

Supporting Information for

**Performance of DFT Methods and Origin of Stereoselectivity in Bipyridine  
*N,N'*-Dioxide Catalyzed Allylation and Propargylation Reactions**

Diana Sepúlveda, Tongxiang Lu, and Steven E. Wheeler\*  
*Department of Chemistry, Texas A&M University, College Station, TX 77843*

Email: [wheeler@chem.tamu.edu](mailto:wheeler@chem.tamu.edu)

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| Method      | BP1                   | BP2 | BP3  | BP4  | BP5  | BP1                   | BP2  | BP3  | BP4  | BP5  |            |           |
|-------------|-----------------------|-----|------|------|------|-----------------------|------|------|------|------|------------|-----------|
|             | (R) Transition States |     |      |      |      | (S) Transition States |      |      |      |      |            |           |
| LPNO-CEPA/1 | 2.9                   | 0.0 | 11.5 | 13.8 | 7.7  | 2.8                   | 5.1  | 3.3  | 7.7  | 10.4 | Mean Error | Max Error |
| MP2         | -1.2                  | 0.0 | -0.7 | -1.6 | -0.9 | -1.3                  | -1.1 | -0.5 | -1.1 | 0.9  | -0.8       | 1.6       |
|             | 6-31G(d)              |     |      |      |      |                       |      |      |      |      |            |           |
| ωB97X-D     | -0.1                  | 0.0 | -2.0 | -1.1 | -1.2 | -0.3                  | -1.5 | -1.0 | -0.8 | -1.0 | -0.9       | 2.0       |
| M06-2X      | -1.3                  | 0.0 | -2.5 | -1.0 | -1.2 | -1.8                  | -0.9 | -1.2 | -1.1 | 3.4  | -0.7       | 2.5       |
| M05-2X      | -1.8                  | 0.0 | -2.3 | -1.3 | -1.4 | -2.2                  | -0.7 | -1.2 | -1.6 | 2.4  | -1.0       | 2.3       |
| B2PLYP-D    | -0.5                  | 0.0 | -2.3 | -2.2 | -1.6 | -0.5                  | -1.5 | -1.4 | -1.7 | -1.3 | -1.3       | 2.3       |
| B2PLYP      | -2.6                  | 0.0 | -2.6 | -3.6 | -2.8 | -2.6                  | -1.3 | -1.3 | -3.1 | -3.4 | -2.3       | 3.6       |
| B97-D       | -0.3                  | 0.0 | -2.9 | -3.3 | -1.7 | -0.3                  | -1.9 | -1.5 | -1.9 | -3.9 | -1.8       | 3.9       |
| B3LYP       | -4.4                  | 0.0 | -3.6 | -5.1 | -3.9 | -4.4                  | -1.1 | -1.6 | -4.4 | -4.4 | -3.3       | 5.1       |
|             | 6-31+G(d,p)           |     |      |      |      |                       |      |      |      |      |            |           |
| ωB97X-D     | -0.1                  | 0.0 | -2.0 | -1.0 | -0.8 | -0.2                  | -1.4 | -0.8 | -0.7 | -1.1 | -0.8       | 2         |
| M06-2X      | -1.1                  | 0.0 | -2.3 | -0.6 | -0.5 | -1.5                  | -0.9 | -0.8 | -0.7 | 3.7  | -0.5       | 2.3       |
| M05-2X      | -1.8                  | 0.0 | -2.3 | -1.0 | -0.8 | -2.0                  | -0.7 | -0.8 | -1.3 | 2.7  | -0.8       | 2.3       |
| B2PLYP-D    | -0.5                  | 0.0 | -1.9 | -1.7 | -0.3 | -0.4                  | -1.7 | -0.7 | -0.9 | 0.0  | -0.8       | 1.9       |
| B2PLYP      | -2.5                  | 0.0 | -2.2 | -3.0 | -1.6 | -2.4                  | -1.6 | -0.6 | -2.3 | -2.1 | -1.8       | 3         |
| B97-D       | -0.6                  | 0.0 | -3.2 | -3.5 | -1.6 | -0.6                  | -1.8 | -1.4 | -2.1 | -4.2 | -1.9       | 4.2       |
| B3LYP       | -4.7                  | 0.0 | -3.8 | -5.3 | -3.7 | -4.7                  | -1.0 | -1.4 | -4.6 | -4.9 | -3.4       | 5.3       |
|             | TZV(2d,2p)            |     |      |      |      |                       |      |      |      |      |            |           |
| ωB97X-D     | -1.0                  | 0.0 | -2.3 | -1.8 | -1.6 | -1.1                  | -1.3 | -1.2 | -1.4 | -2.6 | -1.4       | 2.6       |
| M06-2X      | -2.2                  | 0.0 | -2.6 | -1.4 | -1.5 | -2.6                  | -0.5 | -1.2 | -1.7 | 2.1  | -1.2       | 2.6       |
| M05-2X      | -2.7                  | 0.0 | -2.4 | -1.7 | -1.6 | -3.0                  | -0.4 | -1.2 | -2.0 | 1.4  | -1.4       | 3.0       |
| B2PLYP-D    | -1.4                  | 0.0 | -2.2 | -2.4 | -1.5 | -1.5                  | -1.1 | -1.3 | -1.9 | -1.5 | -1.5       | 2.4       |
| B2PLYP      | -3.5                  | 0.0 | -2.5 | -3.7 | -2.7 | -3.5                  | -0.9 | -1.3 | -3.3 | -3.6 | -2.5       | 3.7       |
| B97-D       | -1.3                  | 0.0 | -3.3 | -3.9 | -2.2 | -1.3                  | -1.6 | -1.7 | -2.5 | -5.2 | -2.3       | 5.2       |
| B3LYP       | -5.3                  | 0.0 | -3.8 | -5.7 | -4.2 | -5.4                  | -0.8 | -1.6 | -5.0 | -6.0 | -3.8       | 6.0       |

**Table S2.** LPNO-CEPA/1 energies (kcal mol<sup>-1</sup>) for the ten TS structures for the propargylation reaction, relative to **BP2(R)**, along with errors in these relative energies from MP2 and eight DFT functionals compared to the LNPO-CEPA/1 results.

| Method      | BP1                   | BP2 | BP3  | BP4  | BP5  | BP1                   | BP2  | BP3  | BP4  | BP5  |            |           |
|-------------|-----------------------|-----|------|------|------|-----------------------|------|------|------|------|------------|-----------|
|             | (R) Transition States |     |      |      |      | (S) Transition States |      |      |      |      |            |           |
| LPNO-CEPA/1 | 2.8                   | 0.0 | 10.0 | 11.4 | 6.2  | 3.7                   | 2.5  | 13.2 | 8.2  | 2.9  | Mean Error | Max Error |
| MP2         | -1.2                  | 0.0 | -0.9 | -1.5 | -1.6 | -1.3                  | -0.5 | -1.3 | -1.2 | -0.7 | -1.0       | 1.6       |
|             |                       |     |      |      |      | 6-31G(d)              |      |      |      |      |            |           |
| ωB97X-D     | -0.4                  | 0.0 | -1.8 | -1.4 | -1.7 | -0.4                  | -1.2 | -1.5 | -0.8 | -1.5 | -1.1       | 1.8       |
| M06-2X      | -1.8                  | 0.0 | -2.1 | -1.5 | -2.1 | -1.5                  | -1.0 | -0.9 | -1.3 | -1.8 | -1.4       | 2.1       |
| M05-2X      | -2.2                  | 0.0 | -2.3 | -1.8 | -2.0 | -2.0                  | -0.7 | -1.0 | -1.6 | -1.8 | -1.5       | 2.3       |
| B2PLYP-D    | -0.8                  | 0.0 | -2.3 | -2.5 | -2.2 | -0.8                  | -1.0 | -1.9 | -1.9 | -2.1 | -1.5       | 2.5       |
| B2PLYP      | -0.7                  | 0.0 | -3.2 | -3.3 | -2.3 | -0.8                  | -1.1 | -3.1 | -2.1 | -2.4 | -1.9       | 3.3       |
| B97-D       | -2.6                  | 0.0 | -2.6 | -3.8 | -2.7 | -2.9                  | -0.9 | -3.0 | -3.3 | -1.6 | -2.3       | 3.8       |
| B3LYP       | -4.5                  | 0.0 | -3.7 | -5.3 | -3.1 | -4.8                  | -0.8 | -4.1 | -4.6 | -1.8 | -3.3       | 5.3       |
|             |                       |     |      |      |      | 6-31+G(d,p)           |      |      |      |      |            |           |
| ωB97X-D     | -0.2                  | 0.0 | -1.7 | -1.4 | -1.1 | -0.3                  | -1.0 | -1.4 | -0.7 | -1.1 | -0.9       | -1.7      |
| M06-2X      | -1.4                  | 0.0 | -1.9 | -1.2 | -1.4 | -1.3                  | -0.7 | -0.7 | -0.9 | -1.2 | -1.1       | -1.9      |
| M05-2X      | -1.9                  | 0.0 | -2.2 | -1.6 | -1.3 | -1.9                  | -0.5 | -0.7 | -1.3 | -1.2 | -1.3       | -2.2      |
| B2PLYP-D    | -0.5                  | 0.0 | -1.8 | -1.9 | -0.8 | -0.7                  | -0.8 | -1.1 | -1.1 | -1.1 | -1.0       | -1.9      |
| B2PLYP      | -0.9                  | 0.0 | -3.5 | -3.6 | -2.0 | -1.1                  | -0.9 | -3.2 | -2.4 | -2.1 | -2.0       | -3.6      |
| B97-D       | -2.3                  | 0.0 | -2.2 | -3.2 | -1.3 | -2.7                  | -0.7 | -2.1 | -2.5 | -0.7 | -1.8       | -3.2      |
| B3LYP       | -4.8                  | 0.0 | -3.8 | -5.5 | -2.8 | -5.2                  | -0.6 | -4.2 | -4.9 | -1.4 | -3.3       | -5.5      |
|             |                       |     |      |      |      | TZV(2d,2p)            |      |      |      |      |            |           |
| ωB97X-D     | -1.1                  | 0.0 | -1.7 | -1.9 | -1.7 | -1.2                  | -0.8 | -2.1 | -1.3 | -1.3 | -1.3       | 2.1       |
| M06-2X      | -2.5                  | 0.0 | -2.0 | -1.9 | -2.2 | -2.3                  | -0.6 | -1.3 | -1.7 | -1.5 | -1.6       | 2.5       |
| M05-2X      | -2.8                  | 0.0 | -2.2 | -2.1 | -1.8 | -2.8                  | -0.3 | -1.3 | -1.9 | -1.5 | -1.7       | 2.8       |
| B2PLYP-D    | -1.6                  | 0.0 | -2.0 | -2.4 | -1.9 | -1.6                  | -0.5 | -2.2 | -2.0 | -1.8 | -1.6       | 2.4       |
| B2PLYP      | -3.8                  | 0.0 | -3.3 | -3.8 | -2.4 | -1.8                  | -1.6 | -0.6 | -2.7 | -2.3 | -2.2       | 3.8       |
| B97-D       | -3.4                  | 0.0 | -2.3 | -3.8 | -2.4 | -3.7                  | -0.4 | -3.2 | -3.4 | -1.4 | -2.4       | 3.8       |
| B3LYP       | -5.3                  | 0.0 | -3.7 | -5.7 | -3.1 | -5.8                  | -0.4 | -4.7 | -5.1 | -1.6 | -3.5       | 5.8       |

