

# Supporting Information for

## Theoretical predictions of aromatic Be-O rings

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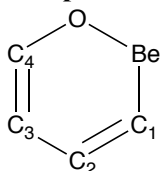
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|                                                                                                                                                              |    |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| Cartesian coordinates of <b>3</b> , <b>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub></b> .....                                                       | 2  |
| Cartesian coordinates of <b>3L</b> , <b>L<sub>1</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub></b> .....                                         | 2  |
| Cartesian coordinates of <b>3L<sub>2</sub></b> , <b>L<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub></b> .....                             | 3  |
| Cartesian coordinates of hydrogenated <b>3L(H<sub>2</sub>)</b> , <b>L<sub>1</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub></b> .....             | 4  |
| Cartesian coordinates of hydrogenated <b>3L<sub>2</sub>(H<sub>2</sub>)</b> , <b>L<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub></b> ..... | 5  |
| Cartesian coordinates of saturated <b>3L(2H<sub>2</sub>)</b> , <b>LBe<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub></b> .....                           | 6  |
| Cartesian coordinates of saturated <b>3L<sub>2</sub>(2H<sub>2</sub>)</b> , <b>L<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub></b> .....   | 7  |
| Cartesian coordinates of <b>4</b> , <b>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub></b> .....                                                       | 9  |
| Cartesian coordinates of <b>4L</b> , <b>L<sub>2</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub></b> .....                                         | 9  |
| Cartesian coordinates of <b>4L<sub>2</sub></b> , <b>L<sub>4</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub></b> .....                             | 10 |
| Cartesian coordinates of <b>5</b> , <b>Be<sub>3</sub>O<sub>3</sub></b> .....                                                                                 | 12 |
| Cartesian coordinates of <b>5L</b> , <b>L<sub>3</sub>Be<sub>3</sub>O<sub>3</sub></b> .....                                                                   | 12 |
| Cartesian coordinates of <b>5L<sub>2</sub></b> , <b>L<sub>6</sub>Be<sub>3</sub>O<sub>3</sub></b> .....                                                       | 13 |
| Cartesian coordinates of non-beryllium compounds .....                                                                                                       | 16 |
| Plots of molecular orbitals .....                                                                                                                            | 17 |
| Plots of NICS-Scan .....                                                                                                                                     | 18 |

## Cartesian Coordinates

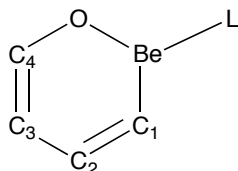
All gas-phase geometries listed have been optimized at the M06-2X/def2-TZVP level of theory with an ultrafine integration grid. Coordinates are given in angstroms. All compounds are neutral with singlet multiplicity.

### Compound 3, Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>



|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 1.212404  | 0.611521  | -0.000007 |
| 6 | -0.128685 | 1.181547  | -0.000024 |
| 6 | -1.266609 | 0.457448  | 0.000228  |
| 6 | 1.522195  | -0.714761 | 0.000066  |
| 1 | 2.012955  | 1.350364  | -0.000183 |
| 1 | -0.228164 | 2.257963  | -0.000303 |
| 1 | -2.245299 | 0.923792  | -0.000188 |
| 1 | 2.567644  | -0.987490 | 0.000081  |
| 4 | 0.053477  | -1.417406 | -0.000081 |
| 8 | -1.294610 | -0.886191 | -0.000082 |

### Compound 3L, (L)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>



### Compound 3CO, (CO)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -1.699407 | 1.192343  | -0.000001 |
| 6 | -2.242831 | -0.148758 | 0.000074  |
| 6 | -1.479548 | -1.264754 | -0.000122 |
| 6 | -0.370951 | 1.493764  | -0.000070 |
| 1 | -2.445419 | 1.986574  | 0.000156  |
| 1 | -3.316299 | -0.279442 | 0.000320  |
| 1 | -1.926112 | -2.254624 | 0.000232  |
| 1 | -0.124187 | 2.549997  | -0.000083 |
| 4 | 0.488179  | 0.080417  | -0.000040 |
| 8 | -0.152306 | -1.257659 | -0.000029 |
| 6 | 2.352500  | -0.017537 | 0.000003  |
| 8 | 3.464896  | 0.025843  | 0.000058  |

### Compound 3PMe<sub>3</sub>, (PMe<sub>3</sub>)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | 2.943585  | 1.148928  | 0.000006  |
| 6  | 3.361408  | -0.239963 | 0.000049  |
| 6  | 2.495139  | -1.275066 | 0.000056  |
| 6  | 1.648695  | 1.561431  | -0.000039 |
| 1  | 3.760894  | 1.870787  | 0.000004  |
| 1  | 4.417832  | -0.473011 | 0.000060  |
| 1  | 2.850013  | -2.302645 | 0.000073  |
| 1  | 1.505710  | 2.638927  | -0.000087 |
| 4  | 0.610756  | 0.249928  | 0.000012  |
| 8  | 1.173529  | -1.145823 | 0.000051  |
| 15 | -1.564533 | 0.070683  | -0.000016 |
| 6  | -2.575762 | 1.582098  | -0.000906 |
| 1  | -3.640045 | 1.344742  | -0.001224 |
| 1  | -2.336643 | 2.174995  | 0.881450  |
| 1  | -2.335983 | 2.174535  | -0.883385 |
| 6  | -2.176339 | -0.877796 | 1.427603  |
| 1  | -3.250329 | -1.053318 | 1.356121  |
| 1  | -1.648492 | -1.830776 | 1.459870  |
| 1  | -1.957586 | -0.334451 | 2.346327  |
| 6  | -2.175785 | -0.879413 | -1.426781 |
| 1  | -1.956952 | -0.336996 | -2.346036 |
| 1  | -1.647593 | -1.832246 | -1.457894 |
| 1  | -3.249734 | -1.055222 | -1.355414 |

### Compound 3pyr, (pyr)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -3.116144 | 1.150722  | -0.000113 |
| 6 | -3.585861 | -0.223212 | 0.000358  |
| 6 | -2.758906 | -1.289069 | 0.000110  |
| 6 | -1.807987 | 1.515032  | -0.000162 |
| 1 | -3.906409 | 1.901936  | -0.000582 |
| 1 | -4.650208 | -0.416631 | 0.000729  |
| 1 | -3.152888 | -2.302415 | 0.000242  |
| 1 | -1.637093 | 2.589970  | -0.001027 |
| 4 | -0.814561 | 0.162189  | -0.000032 |
| 8 | -1.433398 | -1.209945 | -0.000368 |
| 7 | 0.894237  | 0.082814  | 0.000185  |
| 6 | 1.499631  | -1.108868 | 0.000027  |
| 6 | 1.625100  | 1.200369  | 0.000240  |
| 6 | 2.877253  | -1.222552 | -0.000110 |
| 1 | 0.833883  | -1.962817 | -0.000002 |
| 6 | 3.006760  | 1.167716  | 0.000092  |
| 1 | 1.063079  | 2.125532  | 0.000382  |
| 6 | 3.641661  | -0.065345 | -0.000048 |
| 1 | 3.336225  | -2.200664 | -0.000241 |
| 1 | 3.567724  | 2.091024  | 0.000084  |
| 1 | 4.722397  | -0.123585 | -0.000175 |

**Compound 3NHC, (Me<sub>2</sub>NHC)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.150238  | -1.181323 | 0.021227  |
| 6 | 3.676927  | 0.168154  | -0.003226 |
| 6 | 2.888347  | 1.263186  | -0.021878 |
| 6 | 1.826058  | -1.483038 | 0.025672  |
| 1 | 3.905946  | -1.967570 | 0.036993  |
| 1 | 4.747968  | 0.320969  | -0.006163 |
| 1 | 3.322862  | 2.260576  | -0.039169 |
| 1 | 1.616785  | -2.552498 | 0.046912  |
| 4 | 0.842517  | -0.103221 | 0.000571  |
| 8 | 1.564420  | 1.237024  | -0.020872 |
| 6 | -3.100217 | -0.670634 | -0.003826 |
| 6 | -3.089476 | 0.681724  | 0.007235  |
| 1 | -3.916830 | -1.370174 | -0.008724 |
| 1 | -3.894144 | 1.395191  | 0.013658  |
| 6 | -0.952003 | -0.010430 | -0.002409 |
| 7 | -1.786298 | -1.070122 | -0.010149 |
| 7 | -1.768668 | 1.060589  | 0.007672  |
| 6 | -1.335079 | -2.455010 | -0.017568 |
| 1 | -0.686262 | -2.624324 | -0.873315 |
| 1 | -0.773083 | -2.665413 | 0.889502  |
| 1 | -2.206924 | -3.101852 | -0.074987 |
| 6 | -1.315876 | 2.444654  | 0.017682  |
| 1 | -1.683119 | 2.940670  | 0.914992  |
| 1 | -0.229013 | 2.446029  | 0.008134  |
| 1 | -1.698350 | 2.958127  | -0.863256 |

**Compound 3L<sub>2</sub>, (L<sub>2</sub>)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>****Compound 3(CO)<sub>2</sub>, (CO)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -1.761619 | 0.001379  | 1.291981  |
| 6 | -2.480984 | -0.000979 | 0.028748  |
| 6 | -1.863517 | -0.002699 | -1.169507 |
| 6 | -0.412822 | 0.002211  | 1.417600  |
| 1 | -2.394358 | 0.002522  | 2.179458  |
| 1 | -3.561985 | -0.001395 | 0.038436  |
| 1 | -2.435611 | -0.004436 | -2.093671 |
| 1 | -0.027750 | 0.004093  | 2.433634  |
| 4 | 0.324687  | -0.000032 | -0.110468 |
| 8 | -0.546562 | -0.002460 | -1.341221 |
| 6 | 1.559601  | -1.530334 | -0.135404 |
| 8 | 1.995502  | -2.540064 | 0.054480  |
| 6 | 1.557905  | 1.531268  | -0.138292 |
| 8 | 1.992257  | 2.541806  | 0.050898  |

**Compound 3(PMe<sub>3</sub>)<sub>2</sub>, (PMe<sub>3</sub>)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | 0.575408  | 2.552835  | -1.242543 |
| 6  | 0.795363  | 3.165239  | 0.062455  |
| 6  | 0.567185  | 2.519758  | 1.226280  |
| 6  | 0.175735  | 1.272732  | -1.419016 |
| 1  | 0.754267  | 3.210516  | -2.094592 |
| 1  | 1.134639  | 4.191046  | 0.116496  |
| 1  | 0.724840  | 3.034692  | 2.173578  |
| 1  | 0.051852  | 0.973968  | -2.461651 |
| 4  | -0.042105 | 0.409635  | 0.067704  |
| 8  | 0.144748  | 1.272727  | 1.344988  |
| 15 | -2.053381 | -0.511660 | 0.048846  |
| 6  | -2.487777 | -1.299013 | -1.537258 |
| 1  | -3.555663 | -1.511105 | -1.602852 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 1  | -2.199056 | -0.625013 | -2.343951 |
| 1  | -1.930635 | -2.229478 | -1.650448 |
| 6  | -3.198136 | 0.900385  | 0.140343  |
| 1  | -4.237508 | 0.594456  | 0.014813  |
| 1  | -3.068978 | 1.389921  | 1.105743  |
| 1  | -2.919192 | 1.613314  | -0.636285 |
| 6  | -2.726671 | -1.673426 | 1.287906  |
| 1  | -2.173649 | -2.612052 | 1.246981  |
| 1  | -2.598716 | -1.244536 | 2.281672  |
| 1  | -3.785236 | -1.873663 | 1.115936  |
| 15 | 1.677576  | -1.078072 | 0.042501  |
| 6  | 2.052910  | -2.544095 | 1.075758  |
| 1  | 1.379750  | -3.361592 | 0.816368  |
| 1  | 3.083477  | -2.875231 | 0.937360  |
| 1  | 1.897896  | -2.291774 | 2.124714  |
| 6  | 3.024133  | 0.069494  | 0.477580  |
| 1  | 4.007355  | -0.373989 | 0.314375  |
| 1  | 2.908378  | 0.971304  | -0.126619 |
| 1  | 2.911762  | 0.354574  | 1.523622  |
| 6  | 2.148745  | -1.641852 | -1.628053 |
| 1  | 3.168638  | -2.028502 | -1.645942 |
| 1  | 1.464947  | -2.421440 | -1.964979 |
| 1  | 2.066960  | -0.792132 | -2.305973 |

