -0.50403 | 4.49238  | H                  | -0.08556 | 1.58297  | 4.23711  | H                  | -0.24905 | -4.06222 | -1.49143 |
| H                  | 1.58376  | 0.22677  | 4.11665  | H                  | -0.77038 | -0.33911 | 4.47353  | B                  | 0.86114  | -3.58638 | -1.26722 |
| [4.4.3]ch3_plus_oo |          |          |          | [4.4.3]ch3_plus_io |          |          |          | [4.4.3]ch3_plus_ts |          |          |          |
| P                  | 1.03309  | 0.06705  | -0.03337 | P                  | 0.89344  | 0.03909  | -0.00215 | P                  | 1.50127  | -0.36100 | -0.08017 |
| P                  | -2.88021 | 0.02627  | 0.52967  | P                  | -1.83043 | 0.02214  | 0.22386  | P                  | -1.73548 | 0.45874  | 0.51018  |
| C                  | 0.67702  | 1.88293  | -0.15542 | C                  | 0.62667  | 1.86422  | -0.27769 | C                  | 1.73424  | 1.45139  | 0.18388  |
| C                  | -2.27910 | 0.83022  | -1.07015 | C                  | -2.81615 | 1.48550  | -0.30987 | C                  | -1.52383 | 1.91485  | -0.63436 |
| H                  | 1.67967  | 2.30642  | -0.34406 | H                  | 1.57936  | 2.20775  | -0.71809 | H                  | 2.82877  | 1.58526  | 0.11913  |
| H                  | 0.39384  | 2.20908  | 0.85958  | H                  | 0.59579  | 2.29421  | 0.74244  | H                  | 1.46063  | 1.66519  | 1.22988  |
| H                  | -1.51390 | 0.22131  | -1.56441 | H                  | -3.18969 | 1.25786  | -1.32494 | H                  | -1.42455 | 1.51601  | -1.66185 |
| H                  | -3.16308 | 0.76990  | -1.72833 | H                  | -3.69042 | 1.66432  | 0.33918  | H                  | -2.47069 | 2.47773  | -0.60944 |
| C                  | 0.59473  | -0.96391 | -1.50867 | C                  | 0.53226  | -1.10967 | -1.41078 | C                  | 0.52779  | -0.84813 | -1.55626 |
| H                  | 1.57901  | -1.23564 | -1.93025 | H                  | 1.52099  | -1.44077 | -1.77442 | H                  | 1.27868  | -1.05543 | -2.34031 |
| H                  | 0.10751  | -0.33098 | -2.26570 | H                  | 0.09903  | -0.47171 | -2.20347 | H                  | -0.04109 | 0.03413  | -1.88084 |
| C                  | -2.41257 | -1.79711 | 0.23536  | C                  | -2.67541 | -1.54114 | -0.29987 | C                  | -2.51651 | -1.05104 | -0.23500 |
| H                  | -1.89580 | -2.19539 | 1.12662  | H                  | -2.69193 | -2.22426 | 0.56819  | H                  | -2.54352 | -1.78238 | 0.59426  |
| H                  | -3.39657 | -2.29668 | 0.24700  | H                  | -3.72346 | -1.34527 | -0.58483 | H                  | -3.57167 | -0.80484 | -0.44327 |
| C                  | -1.74165 | 0.71904  | 1.87423  | C                  | -1.76263 | -0.02422 | 2.06629  | C                  | -0.88230 | 0.21639  | 2.14687  |
| H                  | -2.42707 | 0.88575  | 2.72290  | H                  | -2.70644 | -0.35833 | 2.52938  | H                  | -1.64373 | 0.26468  | 2.94148  |
| H                  | -1.48585 | 1.73572  | 1.53497  | H                  | -1.53945 | 0.99229  | 2.43920  | H                  | -0.21131 | 1.07662  | 2.31603  |
| C                  | 0.43931  | -0.74344 | 1.50689  | C                  | 0.73806  | -0.54172 | 1.76536  | C                  | 1.20512  | -1.20764 | 1.52683  |
| H                  | -0.01709 | -1.68541 | 1.18020  | H                  | 1.48790  | -1.34697 | 1.86119  | H                  | 1.50488  | -2.25867 | 1.36492  |
| H                  | 1.35943  | -1.01732 | 2.05232  | H                  | 1.14569  | 0.32278  | 2.32596  | H                  | 2.00066  | -0.75820 | 2.15362  |
| C                  | -1.73257 | -2.25280 | -1.08273 | C                  | -1.87739 | -2.17581 | -1.45473 | C                  | -1.89533 | -1.69816 | -1.48408 |
| C                  | -0.19508 | -2.27355 | -1.25243 | C                  | -0.37062 | -2.34953 | -1.15941 | C                  | -0.41156 | -2.06951 | -1.35494 |
| C                  | -1.79468 | 2.29391  | -0.99779 | C                  | -1.86570 | 2.69714  | -0.36864 | C                  | -0.37365 | 2.89060  | -0.34506 |
| C                  | -0.28324 | 2.44615  | -1.22761 | C                  | -0.55112 | 2.39882  | -1.12530 | C                  | 1.03446  | 2.44464  | -0.76612 |
| C                  | -0.50362 | 0.01219  | 2.45761  | C                  | -0.60136 | -0.98748 | 2.37709  | C                  | -0.14407 | -1.12738 | 2.25098  |
| H                  | -2.08620 | 2.78720  | -0.05419 | H                  | -1.63124 | 3.05053  | 0.65213  | H                  | -0.36839 | 3.17869  | 0.72242  |
| H                  | -0.01812 | 2.02721  | -2.21534 | H                  | -0.75475 | 1.72231  | -1.97722 | H                  | 1.02344  | 2.06582  | -1.80398 |

|               |          |          |          |               |          |          |          |               |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| H             | 0.07810  | 0.75371  | 3.03423  | H             | -0.45698 | -1.07854 | 3.46699  | H             | 0.04814  | -1.34673 | 3.31661  |
| H             | -0.00314 | -2.88364 | -2.15267 | H             | 0.01314  | -3.13904 | -1.82674 | H             | -0.16136 | -2.81763 | -2.12380 |
| H             | -2.18203 | -1.72243 | -1.94022 | H             | -1.99583 | -1.57267 | -2.37388 | H             | -2.02645 | -1.03985 | -2.36217 |
| H             | -2.29181 | 2.87471  | -1.79202 | H             | -2.38868 | 3.53038  | -0.86679 | H             | -0.60422 | 3.81669  | -0.89983 |
| H             | -0.04522 | 3.52246  | -1.28922 | H             | -0.19020 | 3.33974  | -1.57410 | H             | 1.67362  | 3.34334  | -0.78797 |
| H             | -2.03207 | -3.30752 | -1.21797 | H             | -2.30881 | -3.16631 | -1.67913 | H             | -2.47695 | -2.61151 | -1.70299 |
| H             | 0.27304  | -2.84046 | -0.42787 | H             | -0.22672 | -2.73778 | -0.13379 | H             | -0.23707 | -2.56486 | -0.38284 |
| H             | -0.83220 | -0.73847 | 3.19673  | H             | -0.85382 | -1.99967 | 2.01697  | H             | -0.80476 | -1.93365 | 1.89537  |
| C             | 2.85490  | -0.01960 | 0.06649  | C             | 2.75515  | 0.04584  | -0.05237 | C             | 3.19219  | -0.96117 | -0.47172 |
| H             | 3.29595  | 0.39295  | -0.85499 | H             | 3.10043  | 0.38011  | -1.04463 | H             | 3.56978  | -0.42563 | -1.35809 |
| H             | 3.20226  | 0.56447  | 0.93409  | H             | 3.15955  | 0.73216  | 0.71032  | H             | 3.86968  | -0.77895 | 0.37750  |
| H             | 3.16499  | -1.07032 | 0.18458  | H             | 3.14722  | -0.96703 | 0.13575  | H             | 3.16128  | -2.04102 | -0.69016 |
| [4.4.3]clf_oo |          |          |          | [4.4.3]clf_io |          |          |          | [4.4.3]clf_ts |          |          |          |
| P             | 1.07504  | 0.07445  | -0.02760 | P             | 0.97153  | 0.04090  | -0.01562 | P             | 0.49696  | -1.69205 | -0.44834 |
| P             | -2.89312 | 0.01230  | 0.52634  | P             | -1.84482 | 0.02311  | 0.19210  | P             | -0.41001 | 1.38606  | 0.73856  |
| C             | 0.67890  | 1.88940  | -0.13414 | C             | 0.64656  | 1.85341  | -0.32870 | C             | 2.17356  | -0.97167 | -0.13399 |
| C             | -2.29640 | 0.84360  | -1.05868 | C             | -2.84281 | 1.50129  | -0.28004 | C             | 0.91323  | 2.21311  | -0.26847 |
| H             | 1.68070  | 2.31027  | -0.33352 | H             | 1.57909  | 2.15852  | -0.83560 | H             | 2.84141  | -1.80581 | -0.41212 |
| H             | 0.41522  | 2.21297  | 0.88737  | H             | 0.69673  | 2.31256  | 0.67786  | H             | 2.27949  | -0.83901 | 0.95619  |
| H             | -1.52298 | 0.24067  | -1.54475 | H             | -3.23329 | 1.31562  | -1.29739 | H             | 0.57874  | 2.16495  | -1.32267 |
| H             | -3.17472 | 0.79447  | -1.72578 | H             | -3.70335 | 1.68347  | 0.38741  | H             | 0.94569  | 3.28086  | 0.00463  |
| C             | 0.58315  | -0.91932 | -1.52018 | C             | 0.54138  | -1.11506 | -1.40427 | C             | -0.48659 | -0.80488 | -1.72564 |
| H             | 1.56648  | -1.17957 | -1.95088 | H             | 1.52905  | -1.45143 | -1.76397 | H             | -0.33070 | -1.40606 | -2.63891 |
| H             | 0.08989  | -0.27098 | -2.26141 | H             | 0.10763  | -0.47887 | -2.19804 | H             | -0.02549 | 0.17943  | -1.89251 |
| C             | -2.39792 | -1.79988 | 0.22006  | C             | -2.70061 | -1.54016 | -0.32405 | C             | -2.13836 | 1.45625  | 0.07600  |
| H             | -1.83718 | -2.17434 | 1.09397  | H             | -2.73801 | -2.21401 | 0.55111  | H             | -2.74541 | 0.96954  | 0.86236  |
| H             | -3.36676 | -2.32730 | 0.26162  | H             | -3.74161 | -1.34872 | -0.63836 | H             | -2.46348 | 2.51106  | 0.06056  |
| C             | -1.74563 | 0.68921  | 1.86564  | C             | -1.77244 | -0.03565 | 2.03671  | C             | -0.11780 | 0.29611  | 2.21068  |
| H             | -2.42431 | 0.89021  | 2.71323  | H             | -2.71487 | -0.37220 | 2.50333  | H             | -0.41740 | 0.82446  | 3.13050  |
| H             | -1.44251 | 1.68771  | 1.51518  | H             | -1.54932 | 0.98177  | 2.40784  | H             | 0.97080  | 0.12779  | 2.28697  |
| C             | 0.45941  | -0.75547 | 1.50214  | C             | 0.73754  | -0.52976 | 1.74655  | C             | -0.31300 | -2.08557 | 1.16159  |
| H             | 0.07289  | -1.72669 | 1.16789  | H             | 1.50174  | -1.32038 | 1.84993  | H             | -1.07054 | -2.84751 | 0.90555  |
| H             | 1.38765  | -0.97307 | 2.05877  | H             | 1.13909  | 0.33762  | 2.30608  | H             | 0.50189  | -2.64715 | 1.65917  |
| C             | -1.73368 | -2.23180 | -1.11408 | C             | -1.87257 | -2.18853 | -1.45276 | C             | -2.44029 | 0.80652  | -1.28656 |
| C             | -0.19748 | -2.23583 | -1.29425 | C             | -0.36665 | -2.34615 | -1.13384 | C             | -2.00000 | -0.65868 | -1.41717 |
| C             | -1.80618 | 2.30455  | -0.95840 | C             | -1.85910 | 2.69060  | -0.31560 | C             | 2.33438  | 1.63765  | -0.15768 |
| C             | -0.29352 | 2.45913  | -1.18865 | C             | -0.56928 | 2.38953  | -1.11737 | C             | 2.60924  | 0.30660  | -0.87599 |
| C             | -0.53671 | -0.06413 | 2.44790  | C             | -0.60369 | -0.98858 | 2.34519  | C             | -0.89270 | -1.02843 | 2.11144  |
| H             | -2.09459 | 2.77851  | -0.00341 | H             | -1.58924 | 2.98943  | 0.71422  | H             | 2.63170  | 1.55305  | 0.90445  |
| H             | -0.03597 | 2.04843  | -2.18208 | H             | -0.80610 | 1.71645  | -1.96371 | H             | 2.19584  | 0.33288  | -1.90014 |
| H             | 0.01756  | 0.64688  | 3.08683  | H             | -0.46461 | -1.08601 | 3.43626  | H             | -0.93856 | -1.48417 | 3.11801  |
| H             | -0.00899 | -2.83158 | -2.20569 | H             | 0.02399  | -3.15427 | -1.77529 | H             | -2.56205 | -1.13028 | -2.23912 |
| H             | -2.19628 | -1.68812 | -1.95687 | H             | -1.97870 | -1.59625 | -2.38086 | H             | -1.97728 | 1.39612  | -2.09929 |
| H             | -2.30834 | 2.90081  | -1.73920 | H             | -2.37089 | 3.56085  | -0.76134 | H             | 3.00830  | 2.39713  | -0.59349 |
| H             | -0.06358 | 3.53826  | -1.24866 | H             | -0.22603 | 3.33297  | -1.57710 | H             | 3.70235  | 0.22715  | -1.00591 |
| H             | -2.03130 | -3.28602 | -1.26280 | H             | -2.29354 | -3.18556 | -1.67329 | H             | -3.53229 | 0.87592  | -1.44626 |
| H             | 0.27619  | -2.81539 | -0.48210 | H             | -0.23456 | -2.70987 | -0.09798 | H             | -2.28575 | -1.21187 | -0.50464 |

|                  |          |          |          |                  |          |          |          |                  |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|----------|------------------|----------|----------|----------|
| H                | -0.89946 | -0.85003 | 3.13448  | H                | -0.84855 | -2.00080 | 1.97844  | H                | -1.93843 | -0.81358 | 1.83637  |
| Cl               | 3.20011  | -0.03780 | 0.06446  | Cl               | 3.07299  | 0.05017  | -0.03898 | Cl               | 0.85041  | -3.61225 | -1.24304 |
| F                | 5.21218  | -0.14709 | 0.14180  | F                | 5.23092  | 0.03860  | -0.07731 | F                | 1.20694  | -5.49136 | -2.04115 |
| [4.4.3]cucl_oo   |          |          |          | [4.4.3]cucl_io   |          |          |          | [4.4.3]cucl_ts   |          |          |          |
| P                | 0.12917  | 0.07435  | 2.11689  | P                | -0.03698 | 0.18510  | 2.14829  | P                | 0.65794  | 0.09689  | 0.15539  |
| P                | 0.12017  | 0.00889  | -2.02855 | P                | -0.23615 | -0.16440 | -0.88805 | P                | -2.94531 | -0.03996 | 0.24321  |
| C                | 0.78213  | -1.63517 | 1.65786  | C                | 0.43738  | -1.60536 | 1.72079  | C                | 0.06796  | 1.87380  | 0.33283  |
| C                | -0.87507 | -1.37886 | -1.22686 | C                | -0.25148 | -1.82705 | -1.69457 | C                | -3.17838 | 1.46633  | -0.81232 |
| H                | 0.98378  | -2.07704 | 2.64692  | H                | 0.52703  | -2.07468 | 2.71500  | H                | 0.99789  | 2.44814  | 0.47215  |
| H                | 1.77421  | -1.48050 | 1.20033  | H                | 1.47414  | -1.52216 | 1.34325  | H                | -0.47413 | 1.93988  | 1.29020  |
| H                | -1.52702 | -0.98022 | -0.44323 | H                | -1.30541 | -2.03376 | -1.95827 | H                | -2.99030 | 1.12254  | -1.84830 |
| H                | -1.54887 | -1.71466 | -2.03454 | H                | 0.35086  | -1.91080 | -2.61641 | H                | -4.22948 | 1.79953  | -0.77487 |
| C                | -1.69918 | 0.22460  | 1.68858  | C                | -1.77616 | 0.64370  | 1.59391  | C                | -0.17921 | -0.67146 | -1.32038 |
| H                | -2.18658 | 0.28787  | 2.67478  | H                | -2.29670 | 0.87851  | 2.53888  | H                | 0.57908  | -0.66823 | -2.12240 |
| H                | -2.06121 | -0.71424 | 1.24221  | H                | -2.23203 | -0.28285 | 1.20412  | H                | -0.99117 | -0.00061 | -1.63021 |
| C                | -0.91239 | 1.53764  | -1.55859 | C                | -1.31062 | 1.04579  | -1.80426 | C                | -3.21868 | -1.70494 | -0.52034 |
| H                | -0.23420 | 2.33160  | -1.19976 | H                | -0.70355 | 1.93128  | -2.06742 | H                | -3.22943 | -2.38818 | 0.35025  |
| H                | -1.26474 | 1.89732  | -2.54171 | H                | -1.70764 | 0.62810  | -2.74611 | H                | -4.23822 | -1.74733 | -0.94182 |
| C                | 1.73936  | 0.05208  | -1.05686 | C                | 1.48371  | 0.50497  | -1.03653 | C                | -2.36492 | -0.01042 | 2.00004  |
| H                | 2.50155  | 0.21062  | -1.84002 | H                | 1.74928  | 0.83646  | -2.05700 | H                | -3.20141 | -0.21910 | 2.68850  |
| H                | 1.89360  | -0.98864 | -0.73313 | H                | 2.19093  | -0.29442 | -0.74710 | H                | -2.03587 | 1.02128  | 2.21548  |
| C                | 0.99385  | 1.39155  | 1.11157  | C                | 1.31222  | 1.29946  | 1.44654  | C                | 0.18278  | -0.69911 | 1.77963  |
| H                | 0.20353  | 1.97991  | 0.63340  | H                | 1.21808  | 2.22962  | 2.03521  | H                | 0.80079  | -1.61193 | 1.84302  |
| H                | 1.45126  | 2.05520  | 1.86321  | H                | 2.21570  | 0.80066  | 1.84946  | H                | 0.65136  | 0.00865  | 2.49192  |
| C                | -2.18772 | 1.42151  | -0.68114 | C                | -2.44983 | 1.44991  | -0.83905 | C                | -2.20053 | -2.21764 | -1.56023 |
| C                | -2.15775 | 1.45596  | 0.86796  | C                | -1.98880 | 1.82331  | 0.59455  | C                | -0.73265 | -2.10569 | -1.11665 |
| C                | -0.10192 | -2.59199 | -0.66833 | C                | 0.20752  | -2.82823 | -0.60517 | C                | -2.27546 | 2.67408  | -0.50733 |
| C                | -0.05577 | -2.66622 | 0.86872  | C                | -0.38890 | -2.55033 | 0.80155  | C                | -0.76813 | 2.52756  | -0.79220 |
| C                | 2.07417  | 1.03086  | 0.08500  | C                | 1.55012  | 1.67285  | -0.03579 | C                | -1.24430 | -1.03423 | 2.25700  |
| H                | 0.92066  | -2.66014 | -1.08063 | H                | 1.31076  | -2.82146 | -0.53198 | H                | -2.41831 | 2.99725  | 0.54102  |
| H                | -1.09059 | -2.67682 | 1.25778  | H                | -1.43025 | -2.19457 | 0.69513  | H                | -0.61691 | 2.02178  | -1.76211 |
| H                | 2.96601  | 0.64310  | 0.61190  | H                | 2.54368  | 2.15483  | -0.08662 | H                | -1.17506 | -1.19528 | 3.35018  |
| H                | -3.21005 | 1.61887  | 1.16419  | H                | -2.77407 | 2.46474  | 1.03017  | H                | -0.11942 | -2.81043 | -1.70161 |
| H                | -2.77514 | 0.54371  | -1.00483 | H                | -3.17997 | 0.62228  | -0.76512 | H                | -2.33030 | -1.67734 | -2.51623 |
| H                | -0.60888 | -3.51203 | -1.00771 | H                | -0.06939 | -3.84939 | -0.92109 | H                | -2.65973 | 3.50538  | -1.12682 |
| H                | 0.36331  | -3.65346 | 1.13597  | H                | -0.45587 | -3.51706 | 1.33080  | H                | -0.36946 | 3.54673  | -0.93319 |
| H                | -2.80924 | 2.29218  | -0.96242 | H                | -2.99840 | 2.30814  | -1.26827 | H                | -2.44856 | -3.27497 | -1.76997 |
| H                | -1.63053 | 2.36217  | 1.21587  | H                | -1.09033 | 2.46337  | 0.54278  | H                | -0.64622 | -2.43264 | -0.06641 |
| H                | 2.39645  | 1.99029  | -0.35912 | H                | 0.82807  | 2.44882  | -0.34369 | H                | -1.55625 | -2.00678 | 1.84086  |
| Cu               | 0.42929  | 0.42025  | 4.19177  | Cu               | 0.10905  | 0.40174  | 4.26535  | Cl               | 4.82747  | -0.09897 | -0.21183 |
| Cl               | 0.71274  | 0.76009  | 6.20661  | Cl               | 0.24470  | 0.61275  | 6.31788  | Cu               | 2.77289  | -0.00481 | -0.02441 |
| [4.4.3]f_plus_oo |          |          |          | [4.4.3]f_plus_io |          |          |          | [4.4.3]f_plus_ts |          |          |          |
| P                | 0.91468  | 0.07306  | -0.02725 | P                | 0.62987  | 0.02686  | 0.02404  | P                | 1.14655  | -0.80208 | -0.10923 |
| P                | -2.87257 | 0.03408  | 0.49926  | P                | -1.78595 | 0.00219  | 0.31170  | P                | -1.42553 | 1.07097  | 0.62269  |
| C                | 0.67427  | 1.88170  | -0.18396 | C                | 0.59476  | 1.85511  | -0.28805 | C                | 2.14417  | 0.71174  | 0.16387  |
| C                | -2.29089 | 0.86115  | -1.10098 | C                | -2.73961 | 1.41255  | -0.37897 | C                | -0.63703 | 2.15001  | -0.69807 |