**Table S3.** Gas-phase electronic energies (in Hartrees) for seven DFT functionals with three different basis sets for the allylation of benzaldehyde catalyzed by (S)-1.

| TS                 | B3LYP        | B97D         | M052X        | M06-2X       | wB97XD       | B2PLYP       | B2PLYP-D     |
|--------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| <b>6-31G</b>       |              |              |              |              |              |              |              |
| BP1(R)             | -2704.340715 | -2703.287041 | -2704.139311 | -2703.638019 | -2703.815078 | -2702.288906 | -2702.349881 |
| BP1(S)             | -2704.340956 | -2703.287289 | -2704.140059 | -2703.639039 | -2703.815597 | -2702.289121 | -2702.350147 |
| BP2(R)             | -2704.325784 | -2703.277490 | -2704.126287 | -2703.626157 | -2703.804412 | -2702.275179 | -2702.338943 |
| BP2(S)             | -2704.335608 | -2703.288283 | -2704.137562 | -2703.637152 | -2703.815907 | -2702.286197 | -2702.350566 |
| BP3(R)             | -2704.338358 | -2703.291174 | -2704.140963 | -2703.640575 | -2703.819546 | -2702.289430 | -2702.353674 |
| BP3(S)             | -2704.332106 | -2703.286163 | -2704.133992 | -2703.633864 | -2703.813785 | -2702.283410 | -2702.347926 |
| BP4(R)             | -2704.332264 | -2703.281666 | -2704.130944 | -2703.630203 | -2703.809192 | -2702.281670 | -2702.343940 |
| BP4(S)             | -2704.328804 | -2703.280857 | -2704.120552 | -2703.618710 | -2703.804576 | -2702.278357 | -2702.339177 |
| BP5(R)             | -2704.324437 | -2703.274360 | -2704.121049 | -2703.620108 | -2703.799305 | -2702.273122 | -2702.335215 |
| BP5(S)             | -2704.333156 | -2703.281881 | -2704.131193 | -2703.630095 | -2703.808530 | -2702.282159 | -2702.344126 |
| <b>6-31+G(d,p)</b> |              |              |              |              |              |              |              |
| BP1(R)             | -2704.421579 | -2703.364447 | -2704.214428 | -2703.704938 | -2703.885979 | -2702.443207 | -2702.507576 |
| BP1(S)             | -2704.421782 | -2703.354214 | -2704.203612 | -2703.694281 | -2703.874886 | -2702.432714 | -2702.496479 |
| BP2(R)             | -2704.406386 | -2703.362304 | -2704.211363 | -2703.702245 | -2703.884177 | -2702.441938 | -2702.506454 |
| BP2(S)             | -2704.415635 | -2703.367494 | -2704.218374 | -2703.708961 | -2703.889996 | -2702.447522 | -2702.511767 |
| BP3(R)             | -2704.418687 | -2703.357636 | -2704.197607 | -2703.686608 | -2703.875269 | -2702.434381 | -2702.495200 |
| BP3(S)             | -2704.412275 | -2703.357751 | -2704.207387 | -2703.697507 | -2703.878918 | -2702.437749 | -2702.500018 |
| BP4(R)             | -2704.412256 | -2703.358535 | -2704.208149 | -2703.697856 | -2703.878803 | -2702.438936 | -2702.500903 |
| BP4(S)             | -2704.409910 | -2703.351031 | -2704.198005 | -2703.687915 | -2703.869645 | -2702.430335 | -2702.492428 |
| BP5(R)             | -2704.405115 | -2703.364056 | -2704.217229 | -2703.706959 | -2703.885886 | -2702.446989 | -2702.508015 |
| BP5(S)             | -2704.413790 | -2703.363845 | -2704.216630 | -2703.706118 | -2703.885536 | -2702.446972 | -2702.507948 |
| <b>TZV(2d,2p)</b>  |              |              |              |              |              |              |              |
| BP1(R)             | -2704.930303 | -2703.869675 | -2704.758338 | -2704.250700 | -2704.376165 | -2703.118985 | -2703.179960 |
| BP1(S)             | -2704.930548 | -2703.869850 | -2704.758973 | -2704.251629 | -2704.376513 | -2703.119237 | -2703.180263 |
| BP2(R)             | -2704.914068 | -2703.858971 | -2704.744034 | -2704.237556 | -2704.364329 | -2703.103633 | -2703.167397 |
| BP2(S)             | -2704.923696 | -2703.869552 | -2704.755164 | -2704.248408 | -2704.375714 | -2703.114778 | -2703.179147 |
| BP3(R)             | -2704.926382 | -2703.872137 | -2704.758590 | -2704.251810 | -2704.379104 | -2703.118050 | -2703.182295 |
| BP3(S)             | -2704.919622 | -2703.866677 | -2704.751204 | -2704.244600 | -2704.373024 | -2703.111461 | -2703.175976 |
| BP4(R)             | -2704.920792 | -2703.863326 | -2704.748890 | -2704.241916 | -2704.369452 | -2703.110149 | -2703.172419 |
| BP4(S)             | -2704.919384 | -2703.863951 | -2704.739792 | -2704.232002 | -2704.366704 | -2703.107316 | -2703.168136 |
| BP5(R)             | -2704.913399 | -2703.856367 | -2704.739319 | -2704.232067 | -2704.359904 | -2703.101988 | -2703.164081 |
| BP5(S)             | -2704.922129 | -2703.863896 | -2704.749579 | -2704.242241 | -2704.369042 | -2703.111036 | -2703.173003 |

**Table S4.** Gas-phase MP2/cc-pVTZ and LPNO-CEPA/1/def2-TZVP electronic energies (in Hartrees) for the allylation of benzaldehyde catalyzed by (S)-**1**.

|        | <b>MP2</b>   | <b>LPNO-CEPA/1</b> |
|--------|--------------|--------------------|
| BP1(R) | -2699.765507 | -2700.063688       |
| BP1(S) | -2699.765962 | -2700.063901       |
| BP2(R) | -2699.751078 | -2700.049922       |
| BP2(S) | -2699.763814 | -2700.063012       |
| BP3(R) | -2699.768257 | -2700.068286       |
| BP3(S) | -2699.761865 | -2700.060204       |
| BP4(R) | -2699.757341 | -2700.056006       |
| BP4(S) | -2699.750370 | -2700.051769       |
| BP5(R) | -2699.748774 | -2700.046273       |
| BP5(S) | -2699.757798 | -2700.056038       |

**Table S5.** Gas-phase electronic energies (in Hartrees) for seven DFT functionals with three different basis sets for the propargylation of benzaldehyde catalyzed by (S)-1.

| TS                 | B3LYP        | B97D         | M052X        | M06-2X       | wB97XD       | B2PLYP       | B2PLYP-D     |
|--------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| <b>6-31G</b>       |              |              |              |              |              |              |              |
| BP1(R)             | -2703.092697 | -2702.036127 | -2702.893623 | -2702.397527 | -2702.758339 | -2702.561875 | -2701.056078 |
| BP1(S)             | -2703.091839 | -2702.034943 | -2702.892046 | -2702.395699 | -2702.757427 | -2702.560545 | -2701.055095 |
| BP2(R)             | -2703.079998 | -2702.028727 | -2702.882391 | -2702.386545 | -2702.745732 | -2702.552698 | -2701.044604 |
| BP2(S)             | -2703.088265 | -2702.038720 | -2702.892887 | -2702.397300 | -2702.754330 | -2702.563573 | -2701.054339 |
| BP3(R)             | -2703.090019 | -2702.039473 | -2702.894656 | -2702.399136 | -2702.756274 | -2702.565789 | -2701.056372 |
| BP3(S)             | -2703.087435 | -2702.037254 | -2702.891898 | -2702.396765 | -2702.753779 | -2702.563839 | -2701.053800 |
| BP4(R)             | -2703.085085 | -2702.033269 | -2702.887990 | -2702.392700 | -2702.751612 | -2702.558604 | -2701.050771 |
| BP4(S)             | -2703.075457 | -2702.023333 | -2702.875173 | -2702.379590 | -2702.740854 | -2702.547191 | -2701.040038 |
| BP5(R)             | -2703.080204 | -2702.026556 | -2702.879395 | -2702.383378 | -2702.745876 | -2702.549873 | -2701.044210 |
| BP5(S)             | -2703.084164 | -2702.029693 | -2702.884006 | -2702.388036 | -2702.749933 | -2702.553855 | -2701.048506 |
| <b>6-31+G(d,p)</b> |              |              |              |              |              |              |              |
| BP1(R)             | -2703.170890 | -2702.110175 | -2702.968046 | -2702.463365 | -2702.828523 | -2702.629808 | -2701.207065 |
| BP1(S)             | -2703.170203 | -2702.109138 | -2702.966648 | -2702.461760 | -2702.827721 | -2702.628605 | -2701.206336 |
| BP2(R)             | -2703.158017 | -2702.102756 | -2702.957041 | -2702.452628 | -2702.815990 | -2702.620693 | -2701.195358 |
| BP2(S)             | -2703.165365 | -2702.111904 | -2702.966801 | -2702.462842 | -2702.823850 | -2702.630967 | -2701.204272 |
| BP3(R)             | -2703.167790 | -2702.113158 | -2702.969460 | -2702.465569 | -2702.826375 | -2702.633908 | -2701.207826 |
| BP3(S)             | -2703.164843 | -2702.110584 | -2702.966328 | -2702.462823 | -2702.823475 | -2702.631549 | -2701.205043 |
| BP4(R)             | -2703.162380 | -2702.106522 | -2702.961666 | -2702.457973 | -2702.821014 | -2702.625881 | -2701.200067 |
| BP4(S)             | -2703.153450 | -2702.097249 | -2702.949572 | -2702.445585 | -2702.810924 | -2702.615152 | -2701.190162 |
| BP5(R)             | -2703.158432 | -2702.100680 | -2702.953842 | -2702.449279 | -2702.816077 | -2702.617909 | -2701.194698 |
| BP5(S)             | -2703.162394 | -2702.103857 | -2702.958427 | -2702.453936 | -2702.820205 | -2702.621949 | -2701.198652 |
| <b>TZV(2d,2p)</b>  |              |              |              |              |              |              |              |
| BP1(R)             | -2703.680395 | -2702.616718 | -2703.509611 | -2703.008095 | -2703.318185 | -2703.121353 | -2701.878370 |
| BP1(S)             | -2703.679700 | -2702.615714 | -2703.508233 | -2703.006414 | -2703.317437 | -2703.120146 | -2701.877389 |
| BP2(R)             | -2703.666373 | -2702.608060 | -2703.497225 | -2702.995819 | -2703.304199 | -2703.110944 | -2701.865227 |
| BP2(S)             | -2703.674267 | -2702.617740 | -2703.507397 | -2703.006300 | -2703.312589 | -2703.121575 | -2701.874938 |
| BP3(R)             | -2703.676363 | -2702.618684 | -2703.509654 | -2703.008557 | -2703.314730 | -2703.124105 | -2701.877412 |
| BP3(S)             | -2703.673017 | -2702.615716 | -2703.506207 | -2703.005505 | -2703.311395 | -2703.121456 | -2701.874079 |
| BP4(R)             | -2703.671473 | -2702.612583 | -2703.502718 | -2703.002132 | -2703.310135 | -2703.116970 | -2701.871386 |
| BP4(S)             | -2703.662785 | -2702.603654 | -2703.490687 | -2702.989602 | -2703.300346 | -2703.106442 | -2701.861467 |
| BP5(R)             | -2703.667284 | -2702.606608 | -2703.494877 | -2702.993410 | -2703.305291 | -2703.109008 | -2701.865220 |
| BP5(S)             | -2703.671358 | -2702.609859 | -2703.499477 | -2702.998170 | -2703.309428 | -2703.113021 | -2701.869684 |