**Compound 3(pyr)<sub>2</sub>, (pyr)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.434076 | 3.131868  | 1.215351  |
| 6 | -0.531166 | 3.637248  | -0.151432 |
| 6 | -0.333413 | 2.871517  | -1.242927 |
| 6 | -0.198919 | 1.838715  | 1.530049  |
| 1 | -0.554226 | 3.891619  | 1.989651  |
| 1 | -0.751171 | 4.684696  | -0.312212 |
| 1 | -0.397941 | 3.313448  | -2.236842 |
| 1 | -0.130380 | 1.652510  | 2.605410  |
| 4 | -0.032786 | 0.822533  | 0.135831  |
| 8 | -0.046525 | 1.577107  | -1.232469 |
| 7 | 1.443519  | -0.215284 | 0.095979  |
| 6 | 2.262463  | -0.165621 | -0.953609 |
| 6 | 1.765945  | -0.974651 | 1.142407  |
| 6 | 3.441085  | -0.893363 | -0.998990 |
| 1 | 1.940042  | 0.491930  | -1.751951 |
| 6 | 2.921778  | -1.732163 | 1.177804  |
| 1 | 1.070668  | -0.949285 | 1.973244  |
| 6 | 3.774572  | -1.690335 | 0.083674  |
| 1 | 4.082133  | -0.826125 | -1.866536 |
| 1 | 3.149204  | -2.332809 | 2.046921  |
| 1 | 4.690534  | -2.266961 | 0.080326  |
| 7 | -1.326848 | -0.455594 | 0.020688  |
| 6 | -1.529486 | -1.071404 | -1.143602 |
| 6 | -2.120643 | -0.729853 | 1.053182  |
| 6 | -2.530685 | -2.010439 | -1.315993 |
| 1 | -0.872226 | -0.768361 | -1.950099 |
| 6 | -3.144002 | -1.659903 | 0.967829  |
| 1 | -1.922846 | -0.157962 | 1.952186  |
| 6 | -3.349367 | -2.312159 | -0.237347 |
| 1 | -2.667648 | -2.485837 | -2.276863 |
| 1 | -3.769515 | -1.854926 | 1.827334  |
| 1 | -4.144500 | -3.039517 | -0.339187 |

**Compound 3(NHC)<sub>2</sub>, (Me<sub>2</sub>NHC)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>4</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 0.638922  | 3.066747  | 1.355182  |
| 6 | 0.774217  | 3.639170  | 0.017726  |
| 6 | 0.426381  | 2.978281  | -1.104883 |
| 6 | 0.304370  | 1.780747  | 1.591644  |
| 1 | 0.806209  | 3.771469  | 2.172345  |
| 1 | 1.122647  | 4.658281  | -0.091025 |
| 1 | 0.503447  | 3.482107  | -2.069813 |
| 1 | 0.205894  | 1.547458  | 2.657807  |
| 4 | 0.033257  | 0.808219  | 0.139712  |
| 8 | -0.037710 | 1.741590  | -1.164517 |
| 6 | 3.151132  | -1.860585 | -0.314685 |
| 6 | 2.432696  | -2.092373 | -1.434727 |
| 1 | 4.079635  | -2.280548 | 0.029471  |
| 1 | 2.609275  | -2.756709 | -2.262041 |
| 6 | 1.346379  | -0.504999 | -0.249949 |
| 7 | 2.470701  | -0.889772 | 0.388851  |
| 7 | 1.341396  | -1.255275 | -1.373707 |
| 6 | 2.917954  | -0.337050 | 1.656300  |
| 1 | 3.976849  | -0.091452 | 1.591075  |
| 1 | 2.341198  | 0.565522  | 1.850844  |
| 1 | 2.766095  | -1.060448 | 2.458713  |
| 6 | 0.296799  | -1.172063 | -2.381684 |
| 1 | -0.520849 | -1.852452 | -2.139050 |
| 1 | -0.066042 | -0.145993 | -2.408450 |
| 1 | 0.715629  | -1.441608 | -3.349435 |
| 6 | -2.940214 | -1.762895 | 1.117601  |
| 6 | -3.586959 | -1.098998 | 0.135835  |
| 1 | -3.267011 | -2.552005 | 1.771356  |
| 1 | -4.591485 | -1.191859 | -0.237370 |
| 7 | -2.692774 | -0.176756 | -0.365480 |
| 7 | -1.675872 | -1.219474 | 1.182733  |
| 6 | -1.506025 | -0.236344 | 0.271142  |
| 6 | -2.999381 | 0.766677  | -1.429130 |
| 1 | -3.256359 | 0.225437  | -2.340102 |
| 1 | -3.840258 | 1.392866  | -1.133218 |
| 1 | -2.115952 | 1.381466  | -1.590970 |
| 6 | -0.635434 | -1.637299 | 2.104520  |
| 1 | -0.003918 | -0.776769 | 2.315747  |
| 1 | -1.093468 | -1.990384 | 3.026548  |
| 1 | -0.032049 | -2.435125 | 1.668737  |

**Hydrogenation of 3L. (3L + H<sub>2</sub>)****Compound 3(H<sub>2</sub>), Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 1.164037  | 0.714852  | 0.224253  |
| 6 | -0.244233 | 1.187596  | -0.089910 |
| 6 | -1.345036 | 0.433822  | -0.098244 |
| 6 | 1.504079  | -0.753919 | -0.189242 |
| 1 | 1.869901  | 1.405474  | -0.242396 |
| 1 | -0.384553 | 2.243586  | -0.282472 |
| 1 | -2.322126 | 0.855346  | -0.303752 |
| 1 | 1.749184  | -0.788444 | -1.254227 |
| 4 | -0.017889 | -1.390909 | 0.058835  |
| 8 | -1.375973 | -0.918757 | 0.138012  |
| 1 | 2.372135  | -1.112763 | 0.358429  |
| 1 | 1.321718  | 0.816384  | 1.303837  |

**Compound 3CO(H<sub>2</sub>), (CO)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 1.752200  | 1.128736  | 0.289820  |
| 6 | 2.212603  | -0.286821 | 0.015943  |
| 6 | 1.410818  | -1.347917 | -0.082929 |
| 6 | 0.363605  | 1.478548  | -0.302023 |
| 1 | 1.719946  | 1.274353  | 1.376959  |
| 1 | 3.276214  | -0.471226 | -0.067763 |
| 1 | 1.811145  | -2.341711 | -0.255508 |
| 1 | 0.469803  | 1.647587  | -1.381001 |
| 4 | -0.506338 | 0.035021  | -0.075388 |
| 8 | 0.055242  | -1.317748 | 0.019970  |
| 6 | -2.412479 | -0.030155 | 0.037307  |
| 8 | -3.521506 | 0.050374  | 0.084147  |
| 1 | 2.518238  | 1.819294  | -0.072785 |
| 1 | -0.000370 | 2.416260  | 0.120006  |

**Compound 3PMe<sub>3</sub>(H<sub>2</sub>), (PMe<sub>3</sub>)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -3.006241 | -1.047602 | 0.294796  |
| 6  | -3.282374 | 0.411645  | 0.011551  |
| 6  | -2.345637 | 1.355014  | -0.099038 |
| 6  | -1.677697 | -1.560906 | -0.307822 |
| 1  | -2.979043 | -1.188311 | 1.383452  |
| 1  | -4.312325 | 0.735243  | -0.076250 |
| 1  | -2.618999 | 2.390265  | -0.284668 |
| 1  | -1.440490 | -2.547964 | 0.095750  |
| 4  | -0.569121 | -0.273332 | -0.084641 |
| 8  | -1.009455 | 1.153629  | 0.005458  |
| 15 | 1.623873  | -0.102204 | 0.013258  |
| 6  | 2.730644  | -1.541099 | 0.138666  |
| 1  | 3.775823  | -1.231516 | 0.168819  |
| 1  | 2.494857  | -2.102226 | 1.042406  |
| 1  | 2.572493  | -2.194759 | -0.718662 |
| 6  | 2.102738  | 0.964112  | 1.406927  |
| 1  | 3.161177  | 1.223380  | 1.364367  |
| 1  | 1.493930  | 1.867025  | 1.361173  |
| 1  | 1.891302  | 0.455823  | 2.347233  |
| 6  | 2.241596  | 0.809129  | -1.436549 |
| 1  | 2.095749  | 0.211881  | -2.336135 |
| 1  | 1.660430  | 1.726097  | -1.533417 |
| 1  | 3.299592  | 1.051597  | -1.330147 |
| 1  | -1.817977 | -1.703775 | -1.388071 |
| 1  | -3.860670 | -1.637169 | -0.050997 |

**Compound 3pyr(H<sub>2</sub>), (pyr)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -3.126038 | 1.071776  | -0.367808 |
| 6 | -3.524073 | -0.348237 | -0.036903 |
| 6 | -2.669322 | -1.358653 | 0.135632  |
| 6 | -1.769911 | 1.499278  | 0.241885  |
| 1 | -3.068051 | 1.168325  | -1.460030 |
| 1 | -4.578617 | -0.585149 | 0.034123  |
| 1 | -3.034560 | -2.359348 | 0.351962  |
| 1 | -1.456588 | 2.450879  | -0.198411 |
| 4 | -0.760881 | 0.114474  | 0.098615  |
| 8 | -1.321931 | -1.272637 | 0.063500  |
| 7 | 0.954010  | 0.072642  | 0.030961  |
| 6 | 1.566398  | -1.112983 | -0.052557 |
| 6 | 1.675798  | 1.194979  | 0.068578  |
| 6 | 2.944161  | -1.213745 | -0.103665 |
| 1 | 0.903355  | -1.969034 | -0.074965 |
| 6 | 3.057211  | 1.174792  | 0.023231  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 1.106768  | 2.113569  | 0.136384  |
| 6 | 3.699623  | -0.051178 | -0.064939 |
| 1 | 3.410527  | -2.185990 | -0.171668 |
| 1 | 3.611909  | 2.101288  | 0.056401  |
| 1 | 4.780224  | -0.099863 | -0.102922 |
| 1 | -1.921379 | 1.702729  | 1.311010  |
| 1 | -3.935779 | 1.741119  | -0.061790 |

**Compound 3NHC(H<sub>2</sub>), (Me<sub>2</sub>NHC)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -3.182472 | 1.007786  | 0.606236  |
| 6 | -3.634522 | -0.268649 | -0.060313 |
| 6 | -2.809236 | -1.240682 | -0.452618 |
| 6 | -1.809255 | 1.507418  | 0.107923  |
| 1 | -3.963016 | 1.764950  | 0.481709  |
| 1 | -4.694658 | -0.434606 | -0.207777 |
| 1 | -3.202267 | -2.144527 | -0.912680 |
| 1 | -1.467163 | 2.317600  | 0.761325  |
| 4 | -0.800965 | 0.102397  | -0.067681 |
| 8 | -1.465282 | -1.230231 | -0.331985 |
| 6 | 3.176885  | 0.610825  | -0.010499 |
| 6 | 3.120513  | -0.731414 | 0.137500  |
| 1 | 4.015115  | 1.282757  | -0.062180 |
| 1 | 3.900487  | -1.464279 | 0.244598  |
| 6 | 1.007336  | 0.017759  | -0.018524 |
| 7 | 1.876760  | 1.045986  | -0.103779 |
| 7 | 1.789366  | -1.070759 | 0.126667  |
| 6 | 1.500061  | 2.439660  | -0.283145 |
| 1 | 0.422781  | 2.489866  | -0.406525 |
| 1 | 1.793135  | 3.018103  | 0.591927  |
| 1 | 1.994688  | 2.839817  | -1.166759 |
| 6 | 1.297565  | -2.435746 | 0.265130  |
| 1 | 1.536818  | -2.810604 | 1.259456  |
| 1 | 0.221003  | -2.425894 | 0.112708  |
| 1 | 1.774039  | -3.065629 | -0.484389 |
| 1 | -1.948812 | 1.964898  | -0.883679 |
| 1 | -3.120170 | 0.831474  | 1.688515  |

**Hydrogenation of 3L<sub>2</sub>. (3L<sub>2</sub> + H<sub>2</sub>)**

**Compound 3(CO)<sub>2</sub>(H<sub>2</sub>), (CO)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|     |           |           |           |
|-----|-----------|-----------|-----------|
| 0 1 |           |           |           |
| 6   | -1.801630 | 0.224502  | 1.143848  |
| 6   | -2.361331 | -0.576070 | -0.009807 |
| 6   | -1.662974 | -0.948708 | -1.085364 |
| 6   | -0.314544 | -0.065578 | 1.440182  |
| 1   | -1.925170 | 1.295700  | 0.931801  |
| 1   | -3.406441 | -0.855960 | 0.019214  |
| 1   | -2.137985 | -1.519145 | -1.879202 |
| 1   | -0.233207 | -1.070542 | 1.870701  |
| 4   | 0.401390  | -0.110142 | -0.153445 |
| 8   | -0.363215 | -0.678202 | -1.317470 |
| 6   | 2.111180  | -0.927917 | 0.025709  |
| 8   | 2.992942  | -1.537182 | 0.334952  |
| 6   | 0.838279  | 1.749064  | -0.435613 |
| 8   | 0.819133  | 2.864593  | -0.395480 |
| 1   | -2.415956 | 0.037248  | 2.029332  |
| 1   | 0.068443  | 0.627834  | 2.192196  |