|              |          |          |          |              |          |          |          |               |          |          |          |
|--------------|----------|----------|----------|--------------|----------|----------|----------|---------------|----------|----------|----------|
| H            | 1.70408  | 2.20316  | -0.42951 | H            | 1.57599  | 2.05598  | -0.74709 | H             | 3.17084  | 0.32357  | 0.03571  |
| H            | 0.46376  | 2.26056  | 0.82998  | H            | 0.62497  | 2.32070  | 0.71594  | H             | 2.03949  | 0.97687  | 1.22877  |
| H            | -1.54759 | 0.25928  | -1.63831 | H            | -3.02375 | 1.11787  | -1.40578 | H             | -0.56893 | 1.60804  | -1.65584 |
| H            | -3.19299 | 0.82529  | -1.73531 | H            | -3.67035 | 1.54505  | 0.20012  | H             | -1.39023 | 2.94107  | -0.84403 |
| C            | 0.56020  | -0.97433 | -1.48605 | C            | 0.50779  | -1.10774 | -1.42707 | C             | 0.21365  | -1.04890 | -1.65575 |
| H            | 1.58313  | -1.22626 | -1.82361 | H            | 1.54757  | -1.39647 | -1.64532 | H             | 0.91093  | -1.65896 | -2.25678 |
| H            | 0.11808  | -0.35311 | -2.27942 | H            | 0.16180  | -0.47605 | -2.26771 | H             | 0.11530  | -0.08071 | -2.16896 |
| C            | -2.36884 | -1.78526 | 0.24824  | C            | -2.58343 | -1.57351 | -0.21704 | C             | -2.64306 | -0.13933 | -0.11214 |
| H            | -1.76193 | -2.12440 | 1.10614  | H            | -2.48597 | -2.29301 | 0.61452  | H             | -2.81804 | -0.90769 | 0.66210  |
| H            | -3.32775 | -2.31836 | 0.35952  | H            | -3.66112 | -1.39064 | -0.37434 | H             | -3.59101 | 0.41956  | -0.19234 |
| C            | -1.73641 | 0.71657  | 1.85211  | C            | -1.74947 | 0.02145  | 2.14645  | C             | -0.60519 | 0.44725  | 2.19655  |
| H            | -2.43076 | 0.94705  | 2.67831  | H            | -2.71401 | -0.28161 | 2.58590  | H             | -1.26344 | 0.79500  | 3.00824  |
| H            | -1.38195 | 1.70333  | 1.51523  | H            | -1.51752 | 1.04645  | 2.48779  | H             | 0.35070  | 0.97880  | 2.33875  |
| C            | 0.49365  | -0.70550 | 1.56237  | C            | 0.70280  | -0.58247 | 1.78389  | C             | 0.66920  | -1.64708 | 1.43631  |
| H            | 0.27102  | -1.75247 | 1.30915  | H            | 1.42122  | -1.41857 | 1.76431  | H             | 0.49669  | -2.69703 | 1.14139  |
| H            | 1.46719  | -0.71613 | 2.08478  | H            | 1.21890  | 0.24861  | 2.29885  | H             | 1.63237  | -1.63444 | 1.98144  |
| C            | -1.75643 | -2.25672 | -1.09353 | C            | -1.89876 | -2.12839 | -1.47831 | C             | -2.35880 | -0.80537 | -1.46508 |
| C            | -0.22429 | -2.29076 | -1.26141 | C            | -0.38723 | -2.36147 | -1.29941 | C             | -1.15632 | -1.75513 | -1.51735 |
| C            | -1.79799 | 2.32162  | -1.00378 | C            | -1.87680 | 2.68468  | -0.41798 | C             | 0.71353  | 2.80202  | -0.36732 |
| C            | -0.28792 | 2.46883  | -1.24180 | C            | -0.53391 | 2.46903  | -1.13822 | C             | 1.93158  | 1.94656  | -0.72593 |
| C            | -0.59186 | -0.09434 | 2.47976  | C            | -0.60615 | -0.95601 | 2.49687  | C             | -0.45724 | -1.07550 | 2.29632  |
| H            | -2.08359 | 2.79749  | -0.04954 | H            | -1.69692 | 3.06275  | 0.60473  | H             | 0.75772  | 3.10324  | 0.69525  |
| H            | -0.03061 | 2.05908  | -2.23487 | H            | -0.69331 | 1.87696  | -2.05985 | H             | 1.89628  | 1.65861  | -1.79168 |
| H            | -0.09129 | 0.55198  | 3.22039  | H            | -0.43303 | -0.96261 | 3.58513  | H             | -0.25931 | -1.34954 | 3.34715  |
| H            | -0.01635 | -2.88617 | -2.16717 | H            | -0.05034 | -3.05594 | -2.08664 | H             | -1.26247 | -2.39947 | -2.40488 |
| H            | -2.21086 | -1.71501 | -1.94118 | H            | -2.06966 | -1.45389 | -2.33781 | H             | -2.25499 | -0.04092 | -2.25654 |
| H            | -2.29618 | 2.91829  | -1.78517 | H            | -2.45080 | 3.46807  | -0.93948 | H             | 0.77804  | 3.73722  | -0.94842 |
| H            | -0.03643 | 3.54232  | -1.28782 | H            | -0.15810 | 3.44849  | -1.47817 | H             | 2.83962  | 2.56198  | -0.61094 |
| H            | -2.07422 | -3.30576 | -1.22535 | H            | -2.38322 | -3.08479 | -1.73605 | H             | -3.26250 | -1.38316 | -1.72820 |
| H            | 0.23426  | -2.86204 | -0.43514 | H            | -0.19424 | -2.88156 | -0.34184 | H             | -1.17037 | -2.43933 | -0.64929 |
| H            | -1.01340 | -0.93421 | 3.05629  | H            | -0.90165 | -1.98367 | 2.22462  | H             | -1.41100 | -1.55743 | 2.03366  |
| F            | 2.53902  | -0.00841 | 0.02149  | F            | 2.34793  | 0.03015  | 0.00199  | F             | 2.39577  | -1.83404 | -0.44166 |
| [4.4.3]hf_oo |          |          |          | [4.4.3]hf_io |          |          |          | [4.4.3]hf_ts_ |          |          |          |
| P            | 0.13769  | 0.07435  | 2.14308  | P            | -0.04392 | 0.19356  | 2.20087  | P             | 0.54002  | -1.90161 | -0.51118 |
| P            | 0.11662  | 0.00378  | -2.04301 | P            | -0.27256 | -0.17748 | -0.90710 | P             | -0.41727 | 1.43138  | 0.67800  |
| C            | 0.77980  | -1.63659 | 1.64730  | C            | 0.41703  | -1.60029 | 1.73277  | C             | 2.12544  | -0.95017 | -0.11159 |
| C            | -0.87624 | -1.37422 | -1.22586 | C            | -0.24300 | -1.83643 | -1.72147 | C             | 0.95815  | 2.33532  | -0.17072 |
| H            | 0.98827  | -2.09166 | 2.63137  | H            | 0.47370  | -2.08688 | 2.72326  | H             | 2.92191  | -1.70000 | -0.25867 |
| H            | 1.77157  | -1.48463 | 1.18701  | H            | 1.46686  | -1.52658 | 1.38997  | H             | 2.11770  | -0.73446 | 0.96962  |
| H            | -1.50208 | -0.96597 | -0.42684 | H            | -1.28864 | -2.07683 | -1.98926 | H             | 0.62809  | 2.43255  | -1.22345 |
| H            | -1.57166 | -1.70424 | -2.01768 | H            | 0.36977  | -1.91363 | -2.63743 | H             | 1.05818  | 3.35994  | 0.22714  |
| C            | -1.69071 | 0.22496  | 1.68405  | C            | -1.77075 | 0.64817  | 1.58266  | C             | -0.47516 | -0.81727 | -1.64891 |
| H            | -2.18769 | 0.30120  | 2.66698  | H            | -2.32175 | 0.88018  | 2.51346  | H             | -0.35131 | -1.25705 | -2.65577 |
| H            | -2.06314 | -0.71538 | 1.24754  | H            | -2.21695 | -0.27689 | 1.17821  | H             | -0.02056 | 0.18199  | -1.67212 |
| C            | -0.90946 | 1.53485  | -1.56909 | C            | -1.33069 | 1.04594  | -1.82781 | C             | -2.13058 | 1.54241  | -0.01437 |
| H            | -0.22857 | 2.32088  | -1.19855 | H            | -0.71372 | 1.92044  | -2.10525 | H             | -2.76329 | 1.14496  | 0.80222  |
| H            | -1.25739 | 1.90530  | -2.54986 | H            | -1.74804 | 0.62870  | -2.76123 | H             | -2.41595 | 2.60396  | -0.11956 |

|                  |          |          |          |                  |          |          |          |                  |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|----------|------------------|----------|----------|----------|
| C                | 1.73437  | 0.05007  | -1.07176 | C                | 1.45160  | 0.48956  | -1.03641 | C                | -0.18227 | 0.37392  | 2.17600  |
| H                | 2.49906  | 0.20318  | -1.85403 | H                | 1.72550  | 0.81510  | -2.05717 | H                | -0.54441 | 0.88827  | 3.08279  |
| H                | 1.88571  | -0.98816 | -0.73958 | H                | 2.15067  | -0.31535 | -0.74190 | H                | 0.90641  | 0.24170  | 2.30573  |
| C                | 0.99394  | 1.38211  | 1.10691  | C                | 1.29928  | 1.28782  | 1.44612  | C                | -0.26632 | -2.07916 | 1.17555  |
| H                | 0.20321  | 1.98069  | 0.64133  | H                | 1.22753  | 2.22531  | 2.02896  | H                | -1.00692 | -2.89044 | 1.04979  |
| H                | 1.46752  | 2.04775  | 1.85023  | H                | 2.20854  | 0.78754  | 1.83606  | H                | 0.56312  | -2.54818 | 1.74250  |
| C                | -2.18584 | 1.41404  | -0.69368 | C                | -2.45238 | 1.47154  | -0.84917 | C                | -2.44522 | 0.78120  | -1.31996 |
| C                | -2.15565 | 1.44934  | 0.85584  | C                | -1.97454 | 1.83250  | 0.58382  | C                | -1.98539 | -0.68685 | -1.32240 |
| C                | -0.10215 | -2.59205 | -0.67900 | C                | 0.23892  | -2.81171 | -0.61626 | C                | 2.34115  | 1.66107  | -0.13444 |
| C                | -0.05457 | -2.67107 | 0.85795  | C                | -0.38044 | -2.54576 | 0.78514  | C                | 2.50383  | 0.32981  | -0.89564 |
| C                | 2.06579  | 1.03483  | 0.06551  | C                | 1.52985  | 1.65861  | -0.03949 | C                | -0.90656 | -0.97909 | 2.04855  |
| H                | 0.92036  | -2.65703 | -1.09234 | H                | 1.34063  | -2.76386 | -0.53362 | H                | 2.66571  | 1.52403  | 0.91429  |
| H                | -1.09082 | -2.68152 | 1.24427  | H                | -1.42361 | -2.19940 | 0.66386  | H                | 1.97463  | 0.39013  | -1.86314 |
| H                | 2.96700  | 0.65357  | 0.58200  | H                | 2.52626  | 2.13469  | -0.10134 | H                | -1.00421 | -1.40542 | 3.06631  |
| H                | -3.20892 | 1.61360  | 1.14971  | H                | -2.74762 | 2.48779  | 1.02184  | H                | -2.56590 | -1.24708 | -2.07424 |
| H                | -2.77028 | 0.53454  | -1.01817 | H                | -3.19678 | 0.65704  | -0.77109 | H                | -1.98837 | 1.30331  | -2.18119 |
| H                | -0.60918 | -3.51018 | -1.02405 | H                | 0.00304  | -3.84522 | -0.92644 | H                | 3.04779  | 2.39314  | -0.56811 |
| H                | 0.36259  | -3.66082 | 1.12115  | H                | -0.44635 | -3.51939 | 1.30319  | H                | 3.57278  | 0.24278  | -1.15695 |
| H                | -2.80982 | 2.28314  | -0.97554 | H                | -2.98863 | 2.34147  | -1.27168 | H                | -3.53968 | 0.83308  | -1.47473 |
| H                | -1.62968 | 2.35926  | 1.19696  | H                | -1.06718 | 2.45858  | 0.52495  | H                | -2.23415 | -1.14361 | -0.34961 |
| H                | 2.37802  | 1.99580  | -0.38388 | H                | 0.81098  | 2.43791  | -0.34668 | H                | -1.94117 | -0.79139 | 1.71503  |
| H                | 0.42307  | 0.43193  | 4.25490  | H                | 0.13773  | 0.39987  | 4.33252  | H                | 0.95081  | -3.87582 | -1.29762 |
| F                | 0.53521  | 0.59523  | 5.19045  | F                | 0.22503  | 0.48326  | 5.28557  | F                | 1.15024  | -4.74594 | -1.64214 |
| [4.4.3]h_plus_oo |          |          |          | [4.4.3]h_plus_io |          |          |          | [4.4.3]h_plus_ts |          |          |          |
| P                | 0.98120  | 0.07878  | -0.03364 | P                | 0.79206  | 0.04999  | 0.01281  | P                | -0.46008 | 1.53476  | -0.58005 |
| P                | -2.88378 | 0.02841  | 0.52505  | P                | -1.83416 | 0.01553  | 0.24924  | P                | 0.39641  | -1.29854 | 0.92293  |
| C                | 0.67500  | 1.90467  | -0.17231 | C                | 0.63142  | 1.86462  | -0.36842 | C                | -2.19393 | 0.98937  | -0.23790 |
| C                | -2.26822 | 0.83275  | -1.06917 | C                | -2.80851 | 1.48429  | -0.28620 | C                | -0.90255 | -2.11684 | -0.14017 |
| H                | 1.68389  | 2.29744  | -0.38861 | H                | 1.56243  | 2.08424  | -0.92274 | H                | -2.80867 | 1.81548  | -0.63572 |
| H                | 0.41978  | 2.24716  | 0.84482  | H                | 0.73831  | 2.37098  | 0.61070  | H                | -2.32341 | 1.00479  | 0.85691  |
| H                | -1.48695 | 0.23285  | -1.55037 | H                | -3.18276 | 1.26514  | -1.30257 | H                | -0.57923 | -2.06374 | -1.19592 |
| H                | -3.13927 | 0.75795  | -1.74286 | H                | -3.68201 | 1.65049  | 0.36750  | H                | -0.88331 | -3.18285 | 0.13725  |
| C                | 0.59669  | -0.97691 | -1.50864 | C                | 0.55606  | -1.13653 | -1.38870 | C                | 0.48093  | 0.63496  | -1.87341 |
| H                | 1.59375  | -1.25489 | -1.89289 | H                | 1.57465  | -1.47609 | -1.64855 | H                | 0.30800  | 1.21239  | -2.79899 |
| H                | 0.13258  | -0.35027 | -2.28560 | H                | 0.19865  | -0.52006 | -2.23522 | H                | 0.00082  | -0.34485 | -2.00968 |
| C                | -2.40967 | -1.79417 | 0.23636  | C                | -2.66002 | -1.54449 | -0.30561 | C                | 2.12603  | -1.36016 | 0.24293  |
| H                | -1.87579 | -2.18384 | 1.12128  | H                | -2.66311 | -2.24492 | 0.54855  | H                | 2.72402  | -0.73033 | 0.92699  |
| H                | -3.38938 | -2.30097 | 0.26486  | H                | -3.71207 | -1.34541 | -0.57362 | H                | 2.48801  | -2.39052 | 0.39963  |
| C                | -1.74455 | 0.71529  | 1.87304  | C                | -1.77993 | -0.03949 | 2.09044  | C                | 0.07816  | 0.00477  | 2.22244  |
| H                | -2.43218 | 0.90191  | 2.71576  | H                | -2.72809 | -0.38290 | 2.53711  | H                | 0.34628  | -0.43332 | 3.19648  |
| H                | -1.46005 | 1.72375  | 1.53221  | H                | -1.57183 | 0.97864  | 2.46745  | H                | -1.00752 | 0.19937  | 2.26402  |
| C                | 0.44410  | -0.74132 | 1.52394  | C                | 0.71486  | -0.52854 | 1.78533  | C                | 0.37254  | 2.21746  | 0.91371  |
| H                | 0.03094  | -1.70537 | 1.20148  | H                | 1.48149  | -1.32162 | 1.84451  | H                | 1.16535  | 2.88142  | 0.52665  |
| H                | 1.38048  | -0.96698 | 2.06208  | H                | 1.12905  | 0.33874  | 2.33604  | H                | -0.41811 | 2.88593  | 1.30734  |
| C                | -1.74159 | -2.24787 | -1.08832 | C                | -1.87261 | -2.14991 | -1.48206 | C                | 2.39632  | -0.95835 | -1.21472 |
| C                | -0.20458 | -2.27943 | -1.25444 | C                | -0.37184 | -2.36335 | -1.18866 | C                | 1.99920  | 0.47420  | -1.59431 |
| C                | -1.80395 | 2.30311  | -0.99102 | C                | -1.86122 | 2.69754  | -0.33138 | C                | -2.34455 | -1.60415 | -0.01059 |