**Table S6.** Gas-phase MP2/cc-pVTZ and LPNO-CEPA/1/def2-TZVP electronic energies (in Hartrees) for the propargylation of benzaldehyde catalyzed by (S)-**1**.

|        | <b>MP2</b>   | <b>LPNO-CEPA/1</b> |
|--------|--------------|--------------------|
| BP1(R) | -2698.522527 | -2698.823273       |
| BP1(S) | -2698.521205 | -2698.821897       |
| BP2(R) | -2698.510483 | -2698.811843       |
| BP2(S) | -2698.521526 | -2698.823102       |
| BP3(R) | -2698.525017 | -2698.827750       |
| BP3(S) | -2698.521823 | -2698.823811       |
| BP4(R) | -2698.517681 | -2698.817896       |
| BP4(S) | -2698.506012 | -2698.806713       |
| BP5(R) | -2698.509231 | -2698.809566       |
| BP5(S) | -2698.513717 | -2698.814607       |

Cartesian coordinates of transition states for  
the allylation and propargylation of  
benzaldehyde catalyzed by (S)-1 optimized at  
the indicated levels of theory

### ALLYLATION - B97D/TZV(2d,2p)

File: A\_BP1\_S\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.01182000  | -2.99995000 | 0.86477000  |
| C  | 4.23872000  | -1.81372000 | 0.74471000  |
| C  | 3.16234000  | -1.79932000 | -0.19517000 |
| C  | 2.87200000  | -2.92804000 | -0.98777000 |
| C  | 3.65405000  | -4.05574000 | -0.84529000 |
| C  | 4.72535000  | -4.09709000 | 0.08381000  |
| N  | 2.41958000  | -0.64049000 | -0.29633000 |
| C  | 2.69801000  | 0.48466000  | 0.40449000  |
| C  | 3.72280000  | 0.48616000  | 1.37731000  |
| C  | 4.47165000  | -0.67107000 | 1.53109000  |
| O  | 1.38597000  | -0.62164000 | -1.16261000 |
| Si | -0.39180000 | -0.73727000 | -0.49911000 |
| Cl | -0.85259000 | 0.79558000  | -2.15374000 |
| C  | 1.92973000  | 1.71255000  | 0.08392000  |
| C  | 2.55855000  | 2.86818000  | -0.43484000 |
| C  | 1.79107000  | 4.01320000  | -0.57544000 |
| C  | 0.43161000  | 4.04508000  | -0.20637000 |
| C  | -0.18514000 | 2.84568000  | 0.26329000  |
| N  | 0.60675000  | 1.71896000  | 0.35424000  |
| C  | -1.55051000 | 2.80798000  | 0.61009000  |
| C  | -2.28919000 | 3.96848000  | 0.49966000  |
| C  | -1.70209000 | 5.17375000  | 0.03612000  |
| C  | -0.37008000 | 5.21256000  | -0.31337000 |
| C  | 3.98606000  | 1.67579000  | 2.26742000  |
| C  | 4.00779000  | 2.84593000  | -0.84775000 |
| O  | 0.03483000  | 0.56950000  | 0.76763000  |
| O  | -2.05295000 | -0.72429000 | 0.12920000  |
| C  | -3.19466000 | -0.74781000 | -0.52909000 |
| C  | -4.41543000 | -0.97591000 | 0.28002000  |
| C  | -4.36117000 | -1.61052000 | 1.53153000  |
| C  | -5.53211000 | -1.79749000 | 2.26480000  |
| C  | -6.76140000 | -1.35871000 | 1.75544000  |
| C  | -6.81741000 | -0.72669000 | 0.50793000  |
| C  | -5.64834000 | -0.53865000 | -0.22957000 |
| C  | -0.76120000 | -2.30694000 | -1.82974000 |
| Cl | 0.19069000  | -2.19620000 | 1.16498000  |
| H  | 2.24611000  | 4.91124000  | -0.98360000 |
| H  | 5.25671000  | -0.70121000 | 2.28191000  |
| H  | -3.30766000 | -0.03631000 | -1.35039000 |
| H  | -3.40322000 | -1.94375000 | 1.91859000  |
| H  | -5.68409000 | -0.04801000 | -1.19938000 |
| H  | -5.48933000 | -2.28491000 | 3.23498000  |
| H  | -7.76847000 | -0.38063000 | 0.11287000  |
| H  | -7.67155000 | -1.50774000 | 2.33004000  |
| H  | 4.19714000  | 3.65075000  | -1.56297000 |
| H  | 4.27695000  | 1.89239000  | -1.31166000 |
| H  | 4.66670000  | 2.99958000  | 0.01368000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.01484000  | 1.34375000  | 3.31042000  |
| H | 3.22015000  | 2.44793000  | 2.17457000  |
| H | 4.96054000  | 2.12037000  | 2.03680000  |
| H | -1.99220000 | 1.87965000  | 0.94693000  |
| H | -3.34104000 | 3.95553000  | 0.76861000  |
| H | 0.09026000  | 6.12700000  | -0.67496000 |
| H | -2.31160000 | 6.06850000  | -0.04461000 |
| H | 2.04940000  | -2.89669000 | -1.68833000 |
| H | 3.44124000  | -4.92890000 | -1.45442000 |
| H | 5.31864000  | -5.00149000 | 0.17631000  |
| H | 5.82659000  | -3.01616000 | 1.58206000  |
| H | 0.02170000  | -2.18778000 | -2.57927000 |
| C | -2.08339000 | -2.15392000 | -2.35118000 |
| H | -0.62798000 | -3.18452000 | -1.19736000 |
| C | -3.22627000 | -2.45372000 | -1.62116000 |
| H | -2.20653000 | -1.58911000 | -3.27289000 |
| H | -4.19715000 | -2.37438000 | -2.10067000 |
| H | -3.15478000 | -3.14899000 | -0.78791000 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.70357100 | 2.72404000  | 0.60132000  |
| C  | -0.34421100 | 2.83114000  | 0.24726000  |
| C  | 0.21337900  | 4.06136000  | -0.21753000 |
| C  | -0.64202100 | 5.19153000  | -0.30308000 |
| C  | -1.96811100 | 5.08672000  | 0.05662000  |
| C  | -2.49620100 | 3.85023100  | 0.50846000  |
| N  | 0.50315900  | 1.74544000  | 0.32708000  |
| C  | 1.81828900  | 1.80189000  | 0.03965000  |
| C  | 2.38662900  | 2.98142000  | -0.49284000 |
| C  | 1.56772900  | 4.09315000  | -0.60857000 |
| C  | 2.64305900  | 0.61544000  | 0.37415000  |
| N  | 2.45903900  | -0.51869000 | -0.33491000 |
| C  | 3.29218900  | -1.61762000 | -0.21868000 |
| C  | 4.31895900  | -1.56633000 | 0.77341000  |
| C  | 4.42897900  | -0.42174000 | 1.58904000  |
| C  | 3.61452900  | 0.68101000  | 1.40107000  |
| C  | 3.14039900  | -2.74399000 | -1.04954000 |
| C  | 4.00028900  | -3.81171000 | -0.88655000 |
| C  | 5.01435900  | -3.79294000 | 0.10332000  |
| C  | 5.17211900  | -2.69204000 | 0.91677000  |
| O  | 1.43096900  | -0.57771000 | -1.20645000 |
| Si | -0.35776100 | -0.75872000 | -0.53430000 |
| Cl | -0.87276100 | 0.75229000  | -2.17947000 |
| C  | 3.70287900  | 1.88995000  | 2.29748000  |
| C  | 3.80611900  | 2.99658000  | -0.99862000 |
| O  | -0.00267100 | 0.56297000  | 0.73585000  |
| O  | -2.05065100 | -0.72199000 | -0.00158000 |
| C  | -2.82996100 | -1.70388900 | 0.40317000  |
| C  | -4.27026100 | -1.37687900 | 0.53684000  |
| C  | -4.84045100 | -0.29086900 | -0.14743000 |
| C  | -6.19548100 | -0.00439900 | 0.01254000  |
| C  | -6.99053100 | -0.79930900 | 0.84860000  |
| C  | -6.42462100 | -1.88373900 | 1.52875000  |
| C  | -5.06910100 | -2.17417900 | 1.37123000  |
| C  | -0.70052100 | -2.35483000 | -1.84866000 |
| Cl | 0.31117900  | -2.19612000 | 1.11916000  |
| H  | 1.97530900  | 5.01368000  | -1.01713000 |
| H  | 5.16949900  | -0.41136000 | 2.38350000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.42633100 | -2.37355900 | 1.16612000  |
| H | -4.21581100 | 0.31979100  | -0.79195000 |
| H | -4.62324100 | -3.01478900 | 1.89771000  |
| H | -6.63477100 | 0.83853100  | -0.51408000 |
| H | -7.03784100 | -2.49916900 | 2.18104000  |
| H | -8.04641100 | -0.57322900 | 0.97002000  |
| H | 2.71986900  | 2.12848000  | 2.71784000  |
| H | 4.05387900  | 2.77599000  | 1.75853000  |
| H | 4.39698900  | 1.69184000  | 3.11792000  |
| H | 4.50221900  | 2.50515000  | -0.31475000 |
| H | 4.13668900  | 4.02543000  | -1.16014000 |
| H | 3.85760900  | 2.46096000  | -1.95473000 |
| H | 5.94756900  | -2.65979000 | 1.67612000  |
| H | 5.67094900  | -4.65037000 | 0.21376000  |
| H | 3.89677900  | -4.67940000 | -1.53082000 |
| H | 2.37307900  | -2.74970000 | -1.81012000 |
| H | -0.22841100 | 6.13003000  | -0.65916000 |
| H | -2.61882100 | 5.95324100  | -0.00950000 |
| H | -3.54505100 | 3.78494100  | 0.78149000  |
| H | -2.09964100 | 1.77073000  | 0.92491000  |
| H | 0.29589900  | -2.75594000 | -2.02331000 |
| H | -1.12228100 | -1.86082000 | -2.72310000 |
| C | -1.59017100 | -3.27015000 | -1.20694000 |
| C | -2.95722100 | -3.04173900 | -1.10701000 |
| H | -1.16056100 | -4.06429000 | -0.60006000 |
| H | -3.59133100 | -3.80128900 | -0.65980000 |
| H | -3.43164100 | -2.38002900 | -1.82788000 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.30945000  | 1.36570800  | -2.06991100 |
| C  | 1.49821000  | 1.87840900  | -1.03977100 |
| C  | 1.97013000  | 2.91395900  | -0.17603100 |
| C  | 3.29097000  | 3.39676800  | -0.36842100 |
| C  | 4.08285000  | 2.88289800  | -1.37253100 |
| C  | 3.58467000  | 1.87126800  | -2.22934100 |
| N  | 0.22161000  | 1.39004900  | -0.82006100 |
| C  | -0.60892000 | 1.91771900  | 0.10217900  |
| C  | -0.15938000 | 2.91073900  | 1.00688900  |
| C  | 1.13091000  | 3.38393900  | 0.85597900  |
| C  | -2.01457000 | 1.44808900  | 0.12810900  |
| N  | -2.23893000 | 0.17859900  | 0.52513900  |
| C  | -3.49797000 | -0.32170000 | 0.79237900  |
| C  | -4.60892000 | 0.54970000  | 0.56900900  |
| C  | -4.37497000 | 1.84008000  | 0.05357900  |
| C  | -3.09232000 | 2.31014000  | -0.17656100 |
| C  | -3.67949100 | -1.63388000 | 1.27019900  |
| C  | -4.96374100 | -2.06583000 | 1.53489900  |
| C  | -6.08387100 | -1.22259000 | 1.32294900  |
| C  | -5.91194000 | 0.05875000  | 0.84671900  |
| O  | -1.17002000 | -0.62734100 | 0.70245900  |
| Si | -0.34523100 | -1.40637100 | -0.79341100 |
| Cl | -0.68384100 | -3.44101100 | 0.12913900  |
| C  | -2.85880000 | 3.65682000  | -0.81229100 |
| C  | -1.05079000 | 3.39200900  | 2.12325900  |
| O  | -0.22083000 | 0.37166900  | -1.57745100 |
| O  | 1.17006900  | -1.07486100 | 0.11886900  |
| C  | 2.13178900  | -1.92758100 | 0.40829900  |
| C  | 3.33810900  | -1.41001200 | 1.09540900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.69164000  | -0.05315200 | 1.07322900  |
| C  | 4.82899000  | 0.38503800  | 1.74898900  |
| C  | 5.62707000  | -0.52818200 | 2.44895900  |
| C  | 5.27861900  | -1.88383200 | 2.47437900  |
| C  | 4.14075900  | -2.32397200 | 1.79888900  |
| C  | 0.75102900  | -2.18486100 | -2.40541100 |
| Cl | -2.25142100 | -1.53508100 | -2.00655100 |
| H  | 1.51316100  | 4.12940900  | 1.54722900  |
| H  | -5.22513000 | 2.47883000  | -0.16944100 |
| H  | 1.82212900  | -2.92356100 | 0.72824900  |
| H  | 3.07090000  | 0.64862800  | 0.53445900  |
| H  | 3.86509900  | -3.37569200 | 1.81759900  |
| H  | 5.09318000  | 1.43875800  | 1.73076900  |
| H  | 5.89132900  | -2.59459200 | 3.02167900  |
| H  | 6.51383000  | -0.18489200 | 2.97473900  |
| H  | -0.46545900 | 3.97721900  | 2.83659900  |
| H  | -1.50639000 | 2.54678900  | 2.64958900  |
| H  | -1.86290900 | 4.02376900  | 1.74767900  |
| H  | -1.98132900 | 4.16777900  | -0.41060100 |
| H  | -3.73490900 | 4.29530000  | -0.67440100 |
| H  | -2.69462000 | 3.52529000  | -1.88927100 |
| H  | -6.76025000 | 0.71385000  | 0.67377900  |
| H  | -7.08138100 | -1.59450000 | 1.53578900  |
| H  | -5.11684100 | -3.07342000 | 1.90922900  |
| H  | -2.82088100 | -2.27663000 | 1.41169900  |
| H  | 3.65911100  | 4.17441800  | 0.29355900  |
| H  | 5.09298000  | 3.25440800  | -1.51281100 |
| H  | 4.21410000  | 1.48369800  | -3.02433100 |
| H  | 1.92030000  | 0.60161900  | -2.72688100 |
| H  | 0.00583900  | -2.76225100 | -2.94914100 |
| C  | 1.82913900  | -2.97558100 | -1.89866100 |
| H  | 1.05656900  | -1.28645100 | -2.94102100 |
| C  | 2.99290900  | -2.44107200 | -1.36478100 |
| H  | 1.64108900  | -4.03503100 | -1.73545100 |
| H  | 3.78442900  | -3.10935200 | -1.04058100 |
| H  | 3.29683900  | -1.43564200 | -1.64517100 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.21486800 | -2.33479100 | 0.66901000  |
| C  | -3.30202900 | -0.93474100 | 0.54495000  |
| C  | -4.56535900 | -0.26711200 | 0.49872000  |
| C  | -5.74247900 | -1.05628200 | 0.58539000  |
| C  | -5.65253800 | -2.42499200 | 0.71613000  |
| C  | -4.38589800 | -3.06070200 | 0.75875000  |
| N  | -2.16985900 | -0.14797100 | 0.46404000  |
| C  | -2.20536000 | 1.19798900  | 0.40218000  |
| C  | -3.43391000 | 1.88483900  | 0.28432000  |
| C  | -4.59599000 | 1.13300800  | 0.33563000  |
| O  | -0.96093900 | -0.74939000 | 0.48860000  |
| Si | 0.00273100  | -0.94480000 | -1.09942000 |
| Cl | 0.16936200  | -3.15692000 | -0.66879000 |
| C  | -0.91619000 | 1.91871000  | 0.52536000  |
| C  | -0.61158100 | 2.69127000  | 1.67124000  |
| C  | 0.57535900  | 3.40168000  | 1.67081000  |
| C  | 1.44543900  | 3.37882100  | 0.55972000  |
| C  | 1.12197900  | 2.55423100  | -0.56053000 |
| N  | -0.04503000 | 1.81502000  | -0.49770000 |
| C  | 1.95633900  | 2.50325100  | -1.69356000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.11291900  | 3.25845200  | -1.70309000 |
| C  | 3.46968900  | 4.06399200  | -0.59377000 |
| C  | 2.65181900  | 4.12556100  | 0.51444000  |
| C  | -3.46400100 | 3.37042900  | 0.03202000  |
| C  | -1.51842100 | 2.66385000  | 2.87472000  |
| O  | -0.32686000 | 0.94818000  | -1.48727000 |
| O  | 1.37796100  | -0.44744900 | -0.07246000 |
| C  | 2.69166100  | -0.43845900 | -0.04759000 |
| C  | 3.42144100  | -1.36946800 | 0.84567000  |
| C  | 2.76275200  | -2.37230900 | 1.57312000  |
| C  | 3.48357200  | -3.18451800 | 2.45028000  |
| C  | 4.86114200  | -3.00275800 | 2.61239000  |
| C  | 5.52036100  | -1.99187700 | 1.90087000  |
| C  | 4.80376100  | -1.17874800 | 1.02609000  |
| C  | 1.22217100  | -1.12750900 | -2.79914000 |
| Cl | -1.83218900 | -1.23448100 | -2.39154000 |
| H  | 0.84939900  | 3.98763100  | 2.54322000  |
| H  | -5.55703000 | 1.63112800  | 0.24367000  |
| H  | 3.12075000  | 0.56862200  | -0.08029000 |
| H  | 1.69410200  | -2.50119900 | 1.45495000  |
| H  | 5.31375100  | -0.39065700 | 0.47669000  |
| H  | 2.96761200  | -3.95812800 | 3.01258000  |
| H  | 6.58795100  | -1.83864700 | 2.03173000  |
| H  | 5.41815200  | -3.63874700 | 3.29510000  |
| H  | -1.09918100 | 3.28298000  | 3.67141000  |
| H  | -1.62423000 | 1.63802900  | 3.24671000  |
| H  | -2.52267100 | 3.03090900  | 2.64218000  |
| H  | -4.49198100 | 3.73712800  | 0.08208000  |
| H  | -3.06604100 | 3.58510900  | -0.96735000 |
| H  | -2.85721100 | 3.92891900  | 0.75009000  |
| H  | 2.90928800  | 4.74634200  | 1.36708000  |
| H  | 4.38874800  | 4.64073200  | -0.62440000 |
| H  | 3.75630900  | 3.23504200  | -2.57736000 |
| H  | 1.67003000  | 1.89472100  | -2.54010000 |
| H  | -6.70575900 | -0.55711300 | 0.54566000  |
| H  | -6.55471800 | -3.02507300 | 0.78388000  |
| H  | -4.33318800 | -4.14051200 | 0.85872000  |
| H  | -2.24424800 | -2.81318100 | 0.68106000  |
| H  | 0.65521100  | -1.86419900 | -3.36493000 |
| C  | 2.50647100  | -1.57720900 | -2.38529000 |
| H  | 1.19356100  | -0.12968900 | -3.23900000 |
| C  | 3.49571100  | -0.72338800 | -1.92492000 |
| H  | 2.63831200  | -2.64620900 | -2.22993000 |
| H  | 4.46782100  | -1.12539800 | -1.66233000 |
| H  | 3.47427000  | 0.31508200  | -2.24239000 |