**Compound 3(PMe<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>), (PMe<sub>3</sub>)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | 1.425576  | -2.544873 | -1.062155 |
| 6  | 1.303077  | -2.913772 | 0.396984  |
| 6  | 0.720710  | -2.168995 | 1.345502  |
| 6  | 0.322409  | -1.586637 | -1.559751 |
| 1  | 2.408401  | -2.083060 | -1.227778 |
| 1  | 1.724522  | -3.857949 | 0.722071  |
| 1  | 0.689341  | -2.540662 | 2.369399  |
| 1  | 0.592234  | -1.198166 | -2.547044 |
| 4  | 0.016117  | -0.432579 | -0.279309 |
| 8  | 0.153919  | -0.963407 | 1.191679  |
| 15 | 1.475754  | 1.255203  | -0.101498 |
| 6  | 1.899424  | 2.557939  | -1.311802 |
| 1  | 2.755767  | 3.146387  | -0.978905 |
| 1  | 2.134997  | 2.093561  | -2.269327 |
| 1  | 1.045893  | 3.220914  | -1.454584 |
| 6  | 3.067668  | 0.406701  | 0.156039  |
| 1  | 3.826992  | 1.084856  | 0.548267  |
| 1  | 2.907931  | -0.422987 | 0.847445  |
| 1  | 3.405940  | -0.006010 | -0.794455 |
| 6  | 1.267356  | 2.189233  | 1.452261  |
| 1  | 0.431421  | 2.882894  | 1.357468  |
| 1  | 1.037747  | 1.471224  | 2.240150  |
| 1  | 2.166776  | 2.749510  | 1.711739  |
| 15 | -2.089487 | 0.277709  | -0.128683 |
| 6  | -2.450481 | 1.134405  | 1.440667  |
| 1  | -2.075557 | 2.157308  | 1.399050  |
| 1  | -3.519735 | 1.154729  | 1.655880  |
| 1  | -1.921995 | 0.602532  | 2.232551  |
| 6  | -3.036434 | -1.269161 | 0.038856  |
| 1  | -4.069242 | -1.082066 | 0.335778  |
| 1  | -3.018307 | -1.804130 | -0.910204 |
| 1  | -2.537819 | -1.886837 | 0.786648  |
| 6  | -3.054630 | 1.222860  | -1.358044 |
| 1  | -4.103984 | 1.296396  | -1.068883 |
| 1  | -2.641535 | 2.226705  | -1.458176 |
| 1  | -2.983615 | 0.726335  | -2.325731 |
| 1  | -0.586729 | -2.183102 | -1.718610 |
| 1  | 1.452683  | -3.470695 | -1.647585 |

**Compound 3(pyr)<sub>2</sub>(H<sub>2</sub>), (pyr)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -1.823384 | 2.165629  | 1.321065  |
| 6 | -1.924711 | 2.807063  | -0.045030 |
| 6 | -1.147574 | 2.530383  | -1.102343 |
| 6 | -0.421761 | 1.600638  | 1.633673  |
| 1 | -2.148917 | 2.901035  | 2.065767  |
| 1 | -2.674426 | 3.576352  | -0.190603 |
| 1 | -1.296639 | 3.088301  | -2.027359 |
| 1 | 0.256093  | 2.444224  | 1.819520  |
| 4 | 0.032879  | 0.788729  | 0.143797  |
| 8 | -0.179172 | 1.610711  | -1.169643 |
| 7 | 1.680005  | 0.138978  | 0.037517  |
| 6 | 2.249178  | 0.029398  | -1.163814 |
| 6 | 2.372689  | -0.190263 | 1.126614  |
| 6 | 3.542771  | -0.437873 | -1.319584 |
| 1 | 1.632923  | 0.353037  | -1.993808 |
| 6 | 3.669795  | -0.668256 | 1.057053  |
| 1 | 1.858459  | -0.038528 | 2.068165  |
| 6 | 4.262477  | -0.795931 | -0.189828 |
| 1 | 3.974247  | -0.510888 | -2.307725 |
| 1 | 4.201536  | -0.922892 | 1.962714  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 5.277446  | -1.161286 | -0.279163 |
| 7 | -1.043969 | -0.672722 | -0.029035 |
| 6 | -1.871618 | -0.749139 | -1.070375 |
| 6 | -1.130821 | -1.584525 | 0.939388  |
| 6 | -2.816298 | -1.757729 | -1.185453 |
| 1 | -1.755348 | 0.035463  | -1.807222 |
| 6 | -2.034802 | -2.629282 | 0.896976  |
| 1 | -0.457166 | -1.446403 | 1.776732  |
| 6 | -2.895702 | -2.715062 | -0.188574 |
| 1 | -3.475926 | -1.780455 | -2.041242 |
| 1 | -2.068659 | -3.349497 | 1.702030  |
| 1 | -3.623497 | -3.513941 | -0.249460 |
| 1 | -0.470843 | 1.038918  | 2.576210  |
| 1 | -2.561105 | 1.351854  | 1.389418  |

**Compound 3(NHC)<sub>2</sub>(H<sub>2</sub>), (Me<sub>2</sub>NHC)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>6</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.199893 | 3.002693  | 1.283235  |
| 6 | -0.069166 | 3.616884  | -0.091422 |
| 6 | 0.199928  | 2.916274  | -1.204614 |
| 6 | 0.729097  | 1.787206  | 1.474495  |
| 1 | -0.020917 | 3.786480  | 2.028315  |
| 1 | -0.160076 | 4.691470  | -0.196701 |
| 1 | 0.311357  | 3.451844  | -2.149897 |
| 1 | 0.566986  | 1.376783  | 2.482139  |
| 4 | 0.406121  | 0.741794  | 0.054855  |
| 8 | 0.330477  | 1.599531  | -1.301518 |
| 6 | 3.147993  | -2.285681 | -0.278674 |
| 6 | 2.456326  | -2.425710 | -1.430281 |
| 1 | 3.988146  | -2.831192 | 0.113162  |
| 1 | 2.571440  | -3.121082 | -2.242849 |
| 6 | 1.556135  | -0.683806 | -0.311355 |
| 7 | 2.581442  | -1.218781 | 0.385504  |
| 7 | 1.495950  | -1.439748 | -1.428581 |
| 6 | 3.039405  | -0.729462 | 1.673588  |
| 1 | 4.092206  | -0.456356 | 1.613476  |
| 1 | 2.449879  | 0.146982  | 1.928317  |
| 1 | 2.912157  | -1.502013 | 2.433046  |
| 6 | 0.506251  | -1.241998 | -2.476612 |
| 1 | -0.361326 | -1.879153 | -2.298893 |
| 1 | 0.213560  | -0.193273 | -2.467686 |
| 1 | 0.950373  | -1.496750 | -3.437274 |
| 6 | -2.847136 | -1.425253 | 1.199826  |
| 6 | -3.445949 | -0.574486 | 0.338446  |
| 1 | -3.252119 | -2.201115 | 1.824753  |
| 1 | -4.479607 | -0.460669 | 0.064638  |
| 7 | -2.450577 | 0.223799  | -0.180980 |
| 7 | -1.505695 | -1.111996 | 1.175434  |
| 6 | -1.241802 | -0.095887 | 0.324260  |
| 6 | -2.674682 | 1.305376  | -1.132587 |
| 1 | -3.747653 | 1.454069  | -1.233280 |
| 1 | -2.200564 | 2.217170  | -0.773432 |
| 1 | -2.240070 | 1.051727  | -2.096928 |
| 6 | -0.482149 | -1.766153 | 1.967843  |
| 1 | 0.243689  | -1.015531 | 2.274623  |
| 1 | -0.941348 | -2.211666 | 2.848033  |
| 1 | 0.020808  | -2.541661 | 1.388028  |
| 1 | 1.762289  | 2.163715  | 1.460835  |
| 1 | -1.241093 | 2.684349  | 1.452732  |

**Double hydrogenation of 3L. (3L + 2H<sub>2</sub>)  
Saturated compound**

**Compound 3(2H<sub>2</sub>), Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 1.129026  | 0.718760  | 0.319371  |
| 6 | -0.195046 | 1.137267  | -0.345279 |
| 6 | -1.421571 | 0.357779  | 0.142838  |
| 6 | 1.622378  | -0.699202 | -0.106426 |
| 1 | 1.889181  | 1.469168  | 0.088170  |
| 1 | -0.381134 | 2.199462  | -0.167446 |
| 1 | -2.300182 | 0.663117  | -0.430415 |
| 1 | 2.397800  | -1.056833 | 0.568684  |
| 4 | 0.104801  | -1.407951 | -0.085374 |
| 8 | -1.270539 | -1.053566 | 0.019729  |
| 1 | 2.056179  | -0.651807 | -1.107979 |
| 1 | 0.991968  | 0.741354  | 1.405183  |
| 1 | -0.104749 | 1.009191  | -1.430113 |
| 1 | -1.612670 | 0.599063  | 1.194558  |

**Compound 3CO(2H<sub>2</sub>), (CO)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -1.732967 | 1.136297  | 0.279730  |
| 6 | -2.115057 | -0.177573 | -0.416435 |
| 6 | -1.377206 | -1.398096 | 0.133563  |
| 6 | -0.284843 | 1.577195  | -0.039823 |
| 1 | -2.455046 | 1.909414  | 0.001250  |
| 1 | -3.188727 | -0.360785 | -0.320120 |
| 1 | -1.657020 | -2.285067 | -0.443095 |
| 1 | 0.031138  | 2.373268  | 0.638105  |
| 4 | 0.547394  | 0.088437  | 0.025769  |
| 8 | 0.028622  | -1.265709 | 0.103393  |
| 6 | 2.478981  | -0.015337 | -0.021748 |
| 8 | 3.591682  | 0.007328  | -0.051581 |
| 1 | -0.256584 | 2.010327  | -1.046633 |
| 1 | -1.839981 | 0.993226  | 1.360594  |
| 1 | -1.902470 | -0.088766 | -1.488284 |
| 1 | -1.696767 | -1.573227 | 1.168887  |

**Compound 3PMe<sub>3</sub>(2H<sub>2</sub>), (PMe<sub>3</sub>)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -2.976554 | -1.064147 | -0.275219 |
| 6  | -3.183524 | 0.289187  | 0.415651  |
| 6  | -2.292392 | 1.396261  | -0.144870 |
| 6  | -1.594296 | -1.672556 | 0.043018  |
| 1  | -3.793982 | -1.736453 | 0.005304  |
| 1  | -4.224395 | 0.613411  | 0.322960  |
| 1  | -2.466138 | 2.321132  | 0.416559  |
| 1  | -1.620500 | -2.099547 | 1.054102  |
| 4  | -0.518476 | -0.331843 | -0.024816 |
| 8  | -0.918128 | 1.089500  | -0.103234 |
| 15 | 1.687470  | -0.117295 | 0.011181  |
| 6  | 2.883580  | -1.488011 | 0.107169  |
| 1  | 3.908742  | -1.115837 | 0.107388  |
| 1  | 2.708531  | -2.059683 | 1.018137  |
| 1  | 2.742787  | -2.153282 | -0.744246 |
| 6  | 2.156624  | 0.975916  | 1.388937  |
| 1  | 3.201441  | 1.280790  | 1.318127  |
| 1  | 1.508051  | 1.851065  | 1.351617  |
| 1  | 1.991957  | 0.464851  | 2.337146  |
| 6  | 2.215740  | 0.828437  | -1.451737 |
| 1  | 2.090346  | 0.221436  | -2.347973 |
| 1  | 1.567816  | 1.701160  | -1.532382 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.257174  | 1.141787  | -1.369176 |
| 1 | -2.588524 | 1.594691  | -1.184366 |
| 1 | -2.977959 | 0.178141  | 1.486993  |
| 1 | -3.068117 | -0.909626 | -1.356572 |
| 1 | -1.385410 | -2.513762 | -0.623888 |

**Compound 3pyr(2H<sub>2</sub>), (pyr)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -3.084994 | 1.105493  | 0.287018  |
| 6 | -3.415997 | -0.202116 | -0.441319 |
| 6 | -2.646983 | -1.406124 | 0.101483  |
| 6 | -1.643218 | 1.577293  | 0.002397  |
| 1 | -3.826564 | 1.863950  | 0.015484  |
| 1 | -4.485374 | -0.422284 | -0.367886 |
| 1 | -2.911691 | -2.295385 | -0.482352 |
| 1 | -1.370843 | 2.380621  | 0.695586  |
| 4 | -0.700011 | 0.130105  | 0.046188  |
| 8 | -1.252098 | -1.241791 | 0.078706  |
| 7 | 1.025890  | 0.078872  | 0.018477  |
| 6 | 1.629368  | -1.113075 | 0.037123  |
| 6 | 1.754884  | 1.195241  | -0.026675 |
| 6 | 3.007402  | -1.226789 | 0.011975  |
| 1 | 0.955949  | -1.960951 | 0.072376  |
| 6 | 3.136883  | 1.163204  | -0.055186 |
| 1 | 1.191516  | 2.119988  | -0.039622 |
| 6 | 3.771168  | -0.070057 | -0.034984 |
| 1 | 3.467488  | -2.204338 | 0.028381  |
| 1 | 3.698199  | 2.085622  | -0.092301 |
| 1 | 4.851798  | -0.128651 | -0.055925 |
| 1 | -1.616413 | 2.032972  | -0.997162 |
| 1 | -3.206424 | 0.932940  | 1.362706  |
| 1 | -3.185921 | -0.086055 | -1.507094 |
| 1 | -2.977197 | -1.595049 | 1.133092  |