|               |          |          |          |               |          |          |          |               |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| C             | -0.29633 | 2.46900  | -1.23318 | C             | -0.57885 | 2.42096  | -1.14596 | C             | -2.68848 | -0.34744 | -0.82075 |
| C             | -0.52985 | -0.01756 | 2.47035  | C             | -0.61054 | -0.99141 | 2.40985  | C             | 0.89263  | 1.28970  | 2.01422  |
| H             | -2.09147 | 2.78579  | -0.04085 | H             | -1.59291 | 3.01507  | 0.69291  | H             | -2.61193 | -1.45266 | 1.05145  |
| H             | -0.03613 | 2.05731  | -2.22509 | H             | -0.81683 | 1.76509  | -2.00568 | H             | -2.36177 | -0.46645 | -1.86941 |
| H             | 0.03581  | 0.70327  | 3.08678  | H             | -0.46692 | -1.07188 | 3.50029  | H             | 0.89862  | 1.86606  | 2.95620  |
| H             | -0.01024 | -2.88857 | -2.15475 | H             | 0.00086  | -3.13367 | -1.88422 | H             | 2.53290  | 0.75576  | -2.51591 |
| H             | -2.18810 | -1.70921 | -1.94203 | H             | -1.98071 | -1.51337 | -2.37974 | H             | 1.90122  | -1.66570 | -1.90492 |
| H             | -2.31482 | 2.88385  | -1.77619 | H             | -2.40271 | 3.54573  | -0.78193 | H             | -3.00170 | -2.41517 | -0.36870 |
| H             | -0.06178 | 3.54639  | -1.28802 | H             | -0.23305 | 3.37150  | -1.58664 | H             | -3.78781 | -0.26435 | -0.86180 |
| H             | -2.04857 | -3.29955 | -1.22896 | H             | -2.32401 | -3.12332 | -1.73870 | H             | 3.48050  | -1.08152 | -1.38735 |
| H             | 0.25658  | -2.84947 | -0.42847 | H             | -0.23923 | -2.79208 | -0.17751 | H             | 2.34888  | 1.17873  | -0.81772 |
| H             | -0.88146 | -0.79162 | 3.17366  | H             | -0.85296 | -2.00835 | 2.05575  | H             | 1.94394  | 1.02867  | 1.81667  |
| H             | 2.38891  | 0.01928  | 0.04253  | H             | 2.23539  | 0.07195  | 0.01009  | H             | -0.69782 | 2.77843  | -1.22527 |
| [4.4.3]lih_oo |          |          |          | [4.4.3]lih_io |          |          |          | [4.4.3]lih_ts |          |          |          |
| P             | 0.14783  | 0.07806  | 2.11975  | P             | -0.04828 | 0.19386  | 2.17285  | P             | 0.53675  | -1.88407 | -0.50955 |
| P             | 0.10753  | 0.00545  | -2.06097 | P             | -0.26004 | -0.17845 | -0.92364 | P             | -0.41864 | 1.44095  | 0.68448  |
| C             | 0.78916  | -1.63414 | 1.62888  | C             | 0.44264  | -1.58731 | 1.68567  | C             | 2.12452  | -0.93209 | -0.12515 |
| C             | -0.88527 | -1.38830 | -1.26540 | C             | -0.24812 | -1.84194 | -1.72995 | C             | 0.94413  | 2.34147  | -0.19009 |
| H             | 1.00396  | -2.09521 | 2.60855  | H             | 0.57489  | -2.08060 | 2.66565  | H             | 2.92626  | -1.67789 | -0.26266 |
| H             | 1.77731  | -1.48189 | 1.16182  | H             | 1.46515  | -1.48145 | 1.27754  | H             | 2.11392  | -0.70535 | 0.95329  |
| H             | -1.54889 | -0.99216 | -0.49003 | H             | -1.29652 | -2.06010 | -2.00612 | H             | 0.59899  | 2.43138  | -1.23863 |
| H             | -1.54699 | -1.73312 | -2.07926 | H             | 0.36773  | -1.92818 | -2.64270 | H             | 1.04362  | 3.36867  | 0.20054  |
| C             | -1.68143 | 0.21870  | 1.66448  | C             | -1.77683 | 0.64621  | 1.55835  | C             | -0.49384 | -0.81100 | -1.64255 |
| H             | -2.19025 | 0.26783  | 2.64275  | H             | -2.33206 | 0.87988  | 2.48633  | H             | -0.37699 | -1.24455 | -2.65287 |
| H             | -2.03400 | -0.71753 | 1.20530  | H             | -2.22008 | -0.28168 | 1.15785  | H             | -0.04250 | 0.18947  | -1.66473 |
| C             | -0.91859 | 1.53491  | -1.58108 | C             | -1.32090 | 1.03822  | -1.84854 | C             | -2.13952 | 1.53992  | 0.00790  |
| H             | -0.23513 | 2.32476  | -1.22311 | H             | -0.70707 | 1.91588  | -2.12251 | H             | -2.76225 | 1.14167  | 0.83170  |
| H             | -1.27459 | 1.89904  | -2.56126 | H             | -1.72979 | 0.61850  | -2.78440 | H             | -2.42987 | 2.60010  | -0.09559 |
| C             | 1.72811  | 0.04243  | -1.09228 | C             | 1.46279  | 0.49224  | -1.04909 | C             | -0.16451 | 0.38275  | 2.17966  |
| H             | 2.49093  | 0.19044  | -1.87706 | H             | 1.73859  | 0.82179  | -2.06775 | H             | -0.52374 | 0.89592  | 3.08809  |
| H             | 1.87585  | -0.99589 | -0.75944 | H             | 2.16595  | -0.30900 | -0.75487 | H             | 0.92568  | 0.25837  | 2.30399  |
| C             | 1.00067  | 1.38567  | 1.08110  | C             | 1.29441  | 1.30078  | 1.43512  | C             | -0.24904 | -2.07447 | 1.18525  |
| H             | 0.20524  | 1.97388  | 0.61089  | H             | 1.21192  | 2.24299  | 2.00888  | H             | -0.98913 | -2.88787 | 1.07126  |
| H             | 1.47342  | 2.06269  | 1.81426  | H             | 2.20497  | 0.80937  | 1.83330  | H             | 0.58981  | -2.53750 | 1.74337  |
| C             | -2.18895 | 1.42094  | -0.69715 | C             | -2.45047 | 1.45833  | -0.87740 | C             | -2.46559 | 0.77705  | -1.29366 |
| C             | -2.14909 | 1.45205  | 0.85162  | C             | -1.98062 | 1.82706  | 0.55572  | C             | -2.00136 | -0.68939 | -1.29985 |
| C             | -0.10907 | -2.59419 | -0.69527 | C             | 0.20592  | -2.83344 | -0.62730 | C             | 2.33161  | 1.67645  | -0.16876 |
| C             | -0.05718 | -2.66167 | 0.84254  | C             | -0.39022 | -2.54115 | 0.77803  | C             | 2.49234  | 0.34192  | -0.92399 |
| C             | 2.06958  | 1.02875  | 0.04028  | C             | 1.53061  | 1.66310  | -0.05232 | C             | -0.88339 | -0.97372 | 2.06155  |
| H             | 0.91178  | -2.66622 | -1.11131 | H             | 1.30910  | -2.82866 | -0.55290 | H             | 2.67242  | 1.54791  | 0.87578  |
| H             | -1.09149 | -2.66545 | 1.23355  | H             | -1.42981 | -2.18210 | 0.66683  | H             | 1.95478  | 0.39346  | -1.88726 |
| H             | 2.97114  | 0.64686  | 0.55553  | H             | 2.52527  | 2.14296  | -0.10814 | H             | -0.96811 | -1.40078 | 3.07988  |
| H             | -3.19978 | 1.61490  | 1.15400  | H             | -2.75837 | 2.47900  | 0.98996  | H             | -2.58645 | -1.25262 | -2.04566 |
| H             | -2.78052 | 0.54515  | -1.01871 | H             | -3.19019 | 0.63960  | -0.80017 | H             | -2.02044 | 1.29962  | -2.16056 |
| H             | -0.61717 | -3.51700 | -1.02580 | H             | -0.07281 | -3.85724 | -0.93323 | H             | 3.02745  | 2.40947  | -0.61738 |
| H             | 0.35482  | -3.65251 | 1.10851  | H             | -0.46043 | -3.50411 | 1.31415  | H             | 3.55891  | 0.25463  | -1.19350 |
| H             | -2.81006 | 2.29366  | -0.97332 | H             | -2.99037 | 2.32350  | -1.30425 | H             | -3.56154 | 0.82410  | -1.43671 |

|                |          |          |          |                |          |          |          |                 |          |          |          |
|----------------|----------|----------|----------|----------------|----------|----------|----------|-----------------|----------|----------|----------|
| H              | -1.62030 | 2.35957  | 1.19471  | H              | -1.07581 | 2.45699  | 0.49958  | H               | -2.23749 | -1.14661 | -0.32420 |
| H              | 2.38250  | 1.98762  | -0.41237 | H              | 0.81059  | 2.43887  | -0.36500 | H               | -1.92206 | -0.79216 | 1.73810  |
| Li             | 0.47691  | 0.49517  | 4.65264  | Li             | 0.14605  | 0.42574  | 4.74495  | H               | 1.39760  | -5.72260 | -2.06355 |
| H              | 0.60166  | 0.74781  | 6.26770  | H              | 0.31494  | 0.55464  | 6.37519  | Li              | 1.02675  | -4.23691 | -1.47025 |
| [4.4.3]oo      |          |          |          | [4.4.3]io      |          |          |          | [4.4.3]ts       |          |          |          |
| P              | 1.89555  | -0.18997 | 0.17953  | P              | 1.87850  | 0.17557  | -0.13239 | P               | 0.40496  | 1.97128  | -0.46327 |
| P              | -2.32544 | 0.22118  | 0.38287  | P              | -1.30108 | -0.03325 | 0.13458  | P               | -0.31324 | -1.49670 | 0.68062  |
| C              | 1.52228  | 1.66301  | -0.03657 | C              | 0.99228  | 1.88636  | -0.14140 | C               | -1.46574 | 1.72917  | -0.19985 |
| C              | -1.69546 | 1.01320  | -1.21914 | C              | -2.43682 | 1.37383  | -0.26104 | C               | -1.86855 | -1.72162 | -0.29944 |
| H              | 2.53300  | 2.08487  | -0.18037 | H              | 1.83891  | 2.58189  | -0.28881 | H               | -1.87806 | 2.74575  | -0.32453 |
| H              | 1.19050  | 2.05726  | 0.93973  | H              | 0.67272  | 2.04222  | 0.90527  | H               | -1.62322 | 1.47556  | 0.86087  |
| H              | -1.15974 | 0.27894  | -1.83547 | H              | -2.89490 | 1.13023  | -1.23793 | H               | -1.51825 | -1.97787 | -1.31851 |
| H              | -2.62390 | 1.23936  | -1.77213 | H              | -3.25449 | 1.55654  | 0.45938  | H               | -2.44670 | -2.58832 | 0.06574  |
| C              | 1.11336  | -1.01503 | -1.33652 | C              | 1.09096  | -0.97609 | -1.42543 | C               | 0.93830  | 0.50714  | -1.51807 |
| H              | 1.98394  | -1.25497 | -1.97171 | H              | 1.95545  | -1.26295 | -2.05429 | H               | 1.10786  | 0.92586  | -2.52778 |
| H              | 0.52056  | -0.29310 | -1.91399 | H              | 0.44204  | -0.35115 | -2.06338 | H               | 0.09871  | -0.19600 | -1.59724 |
| C              | -1.97377 | -1.63629 | 0.16915  | C              | -2.08129 | -1.68344 | -0.23220 | C               | 1.23495  | -2.34902 | 0.12846  |
| H              | -1.54792 | -2.01116 | 1.11615  | H              | -2.09705 | -2.29132 | 0.69131  | H               | 1.89282  | -2.28170 | 1.01618  |
| H              | -2.99337 | -2.05978 | 0.13329  | H              | -3.12421 | -1.59379 | -0.58478 | H               | 1.03452  | -3.42623 | -0.01017 |
| C              | -1.16090 | 0.88823  | 1.70812  | C              | -1.05893 | -0.02580 | 1.97269  | C               | -0.19169 | -0.45499 | 2.20191  |
| H              | -1.84476 | 1.27619  | 2.48435  | H              | -1.94253 | -0.38123 | 2.53543  | H               | -0.15259 | -1.08313 | 3.10898  |
| H              | -0.69153 | 1.78024  | 1.27420  | H              | -0.85882 | 1.01460  | 2.28912  | H               | -1.12847 | 0.12615  | 2.26581  |
| C              | 0.86688  | -0.82883 | 1.62557  | C              | 1.50821  | -0.46016 | 1.62009  | C               | 1.02362  | 1.73709  | 1.30715  |
| H              | 0.35720  | -1.72836 | 1.25778  | H              | 2.24306  | -1.27472 | 1.76582  | H               | 2.04855  | 2.15331  | 1.30299  |
| H              | 1.62368  | -1.20249 | 2.33856  | H              | 1.90701  | 0.38141  | 2.22205  | H               | 0.41775  | 2.50749  | 1.82653  |
| C              | -1.23727 | -2.21826 | -1.06283 | C              | -1.18013 | -2.35358 | -1.29875 | C               | 1.98218  | -1.78902 | -1.10185 |
| C              | 0.30390  | -2.31565 | -1.13020 | C              | 0.34477  | -2.28501 | -1.00854 | C               | 2.20336  | -0.26648 | -1.06753 |
| C              | -0.87218 | 2.31769  | -1.12002 | C              | -1.51999 | 2.61691  | -0.42480 | C               | -2.81048 | -0.50631 | -0.38048 |
| C              | 0.66823  | 2.22058  | -1.20214 | C              | -0.15352 | 2.31996  | -1.10571 | C               | -2.27977 | 0.75688  | -1.08926 |
| C              | -0.10877 | 0.03783  | 2.43649  | C              | 0.16458  | -0.91994 | 2.24607  | C               | 1.04655  | 0.46158  | 2.18040  |
| H              | -1.16589 | 2.90910  | -0.23385 | H              | -1.32819 | 3.06968  | 0.56562  | H               | -3.15936 | -0.23457 | 0.63366  |
| H              | 0.93678  | 1.69345  | -2.13612 | H              | -0.30452 | 1.57864  | -1.91184 | H               | -1.72255 | 0.46090  | -1.99569 |
| H              | 0.47340  | 0.72930  | 3.07520  | H              | 0.32805  | -0.99468 | 3.33802  | H               | 1.22686  | 0.79932  | 3.22065  |
| H              | 0.51162  | -2.95919 | -2.00470 | H              | 0.81127  | -3.11321 | -1.57112 | H               | 3.04420  | -0.00827 | -1.73346 |
| H              | -1.59650 | -1.70997 | -1.97655 | H              | -1.36657 | -1.88101 | -2.28151 | H               | 1.43587  | -2.05219 | -2.02680 |
| H              | -1.16569 | 2.94322  | -1.98292 | H              | -2.06122 | 3.38244  | -1.00941 | H               | -3.71154 | -0.85568 | -0.91917 |
| H              | 1.02046  | 3.25854  | -1.35405 | H              | 0.17379  | 3.24875  | -1.60681 | H               | -3.16202 | 1.30776  | -1.45970 |
| H              | -1.60173 | -3.25871 | -1.15839 | H              | -1.47338 | -3.41494 | -1.40448 | H               | 2.95585  | -2.31234 | -1.15989 |
| H              | 0.68349  | -2.88924 | -0.26519 | H              | 0.52850  | -2.52102 | 0.05388  | H               | 2.52249  | 0.02786  | -0.05375 |
| H              | -0.62420 | -0.63956 | 3.14394  | H              | -0.07013 | -1.94642 | 1.91440  | H               | 1.92619  | -0.15285 | 1.92315  |
| [4.4.4]        |          |          |          |                |          |          |          |                 |          |          |          |
| [4.4.4]agcl_oo |          |          |          | [4.4.4]agcl_io |          |          |          | [4.4.4]agcl_ts_ |          |          |          |
| P              | 0.00000  | 0.00000  | 3.90474  | P              | 0.00000  | 0.00000  | 0.44248  | P               | -0.37253 | 0.00000  | 0.00000  |
| P              | 0.00000  | 0.00000  | -0.46552 | P              | 0.00000  | 0.00000  | -2.67885 | P               | 3.34673  | 0.00001  | 0.00000  |
| C              | 1.69313  | 0.44739  | 3.16206  | C              | -0.28139 | -1.76994 | -0.16908 | C               | 0.32203  | -1.69461 | -0.39461 |
| C              | 1.32281  | -1.17661 | 0.17572  | C              | -1.20677 | -1.20371 | -3.41349 | C               | 3.25756  | -0.75052 | -1.70470 |
| H              | 2.25293  | 0.78878  | 4.04931  | H              | -0.29203 | -2.35893 | 0.76341  | H               | -0.51199 | -2.38936 | -0.20390 |