File: A\_BP3\_S\_B97D.xyz

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -6.16157000 | -0.67068100 | 1.26748000  |
| C | -5.84154000 | 0.58935900  | 0.81116000  |
| C | -4.49126000 | 0.92831900  | 0.53026000  |
| C | -3.48989000 | -0.07087100 | 0.73005000  |
| C | -3.82482000 | -1.35964100 | 1.18893000  |
| C | -5.14852000 | -1.64432100 | 1.45698000  |
| N | -2.17911000 | 0.27691000  | 0.46051000  |
| C | -1.81450000 | 1.51585000  | 0.06722000  |
| C | -2.78383100 | 2.50680900  | -0.20667000 |
| C | -4.11040100 | 2.19226900  | 0.03527000  |
| O | -1.22692000 | -0.65787000 | 0.61285000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -0.39410000 | -1.47546000 | -0.94839000 |
| Cl | 0.66681100  | -2.35270000 | -2.72905000 |
| C  | -0.36377000 | 1.80436000  | -0.01018000 |
| C  | 0.26214900  | 2.69522000  | 0.89205000  |
| C  | 1.60604900  | 2.96532100  | 0.69758000  |
| C  | 2.32936900  | 2.38864100  | -0.36692000 |
| C  | 1.67243000  | 1.46210100  | -1.23504000 |
| N  | 0.34107000  | 1.19030000  | -0.98036000 |
| C  | 2.35972000  | 0.82992100  | -2.28781000 |
| C  | 3.69487000  | 1.12777100  | -2.47472000 |
| C  | 4.37230900  | 2.03832100  | -1.62622000 |
| C  | 3.70474900  | 2.65737100  | -0.59217000 |
| C  | -2.39041100 | 3.82340000  | -0.82639000 |
| C  | -0.49987100 | 3.25423000  | 2.06658000  |
| O  | -0.29524000 | 0.24896000  | -1.71951000 |
| O  | 1.20444000  | -1.19667000 | -0.17621000 |
| C  | 1.53471000  | -1.17045900 | 1.09005000  |
| C  | 2.96904000  | -1.00651900 | 1.39600000  |
| C  | 3.95817000  | -1.27151900 | 0.43454000  |
| C  | 5.29790000  | -1.03940800 | 0.73773000  |
| C  | 5.66075000  | -0.54845800 | 1.99865000  |
| C  | 4.67724000  | -0.28908900 | 2.96047000  |
| C  | 3.33498000  | -0.52033900 | 2.66172000  |
| C  | -0.55467900 | -3.30436000 | 0.06514000  |
| Cl | -2.38799000 | -1.68340000 | -1.96231000 |
| H  | 2.12417900  | 3.62522100  | 1.38746000  |
| H  | -4.87941100 | 2.93183900  | -0.16730000 |
| H  | 0.84739000  | -0.68928000 | 1.78826000  |
| H  | 3.66471000  | -1.63926900 | -0.54312000 |
| H  | 2.56463000  | -0.31642900 | 3.40162000  |
| H  | 6.06189000  | -1.23518800 | -0.00943000 |
| H  | 4.95688000  | 0.09433100  | 3.3772000   |
| H  | 6.70687000  | -0.36748800 | 2.23005000  |
| H  | 0.16521900  | 3.85845000  | 2.68818000  |
| H  | -0.90843100 | 2.44027000  | 2.67691000  |
| H  | -1.34071100 | 3.87995000  | 1.75143000  |
| H  | -3.22301100 | 4.52862900  | -0.76759000 |
| H  | -2.14086100 | 3.67071000  | -1.88390000 |
| H  | -1.51539100 | 4.27131000  | -0.34855000 |
| H  | 4.21184900  | 3.35440100  | 0.06790000  |
| H  | 5.42512900  | 2.24348200  | -1.79333000 |
| H  | 4.23614000  | 0.64758100  | -3.28412000 |
| H  | 1.84091000  | 0.11638100  | -2.91383000 |
| H  | -3.04830900 | -2.10012100 | 1.31838000  |
| H  | -5.41728900 | -2.63371100 | 1.81412000  |
| H  | -6.60816000 | 1.34256800  | 0.65638000  |
| H  | -7.19494000 | -0.92544200 | 1.48142000  |
| H  | -1.61369900 | -3.54315000 | -0.02797000 |
| C  | -0.10327900 | -3.14985000 | 1.41682000  |
| H  | 0.07701100  | -3.95218000 | -0.54358000 |
| C  | 1.23414100  | -3.12012000 | 1.77410000  |
| H  | -0.83221900 | -2.85094000 | 2.16877000  |
| H  | 1.51138100  | -3.02443900 | 2.81939000  |
| H  | 1.97229100  | -3.56492900 | 1.11138000  |