**Compound 3NHC(2H<sub>2</sub>), (Me<sub>2</sub>NHC)Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.159579  | 1.108666  | -0.412913 |
| 6 | 3.530934  | -0.093667 | 0.458414  |
| 6 | 2.794792  | -1.365999 | 0.048400  |
| 6 | 1.706595  | 1.557720  | -0.172539 |
| 1 | 3.877389  | 1.917469  | -0.238331 |
| 1 | 4.606228  | -0.291307 | 0.409596  |
| 1 | 3.082321  | -2.182023 | 0.722825  |
| 1 | 1.409363  | 2.270416  | -0.951547 |
| 4 | 0.747111  | 0.101260  | -0.046840 |
| 8 | 1.398060  | -1.240335 | 0.053319  |
| 6 | -3.248200 | 0.608512  | 0.059693  |
| 6 | -3.191340 | -0.739457 | -0.013820 |
| 1 | -4.086424 | 1.280458  | 0.111624  |
| 1 | -3.971162 | -1.479836 | -0.040385 |
| 6 | -1.075119 | 0.022855  | -0.005358 |
| 7 | -1.947194 | 1.051552  | 0.064019  |
| 7 | -1.859390 | -1.073732 | -0.050758 |
| 6 | -1.576260 | 2.455867  | 0.135483  |
| 1 | -2.029242 | 2.908170  | 1.016509  |
| 1 | -0.495280 | 2.522358  | 0.200158  |
| 1 | -1.921204 | 2.975759  | -0.757407 |
| 6 | -1.371784 | -2.445045 | -0.131971 |
| 1 | -0.284504 | -2.418268 | -0.092804 |
| 1 | -1.766183 | -3.016075 | 0.707442  |
| 1 | -1.708721 | -2.894066 | -1.065535 |
| 1 | 1.675118  | 2.127944  | 0.768727  |
| 1 | 3.282107  | 0.815705  | -1.462292 |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 3.293215 | 0.133624  | 1.504395  |
| 1 | 3.134962 | -1.654133 | -0.957326 |

**Double hydrogenation of 3L<sub>2</sub>. (3L<sub>2</sub> + 2H<sub>2</sub>)  
Saturated compound**

**Compound 3(CO)<sub>2</sub>(2H<sub>2</sub>), (CO)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -1.776163 | -0.128656 | 1.198572  |
| 6 | -2.287641 | 0.784507  | 0.078293  |
| 6 | -1.708788 | 0.439661  | -1.292676 |
| 6 | -0.285108 | 0.111342  | 1.511195  |
| 1 | -2.395534 | 0.014107  | 2.089588  |
| 1 | -3.377784 | 0.729393  | 0.011932  |
| 1 | -2.083758 | 1.152326  | -2.034905 |
| 1 | -0.183909 | 1.090892  | 1.994067  |
| 4 | 0.429950  | 0.138812  | -0.080207 |
| 8 | -0.304543 | 0.443711  | -1.327834 |
| 6 | 1.074349  | -1.795073 | -0.238336 |
| 8 | 0.990847  | -2.908220 | -0.188504 |
| 6 | 2.120570  | 1.065468  | -0.037284 |
| 8 | 2.996893  | 1.728877  | 0.151756  |
| 1 | 0.078999  | -0.620448 | 2.237280  |
| 1 | -1.929181 | -1.170636 | 0.888795  |
| 1 | -2.033073 | 1.822443  | 0.321054  |
| 1 | -2.084442 | -0.551760 | -1.588911 |

**Compound 3(PMe<sub>3</sub>)<sub>2</sub>(2H<sub>2</sub>), (PMe<sub>3</sub>)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -0.606418 | 2.849810  | -1.070936 |
| 6  | 0.159690  | 3.218928  | 0.202448  |
| 6  | -0.200475 | 2.325539  | 1.388170  |
| 6  | -0.129572 | 1.504464  | -1.649529 |
| 1  | -1.672380 | 2.790509  | -0.813774 |
| 1  | 1.236383  | 3.139779  | 0.006257  |
| 1  | -1.257786 | 2.517776  | 1.641335  |
| 1  | -0.795578 | 1.189160  | -2.461356 |
| 4  | 0.003940  | 0.408094  | -0.279493 |
| 8  | 0.001689  | 0.960076  | 1.160556  |
| 15 | -1.765536 | -0.993723 | -0.088404 |
| 6  | -2.438758 | -2.223470 | -1.263899 |
| 1  | -3.412548 | -2.594717 | -0.940569 |
| 1  | -2.540789 | -1.759784 | -2.245254 |
| 1  | -1.749792 | -3.063551 | -1.354099 |
| 6  | -3.139718 | 0.196280  | 0.062535  |
| 1  | -4.078316 | -0.294720 | 0.324334  |
| 1  | -2.873467 | 0.920717  | 0.833062  |
| 1  | -3.254161 | 0.729796  | -0.881477 |
| 6  | -1.840070 | -1.868490 | 1.511825  |
| 1  | -1.192587 | -2.745325 | 1.485623  |
| 1  | -1.467165 | -1.183301 | 2.274018  |
| 1  | -2.855412 | -2.183084 | 1.757907  |
| 15 | 1.910823  | -0.777173 | -0.138039 |
| 6  | 2.023293  | -1.726091 | 1.416321  |
| 1  | 1.440069  | -2.643534 | 1.331175  |
| 1  | 3.054142  | -1.981133 | 1.666519  |
| 1  | 1.589696  | -1.109464 | 2.204628  |
| 6  | 3.186611  | 0.502892  | 0.100652  |
| 1  | 4.157594  | 0.069797  | 0.345085  |
| 1  | 3.269888  | 1.102097  | -0.806311 |
| 1  | 2.853919  | 1.152517  | 0.910780  |
| 6  | 2.681707  | -1.892911 | -1.364494 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.671791  | -2.219496 | -1.042864 |
| 1 | 2.048946  | -2.768067 | -1.513609 |
| 1 | 2.769100  | -1.370468 | -2.317244 |
| 1 | 0.844911  | 1.671402  | -2.130104 |
| 1 | -0.518507 | 3.667635  | -1.795075 |
| 1 | -0.037317 | 4.257167  | 0.487585  |
| 1 | 0.383055  | 2.637038  | 2.265041  |

**Compound 3(pyr)<sub>2</sub>(2H<sub>2</sub>), (pyr)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

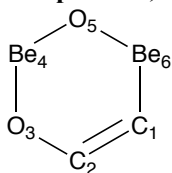
|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 1.615492  | 2.521385  | 1.253035  |
| 6 | 1.396833  | 3.284580  | -0.057445 |
| 6 | 1.291833  | 2.372706  | -1.280277 |
| 6 | 0.399731  | 1.650016  | 1.622867  |
| 1 | 2.502661  | 1.884421  | 1.126702  |
| 1 | 0.473701  | 3.870015  | 0.018210  |
| 1 | 2.257952  | 1.838945  | -1.380853 |
| 1 | 0.621793  | 1.100952  | 2.548726  |
| 4 | 0.026747  | 0.759243  | 0.141950  |
| 8 | 0.231939  | 1.468016  | -1.216788 |
| 7 | 1.086962  | -0.753516 | 0.054983  |
| 6 | 1.589463  | -1.089530 | -1.133106 |
| 6 | 1.419019  | -1.469211 | 1.127753  |
| 6 | 2.440149  | -2.171472 | -1.293190 |
| 1 | 1.286718  | -0.441640 | -1.948151 |
| 6 | 2.258152  | -2.567609 | 1.055670  |
| 1 | 1.002616  | -1.125799 | 2.066677  |
| 6 | 2.777693  | -2.924243 | -0.179788 |
| 1 | 2.830914  | -2.409731 | -2.272415 |
| 1 | 2.503205  | -3.121258 | 1.950990  |
| 1 | 3.442759  | -3.773416 | -0.270924 |
| 7 | -1.621025 | 0.073669  | 0.060200  |
| 6 | -2.249002 | 0.057236  | -1.115666 |
| 6 | -2.246359 | -0.374693 | 1.147001  |
| 6 | -3.538718 | -0.431151 | -1.247268 |
| 1 | -1.677600 | 0.470745  | -1.938489 |
| 6 | -3.532996 | -0.881529 | 1.100813  |
| 1 | -1.687154 | -0.297458 | 2.072068  |
| 6 | -4.188730 | -0.910895 | -0.121182 |
| 1 | -4.020323 | -0.426834 | -2.214847 |
| 1 | -4.009097 | -1.234188 | 2.004613  |
| 1 | -5.198082 | -1.295515 | -0.192008 |
| 1 | -0.431267 | 2.322583  | 1.880431  |
| 1 | 1.874494  | 3.238614  | 2.041202  |
| 1 | 2.216206  | 3.991283  | -0.226106 |
| 1 | 1.191080  | 2.992560  | -2.180920 |

**Compound 3(NHC)<sub>2</sub>(2H<sub>2</sub>), (Me<sub>2</sub>NHC)<sub>2</sub>Be<sub>1</sub>O<sub>1</sub>C<sub>4</sub>H<sub>8</sub>**

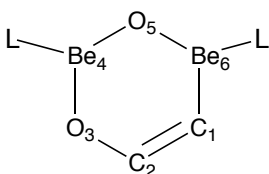
|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.006070 | 2.808466  | 1.528729  |
| 6 | -0.953210 | 3.190380  | 0.388728  |
| 6 | -0.340820 | 2.893359  | -0.980272 |
| 6 | 0.072046  | 1.281702  | 1.698096  |
| 1 | 0.982926  | 3.218658  | 1.285424  |
| 1 | -1.889434 | 2.627066  | 0.500608  |
| 1 | 0.497033  | 3.600914  | -1.125104 |
| 1 | -0.823563 | 0.976599  | 2.260870  |
| 4 | 0.081311  | 0.531894  | 0.031290  |
| 8 | 0.098602  | 1.586561  | -1.144931 |
| 6 | 3.864727  | -0.805036 | -0.274312 |
| 6 | 3.302228  | -2.020405 | -0.439808 |
| 1 | 4.896592  | -0.502428 | -0.253397 |
| 1 | 3.740924  | -2.990021 | -0.594837 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 1.625091  | -0.517609 | -0.202499 |
| 7 | 2.829556  | 0.089171  | -0.135136 |
| 7 | 1.937378  | -1.820456 | -0.395275 |
| 6 | 2.993909  | 1.519777  | 0.078749  |
| 1 | 3.980057  | 1.814167  | -0.274738 |
| 1 | 2.215365  | 2.035302  | -0.479924 |
| 1 | 2.892101  | 1.751865  | 1.137991  |
| 6 | 0.973881  | -2.889648 | -0.560898 |
| 1 | -0.006595 | -2.448120 | -0.709323 |
| 1 | 1.235245  | -3.488074 | -1.432863 |
| 1 | 0.957883  | -3.531850 | 0.320571  |
| 6 | -3.180064 | -1.828356 | 0.673867  |
| 6 | -3.587154 | -1.209728 | -0.455156 |
| 1 | -3.687455 | -2.517936 | 1.325275  |
| 1 | -4.521991 | -1.251106 | -0.985773 |
| 7 | -2.529671 | -0.433346 | -0.878730 |
| 7 | -1.888635 | -1.404623 | 0.900130  |
| 6 | -1.470835 | -0.534397 | -0.048455 |
| 6 | -2.559290 | 0.414358  | -2.062193 |
| 1 | -2.819345 | -0.185085 | -2.934231 |
| 1 | -3.301236 | 1.202095  | -1.930656 |
| 1 | -1.568137 | 0.854818  | -2.170744 |
| 6 | -1.074671 | -1.810041 | 2.030183  |
| 1 | -0.097562 | -1.344095 | 1.925651  |
| 1 | -1.524866 | -1.467853 | 2.961428  |
| 1 | -0.977977 | -2.896081 | 2.050310  |
| 1 | -1.078263 | 3.151370  | -1.761410 |
| 1 | -1.212359 | 4.253671  | 0.426821  |
| 1 | -0.317351 | 3.317236  | 2.449219  |
| 1 | 0.914943  | 1.026672  | 2.357640  |