|                |          |          |          |                |          |          |          |                 |          |          |          |
|----------------|----------|----------|----------|----------------|----------|----------|----------|-----------------|----------|----------|----------|
| H              | 1.59531  | 1.34045  | 2.52887  | H              | 0.63732  | -2.06450 | -0.70388 | H               | 1.09980  | -1.92277 | 0.34539  |
| H              | 0.83189  | -1.94862 | 0.78445  | H              | -2.19551 | -0.70718 | -3.41065 | H               | 2.88779  | 0.04805  | -2.37436 |
| H              | 1.65945  | -1.68984 | -0.73841 | H              | -0.96966 | -1.46315 | -4.46212 | H               | 4.28326  | -0.97513 | -2.04224 |
| C              | -0.45911 | -1.68999 | 3.16206  | C              | -1.39212 | 1.12866  | -0.16908 | C               | 0.32203  | 1.18904  | -1.27027 |
| H              | -0.44337 | -2.34549 | 4.04931  | H              | -1.89688 | 1.43237  | 0.76341  | H               | -0.51198 | 1.37124  | -1.96731 |
| H              | 0.36321  | -2.05181 | 2.52887  | H              | -2.10657 | 0.48032  | -0.70388 | H               | 1.09981  | 0.66226  | -1.83785 |
| C              | -1.68038 | -0.55729 | 0.17572  | C              | -0.43906 | 1.64695  | -3.41349 | C               | 3.25755  | 1.85158  | 0.20239  |
| H              | -2.10350 | 0.25388  | 0.78445  | H              | 0.48532  | 2.25496  | -3.41065 | H               | 2.88778  | 2.03224  | 1.22879  |
| H              | -2.29317 | -0.59221 | -0.73841 | H              | -0.78229 | 1.57133  | -4.46212 | H               | 4.28324  | 2.25621  | 0.17663  |
| C              | 0.35756  | 1.73389  | 0.17572  | C              | 1.64583  | -0.44323 | -3.41349 | C               | 3.25755  | -1.10106 | 1.50232  |
| H              | 0.63372  | 2.28205  | -0.73841 | H              | 1.75195  | -0.10818 | -4.46212 | H               | 4.28325  | -1.28107 | 1.86561  |
| H              | 1.27161  | 1.69475  | 0.78445  | H              | 1.71020  | -1.54778 | -3.41065 | H               | 2.88778  | -2.08027 | 1.14557  |
| C              | -1.23402 | 1.24260  | 3.16206  | C              | 1.67350  | 0.64128  | -0.16908 | C               | 0.32203  | 0.50556  | 1.66487  |
| H              | -1.95852 | 0.71136  | 2.52887  | H              | 1.46925  | 1.58418  | -0.70388 | H               | 1.09980  | 1.26050  | 1.49246  |
| H              | -1.80957 | 1.55671  | 4.04931  | H              | 2.18891  | 0.92656  | 0.76341  | H               | -0.51199 | 1.01811  | 2.17119  |
| C              | -1.82228 | -1.91242 | 0.90605  | C              | -1.49516 | 2.32304  | -2.51600 | C               | 2.41857  | 2.65043  | -0.81577 |
| C              | -1.81350 | -1.90631 | 2.44837  | C              | -1.10819 | 2.39991  | -1.01969 | C               | 0.88457  | 2.53779  | -0.76151 |
| C              | 2.56734  | -0.62193 | 0.90605  | C              | -1.26424 | -2.45637 | -2.51600 | C               | 2.41859  | -2.03169 | -1.88744 |
| C              | 2.55766  | -0.61738 | 2.44837  | C              | -1.52429 | -2.15968 | -1.01969 | C               | 0.88459  | -1.92838 | -1.81704 |
| C              | -0.74507 | 2.53435  | 0.90605  | C              | 2.75939  | 0.13332  | -2.51600 | C               | 2.41858  | -0.61873 | 2.70322  |
| C              | -0.74416 | 2.52369  | 2.44837  | C              | 2.63248  | -0.24023 | -1.01969 | C               | 0.88458  | -0.60941 | 2.57854  |
| H              | 2.83308  | 0.38347  | 0.53326  | H              | -0.32340 | -3.03132 | -2.60816 | H               | 2.75518  | -2.79905 | -1.16513 |
| H              | 2.32598  | -1.63398 | 2.81401  | H              | -2.33388 | -1.41348 | -0.93237 | H               | 0.52013  | -1.17741 | -2.53917 |
| H              | -0.60604 | 3.58728  | 0.60340  | H              | 3.73535  | -0.22704 | -2.88774 | H               | 2.68345  | -1.28266 | 3.54719  |
| H              | 0.25208  | 2.83135  | 2.81401  | H              | 2.39105  | -1.31446 | -0.93237 | H               | 0.52012  | -1.61028 | 2.28924  |
| H              | -2.17999 | -2.90251 | 2.75405  | H              | -1.70002 | 3.21448  | -0.56815 | H               | 0.48445  | 3.33108  | -1.41573 |
| H              | -1.08445 | -2.64525 | 0.53326  | H              | -2.46350 | 1.79573  | -2.60816 | H               | 2.75517  | 2.40857  | -1.84148 |
| H              | 3.40969  | -1.26879 | 0.60340  | H              | -2.06429 | -3.12139 | -2.88774 | H               | 2.68347  | -2.43062 | -2.88440 |
| H              | 3.60364  | -0.43667 | 2.75405  | H              | -1.93381 | -3.07950 | -0.56815 | H               | 0.48447  | -2.89160 | -2.17695 |
| H              | -2.80365 | -2.31849 | 0.60340  | H              | -1.67106 | 3.34843  | -2.88774 | H               | 2.68345  | 3.71329  | -0.66277 |
| H              | -2.57806 | -1.19737 | 2.81401  | H              | -0.05717 | 2.72794  | -0.93237 | H               | 0.52011  | 2.78768  | 0.24992  |
| H              | -1.42366 | 3.33918  | 2.75405  | H              | 3.63383  | -0.13498 | -0.56815 | H               | 0.48445  | -0.43949 | 3.59266  |
| H              | -1.74863 | 2.26178  | 0.53326  | H              | 2.78690  | 1.23559  | -2.60816 | H               | 2.75517  | 0.39049  | 3.00662  |
| Cl             | 0.00000  | 0.00000  | -5.07657 | Cl             | 0.00000  | 0.00000  | 5.06255  | Ag              | -2.69018 | 0.00000  | 0.00000  |
| Ag             | 0.00000  | 0.00000  | -2.78878 | Ag             | 0.00000  | 0.00000  | 2.76848  | Cl              | -4.98060 | 0.00000  | 0.00000  |
| [4.4.4]beh2_oo |          |          |          | [4.4.4]beh2_io |          |          |          | [4.4.4]beh2_ts_ |          |          |          |
| P              | 2.01954  | -0.02273 | -0.34001 | P              | 1.87751  | 0.06276  | 0.19838  | P               | 1.81715  | -0.00800 | 0.25023  |
| P              | -2.45140 | 0.12027  | 0.56245  | P              | -1.25964 | -0.03462 | -0.10693 | P               | -1.84938 | 0.00991  | -0.21338 |
| C              | 1.72271  | 1.58134  | 0.60870  | C              | 1.19234  | -1.24267 | 1.37484  | C               | 1.37065  | -0.05701 | -1.56938 |
| C              | -1.92220 | 1.78843  | -0.20429 | C              | -2.15199 | -0.42916 | 1.47292  | C               | -1.64418 | -1.50838 | -1.27249 |
| H              | 2.70212  | 2.09084  | 0.59639  | H              | 2.10896  | -1.66250 | 1.82615  | H               | 2.30357  | 0.23180  | -2.08683 |
| H              | 1.50214  | 1.36150  | 1.66788  | H              | 0.78224  | -2.04820 | 0.74220  | H               | 0.64657  | 0.74331  | -1.77183 |
| H              | -1.68801 | 1.68051  | -1.27864 | H              | -2.26508 | 0.52349  | 2.02414  | H               | -1.34879 | -2.32565 | -0.58901 |
| H              | -2.83923 | 2.40183  | -0.16595 | H              | -3.16566 | -0.83862 | 1.30548  | H               | -2.62905 | -1.79389 | -1.67900 |
| C              | 0.51298  | -0.10541 | -1.41710 | C              | 1.20723  | 1.77121  | 0.63190  | C               | 1.03744  | -1.49364 | 1.07254  |
| H              | 0.77780  | 0.46210  | -2.32739 | H              | 2.12955  | 2.32851  | 0.87422  | H               | 1.88859  | -2.17794 | 1.23233  |
| H              | -0.25971 | 0.47196  | -0.90740 | H              | 0.65480  | 1.66577  | 1.58148  | H               | 0.37167  | -1.98658 | 0.35158  |

|               |          |          |          |               |          |          |          |                |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|----------------|----------|----------|----------|
| C             | -2.51779 | -1.12946 | -0.86144 | C             | -1.98418 | 1.57121  | -0.69116 | C              | -1.99798 | -0.16466 | 1.63492  |
| H             | -2.52588 | -2.10480 | -0.33589 | H             | -1.88717 | 1.58806  | -1.79319 | H              | -1.65714 | 0.79466  | 2.06599  |
| H             | -3.55323 | -1.00762 | -1.23144 | H             | -3.05907 | 1.67247  | -0.45090 | H              | -3.06525 | -0.25390 | 1.89899  |
| C             | -0.87741 | -0.26081 | 1.50727  | C             | -1.83931 | -1.31378 | -1.32271 | C              | -1.66270 | 1.70066  | -0.97194 |
| H             | -1.01454 | 0.20314  | 2.50166  | H             | -2.85275 | -1.10667 | -1.71435 | H              | -2.66473 | 2.09573  | -1.20994 |
| H             | -0.06178 | 0.28856  | 1.03583  | H             | -1.88544 | -2.27415 | -0.77505 | H              | -1.15685 | 1.55047  | -1.94351 |
| C             | 2.03982  | -1.47918 | 0.83542  | C             | 1.44585  | -0.36229 | -1.59260 | C              | 1.06624  | 1.53532  | 0.98891  |
| H             | 1.98029  | -2.35203 | 0.15664  | H             | 0.93920  | 0.52349  | -2.01081 | H              | 0.23318  | 1.24875  | 1.64470  |
| H             | 3.08379  | -1.47954 | 1.19980  | H             | 2.43343  | -0.40391 | -2.08921 | H              | 1.86602  | 1.92862  | 1.64007  |
| C             | -1.59761 | -1.22585 | -2.10160 | C             | -1.15372 | 2.72314  | -0.08986 | C              | -1.25350 | -1.34017 | 2.29921  |
| C             | -0.10184 | -1.45240 | -1.81813 | C             | 0.36791  | 2.62596  | -0.36060 | C              | 0.28049  | -1.27655 | 2.40369  |
| C             | -0.80049 | 2.60100  | 0.52119  | C             | -1.27443 | -1.39157 | 2.29918  | C              | -0.65816 | -1.42228 | -2.45467 |
| C             | 0.67764  | 2.57876  | 0.01496  | C             | 0.17974  | -0.90035 | 2.50439  | C              | 0.85078  | -1.39043 | -2.15491 |
| C             | -0.40866 | -1.70488 | 1.71985  | C             | -0.80084 | -1.42767 | -2.45736 | C              | -0.92241 | 2.77252  | -0.14706 |
| C             | 1.09668  | -1.68360 | 2.04162  | C             | 0.65195  | -1.64548 | -1.96864 | C              | 0.60214  | 2.65208  | 0.02467  |
| H             | -0.81811 | 2.40012  | 1.60756  | H             | -1.25306 | -2.38931 | 1.82131  | H              | -0.91436 | -0.55149 | -3.08724 |
| H             | 0.69811  | 2.54073  | -1.08819 | H             | 0.16271  | 0.18213  | 2.72508  | H              | 1.13345  | -2.25462 | -1.52944 |
| H             | -0.96577 | -2.17075 | 2.55070  | H             | -1.08460 | -2.27078 | -3.11276 | H              | -1.12771 | 3.73795  | -0.64655 |
| H             | 1.28792  | -0.90296 | 2.80153  | H             | 0.64944  | -2.38177 | -1.14536 | H              | 1.09279  | 2.57654  | -0.96113 |
| H             | 0.40111  | -1.84945 | -2.71611 | H             | 0.77562  | 3.65008  | -0.30420 | H              | 0.58313  | -2.08573 | 3.09078  |
| H             | -1.70731 | -0.31836 | -2.72488 | H             | -1.32183 | 2.77909  | 1.00260  | H              | -1.53688 | -2.28653 | 1.80113  |
| H             | -1.10679 | 3.65765  | 0.42497  | H             | -1.74356 | -1.53805 | 3.28881  | H              | -0.85635 | -2.31033 | -3.08376 |
| H             | 1.07799  | 3.57610  | 0.26837  | H             | 0.56227  | -1.37583 | 3.42408  | H              | 1.36805  | -1.55108 | -3.11650 |
| H             | -1.98723 | -2.06018 | -2.71380 | H             | -1.52417 | 3.67864  | -0.50320 | H              | -1.65691 | -1.41689 | 3.32636  |
| H             | 0.01382  | -2.21657 | -1.03353 | H             | 0.53033  | 2.31204  | -1.40731 | H              | 0.58516  | -0.34188 | 2.90651  |
| H             | 1.39509  | -2.64034 | 2.50798  | H             | 1.20884  | -2.13292 | -2.78704 | H              | 0.94912  | 3.61218  | 0.44392  |
| H             | -0.58795 | -2.33655 | 0.83545  | H             | -0.83441 | -0.52288 | -3.09343 | H              | -1.38783 | 2.85520  | 0.85330  |
| H             | 3.54135  | 1.39664  | -2.30873 | Be            | 4.07341  | -0.02713 | 0.09693  | H              | 4.50088  | 1.26970  | 0.08961  |
| H             | 4.85384  | -0.64004 | -1.41295 | H             | 4.47498  | -1.34432 | 0.20635  | H              | 4.48136  | -1.30896 | 0.03138  |
| Be            | 3.83415  | 0.25918  | -1.58070 | H             | 4.64563  | 1.18836  | -0.21059 | Be             | 4.01722  | -0.01823 | 0.16360  |
| [4.4.4]bh3_oo |          |          |          | [4.4.4]bh3_io |          |          |          | [4.4.4]bh3_ts_ |          |          |          |
| P             | 1.81914  | -0.01574 | -0.04378 | P             | 0.00000  | 0.00000  | 1.81340  | P              | 0.00054  | -0.00132 | 1.96849  |
| P             | -2.50264 | 0.01592  | 0.16191  | P             | 0.00000  | 0.00000  | -1.29606 | P              | -0.00044 | 0.00112  | -1.67613 |
| C             | 1.38416  | 1.77093  | 0.32829  | C             | -1.68678 | -0.60232 | 1.25488  | C              | 0.28802  | 1.73035  | 1.35547  |
| C             | -1.87029 | 1.35121  | -1.03299 | C             | -1.65189 | 0.41646  | -2.03295 | C              | 1.65321  | 0.85307  | -1.58870 |
| H             | 2.38538  | 2.23272  | 0.25530  | H             | -2.18393 | -0.79675 | 2.22200  | H              | 0.11230  | 2.33726  | 2.26093  |
| H             | 1.09946  | 1.86629  | 1.39005  | H             | -1.53804 | -1.59019 | 0.78589  | H              | -0.49750 | 1.99885  | 0.63611  |
| H             | -1.27906 | 0.88568  | -1.83572 | H             | -1.72876 | 1.52009  | -2.04660 | H              | 2.36822  | 0.11085  | -1.18943 |
| H             | -2.78005 | 1.73585  | -1.52452 | H             | -1.75785 | 0.06306  | -3.07571 | H              | 1.98986  | 1.07918  | -2.61447 |
| C             | 1.14454  | -0.43779 | -1.73096 | C             | 0.32177  | 1.76195  | 1.25488  | C              | 1.35587  | -1.11560 | 1.35323  |
| H             | 2.06313  | -0.44247 | -2.34277 | H             | 0.40196  | 2.28971  | 2.22200  | H              | 1.97029  | -1.26753 | 2.25792  |
| H             | 0.53756  | 0.40131  | -2.09955 | H             | -0.60812 | 2.12708  | 0.78589  | H              | 1.98036  | -0.56902 | 0.63360  |
| C             | -1.90417 | -1.62974 | -0.58987 | C             | 1.18661  | 1.22235  | -2.03295 | C              | -0.08938 | -1.85702 | -1.59004 |
| H             | -1.36787 | -2.19088 | 0.19465  | H             | 2.18082  | 0.73711  | -2.04660 | H              | -1.08928 | -2.10543 | -1.18999 |
| H             | -2.85463 | -2.17588 | -0.71995 | H             | 0.93354  | 1.49082  | -3.07571 | H              | -0.06289 | -2.26083 | -2.61614 |
| C             | -1.35402 | 0.35804  | 1.61254  | C             | 0.46528  | -1.63881 | -2.03295 | C              | -1.56508 | 1.00717  | -1.58771 |
| H             | -1.88360 | 1.12855  | 2.19928  | H             | 0.82432  | -1.55387 | -3.07571 | H              | -1.92903 | 1.18696  | -2.61332 |