File: A\_BP3\_R\_B97D.xyz

|   |            |             |            |
|---|------------|-------------|------------|
| C | 4.64321000 | -1.37483000 | 0.93841000 |
| C | 3.29623000 | -1.01033000 | 1.09223000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.94301000  | -0.00820000 | 2.01078000  |
| C  | 3.93222000  | 0.62644000  | 2.75915000  |
| C  | 5.27646000  | 0.26517000  | 2.60025000  |
| C  | 5.63039000  | -0.73574000 | 1.68811000  |
| C  | 2.28418000  | -1.65726000 | 0.23201000  |
| O  | 1.15073000  | -1.01996000 | 0.09042000  |
| Si | -0.35419000 | -1.51128000 | -0.74430000 |
| Cl | -2.34970000 | -1.90909000 | -1.70522000 |
| O  | -1.19308000 | -0.56569000 | 0.72721000  |
| N  | -2.22217000 | 0.26582000  | 0.48935000  |
| C  | -3.49528000 | -0.14827000 | 0.82878000  |
| C  | -4.57838000 | 0.73914000  | 0.54191000  |
| C  | -4.30768000 | 1.96650000  | -0.09071000 |
| C  | -3.01208000 | 2.36178000  | -0.38658000 |
| C  | -1.96190000 | 1.48357000  | -0.04331000 |
| C  | -5.89397000 | 0.32757000  | 0.88788000  |
| C  | -6.10454000 | -0.89269000 | 1.48996000  |
| C  | -5.01210000 | -1.75473000 | 1.76568000  |
| C  | -3.71999000 | -1.39959000 | 1.43702000  |
| C  | -0.53648000 | 1.86930000  | -0.16673000 |
| C  | 0.01141000  | 2.92208000  | 0.60347000  |
| C  | 1.34946000  | 3.22638000  | 0.41886000  |
| C  | 2.14173000  | 2.53692000  | -0.52063000 |
| C  | 1.55507000  | 1.48043000  | -1.28247000 |
| N  | 0.22921000  | 1.17856000  | -1.03509000 |
| C  | 2.30830000  | 0.75080000  | -2.22155000 |
| C  | 3.64271000  | 1.06468000  | -2.38416000 |
| C  | 4.25412000  | 2.09699000  | -1.62939000 |
| C  | 3.51831000  | 2.82278000  | -0.71886000 |
| C  | -2.76071000 | 3.67225000  | -1.09053000 |
| C  | -0.82499000 | 3.64878000  | 1.62486000  |
| O  | -0.33443000 | 0.12716000  | -1.67839000 |
| Cl | 0.72540000  | -2.51208000 | -2.46256000 |
| C  | -0.43380000 | -3.24410000 | 0.42506000  |
| C  | 0.88120000  | -3.80575000 | 0.52375000  |
| H  | 1.19358000  | -4.50517000 | -0.24916000 |
| H  | 1.80708000  | 4.00542000  | 1.02185000  |
| H  | -5.13810000 | 2.61668000  | -0.35233000 |
| H  | 2.67056000  | -2.19689000 | -0.63421000 |
| H  | 1.90006000  | 0.27246000  | 2.11747000  |
| H  | 4.91081000  | -2.14728000 | 0.22131000  |
| H  | 3.65958000  | 1.40634000  | 3.46497000  |
| H  | 6.67278000  | -1.01331000 | 1.55976000  |
| H  | 6.04530000  | 0.76423000  | 3.18379000  |
| H  | -1.14352000 | -3.86815000 | -0.11705000 |
| H  | -1.49608000 | 4.36771000  | 1.14308000  |
| H  | -0.17568000 | 4.19734000  | 2.31186000  |
| H  | -1.44164000 | 2.95170000  | 2.20104000  |
| H  | -3.33837000 | 3.69753000  | -2.02081000 |
| H  | -1.70800000 | 3.82027000  | -1.33910000 |
| H  | -3.09626000 | 4.51053000  | -0.47015000 |
| H  | 3.97208000  | 3.61744000  | -0.13455000 |
| H  | 5.30810000  | 2.31334000  | -1.77340000 |
| H  | 1.83993000  | -0.04863000 | -2.78002000 |
| H  | 4.23443000  | 0.50531000  | -3.10232000 |
| H  | -6.72015000 | 0.99670000  | 0.66758000  |
| H  | -7.11070000 | -1.20276000 | 1.75481000  |
| H  | -5.19487000 | -2.71480000 | 2.23854000  |
| H  | -2.88503000 | -2.05801000 | 1.63018000  |

File: A\_BP4\_S\_B97D.xyz

|                        |             |             |             |
|------------------------|-------------|-------------|-------------|
| C                      | 1.84693000  | -3.32476000 | 1.39192000  |
| H                      | -0.82509000 | -2.87859000 | 1.37569000  |
| H                      | 2.81774000  | -3.80841000 | 1.44115000  |
| H                      | 1.54008000  | -2.75781000 | 2.26761000  |
| File: A_BP4_S_B97D.xyz |             |             |             |
| H                      | -0.98827000 | 1.66918000  | 0.98957000  |
| C                      | -1.61002000 | 1.45726000  | 0.12098000  |
| C                      | -0.98487000 | 0.94352000  | -1.05341000 |
| Si                     | -0.85103100 | -1.06099000 | -0.67670000 |
| O                      | -2.60833100 | -1.09471000 | -0.44702000 |
| C                      | -3.26011100 | -0.42822000 | 0.51972000  |
| C                      | -4.74810100 | -0.52754900 | 0.46756000  |
| C                      | -5.47000100 | -0.37879900 | 1.66065000  |
| C                      | -6.86303100 | -0.46932900 | 1.65128000  |
| C                      | -7.53955100 | -0.70028900 | 0.44888000  |
| C                      | -6.81901100 | -0.84383900 | -0.74410000 |
| C                      | -5.42752100 | -0.75256900 | -0.73872000 |
| O                      | 1.02760900  | -0.95842100 | -1.09486000 |
| N                      | 2.05893900  | -1.14725100 | -0.22978000 |
| C                      | 2.66117900  | -0.06554100 | 0.31664000  |
| C                      | 3.74312900  | -0.22075100 | 1.21562000  |
| C                      | 4.16829900  | -1.50147200 | 1.51377000  |
| C                      | 3.57947900  | -2.63011100 | 0.90775000  |
| C                      | 2.50186900  | -2.44528100 | -0.01161000 |
| C                      | 4.02975800  | -3.95193100 | 1.16347000  |
| C                      | 3.44584800  | -5.02404100 | 0.52441000  |
| C                      | 2.39484800  | -4.81387100 | -0.40051000 |
| C                      | 1.92003900  | -3.54454100 | -0.67048000 |
| C                      | 2.25056000  | 1.27509900  | -0.15502000 |
| N                      | 1.58325000  | 2.04438900  | 0.7500      |
| C                      | 1.21510000  | 3.35926900  | 0.40775000  |
| C                      | 1.53664000  | 3.85256900  | -0.88985000 |
| C                      | 2.23452000  | 3.02471900  | -1.80094000 |
| C                      | 2.60028000  | 1.74241900  | -1.44575000 |
| C                      | 0.52211000  | 4.15346900  | 1.34206000  |
| C                      | 0.14880100  | 5.43643900  | 0.98700000  |
| C                      | 0.45452100  | 5.94961900  | -0.29621000 |
| C                      | 1.13437100  | 5.17538900  | -1.21414000 |
| O                      | 1.25965000  | 1.56337900  | 1.90057000  |
| C                      | 3.35697000  | 0.84275900  | -2.38776000 |
| C                      | 4.40815000  | 0.99585800  | 1.80018000  |
| Cl                     | -1.06229100 | -2.27081000 | -2.39334000 |
| Cl                     | -0.45830100 | -1.82432000 | 1.26637000  |
| H                      | -2.85523100 | -0.55504000 | 1.52748000  |
| H                      | 0.03409000  | 1.26639900  | -1.23706000 |
| C                      | -3.00531000 | 1.41297000  | 0.26875000  |
| H                      | -1.60984000 | 0.96673000  | -1.94954000 |
| H                      | 2.48888000  | 3.40956900  | -2.78382000 |
| H                      | 4.99089900  | -1.64712200 | 2.20840000  |
| H                      | -4.86257100 | -0.86591900 | -1.65874000 |
| H                      | -4.93883100 | -0.20332900 | 2.59323000  |
| H                      | -7.34396100 | -1.02763900 | -1.67745000 |
| H                      | -7.41800100 | -0.36315900 | 2.57912000  |
| H                      | -8.62384100 | -0.76993900 | 0.44010000  |
| H                      | 3.66799000  | 1.40203900  | -3.27378000 |
| H                      | 2.72998900  | 0.00190900  | -2.70608000 |
| H                      | 4.24885900  | 0.42770800  | -1.90340000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.26151000  | 0.70125800  | 2.41565000  |
| H | 3.69599000  | 1.55341900  | 2.41858000  |
| H | 4.76071000  | 1.66564800  | 1.00714000  |
| H | 1.37513100  | 5.56196900  | -2.20035000 |
| H | 0.15197100  | 6.95970900  | -0.55638000 |
| H | -0.38382900 | 6.05637000  | 1.70193000  |
| H | 0.29825000  | 3.74432900  | 2.31940000  |
| H | 4.84491800  | -4.09250200 | 1.86688000  |
| H | 3.79466800  | -6.03302100 | 0.72159000  |
| H | 1.95167800  | -5.66333100 | -0.91126000 |
| H | 1.12165900  | -3.38815100 | -1.38142000 |
| H | -3.43656000 | 1.85622000  | 1.16264000  |
| H | -3.59216000 | 1.53649000  | -0.63911000 |