**Compound 4, Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -1.317433 | -0.075477 | 0.000032  |
| 6 | -0.824680 | 1.178684  | -0.000016 |
| 1 | -2.383154 | -0.296223 | 0.000020  |
| 1 | -1.567658 | 1.964610  | 0.000010  |
| 4 | 0.846268  | 1.153508  | -0.000026 |
| 4 | 0.862738  | -0.969871 | -0.000014 |
| 8 | 1.822109  | 0.096601  | 0.000020  |
| 8 | -0.576176 | -1.224373 | -0.000017 |

**Compound 4L, L<sub>2</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>****Compound 4CO, (CO)<sub>2</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.120794 | 2.158517  | 0.000000  |
| 6 | 1.131612  | 1.658118  | -0.000057 |
| 1 | -0.338320 | 3.227103  | -0.000027 |
| 1 | 1.907055  | 2.417595  | -0.000119 |
| 4 | 1.172033  | -0.033312 | -0.000024 |
| 4 | -1.084565 | -0.059732 | 0.000050  |
| 8 | 0.045865  | -0.969571 | 0.000033  |
| 8 | -1.253954 | 1.419221  | 0.000061  |
| 6 | 2.928031  | -0.873985 | -0.000010 |
| 8 | 3.966104  | -1.277369 | 0.000007  |
| 6 | -2.832917 | -0.879794 | 0.000005  |
| 8 | -3.827290 | -1.378489 | -0.000051 |

**Compound 4PMe<sub>3</sub>, (PMe<sub>3</sub>)<sub>2</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | 0.045352  | 2.782076  | 0.000019  |
| 6  | 1.220367  | 2.119549  | 0.000482  |
| 1  | -0.022470 | 3.872901  | -0.000929 |
| 1  | 2.083120  | 2.784288  | -0.000167 |
| 4  | 1.061307  | 0.411772  | 0.001680  |
| 4  | -1.242204 | 0.706499  | 0.001705  |
| 8  | -0.207067 | -0.337751 | 0.002291  |
| 8  | -1.173649 | 2.208548  | 0.000631  |
| 15 | -3.177706 | -0.349584 | 0.000279  |
| 15 | 3.095821  | -0.509974 | 0.000241  |
| 6  | -3.204576 | -1.490188 | 1.419062  |
| 1  | -4.016123 | -2.214315 | 1.336925  |
| 1  | -2.243663 | -2.004227 | 1.443169  |
| 1  | -3.315669 | -0.923842 | 2.343346  |
| 6  | -4.840239 | 0.395126  | -0.000705 |
| 1  | -4.952063 | 1.026238  | -0.881760 |
| 1  | -5.616803 | -0.370830 | -0.002965 |
| 1  | -4.954427 | 1.023379  | 0.882090  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -3.201709 | -1.487378 | -1.420842 |
| 1 | -4.013464 | -2.211629 | -1.341876 |
| 1 | -3.310859 | -0.919147 | -2.344202 |
| 1 | -2.240758 | -2.001387 | -1.443990 |
| 6 | 3.495822  | -2.290920 | 0.001281  |
| 1 | 3.060416  | -2.757385 | 0.884474  |
| 1 | 3.057965  | -2.758883 | -0.879910 |
| 1 | 4.574179  | -2.456122 | -0.000083 |
| 6 | 4.039804  | 0.129806  | -1.422345 |
| 1 | 3.909978  | 1.211454  | -1.459619 |
| 1 | 5.100027  | -0.113941 | -1.341936 |
| 1 | 3.639954  | -0.291791 | -2.344288 |
| 6 | 4.044016  | 0.132518  | 1.418764  |
| 1 | 5.103966  | -0.111531 | 1.335753  |
| 1 | 3.914461  | 1.214260  | 1.454217  |
| 1 | 3.646817  | -0.287123 | 2.342742  |

**Compound 4pyr, (pyr)<sub>2</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.188780 | 2.936787  | -0.000165 |
| 6 | 1.074053  | 2.469561  | 0.000017  |
| 1 | -0.431142 | 4.002622  | -0.000715 |
| 1 | 1.813195  | 3.269808  | -0.000583 |
| 4 | 1.205327  | 0.757565  | 0.000504  |
| 4 | -1.134251 | 0.667846  | 0.000604  |
| 8 | 0.061199  | -0.188522 | 0.000837  |
| 8 | -1.302190 | 2.173463  | 0.000292  |
| 7 | 2.758061  | -0.032395 | 0.000147  |
| 6 | 2.775784  | -1.366306 | 0.000296  |
| 6 | 3.902665  | 0.650201  | -0.000270 |
| 6 | 3.963315  | -2.076208 | 0.000026  |
| 1 | 1.794305  | -1.825451 | 0.000633  |
| 6 | 5.130962  | 0.013711  | -0.000571 |
| 1 | 3.799981  | 1.728013  | -0.000365 |
| 6 | 5.158629  | -1.372990 | -0.000415 |
| 1 | 3.947296  | -3.156774 | 0.000159  |
| 1 | 6.041406  | 0.595628  | -0.000918 |
| 1 | 6.103887  | -1.900522 | -0.000641 |
| 7 | -2.675016 | -0.106902 | 0.000332  |
| 6 | -3.802283 | 0.606444  | -0.000132 |
| 6 | -2.721088 | -1.439596 | 0.000344  |
| 6 | -5.043435 | -0.004536 | -0.000593 |
| 1 | -3.662669 | 1.680613  | -0.000142 |
| 6 | -3.923969 | -2.122297 | -0.000110 |
| 1 | -1.752208 | -1.924335 | 0.000715  |
| 6 | -5.102251 | -1.390379 | -0.000585 |
| 1 | -5.941091 | 0.596901  | -0.000961 |
| 1 | -3.932947 | -3.202822 | -0.000103 |
| 1 | -6.059332 | -1.896132 | -0.000954 |

**Compound NHC, (Me<sub>2</sub>NHC)<sub>2</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.181451 | 2.912645  | -0.272743 |
| 6 | 1.079225  | 2.442717  | -0.216896 |
| 1 | -0.414026 | 3.975136  | -0.394120 |
| 1 | 1.814446  | 3.241655  | -0.320713 |
| 4 | 1.236972  | 0.724944  | -0.088050 |
| 4 | -1.193963 | 0.645893  | -0.079635 |
| 8 | 0.039545  | -0.175726 | -0.055899 |
| 8 | -1.300048 | 2.167382  | -0.193677 |
| 6 | 5.066371  | -0.539577 | 0.220629  |
| 6 | 4.478520  | -1.668415 | -0.234062 |
| 1 | 6.090607  | -0.326874 | 0.470809  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 4.888504  | -2.636157 | -0.462900 |
| 6 | -4.372914 | -1.773173 | 0.343853  |
| 6 | -5.024157 | -0.608480 | 0.128187  |
| 1 | -4.741683 | -2.766995 | 0.526094  |
| 1 | -6.074921 | -0.383222 | 0.082613  |
| 6 | 2.870536  | -0.105856 | -0.026608 |
| 6 | -2.819310 | -0.171211 | 0.058457  |
| 7 | 4.066815  | 0.397837  | 0.340210  |
| 7 | 3.141078  | -1.380529 | -0.373996 |
| 7 | -4.057229 | 0.353752  | -0.042054 |
| 7 | -3.030400 | -1.481881 | 0.296850  |
| 6 | 4.276185  | 1.762062  | 0.797553  |
| 1 | 3.304167  | 2.212081  | 0.978128  |
| 1 | 4.862108  | 1.750189  | 1.715383  |
| 1 | 4.802714  | 2.335675  | 0.035471  |
| 6 | 2.137148  | -2.322861 | -0.844872 |
| 1 | 1.169974  | -1.823865 | -0.780181 |
| 1 | 2.355819  | -2.610259 | -1.872982 |
| 1 | 2.146975  | -3.209879 | -0.211810 |
| 6 | -1.967567 | -2.457973 | 0.488310  |
| 1 | -1.019222 | -1.922809 | 0.424891  |
| 1 | -2.078570 | -2.929400 | 1.464309  |
| 1 | -2.027260 | -3.219209 | -0.289430 |
| 6 | -4.340504 | 1.758674  | -0.301203 |
| 1 | -3.391822 | 2.290290  | -0.343937 |
| 1 | -4.871664 | 1.854629  | -1.247597 |
| 1 | -4.958498 | 2.156867  | 0.502623  |

**Compound 4L<sub>2</sub>, (L<sub>2</sub>)Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

**Compound 4(PMe<sub>3</sub>)<sub>2</sub>, (PMe<sub>3</sub>)<sub>4</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | 0.006335  | 0.072407  | 2.670227  |
| 6  | -1.060157 | -0.562836 | 2.149733  |
| 1  | 0.230996  | 0.081540  | 3.741649  |
| 1  | -1.662862 | -1.066977 | 2.905682  |
| 4  | -1.345550 | -0.357754 | 0.435305  |
| 4  | 0.810283  | 0.649497  | 0.439865  |
| 8  | -0.310853 | 0.312642  | -0.461205 |
| 8  | 0.929175  | 0.762588  | 1.960662  |
| 15 | 2.037697  | 2.004837  | -0.888688 |
| 15 | -1.838492 | -2.079360 | -0.945486 |
| 6  | 0.846337  | 3.117112  | -1.705998 |
| 1  | 1.272060  | 3.589365  | -2.592482 |
| 1  | -0.018859 | 2.509059  | -1.972938 |
| 1  | 0.528229  | 3.888404  | -1.004119 |
| 6  | 3.462865  | 3.104883  | -0.568464 |
| 1  | 4.293402  | 2.526206  | -0.165284 |
| 1  | 3.785859  | 3.611478  | -1.479292 |
| 1  | 3.178973  | 3.849848  | 0.174709  |
| 6  | 2.612293  | 0.980061  | -2.284939 |
| 1  | 2.895309  | 1.586815  | -3.146280 |
| 1  | 3.466788  | 0.378648  | -1.972535 |
| 1  | 1.795975  | 0.307116  | -2.551572 |
| 6  | -2.172878 | -1.361820 | -2.589465 |
| 1  | -3.188789 | -0.965581 | -2.615216 |
| 1  | -1.472760 | -0.534900 | -2.715560 |
| 1  | -2.049632 | -2.089967 | -3.392661 |
| 6  | -0.228484 | -2.895145 | -1.210642 |
| 1  | 0.047407  | -3.446435 | -0.310309 |
| 1  | -0.242595 | -3.572870 | -2.065895 |
| 1  | 0.501669  | -2.098086 | -1.362479 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -3.000885 | -3.492778 | -0.875289 |
| 1  | -2.895941 | -4.142703 | -1.745586 |
| 1  | -2.810349 | -4.071738 | 0.028345  |
| 1  | -4.024864 | -3.121232 | -0.830458 |
| 15 | -3.133478 | 1.120448  | 0.518692  |
| 15 | 2.684815  | -1.278922 | 0.590380  |
| 6  | 4.142483  | -0.303229 | 1.138386  |
| 1  | 4.880734  | -0.921899 | 1.652651  |
| 1  | 4.620814  | 0.163746  | 0.275007  |
| 1  | 3.788741  | 0.480214  | 1.810604  |
| 6  | 3.522942  | -2.566253 | -0.428800 |
| 1  | 3.902387  | -2.124139 | -1.351223 |
| 1  | 4.352066  | -3.031450 | 0.108566  |
| 1  | 2.800991  | -3.337751 | -0.700268 |
| 6  | 2.356792  | -2.236938 | 2.115983  |
| 1  | 3.243042  | -2.791781 | 2.431443  |
| 1  | 2.053722  | -1.541197 | 2.896959  |
| 1  | 1.528326  | -2.925212 | 1.951383  |
| 6  | -4.232502 | 1.763776  | -0.805219 |
| 1  | -4.976725 | 1.010788  | -1.067027 |
| 1  | -4.745758 | 2.676839  | -0.497671 |
| 1  | -3.632743 | 1.974074  | -1.691677 |
| 6  | -2.166014 | 2.609442  | 0.940283  |
| 1  | -1.489792 | 2.354417  | 1.758265  |
| 1  | -1.560729 | 2.873161  | 0.073211  |
| 1  | -2.805906 | 3.447499  | 1.221563  |
| 6  | -4.280096 | 0.993911  | 1.936309  |
| 1  | -4.816583 | 1.928696  | 2.106968  |
| 1  | -5.000008 | 0.193740  | 1.762860  |
| 1  | -3.690437 | 0.742847  | 2.818226  |