|                    |          |          |          |                    |          |          |          |                     |          |          |          |
|--------------------|----------|----------|----------|--------------------|----------|----------|----------|---------------------|----------|----------|----------|
| H                  | -0.45612 | 0.84129  | 1.22299  | H                  | -0.45206 | -2.25719 | -2.04660 | H                   | -1.27986 | 1.99698  | -1.18714 |
| C                  | 1.20868  | -1.28474 | 1.19220  | C                  | 1.36501  | -1.15964 | 1.25488  | C                   | -1.64273 | -0.61744 | 1.35437  |
| H                  | 0.50820  | -1.95778 | 0.67700  | H                  | 2.14616  | -0.53689 | 0.78589  | H                   | -1.48234 | -1.43101 | 0.63397  |
| H                  | 2.13522  | -1.86352 | 1.34876  | H                  | 1.78197  | -1.49297 | 2.22200  | H                   | -2.08062 | -1.07426 | 2.25915  |
| C                  | -1.14922 | -1.73121 | -1.93698 | C                  | 1.23968  | 2.46326  | -1.11907 | C                   | 1.00314  | -2.57716 | -0.77520 |
| C                  | 0.39299  | -1.76984 | -1.94764 | C                  | 1.53744  | 2.14700  | 0.36663  | C                   | 0.95886  | -2.48609 | 0.75984  |
| C                  | -1.09337 | 2.56081  | -0.44330 | C                  | -2.75308 | -0.15803 | -1.11907 | C                   | 1.73045  | 2.15828  | -0.77224 |
| C                  | 0.44745  | 2.59195  | -0.59364 | C                  | -2.62808 | 0.25796  | 0.36663  | C                   | 1.67348  | 2.07251  | 0.76269  |
| C                  | -0.91721 | -0.79371 | 2.53937  | C                  | 1.51340  | -2.30522 | -1.11907 | C                   | -2.73421 | 0.42044  | -0.77220 |
| C                  | 0.61655  | -0.89474 | 2.56430  | C                  | 1.09064  | -2.40496 | 0.36663  | C                   | -2.63169 | 0.41208  | 0.76274  |
| H                  | -1.36820 | 2.74520  | 0.60928  | H                  | -2.75911 | -1.26279 | -1.18335 | H                   | 0.94712  | 2.85843  | -1.11921 |
| H                  | 0.70892  | 2.39848  | -1.64970 | H                  | -2.36940 | 1.33079  | 0.42152  | H                   | 2.45748  | 1.39097  | 1.13657  |
| H                  | -1.28994 | -0.61861 | 3.56242  | H                  | 1.71744  | -3.32264 | -1.49878 | H                   | -3.62661 | 1.01456  | -1.04472 |
| H                  | 1.05128  | 0.05210  | 2.93364  | H                  | 0.03220  | -2.71735 | 0.42152  | H                   | -2.43352 | 1.43135  | 1.13792  |
| H                  | 0.68045  | -2.12404 | -2.95344 | H                  | 1.97452  | 3.05609  | 0.81465  | H                   | 1.68269  | -3.22802 | 1.13951  |
| H                  | -1.49436 | -0.94919 | -2.63774 | H                  | 0.28595  | 3.02086  | -1.18335 | H                   | 2.00082  | -2.24863 | -1.12292 |
| H                  | -1.44648 | 3.45384  | -0.98944 | H                  | -3.73621 | 0.17397  | -1.49878 | H                   | 2.69088  | 2.63430  | -1.04535 |
| H                  | 0.74202  | 3.64342  | -0.41979 | H                  | -3.63391 | 0.18194  | 0.81465  | H                   | 1.95403  | 3.06986  | 1.14363  |
| H                  | -1.47332 | -2.68384 | -2.39455 | H                  | 2.01877  | 3.14867  | -1.49878 | H                   | 0.93487  | -3.64673 | -1.04906 |
| H                  | 0.75582  | -2.55179 | -1.25751 | H                  | 2.33719  | 1.38657  | 0.42152  | H                   | -0.02300 | -2.82456 | 1.13443  |
| H                  | 0.92096  | -1.67085 | 3.28821  | H                  | 1.65939  | -3.23803 | 0.81465  | H                   | -3.63576 | 0.15589  | 1.14320  |
| H                  | -1.33488 | -1.76822 | 2.22870  | H                  | 2.47316  | -1.75807 | -1.18335 | H                   | -2.94885 | -0.60757 | -1.12049 |
| H                  | 4.10311  | 0.66359  | -0.94115 | B                  | 0.00000  | 0.00000  | 3.75057  | H                   | -0.95047 | 0.70880  | 4.21826  |
| H                  | 4.10660  | 0.14812  | 1.05334  | H                  | -0.25689 | -1.15918 | 4.07192  | H                   | -0.13940 | -1.18280 | 4.21675  |
| H                  | 3.97133  | -1.31674 | -0.38399 | H                  | 1.13232  | 0.35712  | 4.07192  | H                   | 1.09324  | 0.46541  | 4.21757  |
| B                  | 3.75238  | -0.14503 | -0.08636 | H                  | -0.87543 | 0.80206  | 4.07192  | B                   | 0.00104  | -0.00264 | 3.90276  |
| [4.4.4]ch3_plus_oo |          |          |          | [4.4.4]ch3_plus_io |          |          |          | [4.4.4]ch3_plus_ts_ |          |          |          |
| P                  | 1.14425  | 0.07750  | -0.04745 | P                  | 0.00000  | 0.00000  | 0.98375  | P                   | 0.00052  | -0.00120 | 1.79585  |
| P                  | -3.00368 | -0.09443 | 0.18070  | P                  | 0.00000  | 0.00000  | -1.79665 | P                   | -0.00045 | 0.00116  | -1.71381 |
| C                  | 0.77280  | 1.79178  | 0.56527  | C                  | 1.68768  | -0.70765 | 0.65867  | C                   | 0.28755  | 1.76382  | 1.36066  |
| C                  | -2.39235 | 1.39882  | -0.82037 | C                  | 0.82407  | -1.49568 | -2.50708 | C                   | 1.67533  | 0.81695  | -1.52269 |
| H                  | 1.77065  | 2.26483  | 0.51798  | H                  | 2.12096  | -0.86741 | 1.66181  | H                   | 0.13076  | 2.30075  | 2.31319  |
| H                  | 0.52710  | 1.72717  | 1.63839  | H                  | 2.27655  | 0.10015  | 0.18933  | H                   | -0.51515 | 2.08509  | 0.68368  |
| H                  | -1.72651 | 1.06579  | -1.63048 | H                  | 0.09900  | -2.32815 | -2.44595 | H                   | 2.36836  | 0.08094  | -1.07841 |
| H                  | -3.29515 | 1.77682  | -1.32807 | H                  | 1.06635  | -1.34691 | -3.57495 | H                   | 2.04984  | 0.99724  | -2.54293 |
| C                  | 0.67815  | -0.15265 | -1.81977 | C                  | -1.45668 | -1.10775 | 0.65867  | C                   | 1.38511  | -1.13196 | 1.35839  |
| H                  | 1.64510  | -0.11545 | -2.35187 | H                  | -1.81168 | -1.40310 | 1.66181  | H                   | 1.92947  | -1.26537 | 2.31026  |
| H                  | 0.11590  | 0.73485  | -2.14625 | H                  | -1.05154 | -2.02162 | 0.18933  | H                   | 2.06399  | -0.59691 | 0.68112  |
| C                  | -2.38751 | -1.58873 | -0.83538 | C                  | -1.70733 | 0.03418  | -2.50708 | C                   | -0.13166 | -1.85815 | -1.52400 |
| H                  | -1.91578 | -2.32351 | -0.15793 | H                  | -2.06574 | 1.07834  | -2.44595 | H                   | -1.11514 | -2.09067 | -1.07891 |
| H                  | -3.34749 | -2.06415 | -1.10184 | H                  | -1.69963 | -0.25003 | -3.57495 | H                   | -0.16380 | -2.27183 | -2.54453 |
| C                  | -1.92579 | 0.07508  | 1.72855  | C                  | 0.88327  | 1.46150  | -2.50708 | C                   | -1.54487 | 1.04430  | -1.52166 |
| H                  | -2.57825 | 0.65161  | 2.40660  | H                  | 0.63328  | 1.59694  | -3.57495 | H                   | -1.88808 | 1.27976  | -2.54167 |
| H                  | -1.07494 | 0.73354  | 1.52612  | H                  | 1.96674  | 1.24981  | -2.44595 | H                   | -1.25405 | 2.01193  | -1.07612 |
| C                  | 0.60582  | -1.39375 | 0.93185  | C                  | -0.23100 | 1.81539  | 0.65867  | C                   | -1.67147 | -0.63458 | 1.35958  |
| H                  | -0.17123 | -1.88871 | 0.33599  | H                  | -1.22500 | 1.92147  | 0.18933  | H                   | -1.54825 | -1.48954 | 0.68155  |
| H                  | 1.49843  | -2.04241 | 0.87902  | H                  | -0.30928 | 2.27051  | 1.66181  | H                   | -2.05823 | -1.04000 | 2.31154  |

|               |          |          |          |               |          |          |          |                |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|----------------|----------|----------|----------|
| C             | -1.60943 | -1.46116 | -2.16926 | C             | -2.63105 | -0.88056 | -1.68293 | C              | 0.99524  | -2.58312 | -0.76728 |
| C             | -0.06587 | -1.45482 | -2.20695 | C             | -2.65245 | -0.56887 | -0.17266 | C              | 1.00633  | -2.50883 | 0.76696  |
| C             | -1.73086 | 2.57396  | -0.05554 | C             | 2.07811  | -1.83827 | -1.68293 | C              | 1.73958  | 2.15441  | -0.76429 |
| C             | -0.20214 | 2.71840  | -0.20617 | C             | 1.81888  | -2.01265 | -0.17266 | C              | 1.66943  | 2.12495  | 0.76990  |
| C             | -1.41333 | -1.18226 | 2.46145  | C             | 0.55294  | 2.71883  | -1.68293 | C              | -2.73540 | 0.43028  | -0.76423 |
| C             | 0.11940  | -1.25844 | 2.39279  | C             | 0.83357  | 2.58153  | -0.17266 | C              | -2.67507 | 0.38234  | 0.76992  |
| H             | -2.00750 | 2.58602  | 1.01185  | H             | 2.85510  | -1.06504 | -1.82802 | H              | 0.96221  | 2.84152  | -1.14592 |
| H             | 0.06027  | 2.71197  | -1.27944 | H             | 0.95075  | -2.67785 | -0.01457 | H              | 2.46741  | 1.48226  | 1.18259  |
| H             | -1.72050 | -1.15416 | 3.51897  | H             | 1.15090  | 3.56011  | -2.07278 | H              | -3.62211 | 1.03013  | -1.03599 |
| H             | 0.56795  | -0.38312 | 2.89654  | H             | 1.84371  | 2.16230  | -0.01457 | H              | -2.51755 | 1.39424  | 1.18390  |
| H             | 0.21215  | -1.63690 | -3.25935 | H             | -3.55153 | -1.04415 | 0.25405  | H              | 1.77122  | -3.21977 | 1.12185  |
| H             | -1.98317 | -0.59829 | -2.74866 | H             | -2.34990 | -1.94007 | -1.82802 | H              | 1.97860  | -2.25316 | -1.14963 |
| H             | -2.14496 | 3.50976  | -0.46758 | H             | 2.50769  | -2.77676 | -2.07278 | H              | 2.70216  | 2.62262  | -1.03665 |
| H             | 0.06239  | 3.73103  | 0.14682  | H             | 2.68003  | -2.55364 | 0.25405  | H              | 1.90262  | 3.14241  | 1.12609  |
| H             | -1.89838 | -2.34444 | -2.76609 | H             | -3.65859 | -0.78334 | -2.07278 | H              | 0.91914  | -3.65062 | -1.04039 |
| H             | 0.33901  | -2.32008 | -1.65323 | H             | -2.79446 | 0.51555  | -0.01457 | H              | 0.05116  | -2.87886 | 1.18031  |
| H             | 0.47838  | -2.14483 | 2.94140  | H             | 0.87150  | 3.59779  | 0.25405  | H              | -3.67286 | 0.07511  | 1.12556  |
| H             | -1.83964 | -2.11318 | 2.04699  | H             | -0.50520 | 3.00511  | -1.82802 | H              | -2.94170 | -0.58603 | -1.14715 |
| C             | 2.96922  | -0.00106 | 0.00258  | C             | 0.00000  | 0.00000  | 2.83931  | C              | 0.00093  | -0.00245 | 3.62916  |
| H             | 3.39465  | 0.81363  | -0.60428 | H             | 0.11209  | -1.02944 | 3.21812  | H              | -0.84268 | 0.60204  | 4.00020  |
| H             | 3.31077  | 0.10271  | 1.04586  | H             | 0.83548  | 0.61179  | 3.21812  | H              | -0.10088 | -1.03574 | 3.99892  |
| H             | 3.30461  | -0.97173 | -0.39598 | H             | -0.94757 | 0.41765  | 3.21812  | H              | 0.94657  | 0.42558  | 3.99970  |
| [4.4.4]clf_oo |          |          |          | [4.4.4]clf_io |          |          |          | [4.4.4]clf_ts_ |          |          |          |
| P             | 1.18206  | 0.06330  | -0.03502 | P             | 0.00000  | 0.00000  | 1.07870  | P              | 1.06954  | -0.00224 | -0.00147 |
| P             | -3.03491 | -0.07355 | 0.16293  | P             | 0.00000  | 0.00000  | -1.80822 | P              | -2.45897 | 0.00230  | 0.00154  |
| C             | 0.76495  | 1.77452  | 0.58239  | C             | -0.71664 | -1.67261 | 0.67344  | C              | 0.58022  | 0.39016  | 1.73646  |
| C             | -2.39657 | 1.41173  | -0.82946 | C             | -1.47647 | -0.84905 | -2.53517 | C              | -2.32628 | 1.71530  | 0.72946  |
| H             | 1.76626  | 2.24127  | 0.54756  | H             | -0.89335 | -2.10221 | 1.67457  | H              | 1.53255  | 0.27484  | 2.28297  |
| H             | 0.51126  | 1.70673  | 1.65411  | H             | 0.09648  | -2.26316 | 0.21516  | H              | -0.09781 | -0.39318 | 2.10314  |
| H             | -1.71261 | 1.06494  | -1.61693 | H             | -2.31561 | -0.12975 | -2.49450 | H              | -1.88944 | 2.36977  | -0.04555 |
| H             | -3.28299 | 1.79973  | -1.35899 | H             | -1.31804 | -1.11436 | -3.59694 | H              | -3.34972 | 2.08807  | 0.89928  |
| C             | 0.65588  | -0.16091 | -1.80120 | C             | -1.09020 | 1.45693  | 0.67344  | C              | 0.57891  | 1.30723  | -1.20911 |
| H             | 1.62580  | -0.14364 | -2.32878 | H             | -1.37389 | 1.82477  | 1.67457  | H              | 1.53149  | 1.83700  | -1.38480 |
| H             | 0.11356  | 0.73988  | -2.12741 | H             | -2.00819 | 1.04803  | 0.21516  | H              | -0.09704 | 2.01731  | -0.71244 |
| C             | -2.39773 | -1.57465 | -0.82395 | C             | 0.00294  | 1.70318  | -2.53517 | C              | -2.33097 | -0.22397 | -1.84622 |
| H             | -1.85200 | -2.24568 | -0.13870 | H             | 1.04544  | 2.07025  | -2.49450 | H              | -1.89573 | -1.22290 | -2.02655 |
| H             | -3.33601 | -2.11310 | -1.04296 | H             | -0.30604 | 1.69864  | -3.59694 | H              | -3.35543 | -0.26208 | -2.25152 |
| C             | -1.93542 | 0.07380  | 1.68992  | C             | 1.47353  | -0.85413 | -2.53517 | C              | -2.33008 | -1.48495 | 1.12105  |
| H             | -2.53900 | 0.68399  | 2.38391  | H             | 1.62409  | -0.58428 | -3.59694 | H              | -3.35437 | -1.81568 | 1.35913  |
| H             | -1.06533 | 0.68648  | 1.44031  | H             | 1.27017  | -1.94050 | -2.49450 | H              | -1.89218 | -1.14218 | 2.07529  |
| C             | 0.66810  | -1.41204 | 0.97675  | C             | 1.80684  | 0.21567  | 0.67344  | C              | 0.57564  | -1.70224 | -0.53050 |
| H             | -0.01664 | -2.01306 | 0.36204  | H             | 1.91171  | 1.21513  | 0.21516  | H              | -0.10226 | -1.62636 | -1.39218 |
| H             | 1.62305  | -1.96490 | 1.01896  | H             | 2.26724  | 0.27744  | 1.67457  | H              | 1.52684  | -2.12041 | -0.90369 |
| C             | -1.64787 | -1.43865 | -2.17212 | C             | -0.89689 | 2.61794  | -1.68274 | C              | -1.55519 | 0.84909  | -2.63286 |
| C             | -0.10504 | -1.44333 | -2.20638 | C             | -0.54823 | 2.63432  | -0.17887 | C              | -0.02064 | 0.84527  | -2.55424 |
| C             | -1.73130 | 2.57662  | -0.05003 | C             | -1.81875 | -2.08570 | -1.68274 | C              | -1.54990 | 1.85794  | 2.05193  |
| C             | -0.19912 | 2.70775  | -0.18970 | C             | -2.00727 | -1.79193 | -0.17887 | C              | -0.01554 | 1.78767  | 2.00906  |