File: A\_BP4\_R\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.93315900 | 2.50047100  | 0.50714000  |
| C  | -0.59478900 | 2.71276100  | 0.12217000  |
| C  | -0.16775900 | 3.95483000  | -0.43679000 |
| C  | -1.13374800 | 4.98426100  | -0.58829000 |
| C  | -2.44136800 | 4.77472100  | -0.20428000 |
| C  | -2.83904900 | 3.53010100  | 0.34480000  |
| N  | 0.35016100  | 1.70873000  | 0.25802000  |
| C  | 1.65395100  | 1.88565000  | -0.04367000 |
| C  | 2.09736100  | 3.07764000  | -0.66631000 |
| C  | 1.17463100  | 4.09315000  | -0.84940000 |
| C  | 2.60096000  | 0.81783000  | 0.35693000  |
| N  | 2.51716000  | -0.37119000 | -0.27382000 |
| C  | 3.44256000  | -1.38460100 | -0.10616000 |
| C  | 4.49380000  | -1.16230100 | 0.83590000  |
| C  | 4.51548000  | 0.04261900  | 1.56749000  |
| C  | 3.58481000  | 1.04345900  | 1.34785000  |
| C  | 3.35077900  | -2.58716100 | -0.83313000 |
| C  | 4.31325900  | -3.55571100 | -0.62721000 |
| C  | 5.36680900  | -3.36147100 | 0.30105000  |
| C  | 5.45518000  | -2.19011100 | 1.02143000  |
| O  | 1.48589000  | -0.56943000 | -1.12212000 |
| Si | -0.22767000 | -1.01261000 | -0.41121000 |
| Cl | -0.24495100 | -2.89685000 | -1.66949000 |
| C  | 3.56515100  | 2.29845900  | 2.18348000  |
| C  | 3.50593100  | 3.19571900  | -1.18935000 |
| O  | -0.04284000 | 0.52705000  | 0.75472000  |
| O  | -1.88538000 | -1.14184900 | 0.22555000  |
| C  | -2.96264000 | -1.60461900 | -0.37733000 |
| C  | -4.24284000 | -1.48190800 | 0.36448000  |
| C  | -4.37628000 | -0.63488800 | 1.47580000  |
| C  | -5.59745000 | -0.54929800 | 2.14431000  |
| C  | -6.69329000 | -1.30468800 | 1.70974000  |
| C  | -6.56166000 | -2.15568800 | 0.60600000  |
| C  | -5.34226000 | -2.24295800 | -0.06485000 |
| C  | -0.95087000 | 0.12241100  | -2.05306000 |
| Cl | 0.56190000  | -2.13303000 | 1.34560000  |
| H  | 1.48598200  | 5.01641000  | -1.32925000 |
| H  | 5.27841000  | 0.18310900  | 2.32769000  |
| H  | -2.84717100 | -2.52378900 | -0.95542000 |
| H  | -3.51967000 | -0.06698900 | 1.82293000  |
| H  | -5.23582100 | -2.90195800 | -1.92333000 |
| H  | -5.69394000 | 0.10099200  | 3.00951000  |
| H  | -7.40670100 | -2.75102700 | 0.27181000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -7.64308000 | -1.23574700 | 2.23297000  |
| H | 4.38745100  | 2.27714900  | 2.90277000  |
| H | 2.62063100  | 2.36876000  | 2.73558000  |
| H | 3.65855100  | 3.20485900  | 1.57782000  |
| H | 3.70721100  | 4.22559900  | -1.49363000 |
| H | 3.62962100  | 2.54435900  | -2.06329000 |
| H | 4.25495100  | 2.89403900  | -0.45310000 |
| H | 6.25391000  | -2.03092100 | 1.73948000  |
| H | 6.10476900  | -4.14474100 | 0.44452000  |
| H | 4.25686900  | -4.48573100 | -1.18457000 |
| H | 2.53197900  | -2.73516000 | -1.52476000 |
| H | -0.81973800 | 5.93247100  | -1.01377000 |
| H | -3.17529800 | 5.56576100  | -0.32270000 |
| H | -3.87216900 | 3.38102100  | 0.64362000  |
| H | -2.21953900 | 1.54374100  | 0.92214000  |
| H | -0.11888000 | 0.08900000  | -2.75575000 |
| H | -1.12784000 | 1.11735100  | -1.64994000 |
| C | -2.14095000 | -0.50019900 | -2.53193000 |
| C | -3.37242000 | -0.35323900 | -1.90448000 |
| H | -2.04262000 | -1.28080900 | -3.28273000 |
| H | -4.25035000 | -0.81604800 | -2.34436000 |
| H | -3.55165000 | 0.53238100  | -1.29987000 |

File: A\_BP5\_S\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.04501000  | -2.78254100 | -0.92693900 |
| C  | 3.20853000  | -1.66592100 | -0.08193900 |
| C  | 4.18113000  | -1.66062100 | 0.96384100  |
| C  | 4.98671000  | -2.81733100 | 1.13597100  |
| C  | 4.82769000  | -3.90456100 | 0.30438100  |
| C  | 3.85616000  | -3.88276100 | -0.72796900 |
| N  | 2.41897000  | -0.53794100 | -0.23070900 |
| C  | 2.59392000  | 0.58503900  | 0.50411100  |
| C  | 3.51723000  | 0.60489900  | 1.57674100  |
| C  | 4.28606000  | -0.52682100 | 1.79343100  |
| C  | 1.82952000  | 1.79888900  | 0.12716100  |
| N  | 0.48475000  | 1.75457000  | 0.26213100  |
| C  | -0.33092000 | 2.85534000  | 0.10275100  |
| C  | 0.29006100  | 4.08951000  | -0.26051900 |
| C  | 1.67996100  | 4.11316000  | -0.47922900 |
| C  | 2.46809000  | 2.98668900  | -0.29379900 |
| C  | -1.72515000 | 2.76022000  | 0.28367100  |
| C  | -2.48980000 | 3.89712000  | 0.12328100  |
| C  | -1.89789900 | 5.13826000  | -0.22778900 |
| C  | -0.53761900 | 5.23361000  | -0.42125900 |
| O  | -0.08309000 | 0.57978000  | 0.59167100  |
| Si | -0.36534000 | -0.74780000 | -0.75480900 |
| Cl | -0.50100000 | -2.44174000 | -2.24950900 |
| C  | 3.94823000  | 3.04399900  | -0.57942900 |
| C  | 3.64577000  | 1.81031900  | 2.47223100  |
| O  | 1.48658000  | -0.54502000 | -1.20126900 |
| O  | -2.08981000 | -0.69039000 | -0.29762900 |
| C  | -2.94235000 | -1.68530000 | -0.17460900 |
| C  | -4.28640000 | -1.34655000 | 0.35256100  |
| C  | -4.49714000 | -0.23593000 | 1.18513100  |
| C  | -5.77996000 | 0.05673000  | 1.64442100  |
| C  | -6.86055000 | -0.75921900 | 1.28328100  |
| C  | -6.65253000 | -1.87060900 | 0.45957100  |
| C  | -5.36873000 | -2.16669000 | -0.00097900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.00314000  | -2.11580000 | 0.81991100  |
| Cl | -0.74643000 | 0.75884000  | -2.36021900 |
| H  | 4.98984000  | -0.54436100 | 2.62075100  |
| H  | 2.14422100  | 5.03892900  | -0.80811900 |
| H  | -2.92644000 | -2.45069000 | -0.95340900 |
| H  | -3.65542000 | 0.38803000  | 1.46785100  |
| H  | -5.20099000 | -3.02733000 | -0.64397900 |
| H  | -5.94071000 | 0.91947000  | 2.28520100  |
| H  | -7.48847000 | -2.50328900 | 0.17464100  |
| H  | -7.85950000 | -0.52849900 | 1.64314100  |
| H  | 2.68490000  | 2.31355900  | 2.61101100  |
| H  | 4.34871000  | 2.53711900  | 2.05100100  |
| H  | 4.02809000  | 1.50207900  | 3.44891100  |
| H  | 4.41441000  | 2.05673900  | -0.57121900 |
| H  | 4.45806000  | 3.67799900  | 0.15453100  |
| H  | 4.10656000  | 3.49027900  | -1.56672900 |
| H  | -0.07355900 | 6.17437000  | -0.70126900 |
| H  | -2.52716900 | 6.01431000  | -0.35120900 |
| H  | -3.56543000 | 3.83712000  | 0.25872100  |
| H  | -2.16587000 | 1.80197000  | 0.52040100  |
| H  | 5.72571000  | -2.81990100 | 1.93149100  |
| H  | 5.44783900  | -4.78571100 | 0.43669100  |
| H  | 3.74503900  | -4.74664100 | -1.37610900 |
| H  | 2.29021000  | -2.76092100 | -1.70292900 |
| H  | 0.96609000  | -2.55575000 | 0.56901100  |
| C  | -1.05069000 | -3.07927000 | 0.83293100  |
| H  | 0.04073000  | -1.48479000 | 1.70856100  |
| C  | -2.30085000 | -2.82482000 | 1.37850100  |
| H  | -0.93698100 | -3.96561000 | 0.21274100  |
| H  | -3.04709000 | -3.61338000 | 1.39689100  |
| H  | -2.39691000 | -2.05220000 | 2.13756100  |