**Compound 4(pyr)<sub>2</sub>, (pyr)<sub>4</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

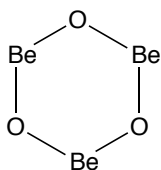
|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 0.316139  | -0.469982 | 2.839449  |
| 6 | -0.904384 | -0.222824 | 2.321740  |
| 1 | 0.511466  | -0.476689 | 3.918896  |
| 1 | -1.644940 | -0.041976 | 3.107547  |
| 4 | -1.110920 | -0.474726 | 0.577287  |
| 4 | 1.256134  | -0.611775 | 0.563629  |
| 8 | 0.055976  | -0.912980 | -0.300464 |
| 8 | 1.422657  | -0.731029 | 2.124181  |
| 7 | -2.521544 | -1.565592 | 0.227813  |
| 6 | -2.308587 | -2.573256 | -0.615422 |
| 6 | -3.697681 | -1.454198 | 0.839727  |
| 6 | -3.289308 | -3.514811 | -0.889941 |
| 1 | -1.308955 | -2.584512 | -1.037987 |
| 6 | -4.730811 | -2.347775 | 0.619494  |
| 1 | -3.786914 | -0.626458 | 1.533523  |
| 6 | -4.519774 | -3.397371 | -0.263921 |
| 1 | -3.084338 | -4.324646 | -1.576164 |
| 1 | -5.672640 | -2.227151 | 1.135890  |
| 1 | -5.304459 | -4.118497 | -0.454549 |
| 7 | 2.740391  | -1.344573 | -0.106663 |
| 6 | 3.847301  | -1.464804 | 0.622178  |
| 6 | 2.704338  | -1.817938 | -1.349555 |
| 6 | 4.991011  | -2.060269 | 0.116392  |
| 1 | 3.771436  | -1.083289 | 1.633530  |
| 6 | 3.805910  | -2.424719 | -1.930603 |
| 1 | 1.744372  | -1.701893 | -1.841108 |
| 6 | 4.968266  | -2.543593 | -1.183498 |
| 1 | 5.874686  | -2.146618 | 0.732713  |
| 1 | 3.747942  | -2.800483 | -2.942486 |
| 1 | 5.845709  | -3.015488 | -1.607300 |

|   |           |          |           |
|---|-----------|----------|-----------|
| 7 | 1.557336  | 1.261473 | 0.300003  |
| 6 | 1.289172  | 1.778311 | -0.896841 |
| 6 | 1.776408  | 2.074615 | 1.328151  |
| 6 | 1.258259  | 3.143204 | -1.125305 |
| 1 | 1.059684  | 1.050339 | -1.666907 |
| 6 | 1.754175  | 3.456523 | 1.192107  |
| 1 | 1.953793  | 1.577428 | 2.274155  |
| 6 | 1.496483  | 3.997129 | -0.056703 |
| 1 | 1.038457  | 3.524385 | -2.113000 |
| 1 | 1.929978  | 4.086779 | 2.052720  |
| 1 | 1.470657  | 5.070777 | -0.196066 |
| 7 | -1.763934 | 1.125297 | -0.186040 |
| 6 | -1.829810 | 2.250616 | 0.517984  |
| 6 | -1.949119 | 1.166938 | -1.503707 |
| 6 | -2.105687 | 3.475539 | -0.074969 |
| 1 | -1.629526 | 2.136394 | 1.578270  |
| 6 | -2.237381 | 2.342621 | -2.174971 |
| 1 | -1.832683 | 0.218721 | -2.016743 |
| 6 | -2.319553 | 3.519493 | -1.442313 |
| 1 | -2.144295 | 4.370984 | 0.529831  |
| 1 | -2.388375 | 2.334668 | -3.245641 |
| 1 | -2.538929 | 4.458376 | -1.935147 |

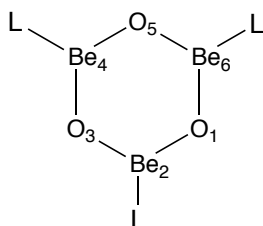
**Compound 4(NHC)<sub>2</sub>, (Me<sub>2</sub>NHC)<sub>4</sub>Be<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>2</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.138523 | 0.067189  | 2.799100  |
| 6 | 1.080442  | 0.253548  | 2.251294  |
| 1 | -0.313864 | 0.188894  | 3.878645  |
| 1 | 1.810047  | 0.546690  | 3.016306  |
| 4 | 1.270582  | -0.042793 | 0.480215  |
| 4 | -1.273725 | -0.227099 | 0.538983  |
| 8 | -0.026492 | -0.275727 | -0.355642 |
| 8 | -1.256696 | -0.259622 | 2.145146  |
| 6 | 3.886034  | 3.037305  | -0.285848 |
| 6 | 2.839282  | 3.451413  | -1.032662 |
| 1 | 4.831256  | 3.505088  | -0.073566 |
| 1 | 2.688880  | 4.353805  | -1.598661 |
| 6 | -3.619208 | -3.276205 | -0.928670 |
| 6 | -4.454620 | -2.771228 | 0.006589  |
| 1 | -3.734163 | -4.104609 | -1.605371 |
| 1 | -5.443813 | -3.070748 | 0.305204  |
| 6 | 2.294448  | 1.432610  | -0.171113 |
| 6 | -2.557639 | -1.547873 | 0.063399  |
| 7 | 3.530724  | 1.808303  | 0.227839  |
| 7 | 1.887732  | 2.456133  | -0.951248 |
| 7 | -3.784144 | -1.723273 | 0.598147  |
| 7 | -2.471512 | -2.514238 | -0.874074 |
| 6 | 4.353969  | 0.993576  | 1.100172  |
| 1 | 3.691952  | 0.433937  | 1.757755  |
| 1 | 4.964647  | 0.299770  | 0.519860  |
| 1 | 5.001140  | 1.638789  | 1.692103  |
| 6 | 0.572275  | 2.495566  | -1.567686 |
| 1 | 0.105690  | 1.528962  | -1.350157 |
| 1 | -0.023826 | 3.301503  | -1.134115 |
| 1 | 0.669919  | 2.659570  | -2.642299 |
| 6 | -1.283000 | -2.722738 | -1.685849 |
| 1 | -0.548121 | -1.978546 | -1.355053 |
| 1 | -0.904972 | -3.733943 | -1.532579 |
| 1 | -1.526042 | -2.588338 | -2.741816 |
| 6 | -4.302152 | -0.885801 | 1.666943  |
| 1 | -3.446316 | -0.449708 | 2.182091  |
| 1 | -4.941491 | -0.101247 | 1.259210  |
| 1 | -4.878963 | -1.499304 | 2.357719  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.500865  | -2.977833 | -1.301145 |
| 6 | 3.743746  | -3.350379 | -0.025433 |
| 1 | 3.806656  | -3.416296 | -2.234842 |
| 1 | 4.299747  | -4.179646 | 0.375235  |
| 6 | -2.962708 | 3.053952  | -1.290895 |
| 6 | -2.786473 | 3.587193  | -0.060133 |
| 1 | -3.310737 | 3.494915  | -2.208367 |
| 1 | -2.949526 | 4.585919  | 0.304683  |
| 6 | -2.186866 | 1.413632  | 0.060775  |
| 6 | 2.450701  | -1.495443 | 0.048498  |
| 7 | -2.591283 | 1.731202  | -1.189560 |
| 7 | -2.318781 | 2.569259  | 0.742684  |
| 7 | 2.711614  | -1.850927 | -1.230444 |
| 7 | 3.094512  | -2.434082 | 0.775703  |
| 6 | 2.205732  | -1.106619 | -2.371603 |
| 1 | 2.943567  | -0.376509 | -2.708363 |
| 1 | 1.989659  | -1.800575 | -3.183841 |
| 1 | 1.292157  | -0.603628 | -2.046105 |
| 6 | 3.083075  | -2.476398 | 2.227524  |
| 1 | 2.804291  | -3.474906 | 2.562811  |
| 1 | 4.070945  | -2.229595 | 2.620231  |
| 1 | 2.346616  | -1.750461 | 2.573128  |
| 6 | -1.918425 | 2.717503  | 2.136298  |
| 1 | -0.855689 | 2.495093  | 2.236413  |
| 1 | -2.130403 | 3.737737  | 2.450222  |
| 1 | -2.464613 | 2.007296  | 2.751936  |
| 6 | -2.539030 | 0.777360  | -2.283184 |
| 1 | -3.440502 | 0.163252  | -2.306048 |
| 1 | -2.444704 | 1.317187  | -3.224393 |
| 1 | -1.664933 | 0.143418  | -2.122355 |

**Compound 5, Be<sub>3</sub>O<sub>3</sub>**

|   |           |           |          |
|---|-----------|-----------|----------|
| 8 | 1.371926  | 0.792082  | 0.000000 |
| 8 | -1.371926 | 0.792082  | 0.000000 |
| 8 | 0.000000  | -1.584164 | 0.000000 |
| 4 | 0.000000  | 1.268513  | 0.000000 |
| 4 | -1.098565 | -0.634257 | 0.000000 |
| 4 | 1.098565  | -0.634257 | 0.000000 |

**Compound 5L, L<sub>3</sub>Be<sub>3</sub>O<sub>3</sub>****Compound 5CO, (CO)<sub>3</sub>Be<sub>3</sub>O<sub>3</sub>**

|   |           |           |          |
|---|-----------|-----------|----------|
| 8 | 1.363643  | 0.787604  | 0.000000 |
| 8 | -1.363907 | 0.787147  | 0.000000 |
| 8 | 0.000264  | -1.574752 | 0.000000 |
| 4 | 0.000000  | 1.337467  | 0.000000 |
| 4 | -1.158280 | -0.668733 | 0.000000 |
| 4 | 1.158280  | -0.668733 | 0.000000 |
| 6 | 2.871588  | -1.654241 | 0.000000 |
| 8 | 3.837588  | -2.208523 | 0.000000 |
| 6 | -0.003180 | 3.313989  | 0.000000 |
| 8 | -0.006157 | 4.427710  | 0.000000 |
| 6 | -2.868409 | -1.659748 | 0.000000 |
| 8 | -3.831431 | -2.219188 | 0.000000 |

**Compound 5PMe<sub>3</sub>, (PMe<sub>3</sub>)<sub>3</sub>Be<sub>3</sub>O<sub>3</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -1.435950 | 0.651225  | 0.000000  |
| 8  | 0.154113  | -1.569606 | 0.000000  |
| 8  | 1.282412  | 0.917819  | 0.000000  |
| 4  | -1.119675 | -0.793711 | 0.000000  |
| 4  | 1.247345  | -0.573288 | 0.000000  |
| 4  | -0.127072 | 1.366360  | 0.000000  |
| 15 | 3.475097  | -0.933258 | 0.000000  |
| 15 | -2.545757 | -2.542445 | 0.000000  |
| 15 | -0.929103 | 3.475638  | 0.000000  |
| 6  | -0.103673 | 5.106806  | 0.000000  |
| 1  | 0.530018  | 5.193585  | 0.882313  |
| 1  | 0.530018  | 5.193585  | -0.882313 |
| 1  | -0.831496 | 5.919757  | 0.000000  |
| 6  | -2.073157 | 3.589558  | -1.414645 |
| 1  | -2.649584 | 2.664600  | -1.428026 |
| 1  | -2.737135 | 4.451053  | -1.328288 |
| 1  | -1.507176 | 3.660515  | -2.343329 |
| 6  | -2.073157 | 3.589558  | 1.414645  |
| 1  | -2.737135 | 4.451053  | 1.328288  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -2.649584 | 2.664600  | 1.428026  |
| 1 | -1.507176 | 3.660515  | 2.343329  |
| 6 | -4.371164 | -2.641787 | 0.000000  |
| 1 | -4.712168 | -3.678290 | 0.000000  |
| 1 | -4.762748 | -2.136086 | 0.882321  |
| 1 | -4.762748 | -2.136086 | -0.882321 |
| 6 | -2.073157 | -3.590587 | 1.414591  |
| 1 | -2.487595 | -4.596178 | 1.327861  |
| 1 | -0.983927 | -3.627762 | 1.428342  |
| 1 | -2.417728 | -3.136002 | 2.343267  |
| 6 | 4.475254  | -2.463523 | 0.000000  |
| 1 | 4.233662  | -3.055746 | 0.882311  |
| 1 | 4.233662  | -3.055746 | -0.882311 |
| 1 | 5.543173  | -2.239563 | 0.000000  |
| 6 | 4.145584  | 0.000706  | -1.414638 |
| 1 | 3.632227  | 0.962100  | -1.428229 |
| 1 | 5.223546  | 0.145596  | -1.328069 |
| 1 | 3.924544  | -0.525175 | -2.343299 |
| 6 | 4.145584  | 0.000706  | 1.414638  |
| 1 | 5.223546  | 0.145596  | 1.328069  |
| 1 | 3.632227  | 0.962100  | 1.428229  |
| 1 | 3.924544  | -0.525175 | 2.343299  |
| 6 | -2.073157 | -3.590587 | -1.414591 |
| 1 | -0.983927 | -3.627762 | -1.428342 |
| 1 | -2.487595 | -4.596178 | -1.327861 |
| 1 | -2.417728 | -3.136002 | -2.343267 |