|                |          |          |          |                |          |          |          |                 |          |          |          |
|----------------|----------|----------|----------|----------------|----------|----------|----------|-----------------|----------|----------|----------|
| C              | -1.44449 | -1.19792 | 2.41157  | C              | 2.71564  | -0.53224 | -1.68274 | C               | -1.55702 | -2.70362 | 0.58322  |
| C              | 0.09054  | -1.26512 | 2.40034  | C              | 2.55550  | -0.84238 | -0.17887 | C               | -0.02248 | -2.63546 | 0.54356  |
| H              | -2.01338 | 2.57757  | 1.01642  | H              | -1.03549 | -2.85776 | -1.80222 | H               | -1.92294 | 1.11843  | 2.78502  |
| H              | 0.06642  | 2.69933  | -1.26231 | H              | -2.65601 | -0.90675 | -0.05014 | H               | 0.38709  | 2.54096  | 1.30935  |
| H              | -1.79537 | -1.19589 | 3.45674  | H              | 3.56948  | -1.11398 | -2.07244 | H               | -1.83345 | -3.55580 | 1.23091  |
| H              | 0.51426  | -0.38431 | 2.91576  | H              | 2.11327  | -1.84679 | -0.05014 | H               | 0.38091  | -2.40723 | 1.54573  |
| H              | 0.17430  | -1.62494 | -3.25934 | H              | -0.99034 | 3.54758  | 0.25441  | H               | 0.34151  | 1.55250  | -3.32004 |
| H              | -2.02007 | -0.56643 | -2.73902 | H              | -1.95715 | 2.32564  | -1.80222 | H               | -1.92639 | 1.85415  | -2.35806 |
| H              | -2.14114 | 3.51820  | -0.45515 | H              | -2.74948 | -2.53427 | -2.07244 | H               | -1.82414 | 2.84528  | 2.46674  |
| H              | 0.06621  | 3.72186  | 0.16098  | H              | -2.57712 | -2.63145 | 0.25441  | H               | 0.34761  | 2.09629  | 3.00437  |
| H              | -1.95028 | -2.31456 | -2.77417 | H              | -0.82000 | 3.64825  | -2.07244 | H               | -1.83215 | 0.71498  | -3.69466 |
| H              | 0.28456  | -2.31816 | -1.65678 | H              | 0.54273  | 2.75354  | -0.05014 | H               | 0.38009  | -0.13782 | -2.85773 |
| H              | 0.42604  | -2.14400 | 2.97731  | H              | 3.56747  | -0.91613 | 0.25441  | H               | 0.33790  | -3.65271 | 0.31312  |
| H              | -1.84887 | -2.12157 | 1.96016  | H              | 2.99264  | 0.53212  | -1.80222 | H               | -1.93093 | -2.96772 | -0.42371 |
| Cl             | 3.31173  | 0.00514  | -0.03164 | Cl             | 0.00000  | 0.00000  | 3.17213  | Cl              | 3.17597  | -0.00492 | -0.00326 |
| F              | 5.32929  | -0.05936 | -0.04927 | F              | 0.00000  | 0.00000  | 5.32430  | F               | 5.24578  | -0.00756 | -0.00501 |
| [4.4.4]cucl_oo |          |          |          | [4.4.4]cucl_io |          |          |          | [4.4.4]cucl_ts_ |          |          |          |
| P              | 0.00000  | 0.00000  | 3.60091  | P              | 0.00000  | 0.00000  | 0.74099  | P               | 0.73144  | 0.00003  | 0.00003  |
| P              | 0.00000  | 0.00000  | -0.77179 | P              | 0.00000  | 0.00000  | -2.38855 | P               | -2.99073 | -0.00004 | -0.00005 |
| C              | 1.05209  | 1.39948  | 2.85766  | C              | 0.39915  | -1.74520 | 0.12452  | C               | 0.03266  | -0.73567 | -1.57438 |
| C              | 1.76615  | -0.10395 | -0.12859 | C              | -0.66324 | -1.56992 | -3.12441 | C               | -2.90417 | -1.82245 | -0.38473 |
| H              | 1.27954  | 2.01536  | 3.74431  | H              | 0.60748  | -2.29630 | 1.05705  | H               | 0.86528  | -0.69093 | -2.29509 |
| H              | 0.42210  | 2.03859  | 2.22320  | H              | 1.36254  | -1.67612 | -0.40802 | H               | -0.74668 | -0.05952 | -1.94832 |
| H              | 1.86145  | -1.01501 | 0.47827  | H              | -1.76617 | -1.48171 | -3.12521 | H               | -2.53641 | -2.31358 | 0.53531  |
| H              | 2.34604  | -0.29647 | -1.04471 | H              | -0.34246 | -1.72253 | -4.17181 | H               | -3.92996 | -2.19805 | -0.53706 |
| C              | 0.68594  | -1.61088 | 2.85766  | C              | -1.71096 | 0.52692  | 0.12452  | C               | 0.03266  | -0.99558 | 1.42440  |
| H              | 1.10558  | -2.11579 | 3.74431  | H              | -2.29239 | 0.62206  | 1.05705  | H               | 0.86533  | -1.64198 | 1.74610  |
| H              | 1.55442  | -1.38485 | 2.22320  | H              | -2.13283 | -0.34194 | -0.40802 | H               | -0.74657 | -1.65760 | 1.02577  |
| C              | -0.97310 | -1.47756 | -0.12859 | C              | -1.02797 | 1.35934  | -3.12441 | C               | -2.90427 | 0.57802  | 1.77054  |
| H              | -1.80975 | -1.10456 | 0.47827  | H              | -0.40012 | 2.27040  | -3.12521 | H               | -2.53648 | 1.62036  | 1.73589  |
| H              | -1.42977 | -1.88349 | -1.04471 | H              | -1.32052 | 1.15785  | -4.17181 | H               | -3.93009 | 0.63392  | 2.17192  |
| C              | -0.79305 | 1.58151  | -0.12859 | C              | 1.69121  | 0.21058  | -3.12441 | C               | -2.90425 | 1.24436  | -1.38591 |
| H              | -0.91626 | 2.17997  | -1.04471 | H              | 1.66299  | 0.56468  | -4.17181 | H               | -3.93007 | 1.56408  | -1.63497 |
| H              | -0.05170 | 2.11957  | 0.47827  | H              | 2.16628  | -0.78869 | -3.12521 | H               | -2.53653 | 0.69320  | -2.27131 |
| C              | -1.73804 | 0.21140  | 2.85766  | C              | 1.31181  | 1.21827  | 0.12452  | C               | 0.03266  | 1.73137  | 0.15007  |
| H              | -1.97652 | -0.65375 | 2.22320  | H              | 0.77029  | 2.01805  | -0.40802 | H               | -0.74661 | 1.71716  | 0.92267  |
| H              | -2.38512 | 0.10043  | 3.74431  | H              | 1.68491  | 1.67424  | 1.05705  | H               | 0.86531  | 2.33318  | 0.54907  |
| C              | -0.24641 | -2.62975 | 0.60199  | C              | -2.25808 | 1.59090  | -2.22354 | C               | -2.06311 | -0.25184 | 2.76194  |
| C              | -0.24391 | -2.61946 | 2.14432  | C              | -1.92311 | 1.81024  | -0.72858 | C               | -0.52924 | -0.21929 | 2.63926  |
| C              | 2.40064  | 1.10148  | 0.60199  | C              | -0.24872 | -2.75100 | -2.22354 | C               | -2.06293 | -2.26608 | -1.59907 |
| C              | 2.39047  | 1.09850  | 2.14432  | C              | -0.60616 | -2.57058 | -0.72858 | C               | -0.52907 | -2.17598 | -1.50953 |
| C              | -2.15423 | 1.52828  | 0.60199  | C              | 2.50680  | 1.16011  | -2.22354 | C               | -2.06304 | 2.51784  | -1.16290 |
| C              | -2.14656 | 1.52096  | 2.14432  | C              | 2.52927  | 0.76034  | -0.72858 | C               | -0.52917 | 2.39530  | -1.12968 |
| H              | 1.98651  | 2.05567  | 0.23009  | H              | 0.83961  | -2.93016 | -2.31180 | H               | -2.39772 | -1.71733 | -2.49950 |
| H              | 2.83744  | 0.15634  | 2.50966  | H              | -1.63548 | -2.17868 | -0.64678 | H               | -0.16679 | -2.72649 | -0.62424 |
| H              | -2.69757 | 2.44095  | 0.29954  | H              | 3.54659  | 1.19452  | -2.59552 | H               | -2.32851 | 3.20699  | -1.98630 |
| H              | -1.55411 | 2.37913  | 2.50966  | H              | 2.70453  | -0.32703 | -0.64678 | H               | -0.16690 | 1.90388  | -2.04910 |

|                  |          |          |          |                  |          |          |          |                   |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|----------|-------------------|----------|----------|----------|
| H                | 0.08467  | -3.62861 | 2.45079  | H                | -2.77379 | 2.34834  | -0.27631 | H                 | -0.12757 | -0.69357 | 3.55098  |
| H                | 0.78700  | -2.74820 | 0.23009  | H                | -2.95740 | 0.73795  | -2.31180 | H                 | -2.39787 | -1.30602 | 2.73685  |
| H                | 3.46271  | 1.11569  | 0.29954  | H                | -0.73881 | -3.66869 | -2.59552 | H                 | -2.32836 | -3.32376 | -1.78415 |
| H                | 3.10013  | 1.88763  | 2.45079  | H                | -0.64682 | -3.57634 | -0.27631 | H                 | -0.12735 | -2.72839 | -2.37612 |
| H                | -0.76514 | -3.55664 | 0.29954  | H                | -2.80777 | 2.47417  | -2.59552 | H                 | -2.32863 | 0.11667  | 3.77045  |
| H                | -1.28333 | -2.53547 | 2.50966  | H                | -1.06905 | 2.50571  | -0.64678 | H                 | -0.16701 | 0.82267  | 2.67341  |
| H                | -3.18480 | 1.74098  | 2.45079  | H                | 3.42061  | 1.22800  | -0.27631 | H                 | -0.12750 | 3.42202  | -1.17481 |
| H                | -2.77351 | 0.69253  | 0.23009  | H                | 2.11778  | 2.19221  | -2.31180 | H                 | -2.39782 | 3.02321  | -0.23742 |
| Cu               | 0.00000  | 0.00000  | -2.89710 | Cu               | 0.00000  | 0.00000  | 2.87041  | Cl                | 4.91814  | 0.00000  | -0.00001 |
| Cl               | 0.00000  | 0.00000  | -4.96004 | Cl               | 0.00000  | 0.00000  | 4.93832  | Cu                | 2.85290  | 0.00000  | 0.00002  |
| [4.4.4]f_plus_oo |          |          |          | [4.4.4]f_plus_io |          |          |          | [4.4.4]f_plus_ts_ |          |          |          |
| P                | 1.02538  | 0.06161  | -0.03978 | P                | 0.00000  | 0.00000  | 0.66564  | P                 | 1.59254  | -0.02019 | 0.08032  |
| P                | -3.01304 | -0.06260 | 0.14914  | P                | 0.00000  | 0.00000  | -1.75761 | P                 | -2.45121 | -0.05897 | 0.00504  |
| C                | 0.76161  | 1.77681  | 0.56323  | C                | 1.72554  | -0.67162 | 0.59090  | C                 | 1.29716  | 0.86103  | -1.49419 |
| C                | -2.37198 | 1.42977  | -0.83667 | C                | 0.72596  | -1.55886 | -2.41240 | C                 | -1.76352 | -0.71505 | -1.65040 |
| H                | 1.78916  | 2.17603  | 0.46556  | H                | 2.03231  | -0.78107 | 1.64233  | H                 | 2.33432  | 1.07428  | -1.81458 |
| H                | 0.54891  | 1.73679  | 1.64385  | H                | 2.35743  | 0.11912  | 0.14579  | H                 | 0.84011  | 1.83431  | -1.26023 |
| H                | -1.69740 | 1.10109  | -1.64137 | H                | -0.01177 | -2.36342 | -2.24261 | H                 | -1.21895 | -1.65893 | -1.47760 |
| H                | -3.26598 | 1.81337  | -1.35536 | H                | 0.86243  | -1.46141 | -3.50481 | H                 | -2.68803 | -1.02890 | -2.16329 |
| C                | 0.63386  | -0.18609 | -1.80848 | C                | -1.44441 | -1.15856 | 0.59090  | C                 | 1.18641  | -1.80801 | 0.02388  |
| H                | 1.64827  | -0.19691 | -2.24971 | H                | -1.69258 | -1.36950 | 1.64233  | H                 | 2.19670  | -2.22973 | -0.13378 |
| H                | 0.14495  | 0.72661  | -2.18109 | H                | -1.07555 | -2.10116 | 0.14579  | H                 | 0.63021  | -1.96991 | -0.91135 |
| C                | -2.36039 | -1.57455 | -0.81615 | C                | -1.71300 | 0.15073  | -2.41240 | C                 | -1.47780 | -0.93471 | 1.37377  |
| H                | -1.76980 | -2.21801 | -0.14198 | H                | -2.04090 | 1.19190  | -2.24261 | H                 | -0.60284 | -0.34033 | 1.66158  |
| H                | -3.28915 | -2.14465 | -0.98547 | H                | -1.69684 | -0.01618 | -3.50481 | H                 | -2.15498 | -0.87032 | 2.24246  |
| C                | -1.95208 | 0.07323  | 1.71238  | C                | 0.98704  | 1.40813  | -2.41240 | C                 | -1.73868 | 1.69710  | 0.14089  |
| H                | -2.59823 | 0.63953  | 2.40458  | H                | 0.83441  | 1.47759  | -3.50481 | H                 | -2.59793 | 2.35319  | -0.07516 |
| H                | -1.09330 | 0.73134  | 1.53614  | H                | 2.05267  | 1.17152  | -2.24261 | H                 | -1.02451 | 1.88906  | -0.67383 |
| C                | 0.69468  | -1.40484 | 1.01120  | C                | -0.28113 | 1.83017  | 0.59090  | C                 | 1.31598  | 0.99871  | 1.58378  |
| H                | 0.11110  | -2.10341 | 0.39339  | H                | -1.28188 | 1.98204  | 0.14579  | H                 | 1.04284  | 0.32711  | 2.41380  |
| H                | 1.71550  | -1.82473 | 1.08203  | H                | -0.33973 | 2.15057  | 1.64233  | H                 | 2.35205  | 1.33189  | 1.78461  |
| C                | -1.66582 | -1.44198 | -2.19182 | C                | -2.66282 | -0.82932 | -1.69913 | C                 | -1.04046 | -2.40033 | 1.17314  |
| C                | -0.12739 | -1.45930 | -2.24585 | C                | -2.70076 | -0.66932 | -0.17008 | C                 | 0.48879  | -2.52818 | 1.19839  |
| C                | -1.71979 | 2.59839  | -0.05361 | C                | 2.04962  | -1.89141 | -1.69913 | C                 | -0.99193 | 0.18690  | -2.64216 |
| C                | -0.19131 | 2.73529  | -0.19654 | C                | 1.93003  | -2.00427 | -0.17008 | C                 | 0.54682  | 0.13960  | -2.63803 |
| C                | -1.45992 | -1.21271 | 2.40788  | C                | 0.61320  | 2.72073  | -1.69913 | C                 | -1.11718 | 2.13204  | 1.49320  |
| C                | 0.07330  | -1.28137 | 2.41954  | C                | 0.77073  | 2.67359  | -0.17008 | C                 | 0.41842  | 2.26131  | 1.51881  |
| H                | -2.00255 | 2.59690  | 1.01233  | H                | 2.81849  | -1.13890 | -1.95169 | H                 | -1.32748 | 1.23653  | -2.57204 |
| H                | 0.07798  | 2.74136  | -1.26771 | H                | 1.14431  | -2.73325 | 0.09840  | H                 | 0.89931  | -0.90233 | -2.73477 |
| H                | -1.81129 | -1.23149 | 3.45161  | H                | 1.25933  | 3.52008  | -2.09863 | H                 | -1.49320 | 3.14311  | 1.72258  |
| H                | 0.49279  | -0.41443 | 2.96021  | H                | 1.79491  | 2.35763  | 0.09840  | H                 | 0.74717  | 2.89769  | 0.67805  |
| H                | 0.15770  | -1.60535 | -3.30168 | H                | -3.54203 | -1.27078 | 0.21251  | H                 | 0.77689  | -3.58959 | 1.11480  |
| H                | -2.04317 | -0.56549 | -2.74733 | H                | -2.39556 | -1.87143 | -1.95169 | H                 | -1.42816 | -2.83290 | 0.23444  |
| H                | -2.13020 | 3.53933  | -0.45666 | H                | 2.41882  | -2.85065 | -2.09863 | H                 | -1.28581 | -0.13657 | -3.65562 |
| H                | 0.09045  | 3.73485  | 0.17809  | H                | 2.87154  | -2.43210 | 0.21251  | H                 | 0.88857  | 0.64475  | -3.55749 |
| H                | -1.98333 | -2.31359 | -2.78979 | H                | -3.67815 | -0.66943 | -2.09863 | H                 | -1.44958 | -3.02684 | 1.98140  |
| H                | 0.26555  | -2.34541 | -1.71704 | H                | -2.93922 | 0.37562  | 0.09840  | H                 | 0.88775  | -2.17859 | 2.16716  |