File: A\_BP5\_R\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.69275000 | 2.82967000  | 0.19633000  |
| C  | -0.29021000 | 2.86236100  | 0.07038000  |
| C  | 0.38672900  | 4.07998100  | -0.25221000 |
| C  | -0.38727100 | 5.26025100  | -0.41953000 |
| C  | -1.75550100 | 5.22093000  | -0.27410000 |
| C  | -2.40639100 | 3.99865000  | 0.03117000  |
| N  | 0.48138000  | 1.72870100  | 0.24299000  |
| C  | 1.83209000  | 1.73361100  | 0.14257000  |
| C  | 2.52256900  | 2.90349200  | -0.24494000 |
| C  | 1.78102900  | 4.05992100  | -0.43031000 |
| O  | -0.12804000 | 0.56498100  | 0.55085000  |
| Si | -0.38952000 | -0.77435900 | -0.81196000 |
| Cl | -0.50481900 | -2.44452900 | -2.32673000 |
| C  | 2.56341000  | 0.49361200  | 0.49775000  |
| C  | 3.46981000  | 0.45804200  | 1.58430000  |
| C  | 4.23070000  | -0.68642800 | 1.75688000  |
| C  | 4.12692100  | -1.78266800 | 0.87699000  |
| C  | 3.16426100  | -1.73622800 | -0.17766000 |
| N  | 2.39461000  | -0.58976900 | -0.29247000 |
| C  | 2.98003100  | -2.82357800 | -1.05394000 |
| C  | 3.77043100  | -3.94383800 | -0.88548000 |
| C  | 4.73902100  | -4.01382800 | 0.14728000  |
| C  | 4.91282100  | -2.95685800 | 1.01461000  |
| C  | 4.00941900  | 2.91584200  | -0.50292000 |
| C  | 3.58216000  | 1.61949200  | 2.53783000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | 1.46075000  | -0.54876900 | -1.25818000 |
| O  | -2.14137000 | -0.87570000 | -0.46704000 |
| C  | -2.79408000 | -0.72662000 | 0.66111000  |
| C  | -4.24364000 | -1.02632000 | 0.64050000  |
| C  | -4.80860900 | -1.85256000 | -0.34438000 |
| C  | -6.18076900 | -2.09793100 | -0.33828000 |
| C  | -6.99568900 | -1.52668100 | 0.64794000  |
| C  | -6.43405000 | -0.70319100 | 1.63049000  |
| C  | -5.06119000 | -0.45624000 | 1.62932000  |
| C  | -0.02245900 | -2.16606900 | 0.75010000  |
| Cl | -0.78969000 | 0.75518100  | -2.38787000 |
| H  | 4.92301000  | -0.74684800 | 2.59177000  |
| H  | 2.28548900  | 4.97394100  | -0.73136000 |
| H  | -2.50111000 | 0.09783000  | 1.31455000  |
| H  | -4.17010900 | -2.28600000 | -1.10773000 |
| H  | -4.61758000 | 0.18353000  | 2.38879000  |
| H  | -6.61836900 | -2.73304100 | -1.10353000 |
| H  | -7.06468000 | -0.25419100 | 2.39269000  |
| H  | -8.06477900 | -1.72078100 | 0.64837000  |
| H  | 4.02185000  | 1.28029200  | 3.47933000  |
| H  | 2.60287000  | 2.06177200  | 2.74372000  |
| H  | 4.22731000  | 2.40505200  | 2.13024000  |
| H  | 4.44857000  | 1.91685200  | -0.48562000 |
| H  | 4.52349900  | 3.53822200  | 0.23787000  |
| H  | 4.19702900  | 3.35517200  | -1.48829000 |
| H  | 5.64544100  | -2.99916800 | 1.81483000  |
| H  | 5.34294100  | -4.90961800 | 0.25416000  |
| H  | 3.64413100  | -4.78682800 | -1.55790000 |
| H  | 2.22685100  | -2.76611900 | -1.82950000 |
| H  | 0.12616900  | 6.18439100  | -0.66672000 |
| H  | -2.34394100 | 6.12409000  | -0.40232000 |
| H  | -3.48761100 | 3.97639000  | 0.12610000  |
| H  | -2.19256000 | 1.89582000  | 0.39761000  |
| H  | 1.03354100  | -2.07207900 | 0.98915000  |
| H  | -0.25637900 | -3.11414900 | 0.26776000  |
| C  | -0.85853900 | -1.86382900 | 1.86862000  |
| C  | -2.19401900 | -2.22815000 | 1.92640000  |
| H  | -0.48942000 | -1.15467900 | 2.60805000  |
| H  | -2.77697900 | -2.00395000 | 2.81425000  |
| H  | -2.54531900 | -3.05160000 | 1.30967000  |

# PROPARGYLATION - B97D/TZV(2d,2p)

File: p\_bp2\_s\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.54412000  | -0.51188000 | 2.53655000  |
| C  | 4.63755000  | 0.40963000  | 1.99881000  |
| C  | 3.53090000  | -0.03535000 | 1.27776000  |
| C  | 3.32080000  | -1.40904000 | 1.08845000  |
| C  | 4.22983100  | -2.33184000 | 1.63359000  |
| C  | 5.33495100  | -1.88459000 | 2.35611000  |
| C  | 2.15387100  | -1.93273100 | 0.33772000  |
| O  | 1.14243000  | -1.10786100 | 0.14107000  |
| Si | -0.37214900 | -1.43552100 | -0.76835000 |
| O  | -1.19542000 | -0.66340100 | 0.72276000  |
| N  | -2.23952000 | 0.17378900  | 0.54082000  |
| C  | -1.98098000 | 1.44333900  | 0.16543000  |
| C  | -3.03545000 | 2.33546900  | -0.13869000 |
| C  | -4.33138000 | 1.88852900  | 0.05688000  |
| C  | -4.60234000 | 0.59414900  | 0.54539000  |
| C  | -3.51427000 | -0.30266100 | 0.77872000  |
| C  | -0.56454000 | 1.87825900  | 0.11065000  |
| C  | -0.05969000 | 2.88350900  | 0.96988000  |
| C  | 1.22393000  | 3.34618900  | 0.73447000  |
| C  | 2.0200      | 2.82123900  | -0.30431000 |
| C  | 1.50820000  | 1.74754900  | -1.09636000 |
| N  | 0.22232000  | 1.31737900  | -0.83178000 |
| O  | -0.28531000 | 0.30813900  | -1.56534000 |
| C  | 0.70620100  | -2.13122100 | -2.38022000 |
| C  | 1.92284100  | -2.37623100 | -2.11488000 |
| C  | 3.06642100  | -2.40472000 | -1.37524000 |
| Cl | -2.27042900 | -1.62496100 | -1.97490000 |
| Cl | -0.65367900 | -3.47275100 | 0.12748000  |
| C  | -0.85025000 | 3.36275900  | 2.16003000  |
| H  | 1.63872000  | 4.11959900  | 1.37456000  |
| C  | -2.74843000 | 3.70269900  | -0.70585000 |
| H  | -5.16318000 | 2.54677900  | -0.17736000 |
| C  | -5.92050000 | 0.12342900  | 0.78247000  |
| H  | 1.88649100  | -2.96574100 | 0.56993000  |
| H  | 2.82139000  | 0.67284900  | 0.87236000  |
| H  | 4.06315100  | -3.39721000 | 1.49398000  |
| H  | 4.79194000  | 1.47509000  | 2.14515000  |
| H  | 6.03024100  | -2.60314000 | 2.78065000  |
| H  | 6.40608000  | -0.16295000 | 3.09851000  |
| H  | 3.79162100  | -1.60682000 | -1.53341000 |
| H  | 3.49183100  | -3.36643000 | -1.09272000 |
| H  | 0.15499100  | -2.21713100 | -3.30679000 |
| C  | 3.34377000  | 3.26727000  | -0.55880000 |
| H  | -0.47160000 | 4.33011900  | 2.49964000  |
| H  | -0.73774000 | 2.64211900  | 2.98008000  |
| H  | -1.91826000 | 3.45218900  | 1.95297000  |
| H  | -3.67610000 | 4.15438900  | -1.06590000 |
| H  | -2.04259000 | 3.63518900  | -1.54056000 |
| H  | -2.31123000 | 4.37169900  | 0.04287000  |
| C  | -6.12774000 | -1.16270200 | 1.23146000  |
| H  | -6.75226000 | 0.79703800  | 0.60097000  |
| H  | -7.13698900 | -1.51886200 | 1.41366000  |
| C  | -5.02953900 | -2.03152100 | 1.45384000  |
| C  | -3.73133900 | -1.62001100 | 1.22696000  |
| H  | -5.21092900 | -3.04306100 | 1.80404000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.88875900 | -2.28294100 | 1.37355000  |
| C | 4.10299000  | 2.66690000  | -1.53951000 |
| H | 3.74242000  | 4.07875000  | 0.04213000  |
| H | 5.11722000  | 3.00628000  | -1.72529000 |
| C | 3.57178000  | 1.60122000  | -2.30817000 |
| C | 2.28843000  | 1.13747900  | -2.09738000 |
| H | 4.18431000  | 1.13839000  | -3.07572000 |
| H | 1.87513000  | 0.31830900  | -2.67008000 |

File: p\_bp2\_R\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.93083100  | -2.67064800 | 2.81775000  |
| C  | 3.63734100  | -3.12120900 | 2.52476000  |
| C  | 2.86748100  | -2.47114900 | 1.56039000  |
| C  | 3.39433100  | -1.36061900 | 0.88306000  |
| C  | 4.69167000  | -0.90949900 | 1.17766000  |
| C  | 5.45626100  | -1.56078800 | 2.14502000  |
| C  | 2.60982000  | -0.62698900 | -0.14147000 |
| O  | 1.29390000  | -0.71744000 | -0.07714000 |
| Si | -0.12133000 | -1.05448000 | -1.09847000 |
| O  | -1.04470000 | -0.79038000 | 0.49473000  |
| N  | -2.18550000 | -0.07017100 | 0.50037000  |
| C  | -2.09612000 | 1.27779900  | 0.47192000  |
| C  | -3.26313100 | 2.07457900  | 0.44494000  |
| C  | -4.48739000 | 1.42807800  | 0.50600000  |
| C  | -4.58138000 | 0.02676800  | 0.60704000  |
| C  | -3.38299000 | -0.75180100 | 0.59567000  |
| C  | -0.74366100 | 1.88842000  | 0.49667000  |
| C  | -0.29701100 | 2.70228000  | 1.56208000  |
| C  | 0.94074900  | 3.31446000  | 1.43355000  |
| C  | 1.72065900  | 3.17148000  | 0.27002000  |
| C  | 1.24966900  | 2.32125000  | -0.77671000 |
| N  | 0.04678000  | 1.67582000  | -0.58047000 |
| O  | -0.37348000 | 0.79835000  | -1.51492000 |
| C  | 1.03330100  | -1.27596000 | -2.79916000 |
| C  | 2.27216100  | -1.33328900 | -2.55058000 |
| C  | 3.41556100  | -1.35971900 | -1.80629000 |
| Cl | -1.97930900 | -1.30727100 | -2.36160000 |
| Cl | -0.03471900 | -3.26241000 | -0.66731000 |
| C  | -1.10011100 | 2.87786000  | 2.82638000  |
| H  | 1.32084900  | 3.92391000  | 2.24865000  |
| C  | -3.18158100 | 3.57493900  | 0.32885000  |
| H  | -5.40092100 | 2.01468800  | 0.47197000  |
| C  | -5.82402000 | -0.65538200 | 0.69497000  |
| H  | 2.98361000  | 0.38018100  | -0.34675000 |
| H  | 1.86375100  | -2.80891900 | 1.32540000  |
| H  | 5.09194000  | -0.04497800 | 0.65232000  |
| H  | 3.22925100  | -3.97947900 | 3.05159000  |
| H  | 6.45631100  | -1.20491800 | 2.37651000  |
| H  | 5.52623100  | -3.18031800 | 3.57044000  |
| H  | 4.17041000  | -0.59344900 | -1.97679000 |
| H  | 3.81027100  | -2.33846900 | -1.53512000 |
| H  | 0.46842100  | -1.40214000 | -3.71164000 |
| C  | 2.97439900  | 3.81711100  | 0.09405000  |
| H  | -0.45566100 | 2.69044000  | 3.69152000  |
| H  | -1.95371100 | 2.19924900  | 2.87802000  |
| H  | -1.46710100 | 3.90728900  | 2.90563000  |
| H  | -3.01806100 | 4.03507900  | 1.30935000  |
| H  | -4.12125100 | 3.96355900  | -0.07231000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.36376100 | 3.88292900  | -0.32903000 |
| C | 3.69423900  | 3.63342100  | -1.06636000 |
| H | 3.34341900  | 4.45819100  | 0.88884000  |
| H | 4.64913900  | 4.13257100  | -1.19818000 |
| C | 3.19439900  | 2.79842100  | -2.09802000 |
| C | 1.98896900  | 2.13866100  | -1.96326000 |
| H | 3.76934900  | 2.67222100  | -3.01023000 |
| H | 1.60663000  | 1.48552000  | -2.73581000 |
| C | -5.85541900 | -2.03005200 | 0.77613000  |
| H | -6.73810000 | -0.06945200 | 0.69671000  |
| H | -6.80640900 | -2.54919200 | 0.84492000  |
| C | -4.65026900 | -2.77807200 | 0.76766000  |
| C | -3.42053900 | -2.15817100 | 0.67385000  |
| H | -4.69377900 | -3.86119200 | 0.82892000  |
| H | -2.49776900 | -2.72288100 | 0.64501000  |