**Compound 5pyr, (pyr)<sub>3</sub>Be<sub>3</sub>O<sub>3</sub>**

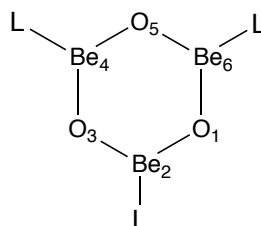
|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -1.575976 | 0.120694  | -0.000068 |
| 8 | 0.892695  | 1.304527  | -0.000115 |
| 8 | 0.683593  | -1.425267 | -0.000108 |
| 4 | -0.598318 | 1.247772  | -0.000105 |
| 4 | 1.379928  | -0.105712 | -0.000107 |
| 4 | -0.781304 | -1.142114 | -0.000061 |
| 7 | 3.125247  | -0.239460 | -0.000031 |
| 6 | 3.695990  | -1.442423 | 0.000029  |
| 6 | 3.873128  | 0.862167  | -0.000010 |
| 6 | 5.072483  | -1.590513 | 0.000116  |
| 1 | 2.994826  | -2.268752 | 0.000010  |
| 6 | 5.256063  | 0.798066  | 0.000070  |
| 1 | 3.306499  | 1.785965  | -0.000062 |
| 6 | 5.861977  | -0.449861 | 0.000137  |
| 1 | 5.512014  | -2.577862 | 0.000167  |
| 1 | 5.841343  | 1.706627  | 0.000082  |
| 1 | 6.941475  | -0.532886 | 0.000202  |
| 7 | -1.769921 | -2.586695 | 0.000023  |
| 6 | -1.190021 | -3.785271 | 0.000009  |
| 6 | -3.097066 | -2.479257 | 0.000133  |
| 6 | -1.937133 | -4.950795 | 0.000107  |
| 1 | -0.106704 | -3.756603 | -0.000079 |
| 6 | -3.913692 | -3.597167 | 0.000240  |
| 1 | -3.461913 | -1.458800 | 0.000136  |
| 6 | -3.320827 | -4.851347 | 0.000221  |
| 1 | -1.443058 | -5.912007 | 0.000095  |
| 1 | -4.988507 | -3.483985 | 0.000331  |
| 1 | -3.932576 | -5.744641 | 0.000304  |
| 7 | -1.355126 | 2.826098  | -0.000082 |
| 6 | -2.683102 | 2.922873  | -0.000079 |
| 6 | -0.598793 | 3.921919  | -0.000099 |
| 6 | -3.319230 | 4.152505  | -0.000092 |
| 1 | -3.199682 | 1.970228  | -0.000067 |
| 6 | -1.158941 | 5.187955  | -0.000111 |

|   |           |          |           |
|---|-----------|----------|-----------|
| 1 | 0.467438  | 3.727989 | -0.000104 |
| 6 | -2.541563 | 5.301267 | -0.000109 |
| 1 | -4.398708 | 4.205044 | -0.000092 |
| 1 | -0.523721 | 6.062328 | -0.000124 |
| 1 | -3.009487 | 6.277618 | -0.000123 |

**Compound 5NHC, (Me<sub>2</sub>NHC)<sub>3</sub>Be<sub>3</sub>O<sub>3</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -1.359665 | 0.785003  | 0.000000  |
| 8 | 1.359665  | 0.785003  | 0.000000  |
| 8 | 0.000000  | -1.570006 | 0.000000  |
| 4 | 0.000000  | 1.428693  | 0.000000  |
| 4 | 1.237285  | -0.714347 | 0.000000  |
| 4 | -1.237285 | -0.714347 | 0.000000  |
| 6 | 4.370212  | -3.281336 | 0.161000  |
| 6 | 5.026827  | -2.144047 | -0.161000 |
| 1 | 4.729291  | -4.280878 | 0.331623  |
| 1 | 6.071994  | -1.955247 | -0.331623 |
| 6 | -4.370212 | -3.281336 | -0.161000 |
| 6 | -5.026827 | -2.144047 | 0.161000  |
| 1 | -4.729291 | -4.280878 | -0.331623 |
| 1 | -6.071994 | -1.955247 | 0.331623  |
| 6 | -0.656614 | 5.425383  | -0.161000 |
| 6 | 0.656614  | 5.425383  | 0.161000  |
| 1 | -1.342703 | 6.236125  | -0.331623 |
| 1 | 1.342703  | 6.236125  | 0.331623  |
| 6 | 0.000000  | 3.277147  | 0.000000  |
| 6 | -2.838092 | -1.638573 | 0.000000  |
| 6 | 2.838092  | -1.638573 | 0.000000  |
| 7 | 3.038645  | -2.948006 | 0.252212  |
| 7 | 4.072371  | -1.157540 | -0.252212 |
| 7 | 1.033726  | 4.105547  | 0.252212  |
| 7 | -1.033726 | 4.105547  | -0.252212 |
| 7 | -4.072371 | -1.157540 | 0.252212  |
| 7 | -3.038645 | -2.948006 | -0.252212 |
| 6 | -1.968119 | -3.874023 | -0.587450 |
| 1 | -2.144433 | -4.297088 | -1.576364 |
| 1 | -1.037381 | -3.303200 | -0.567746 |
| 1 | -1.935620 | -4.677966 | 0.148287  |
| 6 | -4.339062 | 0.232571  | 0.587450  |
| 1 | -4.793604 | 0.291411  | 1.576364  |
| 1 | -3.379346 | 0.753201  | 0.567746  |
| 1 | -5.019047 | 0.662686  | -0.148287 |
| 6 | 2.370943  | 3.641453  | 0.587450  |
| 1 | 2.649171  | 4.005677  | 1.576364  |
| 1 | 2.341965  | 2.549999  | 0.567746  |
| 1 | 3.083427  | 4.015279  | -0.148287 |
| 6 | -2.370943 | 3.641453  | -0.587450 |
| 1 | -2.341965 | 2.549999  | -0.567746 |
| 1 | -3.083427 | 4.015279  | 0.148287  |
| 1 | -2.649171 | 4.005677  | -1.576364 |
| 6 | 4.339062  | 0.232571  | -0.587450 |
| 1 | 4.793604  | 0.291411  | -1.576364 |
| 1 | 3.379346  | 0.753201  | -0.567746 |
| 1 | 5.019047  | 0.662686  | 0.148287  |
| 6 | 1.968119  | -3.874023 | 0.587450  |
| 1 | 1.037381  | -3.303200 | 0.567746  |
| 1 | 1.935620  | -4.677966 | -0.148287 |
| 1 | 2.144433  | -4.297088 | 1.576364  |

**Compound 5L<sub>2</sub>, L<sub>6</sub>Be<sub>3</sub>O<sub>3</sub>**



**Compound 5(CO)<sub>2</sub>, (CO)<sub>6</sub>Be<sub>3</sub>O<sub>3</sub>**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | 0.812972  | 1.377686  | 0.909512  |
| 8 | -1.031820 | -0.574134 | 0.460578  |
| 8 | 1.448341  | -0.764725 | -0.645698 |
| 4 | -0.478318 | 0.680890  | 0.999642  |
| 4 | 0.066235  | -1.161366 | -0.328666 |
| 4 | 1.642707  | 0.519964  | 0.047208  |
| 6 | 3.396624  | 1.325885  | -0.341394 |
| 8 | 4.369521  | 1.804037  | -0.596070 |
| 6 | -3.291552 | 0.826098  | -0.642426 |
| 8 | -3.552311 | 0.131732  | -1.482335 |
| 6 | -0.448019 | -2.864548 | -1.170764 |
| 8 | -0.727529 | -3.844975 | -1.618740 |
| 6 | 0.610816  | 1.915211  | -2.204724 |
| 8 | -0.481844 | 1.784877  | -2.417420 |
| 6 | 0.980850  | -2.737519 | 1.804165  |
| 8 | 1.474450  | -2.302615 | 2.710624  |
| 6 | -1.787307 | 1.682014  | 2.074956  |
| 8 | -2.523151 | 2.258017  | 2.680597  |

**Compound 5(PMe<sub>3</sub>)<sub>2</sub>, (PMe<sub>3</sub>)<sub>6</sub>Be<sub>3</sub>O<sub>3</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -1.123694 | -0.028134 | 0.211114  |
| 8  | 0.907796  | 1.710724  | 0.694313  |
| 8  | 1.170580  | -0.183369 | -1.242325 |
| 4  | -0.429786 | 1.107944  | 0.898074  |
| 4  | 1.611917  | 0.939830  | -0.365410 |
| 4  | -0.227297 | -0.530346 | -0.856558 |
| 15 | 3.640152  | -1.461155 | 1.068276  |
| 15 | -1.711587 | 1.781866  | 2.603080  |
| 15 | -1.787142 | -3.203130 | 0.833958  |
| 6  | -2.467008 | -4.802084 | 1.461732  |
| 1  | -2.920082 | -5.357538 | 0.639287  |
| 1  | -1.659240 | -5.409978 | 1.870986  |
| 1  | -3.219888 | -4.645692 | 2.237780  |
| 6  | -1.370545 | -2.412168 | 2.441133  |
| 1  | -1.098963 | -1.378272 | 2.223121  |
| 1  | -2.220803 | -2.443829 | 3.128262  |
| 1  | -0.518963 | -2.914544 | 2.900804  |
| 6  | -3.366166 | -2.322074 | 0.494288  |
| 1  | -4.020589 | -2.331235 | 1.370207  |
| 1  | -3.107605 | -1.293811 | 0.234208  |
| 1  | -3.894447 | -2.789320 | -0.337528 |
| 6  | -3.376260 | 1.063243  | 2.449155  |
| 1  | -4.031447 | 1.363637  | 3.268073  |
| 1  | -3.798134 | 1.380178  | 1.494936  |
| 1  | -3.278508 | -0.022737 | 2.427125  |
| 6  | -2.023347 | 3.562277  | 2.836746  |
| 1  | -2.696863 | 3.742747  | 3.675906  |
| 1  | -1.074875 | 4.068803  | 3.014669  |
| 1  | -2.459187 | 3.957400  | 1.919519  |