|                  |          |          |          |                  |          |          |          |                   |          |          |          |
|------------------|----------|----------|----------|------------------|----------|----------|----------|-------------------|----------|----------|----------|
| H                | 0.40353  | -2.17584 | 2.97404  | H                | 0.67049  | 3.70288  | 0.21251  | H                 | 0.69065  | 2.82244  | 2.42979  |
| H                | -1.86340 | -2.12765 | 1.94026  | H                | -0.42293 | 3.01033  | -1.95169 | H                 | -1.45901 | 1.50308  | 2.33210  |
| F                | 2.65381  | 0.02883  | -0.06305 | F                | 0.00000  | 0.00000  | 2.38492  | F                 | 3.21922  | -0.10249 | 0.10277  |
| [4.4.4]hf_oo     |          |          |          | [4.4.4]hf_io     |          |          |          | [4.4.4]hf_ts_     |          |          |          |
| P                | 1.97081  | -0.00268 | -0.06028 | P                | 0.00000  | 0.00000  | 1.79242  | P                 | 0.00058  | -0.00143 | 2.10885  |
| P                | -2.43938 | -0.02616 | 0.23100  | P                | 0.00000  | 0.00000  | -1.42634 | P                 | -0.00044 | 0.00113  | -1.67319 |
| C                | 1.43680  | 1.78828  | 0.26732  | C                | -0.28760 | -1.75385 | 1.11391  | C                 | 0.27467  | 1.70101  | 1.34967  |
| C                | -1.82191 | 1.29167  | -0.98615 | C                | -1.17987 | -1.23066 | -2.16421 | C                 | 1.63636  | 0.88748  | -1.60513 |
| H                | 2.40754  | 2.30930  | 0.17647  | H                | -0.30745 | -2.36792 | 2.03244  | H                 | 0.02907  | 2.40670  | 2.16232  |
| H                | 1.17977  | 1.87969  | 1.33837  | H                | 0.63414  | -2.04524 | 0.58279  | H                 | -0.47456 | 1.85883  | 0.56327  |
| H                | -1.19009 | 0.81300  | -1.74846 | H                | -2.17472 | -0.74645 | -2.18370 | H                 | 2.36941  | 0.14003  | -1.24821 |
| H                | -2.72536 | 1.63291  | -1.51968 | H                | -0.92544 | -1.50720 | -3.20466 | H                 | 1.94601  | 1.14935  | -2.63119 |
| C                | 1.27026  | -0.43950 | -1.75845 | C                | -1.37508 | 1.12599  | 1.11391  | C                 | 1.33713  | -1.08941 | 1.34749  |
| H                | 2.15142  | -0.47562 | -2.42127 | H                | -1.89695 | 1.45022  | 2.03244  | H                 | 2.07188  | -1.23020 | 2.15930  |
| H                | 0.65724  | 0.39843  | -2.12515 | H                | -2.08830 | 0.47344  | 0.58279  | H                 | 1.84764  | -0.51886 | 0.56102  |
| C                | -1.89619 | -1.65324 | -0.60608 | C                | -0.47584 | 1.63713  | -2.16421 | C                 | -0.05118 | -1.85961 | -1.60653 |
| H                | -1.50240 | -2.33519 | 0.17009  | H                | 0.44091  | 2.25659  | -2.18370 | H                 | -1.06466 | -2.12100 | -1.24881 |
| H                | -2.87950 | -2.08629 | -0.86580 | H                | -0.84255 | 1.55505  | -3.20466 | H                 | 0.01976  | -2.25791 | -2.63297 |
| C                | -1.30215 | 0.35030  | 1.69087  | C                | 1.65571  | -0.40647 | -2.16421 | C                 | -1.58646 | 0.97539  | -1.60420 |
| H                | -1.89266 | 1.08455  | 2.26656  | H                | 1.76799  | -0.04785 | -3.20466 | H                 | -1.96788 | 1.11391  | -2.63015 |
| H                | -0.42548 | 0.88953  | 1.32112  | H                | 1.73381  | -1.51014 | -2.18370 | H                 | -1.30573 | 1.98350  | -1.24596 |
| C                | 1.06501  | -1.23043 | 1.03368  | C                | 1.66268  | 0.62786  | 1.11391  | C                 | -1.61068 | -0.61433 | 1.34861  |
| H                | 0.14189  | -1.52421 | 0.52584  | H                | 1.45416  | 1.57180  | 0.58279  | H                 | -1.37260 | -1.34110 | 0.56134  |
| H                | 1.73255  | -2.10942 | 0.99932  | H                | 2.20441  | 0.91770  | 2.03244  | H                 | -2.09918 | -1.18088 | 2.16046  |
| C                | -1.05899 | -1.73564 | -1.91133 | C                | -1.51803 | 2.30372  | -1.24235 | C                 | 1.01390  | -2.57956 | -0.75337 |
| C                | 0.48953  | -1.77106 | -1.91817 | C                | -1.09251 | 2.38620  | 0.24479  | C                 | 0.92900  | -2.47054 | 0.78007  |
| C                | -1.08048 | 2.53108  | -0.41972 | C                | -1.23606 | -2.46651 | -1.24235 | C                 | 1.72716  | 2.16878  | -0.75035 |
| C                | 0.45163  | 2.58853  | -0.62457 | C                | -1.52026 | -2.13924 | 0.24479  | C                 | 1.67492  | 2.03882  | 0.78292  |
| C                | -0.81008 | -0.77164 | 2.63242  | C                | 2.75409  | 0.16279  | -1.24235 | C                 | -2.74165 | 0.41231  | -0.75034 |
| C                | 0.71862  | -0.89170 | 2.50135  | C                | 2.61276  | -0.24696 | 0.24479  | C                 | -2.60326 | 0.43013  | 0.78299  |
| H                | -1.32433 | 2.71097  | 0.64097  | H                | -0.28683 | -3.03127 | -1.31025 | H                 | 0.94565  | 2.88263  | -1.07268 |
| H                | 0.67215  | 2.38920  | -1.68934 | H                | -2.31680 | -1.37555 | 0.29580  | H                 | 2.44850  | 1.32974  | 1.12535  |
| H                | -1.08844 | -0.54233 | 3.67481  | H                | 3.73811  | -0.17775 | -1.61284 | H                 | -3.63518 | 1.00763  | -1.01758 |
| H                | 1.19058  | 0.05024  | 2.83570  | H                | 2.34966  | -1.31864 | 0.29580  | H                 | -2.37603 | 1.45418  | 1.12674  |
| H                | 0.75738  | -2.15872 | -2.91755 | H                | -1.65461 | 3.21979  | 0.70060  | H                 | 1.62503  | -3.22332 | 1.18911  |
| H                | -1.39663 | -0.95694 | -2.61933 | H                | -2.48174 | 1.76404  | -1.31025 | H                 | 2.02255  | -2.25943 | -1.07645 |
| H                | -1.47494 | 3.41239  | -0.95626 | H                | -2.02299 | -3.14842 | -1.61284 | H                 | 2.68922  | 2.64515  | -1.01818 |
| H                | 0.73537  | 3.64671  | -0.47214 | H                | -1.96112 | -3.04283 | 0.70060  | H                 | 1.97876  | 3.01749  | 1.19324  |
| H                | -1.36635 | -2.68933 | -2.38020 | H                | -1.71512 | 3.32617  | -1.61284 | H                 | 0.94515  | -3.65071 | -1.02196 |
| H                | 0.85121  | -2.53781 | -1.21206 | H                | -0.03286 | 2.69418  | 0.29580  | H                 | -0.07154 | -2.78620 | 1.12325  |
| H                | 1.10271  | -1.68252 | 3.16734  | H                | 3.61572  | -0.17697 | 0.70060  | H                 | -3.60280 | 0.20342  | 1.19284  |
| H                | -1.27208 | -1.74801 | 2.39695  | H                | 2.76857  | 1.26723  | -1.31025 | H                 | -2.96905 | -0.62102 | -1.07399 |
| F                | 5.08039  | -0.25803 | 0.14109  | H                | 0.00000  | 0.00000  | 3.93872  | H                 | 0.00114  | -0.00291 | 4.27754  |
| H                | 4.13019  | -0.18217 | 0.08891  | F                | 0.00000  | 0.00000  | 4.89913  | F                 | 0.00138  | -0.00356 | 5.23366  |
| [4.4.4]h_plus_oo |          |          |          | [4.4.4]h_plus_io |          |          |          | [4.4.4]h_plus_ts_ |          |          |          |
| P                | 1.08618  | 0.08035  | -0.03557 | P                | 0.00000  | 0.00000  | 0.87786  | P                 | 0.00010  | -0.00008 | 1.73683  |

|               |          |          |          |               |          |          |          |               |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| P             | -3.01160 | -0.07630 | 0.17661  | P             | 0.00000  | 0.00000  | -1.79283 | P             | -0.00010 | 0.00008  | -1.72094 |
| C             | 0.76182  | 1.81087  | 0.56529  | C             | 1.69855  | -0.71761 | 0.64964  | C             | -1.78395 | 0.28441  | 1.37508  |
| C             | -2.36453 | 1.39974  | -0.82446 | C             | 0.80802  | -1.50718 | -2.49128 | C             | -0.81667 | 1.67483  | -1.49657 |
| H             | 1.76931  | 2.25913  | 0.49199  | H             | 2.07130  | -0.88436 | 1.67574  | H             | -2.27455 | 0.15805  | 2.35596  |
| H             | 0.53313  | 1.75675  | 1.64283  | H             | 2.31796  | 0.08708  | 0.21323  | H             | -2.13504 | -0.53839 | 0.73722  |
| H             | -1.65895 | 1.05466  | -1.59453 | H             | 0.08259  | -2.33696 | -2.40697 | H             | -0.09633 | 2.36104  | -1.01910 |
| H             | -3.24264 | 1.76479  | -1.38245 | H             | 1.02511  | -1.36591 | -3.56564 | H             | -0.97253 | 2.06902  | -2.51320 |
| C             | 0.68347  | -0.17512 | -1.82365 | C             | -1.47075 | -1.11218 | 0.64964  | C             | 1.13847  | 1.40272  | 1.37502  |
| H             | 1.67186  | -0.18952 | -2.31441 | H             | -1.80153 | -1.35162 | 1.67574  | H             | 1.27450  | 1.89068  | 2.35593  |
| H             | 0.17260  | 0.73030  | -2.18563 | H             | -1.08357 | -2.05096 | 0.21323  | H             | 0.60141  | 2.11826  | 0.73730  |
| C             | -2.39216 | -1.57798 | -0.82591 | C             | -1.70927 | 0.05383  | -2.49128 | C             | 1.85859  | -0.13013 | -1.49680 |
| H             | -1.88653 | -2.29035 | -0.14993 | H             | -2.06516 | 1.09695  | -2.40697 | H             | 2.09275  | -1.09709 | -1.01941 |
| H             | -3.34498 | -2.07940 | -1.06767 | H             | -1.69547 | -0.20482 | -3.56564 | H             | 2.27777  | -0.19219 | -2.51348 |
| C             | -1.93479 | 0.07225  | 1.72831  | C             | 0.90125  | 1.45336  | -2.49128 | C             | -1.04220 | -1.54447 | -1.49667 |
| H             | -2.57924 | 0.64846  | 2.41403  | H             | 0.67035  | 1.57073  | -3.56564 | H             | -1.30572 | -1.87642 | -2.51332 |
| H             | -1.07666 | 0.72532  | 1.53466  | H             | 1.98257  | 1.24001  | -2.40697 | H             | -1.99661 | -1.26378 | -1.01910 |
| C             | 0.63101  | -1.41192 | 0.96226  | C             | -0.22781 | 1.82979  | 0.64964  | C             | 0.64573  | -1.68734 | 1.37491  |
| H             | -0.08767 | -1.97409 | 0.35102  | H             | -1.23440 | 1.96388  | 0.21323  | H             | 1.53387  | -1.57998 | 0.73708  |
| H             | 1.57362  | -1.98684 | 0.94815  | H             | -0.26977 | 2.23598  | 1.67574  | H             | 1.00042  | -2.04914 | 2.35577  |
| C             | -1.63559 | -1.44268 | -2.17090 | C             | -2.63598 | -0.88051 | -1.69372 | C             | 2.56958  | 1.02426  | -0.76995 |
| C             | -0.09293 | -1.45606 | -2.21567 | C             | -2.67455 | -0.59471 | -0.18013 | C             | 2.51190  | 1.04954  | 0.76393  |
| C             | -1.73732 | 2.58543  | -0.04781 | C             | 2.08054  | -1.84256 | -1.69372 | C             | -2.17187 | 1.71327  | -0.76968 |
| C             | -0.21144 | 2.74387  | -0.19803 | C             | 1.85230  | -2.01887 | -0.18013 | C             | -2.16485 | 1.65050  | 0.76419  |
| C             | -1.43741 | -1.20086 | 2.44382  | C             | 0.55544  | 2.72308  | -1.69372 | C             | -0.39785 | -2.73741 | -0.76997 |
| C             | 0.09547  | -1.28488 | 2.40572  | C             | 0.82224  | 2.61358  | -0.18013 | C             | -0.34691 | -2.70016 | 0.76391  |
| H             | -2.01435 | 2.58353  | 1.01946  | H             | 2.85056  | -1.06607 | -1.85639 | H             | -2.83649 | 0.92242  | -1.16285 |
| H             | 0.05061  | 2.74556  | -1.27139 | H             | 1.00417  | -2.70546 | -0.00416 | H             | -1.54559 | 2.46403  | 1.18215  |
| H             | -1.76152 | -1.19193 | 3.49653  | H             | 1.15471  | 3.55819  | -2.09420 | H             | -0.98245 | -3.63070 | -1.05244 |
| H             | 0.54015  | -0.42029 | 2.93027  | H             | 1.84092  | 2.22237  | -0.00416 | H             | -1.36106 | -2.57072 | 1.18196  |
| H             | 0.18219  | -1.63154 | -3.27009 | H             | -3.56201 | -1.10127 | 0.23471  | H             | 3.20759  | 1.83381  | 1.10673  |
| H             | -2.00610 | -0.57135 | -2.73906 | H             | -2.34853 | -1.93562 | -1.85639 | H             | 2.21695  | 1.99527  | -1.16305 |
| H             | -2.16564 | 3.51730  | -0.45322 | H             | 2.50413  | -2.77910 | -2.09420 | H             | -2.65320 | 2.66621  | -1.05208 |
| H             | 0.05474  | 3.75241  | 0.16514  | H             | 2.73473  | -2.53415 | 0.23471  | H             | -3.19187 | 1.86082  | 1.10710  |
| H             | -1.93672 | -2.31768 | -2.77347 | H             | -3.65884 | -0.77909 | -2.09420 | H             | 3.63548  | 0.96463  | -1.05247 |
| H             | 0.30055  | -2.33222 | -1.67114 | H             | -2.84509 | 0.48310  | -0.00416 | H             | 2.90688  | 0.10649  | 1.18184  |
| H             | 0.43618  | -2.18144 | 2.94986  | H             | 0.82727  | 3.63542  | 0.23471  | H             | -0.01551 | -3.69479 | 1.10664  |
| H             | -1.86116 | -2.12194 | 2.00600  | H             | -0.50203 | 3.00169  | -1.85639 | H             | 0.61934  | -2.91751 | -1.16321 |
| H             | 2.49615  | 0.04210  | 0.00094  | H             | 0.00000  | 0.00000  | 2.31710  | H             | 0.00014  | -0.00013 | 3.15520  |
| [4.4.4]lih_oo |          |          |          | [4.4.4]lih_io |          |          |          | [4.4.4]lih_ts |          |          |          |
| P             | 1.90138  | 0.00696  | -0.06946 | P             | 0.00000  | 0.00000  | 1.98830  | P             | 0.00106  | -0.00154 | 2.07813  |
| P             | -2.50115 | -0.03187 | 0.23470  | P             | 0.00000  | 0.00000  | -1.21659 | P             | -0.00057 | 0.00108  | -1.69918 |
| C             | 1.37323  | 1.79814  | 0.26016  | C             | -0.93730 | -1.51337 | 1.31825  | C             | 0.27475  | 1.70334  | 1.32728  |
| C             | -1.89567 | 1.29322  | -0.98188 | C             | -1.56487 | -0.67833 | -1.95200 | C             | 1.63721  | 0.88725  | -1.62456 |
| H             | 2.33931  | 2.32741  | 0.16997  | H             | -1.18578 | -2.08143 | 2.23299  | H             | 0.02418  | 2.41319  | 2.13464  |
| H             | 1.11472  | 1.88482  | 1.33110  | H             | -0.19670 | -2.12847 | 0.78071  | H             | -0.47333 | 1.85385  | 0.53873  |
| H             | -1.27616 | 0.81927  | -1.75751 | H             | -2.29578 | 0.15227  | -1.96913 | H             | 2.37055  | 0.13958  | -1.26853 |
| H             | -2.80656 | 1.63750  | -1.50033 | H             | -1.43769 | -1.02897 | -2.99324 | H             | 1.94717  | 1.14898  | -2.65035 |

|           |          |          |          |           |          |          |          |            |          |          |          |
|-----------|----------|----------|----------|-----------|----------|----------|----------|------------|----------|----------|----------|
| C         | 1.20320  | -0.42908 | -1.76765 | C         | -0.84197 | 1.56841  | 1.31825  | C          | 1.33972  | -1.09021 | 1.32452  |
| H         | 2.07565  | -0.45075 | -2.44213 | H         | -1.20968 | 2.06763  | 2.23299  | H          | 2.08123  | -1.22827 | 2.13049  |
| H         | 0.57725  | 0.40534  | -2.11891 | H         | -1.74496 | 1.23458  | 0.78071  | H          | 1.84247  | -0.51712 | 0.53531  |
| C         | -1.95221 | -1.65641 | -0.60611 | C         | 0.19498  | 1.69438  | -1.95200 | C          | -0.05195 | -1.86042 | -1.62567 |
| H         | -1.55990 | -2.34171 | 0.16806  | H         | 1.27976  | 1.91207  | -1.96913 | H          | -1.06570 | -2.12184 | -1.26859 |
| H         | -2.93556 | -2.08855 | -0.86697 | H         | -0.17227 | 1.75956  | -2.99324 | H          | 0.01847  | -2.25904 | -2.65181 |
| C         | -1.37396 | 0.35257  | 1.70264  | C         | 1.36989  | -1.01605 | -1.95200 | C          | -1.58681 | 0.97641  | -1.62301 |
| H         | -1.98207 | 1.07059  | 2.28041  | H         | 1.60996  | -0.73059 | -2.99324 | H          | -1.96843 | 1.11562  | -2.64858 |
| H         | -0.50516 | 0.91337  | 1.34519  | H         | 1.01602  | -2.06434 | -1.96913 | H          | -1.30582 | 1.98472  | -1.26540 |
| C         | 0.99071  | -1.21504 | 1.02234  | C         | 1.77927  | -0.05504 | 1.31825  | C          | -1.61210 | -0.61589 | 1.32609  |
| H         | 0.05881  | -1.47912 | 0.51489  | H         | 1.94166  | 0.89389  | 0.78071  | H          | -1.36822 | -1.33745 | 0.53619  |
| H         | 1.63392  | -2.11125 | 0.97469  | H         | 2.39546  | 0.01380  | 2.23299  | H          | -2.10146 | -1.18943 | 2.13237  |
| C         | -1.11667 | -1.73708 | -1.91262 | C         | -0.51196 | 2.71241  | -1.03352 | C          | 1.01355  | -2.58068 | -0.77356 |
| C         | 0.43179  | -1.76721 | -1.92229 | C         | -0.09347 | 2.62581  | 0.45504  | C          | 0.92930  | -2.47212 | 0.75985  |
| C         | -1.14888 | 2.53144  | -0.42046 | C         | -2.09303 | -1.79957 | -1.03352 | C          | 1.72813  | 2.16894  | -0.77067 |
| C         | 0.38212  | 2.59130  | -0.63184 | C         | -2.22729 | -1.39385 | 0.45504  | C          | 1.67655  | 2.03956  | 0.76257  |
| C         | -0.86730 | -0.76749 | 2.63922  | C         | 2.60499  | -0.91283 | -1.03352 | C          | -2.74233 | 0.41318  | -0.76996 |
| C         | 0.66070  | -0.88017 | 2.49471  | C         | 2.32076  | -1.23196 | 0.45504  | C          | -2.60434 | 0.43084  | 0.76328  |
| H         | -1.38874 | 2.71386  | 0.64067  | H         | -1.43685 | -2.68763 | -1.10529 | H          | 0.94703  | 2.88316  | -1.09270 |
| H         | 0.60081  | 2.39162  | -1.69671 | H         | -2.67207 | -0.38450 | 0.51255  | H          | 2.44957  | 1.33033  | 1.10575  |
| H         | -1.13582 | -0.53916 | 3.68416  | H         | 3.37970  | -1.60870 | -1.40302 | H          | -3.63565 | 1.00882  | -1.03609 |
| H         | 1.12972  | 0.06431  | 2.82586  | H         | 1.66902  | -2.12183 | 0.51255  | H          | -2.37661 | 1.45439  | 1.10799  |
| H         | 0.70112  | -2.15431 | -2.92113 | H         | -0.29796 | 3.60949  | 0.91182  | H          | 1.62550  | -3.22375 | 1.17000  |
| H         | -1.45771 | -0.96006 | -2.62070 | H         | -1.60913 | 2.58816  | -1.10529 | H          | 2.02227  | -2.26133 | -1.09673 |
| H         | -1.54437 | 3.41218  | -0.95686 | H         | -3.08303 | -2.12255 | -1.40302 | H          | 2.69019  | 2.64513  | -1.03774 |
| H         | 0.66456  | 3.64979  | -0.48127 | H         | -2.97693 | -2.06279 | 0.91182  | H          | 1.97949  | 3.01775  | 1.17397  |
| H         | -1.42113 | -2.69200 | -2.38035 | H         | -0.29667 | 3.73126  | -1.40302 | H          | 0.94437  | -3.65178 | -1.04115 |
| H         | 0.79870  | -2.53082 | -1.21566 | H         | 1.00305  | 2.50633  | 0.51255  | H          | -0.07098 | -2.78712 | 1.10415  |
| H         | 1.05652  | -1.66969 | 3.15496  | H         | 3.27489  | -1.54670 | 0.91182  | H          | -3.60287 | 0.20344  | 1.17449  |
| H         | -1.32743 | -1.74574 | 2.40846  | H         | 3.04598  | 0.09947  | -1.10529 | H          | -2.97049 | -0.61985 | -1.09357 |
| Li        | 4.47613  | -0.22359 | 0.11064  | Li        | 0.00000  | 0.00000  | 4.57297  | Li         | 0.00002  | -0.00319 | 4.66451  |
| H         | 6.10977  | -0.35201 | 0.16366  | H         | 0.00000  | 0.00000  | 6.21794  | H          | -0.00292 | -0.00328 | 6.30636  |
| [4.4.4]oo |          |          |          | [4.4.4]io |          |          |          | [4.4.4]ts_ |          |          |          |
| P         | 2.19839  | -0.43470 | 0.08822  | P         | 0.00000  | 0.00000  | 1.98307  | P          | -0.00087 | -0.00031 | 2.06884  |
| P         | -2.19845 | 0.43513  | 0.08322  | P         | 0.00000  | 0.00000  | -1.29100 | P          | 0.00062  | 0.00011  | -1.77148 |
| C         | 1.96384  | 1.43996  | -0.18748 | C         | -0.98199 | -1.46845 | 1.23967  | C          | -0.74152 | -1.53800 | 1.24145  |
| C         | -1.36125 | 1.19754  | -1.44090 | C         | -1.58743 | -0.62193 | -2.03124 | C          | -1.81795 | -0.39737 | -1.71796 |
| H         | 3.00997  | 1.74810  | -0.36921 | H         | -1.24538 | -2.05504 | 2.13884  | H          | -0.69338 | -2.32017 | 2.01948  |
| H         | 1.71293  | 1.90517  | 0.78383  | H         | -0.26212 | -2.09160 | 0.68322  | H          | -0.07177 | -1.86169 | 0.43477  |
| H         | -0.86802 | 0.40342  | -2.02149 | H         | -2.28553 | 0.23657  | -2.05245 | H          | -2.31261 | 0.53138  | -1.37619 |
| H         | -2.19431 | 1.55221  | -2.07163 | H         | -1.47382 | -0.98239 | -3.07120 | H          | -2.18206 | -0.57524 | -2.74439 |
| C         | 1.36374  | -1.20438 | -1.43373 | C         | -0.78072 | 1.58465  | 1.23967  | C          | -0.96185 | 1.41066  | 1.24216  |
| H         | 2.19789  | -1.56246 | -2.06107 | H         | -1.15702 | 2.10605  | 2.13884  | H          | -1.66300 | 1.75994  | 2.02052  |
| H         | 0.87201  | -0.41286 | -2.01913 | H         | -1.68032 | 1.27280  | 0.68322  | H          | -1.57744 | 0.99309  | 0.43544  |
| C         | -1.96361 | -1.44078 | -0.18360 | C         | 0.25511  | 1.68572  | -2.03124 | C          | 0.56563  | 1.77375  | -1.71679 |
| H         | -1.71405 | -1.90174 | 0.79007  | H         | 1.34764  | 1.86104  | -2.05245 | H          | 1.61706  | 1.73765  | -1.37438 |
| H         | -3.00946 | -1.74978 | -0.36549 | H         | -0.11387 | 1.76756  | -3.07120 | H          | 0.59426  | 2.17852  | -2.74300 |

|   |          |          |          |   |          |          |          |   |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|---|----------|----------|----------|
| C | -1.01164 | 1.04704  | 1.41686  | C | 1.33232  | -1.06379 | -2.03124 | C | 1.25410  | -1.37599 | -1.71707 |
| H | -1.45056 | 2.02183  | 1.69387  | H | 1.58769  | -0.78517 | -3.07120 | H | 1.59089  | -1.60247 | -2.74325 |
| H | -0.04781 | 1.26721  | 0.94940  | H | 0.93789  | -2.09761 | -2.05245 | H | 0.69693  | -2.26875 | -1.37558 |
| C | 1.00915  | -1.04037 | 1.42244  | C | 1.76271  | -0.11620 | 1.23967  | C | 1.70188  | 0.12700  | 1.24290  |
| H | 0.04597  | -1.26164 | 0.95420  | H | 1.94244  | 0.81879  | 0.68322  | H | 1.64832  | 0.86920  | 0.43644  |
| H | 1.44687  | -2.01438 | 1.70404  | H | 2.40241  | -0.05101 | 2.13884  | H | 2.35460  | 0.55932  | 2.02169  |
| C | -1.14470 | -2.08064 | -1.33747 | C | -0.40678 | 2.72949  | -1.10678 | C | -0.23863 | 2.76426  | -0.84757 |
| C | 0.37084  | -2.37896 | -1.22430 | C | 0.00894  | 2.61718  | 0.38189  | C | -0.17440 | 2.62170  | 0.68480  |
| C | -0.36909 | 2.37342  | -1.23538 | C | -2.16042 | -1.71703 | -1.10678 | C | -2.27443 | -1.58887 | -0.84878 |
| C | 1.14658  | 2.07473  | -1.34525 | C | -2.27102 | -1.30085 | 0.38189  | C | -2.18386 | -1.46173 | 0.68362  |
| C | -0.74226 | 0.21691  | 2.69237  | C | 2.56720  | -1.01246 | -1.10678 | C | 2.51356  | -1.17532 | -0.84701 |
| C | 0.73840  | -0.20486 | 2.69409  | C | 2.26208  | -1.31633 | 0.38189  | C | 2.35724  | -1.16025 | 0.68531  |
| H | -0.57499 | 2.92468  | -0.30212 | H | -1.54072 | -2.63124 | -1.17758 | H | -1.73109 | -2.50079 | -1.16129 |
| H | 1.32601  | 1.51018  | -2.27871 | H | -2.67314 | -0.27312 | 0.43271  | H | -2.71590 | -0.55229 | 1.01285  |
| H | -0.97649 | 0.81284  | 3.59088  | H | 3.31415  | -1.74000 | -1.47419 | H | 3.20009  | -2.00141 | -1.11380 |
| H | 1.37353  | 0.69877  | 2.74402  | H | 1.57309  | -2.17845 | 0.43271  | H | 1.83557  | -2.07571 | 1.01443  |
| H | 0.57596  | -3.10744 | -2.02955 | H | -0.15063 | 3.60882  | 0.84084  | H | -0.61444 | 3.54264  | 1.10609  |
| H | -1.32294 | -1.52026 | -2.27366 | H | -1.50836 | 2.64992  | -1.17758 | H | -1.29992 | 2.74949  | -1.16051 |
| H | -0.57333 | 3.09830  | -2.04409 | H | -3.16396 | -2.00013 | -1.47419 | H | -3.33301 | -1.77011 | -1.11618 |
| H | 1.62433  | 3.05779  | -1.51778 | H | -3.05001 | -1.93486 | 0.84084  | H | -2.76160 | -2.30318 | 1.10483  |
| H | -1.62220 | -3.06447 | -1.50624 | H | -0.15019 | 3.74013  | -1.47419 | H | 0.13349  | 3.77186  | -1.11442 |
| H | 0.57541  | -2.92618 | -0.28839 | H | 1.10004  | 2.45156  | 0.43271  | H | 0.87908  | 2.62765  | 1.01448  |
| H | 0.97169  | -0.79689 | 3.59541  | H | 3.20064  | -1.67396 | 0.84084  | H | 3.37465  | -1.23975 | 1.10699  |
| H | -1.37752 | -0.68644 | 2.74549  | H | 3.04908  | -0.01869 | -1.17758 | H | 3.03176  | -0.24881 | -1.15932 |

**Table S2.** P...P distances in Å, pyramidalisation (pyr) in degrees calculated at MP2/jul-cc-pVDZ computational level.

| System                       | P...P   |        | P1      | P2*     | P1     | P2*    |
|------------------------------|---------|--------|---------|---------|--------|--------|
| [3.3.3]                      | out:out | in:out | out:out | out:out | in:out | in:out |
| PP                           | 4.143   |        | 314.9   |         |        |        |
| F <sup>+</sup>               | 3.728   | 2.339  | 319.7   | 345.3   | 351.2  | 359.2  |
| H <sup>+</sup>               | 3.809   | 2.462  | 317.9   | 341.5   | 352.2  | 357.1  |
| CH <sub>3</sub> <sup>+</sup> | 3.854   | 2.507  | 317.4   | 338.2   | 351.7  | 355.0  |
| ClF                          | 3.913   | 2.543  | 317.2   | 333.6   | 351.2  | 353.0  |
| AgCl                         | 4.047   |        | 315.3   | 324.1   |        |        |
| CuCl                         | 4.051   |        | 315.3   | 323.6   |        |        |
| BH <sub>3</sub>              | 3.992   |        | 316.5   | 327.3   |        |        |
| BeH <sub>2</sub>             | 4.024   |        | 316.0   | 325.1   |        |        |
| LiH                          | 4.084   |        | 315.2   | 320.5   |        |        |
| HF                           | 4.091   |        | 315.3   | 319.7   |        |        |
| [4.3.3]                      |         |        |         |         |        |        |
| -                            | 4.246   | 3.198  | 315.4   | 315.4   | 333.7  | 326.4  |
| F <sup>+</sup>               | 3.822   | 2.396  | 316.9   | 350.2   | 339.1  | 359.9  |
| H <sup>+</sup>               | 3.886   | 2.547  | 315.3   | 347.9   | 338.5  | 357.9  |
| CH <sub>3</sub> <sup>+</sup> | 3.755   | 2.621  | 316.2   | 340.6   | 337.3  | 355.2  |
| ClF                          | 3.807   | 2.681  | 315.2   | 337.2   | 336.3  | 352.5  |
| AgCl                         | 3.938   | 2.938  | 315.9   | 325.2   | 335.3  | 338.4  |
| CuCl                         | 3.943   | 2.951  | 315.8   | 324.8   | 335.3  | 337.4  |
| BH <sub>3</sub>              | 3.894   | 2.924  | 315.3   | 329.8   | 336.3  | 339.9  |
| BeH <sub>2</sub>             | 3.92    | 2.962  | 315.5   | 327.3   | 336.1  | 337.6  |
| LiH                          | 3.981   | 3.014  | 315.6   | 321.4   | 335.0  | 332.9  |
| HF                           | 3.989   | 3.028  | 315.5   | 320.8   | 334.9  | 331.9  |
| [4.4.3]                      |         |        |         |         |        |        |
| -                            | 4.042   | 3.083  | 316.6   | 316.6   | 323.5  | 322.4  |
| F <sup>+</sup>               | 3.824   | 2.433  | 314.4   | 350.0   | 328.8  | 359.9  |
| H <sup>+</sup>               | 3.905   | 2.637  | 313.7   | 345.8   | 326.4  | 357.9  |
| CH <sub>3</sub> <sup>+</sup> | 3.954   | 2.733  | 314.4   | 341.9   | 325.5  | 354.1  |
| ClF                          | 4.007   | 2.824  | 313.2   | 339.0   | 324.0  | 350.8  |
| AgCl                         | 4.145   | 3.054  | 316.6   | 326.1   | 323.4  | 336.5  |
| CuCl                         | 4.146   | 3.063  | 314.7   | 326.7   | 324.0  | 334.4  |
| BH <sub>3</sub>              | 4.088   | 3.036  | 313.0   | 332.5   | 323.8  | 338.9  |
| BeH <sub>2</sub>             | 4.116   | 3.073  | 313.2   | 330.2   | 323.5  | 337.4  |

|                              |       |       |       |       |       |       |
|------------------------------|-------|-------|-------|-------|-------|-------|
| LiH                          | 4.182 | 3.126 | 314.7 | 323.6 | 324.0 | 329.8 |
| HF                           | 4.187 | 3.138 | 313.9 | 323.5 | 323.5 | 329.7 |
| [4.4.4]                      |       |       |       |       |       |       |
| -                            | 4.482 | 3.274 | 312.3 | 312.2 | 315.6 | 317.8 |
| F <sup>+</sup>               | 4.045 | 2.423 | 311.1 | 350.6 | 324.2 | 359.5 |
| H <sup>+</sup>               | 4.106 | 2.671 | 311.1 | 346.8 | 319.8 | 355.5 |
| CH <sub>3</sub> <sup>+</sup> | 4.158 | 2.780 | 312.3 | 342.1 | 318.5 | 351.0 |
| ClF                          | 4.224 | 2.887 | 309.6 | 340.3 | 316.8 | 346.2 |
| AgCl                         | 4.37  | 3.121 | 327.1 | 317.2 | 316.1 | 330.3 |
| CuCl                         | 4.373 | 3.130 | 326.9 | 317.2 | 316.0 | 329.8 |
| BH <sub>3</sub>              | 4.327 | 3.109 | 309.2 | 333.1 | 315.8 | 334.6 |
| BeH <sub>2</sub>             | 4.563 | 3.153 | 310.8 | 321.8 | 316.0 | 331.3 |
| LiH                          | 4.413 | 3.205 | 312.3 | 319.2 | 316.1 | 324.9 |
| HF                           | 4.42  | 3.219 | 311.6 | 319.2 | 315.8 | 324.0 |

\* P2 is the atom involved in the interaction with the Lewis acids.

**Table S3.** Electron density ( $\rho_{\text{BCP}}$ ), Laplacian ( $\nabla^2\rho_{\text{BCP}}$ ) and total electron energy density ( $H_{\text{BCP}}$ ) (au) at the P $\cdots$ P BCP, at MP2/jul-cc-pVDZ computational level.

|                              |                     |                             |                  |
|------------------------------|---------------------|-----------------------------|------------------|
| [3.3.3]                      | $\rho_{\text{BCP}}$ | $\nabla^2\rho_{\text{BCP}}$ | $H_{\text{BCP}}$ |
| ClF                          | 0.0689              | -0.0155                     | -0.0283          |
| H <sup>+</sup>               | 0.0825              | -0.0603                     | -0.0402          |
| F <sup>+</sup>               | 0.1031              | -0.1380                     | -0.0657          |
| CH <sub>3</sub> <sup>+</sup> | 0.0759              | -0.0397                     | -0.0341          |
| [4.3.3]                      |                     |                             |                  |
| -                            | 0.0244              | 0.0537                      | -0.0012          |
| BH <sub>3</sub>              | 0.0313              | 0.0527                      | -0.0038          |
| BeH <sub>2</sub>             | 0.0297              | 0.0532                      | -0.0031          |
| LiH                          | 0.0274              | 0.0536                      | -0.0022          |
| CuCl                         | 0.0301              | 0.0529                      | -0.0032          |
| AgCl                         | 0.0311              | 0.0519                      | -0.0036          |
| HF                           | 0.0267              | 0.0538                      | -0.0019          |
| ClF                          | 0.0508              | 0.0240                      | -0.0145          |
| H <sup>+</sup>               | 0.0682              | -0.0206                     | -0.0274          |
| F <sup>+</sup>               | 0.0913              | -0.0987                     | -0.0514          |
| CH <sub>3</sub> <sup>+</sup> | 0.0590              | 0.0024                      | -0.0203          |
| [4.4.3]                      |                     |                             |                  |
| -                            | 0.0204              | 0.0476                      | -0.0002          |
| BH <sub>3</sub>              | 0.0253              | 0.0495                      | -0.0017          |
| BeH <sub>2</sub>             | 0.0243              | 0.0485                      | -0.0014          |
| LiH                          | 0.0226              | 0.0486                      | -0.0008          |
| CuCl                         | 0.0246              | 0.0496                      | -0.0014          |
| AgCl                         | 0.0252              | 0.0486                      | -0.0016          |
| HF                           | 0.0221              | 0.0482                      | -0.0007          |
| ClF                          | 0.0380              | 0.0395                      | -0.0071          |
| H <sup>+</sup>               | 0.0567              | 0.0047                      | -0.0183          |
| F <sup>+</sup>               | 0.0844              | -0.0767                     | -0.0441          |
| CH <sub>3</sub> <sup>+</sup> | 0.0468              | 0.0240                      | -0.0120          |
| [4.4.4]                      |                     |                             |                  |
| -                            | 0.0183              | 0.0459                      | 0.0002           |
| BH <sub>3</sub>              | 0.0225              | 0.0495                      | -0.0008          |
| BeH <sub>2</sub>             | 0.0215              | 0.0483                      | -0.0005          |
| LiH                          | 0.0201              | 0.0475                      | -0.0002          |
| CuCl                         | 0.0221              | 0.0496                      | -0.0006          |
| AgCl                         | 0.0227              | 0.0495                      | -0.0008          |
| HF                           | 0.0196              | 0.0472                      | -0.0001          |
| ClF                          | 0.0337              | 0.0461                      | -0.0049          |
| H <sup>+</sup>               | 0.0529              | 0.0152                      | -0.0158          |
| F <sup>+</sup>               | 0.0855              | -0.0783                     | -0.0464          |
| CH <sub>3</sub> <sup>+</sup> | 0.0426              | 0.0329                      | -0.0095          |