|                                                                                  |           |           |           |   |           |           |           |
|----------------------------------------------------------------------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 6                                                                                | -1.196149 | 1.249561  | 4.274662  | 4 | -0.895827 | -0.954337 | -0.793167 |
| 1                                                                                | -1.094582 | 0.163821  | 4.289114  | 7 | 1.613504  | -1.850871 | 2.199483  |
| 1                                                                                | -0.225025 | 1.686744  | 4.506267  | 6 | 1.681063  | -3.177969 | 2.165643  |
| 1                                                                                | -1.920339 | 1.552959  | 5.032346  | 6 | 2.030623  | -1.185230 | 3.271267  |
| 6                                                                                | 4.661348  | -2.689932 | 1.992052  | 6 | 2.199487  | -3.907581 | 3.224001  |
| 1                                                                                | 5.683352  | -2.679507 | 1.611553  | 1 | 1.282595  | -3.619853 | 1.258514  |
| 1                                                                                | 4.692913  | -2.423902 | 3.049142  | 6 | 2.561956  | -1.838508 | 4.373101  |
| 1                                                                                | 4.257904  | -3.700354 | 1.892890  | 1 | 1.898476  | -0.110169 | 3.201021  |
| 6                                                                                | 1.984232  | -1.903368 | 1.732146  | 6 | 2.649397  | -3.222531 | 4.343657  |
| 1                                                                                | 1.216936  | -1.343773 | 1.195900  | 1 | 2.244296  | -4.986500 | 3.171257  |
| 1                                                                                | 1.784607  | -2.973001 | 1.625065  | 1 | 2.894030  | -1.273864 | 5.233283  |
| 1                                                                                | 1.930533  | -1.629994 | 2.787304  | 1 | 3.058667  | -3.763176 | 5.187939  |
| 6                                                                                | 3.561763  | -2.291090 | -0.568307 | 7 | -2.492706 | -0.780399 | 0.344080  |
| 1                                                                                | 3.219750  | -3.325445 | -0.478382 | 6 | -2.443989 | -1.319617 | 1.556639  |
| 1                                                                                | 2.862959  | -1.721110 | -1.184438 | 6 | -3.442981 | 0.104679  | 0.061417  |
| 1                                                                                | 4.548978  | -2.282893 | -1.033826 | 6 | -3.371292 | -1.003135 | 2.541910  |
| 15                                                                               | -0.865785 | -1.808709 | -2.578491 | 1 | -1.610488 | -1.998567 | 1.704299  |
| 15                                                                               | -2.537294 | 2.695542  | -1.066348 | 6 | -4.412649 | 0.475143  | 0.978484  |
| 15                                                                               | 3.591439  | 1.956029  | -0.538180 | 1 | -3.384056 | 0.544574  | -0.928263 |
| 6                                                                                | -2.436508 | -2.681456 | -2.904519 | 6 | -4.373037 | -0.093922 | 2.244502  |
| 1                                                                                | -2.439620 | -3.116106 | -3.905409 | 1 | -3.298450 | -1.457697 | 3.520485  |
| 1                                                                                | -2.556678 | -3.476394 | -2.168441 | 1 | -5.167173 | 1.202257  | 0.710962  |
| 1                                                                                | -3.272603 | -1.987987 | -2.808455 | 1 | -5.108523 | 0.178921  | 2.991397  |
| 6                                                                                | 0.379721  | -3.116864 | -2.801779 | 7 | -1.250777 | 2.362489  | 0.702609  |
| 1                                                                                | 0.294412  | -3.824652 | -1.976549 | 6 | -2.026347 | 3.105446  | -0.080844 |
| 1                                                                                | 0.253426  | -3.637383 | -3.752334 | 6 | -1.484888 | 2.310484  | 2.009654  |
| 1                                                                                | 1.362870  | -2.648895 | -2.758504 | 6 | -3.070656 | 3.863611  | 0.421580  |
| 6                                                                                | -0.648704 | -0.785592 | -4.074084 | 1 | -1.794910 | 3.052606  | -1.139016 |
| 1                                                                                | -1.441517 | -0.037357 | -4.117066 | 6 | -2.518832 | 3.030118  | 2.594877  |
| 1                                                                                | 0.307103  | -0.269766 | -3.978173 | 1 | -0.811635 | 1.646305  | 2.544244  |
| 1                                                                                | -0.665595 | -1.384352 | -4.986000 | 6 | -3.317652 | 3.823469  | 1.787784  |
| 6                                                                                | 3.373130  | 3.564631  | -1.378524 | 1 | -3.677900 | 4.463713  | -0.242133 |
| 1                                                                                | 2.533662  | 4.076491  | -0.907086 | 1 | -2.691428 | 2.960949  | 3.660197  |
| 1                                                                                | 4.267943  | 4.184515  | -1.303933 | 1 | -4.130484 | 4.398394  | 2.214046  |
| 1                                                                                | 3.132158  | 3.402620  | -2.429143 | 7 | 2.492604  | -0.780080 | -0.344097 |
| 6                                                                                | 4.129023  | 2.462362  | 1.123100  | 6 | 3.442922  | 0.104988  | -0.061557 |
| 1                                                                                | 4.437086  | 1.573292  | 1.672268  | 6 | 2.443610  | -1.319135 | -1.556715 |
| 1                                                                                | 4.947917  | 3.182076  | 1.082001  | 6 | 4.412361  | 0.475601  | -0.978808 |
| 1                                                                                | 3.261333  | 2.893894  | 1.622130  | 1 | 3.384240  | 0.544752  | 0.928197  |
| 6                                                                                | 5.108387  | 1.295614  | -1.307270 | 6 | 3.370663  | -1.002499 | -2.542173 |
| 1                                                                                | 5.924994  | 2.017646  | -1.259486 | 1 | 1.610112  | -1.998108 | -1.704273 |
| 1                                                                                | 5.396660  | 0.387142  | -0.778207 | 6 | 4.372461  | -0.093304 | -2.244890 |
| 1                                                                                | 4.909385  | 1.042535  | -2.348529 | 1 | 5.166934  | 1.202694  | -0.711368 |
| 6                                                                                | -1.054085 | 2.693528  | -2.153159 | 1 | 3.297593  | -1.456939 | -3.520788 |
| 1                                                                                | -0.448393 | 3.575221  | -1.940592 | 1 | 5.107761  | 0.179653  | -2.991927 |
| 1                                                                                | -0.442217 | 1.814884  | -1.943010 | 7 | -1.612994 | -1.851387 | -2.199191 |
| 1                                                                                | -1.338253 | 2.696492  | -3.208801 | 6 | -2.029806 | -1.185978 | -3.271238 |
| 6                                                                                | -3.421174 | 1.238595  | -1.760187 | 6 | -1.680399 | -3.178489 | -2.165158 |
| 1                                                                                | -4.432688 | 1.185817  | -1.353792 | 6 | -2.560658 | -1.839504 | -4.373157 |
| 1                                                                                | -3.481224 | 1.286863  | -2.850910 | 1 | -1.897805 | -0.110889 | -3.201136 |
| 1                                                                                | -2.874354 | 0.348499  | -1.444631 | 6 | -2.198356 | -3.908340 | -3.223581 |
| 6                                                                                | -3.492382 | 4.043672  | -1.892025 | 1 | -1.282190 | -3.620178 | -1.257821 |
| 1                                                                                | -3.574351 | 3.882445  | -2.969414 | 6 | -2.647945 | -3.223532 | -4.343514 |
| 1                                                                                | -4.495115 | 4.098932  | -1.466456 | 1 | -2.892481 | -1.275044 | -5.233557 |
| 1                                                                                | -2.999935 | 5.000893  | -1.716385 | 1 | -2.243053 | -4.987256 | -3.170671 |
| <b>Compound 5(pyr)<sub>2</sub>, (pyr)<sub>6</sub>Be<sub>3</sub>O<sub>3</sub></b> |           |           |           | 1 | -3.056839 | -3.764369 | -5.187855 |
| 8                                                                                | -0.646792 | 0.494737  | -1.218416 | 7 | 1.250357  | 2.362678  | -0.702632 |
| 8                                                                                | 0.646787  | 0.494995  | 1.218596  | 6 | 2.025988  | 3.105639  | 0.080758  |
| 8                                                                                | 0.000024  | -1.905680 | 0.000313  | 6 | 1.484194  | 2.310875  | -2.009732 |
| 4                                                                                | -0.000054 | 1.167519  | 0.000045  | 6 | 3.070083  | 3.864014  | -0.421793 |
| 4                                                                                | 0.895841  | -0.954131 | 0.793559  | 1 | 1.794782  | 3.052618  | 1.138971  |
|                                                                                  |           |           |           | 6 | 2.517900  | 3.030741  | -2.595085 |
|                                                                                  |           |           |           | 1 | 0.810928  | 1.646658  | -2.544261 |

|   |          |          |           |
|---|----------|----------|-----------|
| 6 | 3.316779 | 3.824101 | -1.788059 |
| 1 | 3.677392 | 4.464109 | 0.241867  |
| 1 | 2.690275 | 2.961741 | -3.660452 |
| 1 | 4.129434 | 4.399202 | -2.214420 |

**Non-beryllium compounds****azaborine**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -1.320476 | -0.487641 | -0.000007 |
| 6 | -0.195386 | -1.357308 | 0.000007  |
| 6 | 1.060584  | -0.842275 | -0.000016 |
| 6 | -1.184764 | 0.871347  | -0.000005 |
| 1 | -2.305247 | -0.945074 | 0.000019  |
| 1 | -0.325821 | -2.429556 | 0.000029  |
| 1 | 1.939071  | -1.474222 | 0.000002  |
| 1 | -2.085635 | 1.473621  | 0.000005  |
| 5 | 0.206553  | 1.465868  | 0.000003  |
| 1 | 0.499313  | 2.618786  | 0.000007  |
| 7 | 1.265255  | 0.503258  | 0.000004  |
| 1 | 2.229032  | 0.799561  | 0.000018  |

**phosphole**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 6  | -0.045681 | -1.277808 | 0.048675  |
| 6  | -1.273609 | -0.727981 | 0.002133  |
| 6  | -1.273609 | 0.727981  | 0.002134  |
| 6  | -0.045680 | 1.277808  | 0.048675  |
| 1  | 0.157395  | -2.338376 | 0.045198  |
| 1  | -2.191063 | -1.302109 | -0.033833 |
| 1  | -2.191062 | 1.302110  | -0.033833 |
| 1  | 0.157396  | 2.338376  | 0.045195  |
| 15 | 1.208499  | 0.000000  | -0.120467 |
| 1  | 1.771337  | -0.000002 | 1.174568  |

**furan**

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 1.087199  | -0.346829 | -0.000146 |
| 6 | 0.716479  | 0.952735  | 0.000124  |
| 6 | -0.716287 | 0.952868  | -0.000045 |
| 6 | -1.087268 | -0.346626 | -0.000132 |
| 8 | -0.000115 | -1.149917 | 0.000183  |
| 1 | 2.041500  | -0.843318 | -0.000216 |
| 1 | 1.372094  | 1.806203  | 0.000229  |
| 1 | -1.371729 | 1.806466  | -0.000076 |
| 1 | -2.041681 | -0.842900 | -0.000207 |

**benzene**

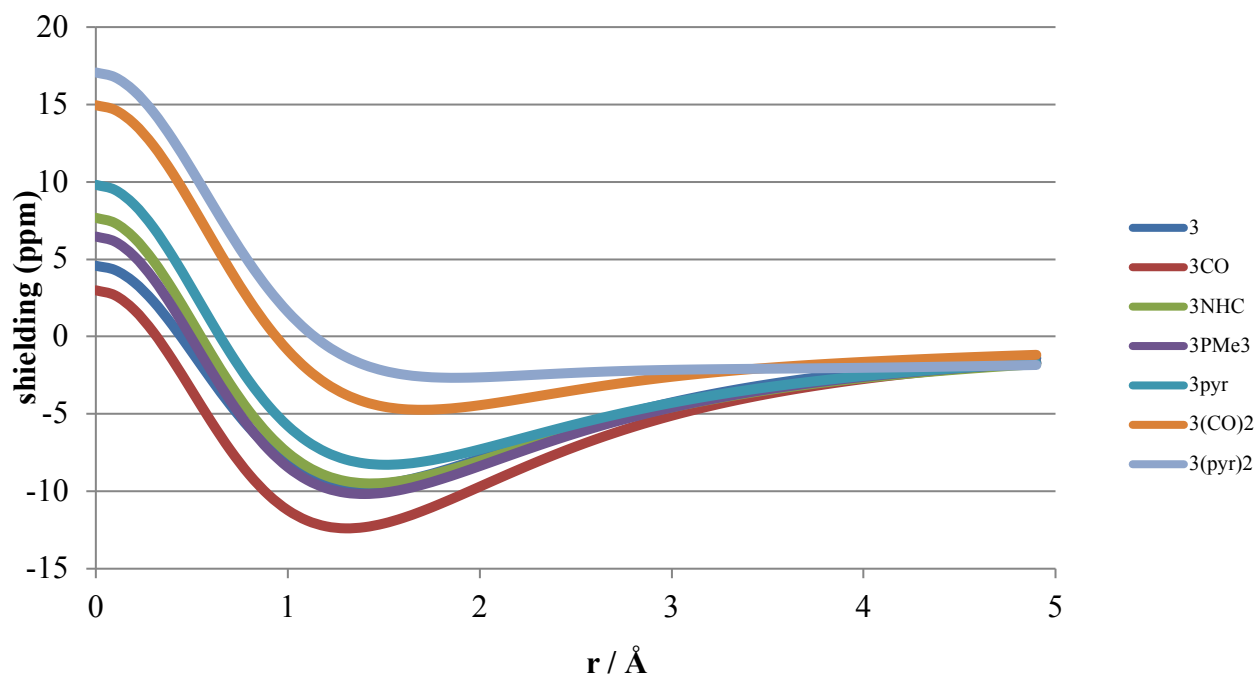
|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.331118 | -1.348459 | 0.000001  |
| 6 | 1.002321  | -0.960928 | 0.000009  |
| 6 | 1.333400  | 0.387469  | -0.000001 |
| 6 | 0.331055  | 1.348475  | 0.000001  |
| 6 | -1.002276 | 0.960975  | 0.000003  |
| 6 | -1.333382 | -0.387532 | -0.000007 |
| 1 | -0.589157 | -2.399636 | -0.000007 |
| 1 | 1.783560  | -1.710083 | -0.000008 |
| 1 | 2.372757  | 0.689632  | -0.000024 |
| 1 | 0.589234  | 2.399617  | -0.000005 |
| 1 | -1.783612 | 1.710028  | 0.000007  |
| 1 | -2.372779 | -0.689558 | 0.000000  |



## Molecular Orbitals

|      | LUMO | HOMO | HOMO-1 | HOMO-2 |
|------|------|------|--------|--------|
| 3    |      |      |        |        |
| 3CO  |      |      |        |        |
| 3pyr |      |      |        |        |
| 4    |      |      |        |        |
| 4CO  |      |      |        |        |
| 4pyr |      |      |        |        |
| 5    |      |      |        |        |
| 5CO  |      |      |        |        |
| 5pyr |      |      |        |        |

NICS-Scan plots (NICS(1)<sub>zz</sub>, ppm) for compounds 3, 3L and 3L<sub>2</sub>.



NICS-Scan plots (NICS(1)<sub>zz</sub>, ppm) for compounds 4, 4L and 4L<sub>2</sub>.