File: p\_bp3\_S\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.57218000  | -0.43399800 | 2.10843000  |
| C  | 5.23832000  | -0.88057800 | 0.82374000  |
| C  | 3.91354000  | -1.17346900 | 0.50503000  |
| C  | 2.91149000  | -1.01419900 | 1.47454000  |
| C  | 3.24770000  | -0.57221900 | 2.76374000  |
| C  | 4.57471000  | -0.27970900 | 3.07839000  |
| C  | 1.48337000  | -1.26057000 | 1.15699000  |
| O  | 1.17701000  | -1.22564000 | -0.12935000 |
| Si | -0.40317000 | -1.49831100 | -0.90763000 |
| O  | -1.20885000 | -0.65077100 | 0.62023000  |
| N  | -2.16148000 | 0.28180900  | 0.45141000  |
| C  | -1.79677100 | 1.51935900  | 0.04009000  |
| C  | -2.77139100 | 2.50969900  | -0.20814000 |
| C  | -4.09750100 | 2.18876800  | 0.04096000  |
| C  | -4.47308100 | 0.92808800  | 0.53975000  |
| C  | -3.46549000 | -0.06487200 | 0.74279000  |
| C  | -0.34429100 | 1.79745900  | -0.07208000 |
| C  | 0.30092900  | 2.72807000  | 0.77499000  |
| C  | 1.64880900  | 2.96715000  | 0.56154000  |
| C  | 2.35820900  | 2.33364100  | -0.47747000 |
| C  | 1.68088900  | 1.38108000  | -1.29983000 |
| N  | 0.34951900  | 1.13785000  | -1.02378000 |
| O  | -0.30011000 | 0.17962000  | -1.73210000 |
| C  | -0.62828900 | -3.29809100 | 0.09451000  |
| C  | 0.15785100  | -3.40015000 | 1.08276000  |
| C  | 1.21183100  | -3.07543000 | 1.89446000  |
| Cl | -2.40507000 | -1.74341100 | -1.89731000 |
| Cl | 0.62771100  | -2.50258000 | -2.62086000 |
| C  | -0.44367200 | 3.40328900  | 1.89763000  |
| H  | 2.17799800  | 3.65496000  | 1.21508000  |
| C  | -2.41133200 | 3.86628900  | -0.76041000 |
| H  | -4.86907100 | 2.92778800  | -0.15549000 |
| C  | -5.82134100 | 0.58610700  | 0.83174000  |
| C  | -3.78981000 | -1.34945200 | 1.22420000  |
| H  | 0.77483000  | -0.77958000 | 1.83652000  |
| H  | 3.64129000  | -1.50372900 | -0.49163000 |
| H  | 2.46686000  | -0.44828900 | 3.51050000  |
| H  | 6.01200000  | -0.99316800 | 0.06943000  |
| H  | 4.83101000  | 0.07060100  | 4.07434000  |
| H  | 6.60596000  | -0.20462800 | 2.35218000  |
| H  | 2.15731100  | -3.58239000 | 1.70104000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.02120100  | -2.84543000 | 2.94223000  |
| H | -1.36630900 | -3.96357100 | -0.33037000 |
| C | 3.73511900  | 2.57586100  | -0.72457000 |
| H | -1.14263100 | 2.71690900  | 2.38510000  |
| H | -1.01673200 | 4.26074900  | 1.52876000  |
| H | 0.26725800  | 3.76983000  | 2.64267000  |
| H | -1.36945200 | 3.92358900  | -1.08150000 |
| H | -2.59020200 | 4.64511900  | -0.01068000 |
| H | -3.05037200 | 4.08570800  | -1.62196000 |
| C | 4.38503900  | 1.90906100  | -1.73928000 |
| H | 4.25577800  | 3.29287100  | -0.09737000 |
| H | 5.43839900  | 2.09446200  | -1.92475000 |
| C | 3.68810900  | 0.97262100  | -2.54314000 |
| C | 2.35178900  | 0.69831100  | -2.33215000 |
| H | 4.21565900  | 0.45314100  | -3.33720000 |
| H | 1.82047000  | -0.03373000 | -2.92539000 |
| C | -5.11056000 | -1.63474200 | 1.50383000  |
| H | -3.00685000 | -2.08363200 | 1.35899000  |
| H | -5.37306900 | -2.61979200 | 1.87742000  |
| C | -6.13114000 | -0.66906300 | 1.30554000  |
| H | -6.59211100 | 1.33436700  | 0.67362000  |
| H | -7.16170000 | -0.92710300 | 1.52902000  |

File: p\_bp3\_R\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.30597000  | 0.15141800  | 2.49893000  |
| C  | 3.97784100  | 0.57026900  | 2.65100000  |
| C  | 2.95697000  | -0.07047100 | 1.95163000  |
| C  | 3.26219000  | -1.13561100 | 1.08993000  |
| C  | 4.59132000  | -1.56027200 | 0.94537000  |
| C  | 5.61130000  | -0.91407200 | 1.64480000  |
| C  | 2.20950900  | -1.80648000 | 0.28642000  |
| O  | 1.14176000  | -1.06936000 | 0.04043000  |
| Si | -0.36035000 | -1.49202900 | -0.80397000 |
| O  | -1.18331000 | -0.60300900 | 0.69245000  |
| N  | -2.20527000 | 0.24769200  | 0.47938000  |
| C  | -1.93175900 | 1.47120200  | -0.02958000 |
| C  | -2.97375900 | 2.36648200  | -0.35660000 |
| C  | -4.27143900 | 1.98255300  | -0.05644000 |
| C  | -4.55362900 | 0.74630300  | 0.55606000  |
| C  | -3.47990000 | -0.15891800 | 0.81940000  |
| C  | -0.50137900 | 1.84686100  | -0.13925000 |
| C  | 0.05745200  | 2.86087100  | 0.67422000  |
| C  | 1.39740200  | 3.16119000  | 0.49737000  |
| C  | 2.18431200  | 2.49792000  | -0.46569000 |
| C  | 1.59066100  | 1.46905000  | -1.25919000 |
| N  | 0.26019100  | 1.17805100  | -1.02668000 |
| O  | -0.31319000 | 0.14947100  | -1.70113000 |
| C  | -0.55336100 | -3.24012900 | 0.30222000  |
| C  | 0.49859900  | -3.51955900 | 0.94966000  |
| C  | 1.76605900  | -3.34670000 | 1.43684000  |
| Cl | -2.35286100 | -1.85199800 | -1.77916000 |
| Cl | 0.70531900  | -2.52191000 | -2.49119000 |
| C  | -0.76931800 | 3.53796100  | 1.73688000  |
| H  | 1.86233200  | 3.91266000  | 1.12897000  |
| C  | -2.70366800 | 3.66147200  | -1.08024000 |
| H  | -5.09470800 | 2.64848300  | -0.29934000 |
| C  | -5.87082000 | 0.34193400  | 0.90258000  |
| H  | 2.57722900  | -2.40802100 | -0.54897000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.92604000  | 0.25179000  | 2.05653000  |
| H | 4.82172900  | -2.38243200 | 0.27184000  |
| H | 3.74231100  | 1.39958900  | 3.31242000  |
| H | 6.64123000  | -1.23672300 | 1.52110000  |
| H | 6.10004100  | 0.65550800  | 3.04300000  |
| H | 2.54364800  | -4.04314100 | 1.12531000  |
| H | 1.86395900  | -2.97867000 | 2.45814000  |
| H | -1.51271200 | -3.73079800 | 0.22111000  |
| C | 2.34162100  | 0.75167000  | -2.20935000 |
| C | 3.56411200  | 2.77541900  | -0.65053000 |
| H | -0.12285800 | 4.13659100  | 2.38330000  |
| H | -1.29518800 | 2.79901100  | 2.35083000  |
| H | -1.52336800 | 4.19969200  | 1.29790000  |
| H | -3.41258700 | 4.42992200  | -0.75934000 |
| H | -2.83719800 | 3.50501200  | -2.15799000 |
| H | -1.68747800 | 4.02837200  | -0.92580000 |
| C | 4.29673100  | 2.06566900  | -1.57632000 |
| H | 4.02346200  | 3.54884900  | -0.04257000 |
| H | 5.35347100  | 2.27507800  | -1.70998000 |
| C | 3.67976100  | 1.05702900  | -2.35807000 |
| H | 1.86907000  | -0.03241000 | -2.78613000 |
| H | 4.27060100  | 0.50795900  | -3.08479000 |
| C | -6.09002000 | -0.88848600 | 1.48146000  |
| H | -6.69180900 | 1.02312400  | 0.70070000  |
| H | -7.09797000 | -1.19368600 | 1.74509000  |
| C | -5.00520100 | -1.76615700 | 1.73711000  |
| C | -3.71094000 | -1.41771700 | 1.40896000  |
| H | -5.19563100 | -2.73143700 | 2.19613000  |
| H | -2.87673100 | -2.08069800 | 1.59364000  |

File: p\_bp4\_S\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.81275400 | -2.33264800 | 0.82517800  |
| C  | -5.79581300 | -3.00658400 | 0.13658500  |
| C  | -4.55049500 | -2.40505300 | -0.04228700 |
| C  | -4.31671900 | -1.12178900 | 0.47477200  |
| C  | -5.33628500 | -0.44624400 | 1.16268400  |
| C  | -6.58046500 | -1.05267300 | 1.34071900  |
| C  | -3.00491400 | -0.44165600 | 0.29773000  |
| O  | -1.96744600 | -1.24410800 | 0.11321700  |
| Si | -0.31475600 | -0.97795400 | -0.41781000 |
| O  | 1.40774500  | -0.61338200 | -1.12166000 |
| N  | 2.45500700  | -0.50612400 | -0.27783400 |
| C  | 2.60319200  | 0.65608900  | 0.38073900  |
| C  | 3.61529400  | 0.81838500  | 1.35187100  |
| C  | 4.50066700  | -0.23219100 | 1.53003100  |
| C  | 4.40292200  | -1.42029700 | 0.77595900  |
| C  | 3.32555500  | -1.57020800 | -0.15150400 |
| C  | 1.71439100  | 1.77282600  | -0.01469900 |
| C  | 2.22994900  | 2.88167200  | -0.72648900 |
| C  | 1.37700600  | 3.94140300  | -0.97716500 |
| C  | 0.06253400  | 3.95596500  | -0.46645200 |
| C  | -0.42183600 | 2.81593300  | 0.24499800  |
| N  | 0.41374700  | 1.71276900  | 0.34405500  |
| O  | -0.08134200 | 0.55485700  | 0.82412500  |
| C  | -0.92428000 | 0.34748000  | -1.91570200 |
| C  | -2.12692300 | 0.70183000  | -1.77021300 |
| C  | -3.39645600 | 0.66601900  | -1.25354400 |
| Cl | 0.42583900  | -2.23681100 | 1.23434500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Cl | -0.45119800 | -2.65242100 | -1.91138900 |
| C  | 3.64226300  | 2.85827700  | -1.25337300 |
| H  | 1.72876100  | 4.78834300  | -1.55916100 |
| C  | 3.67398400  | 2.06412600  | 2.19742000  |
| H  | 5.29022500  | -0.14378800 | 2.27069500  |
| C  | 5.31400100  | -2.49962900 | 0.91974800  |
| H  | -2.83909400 | 0.38246000  | 0.99068500  |
| H  | -3.75455700 | -2.92033600 | -0.57062200 |
| H  | -5.14892500 | 0.54782000  | 1.56316600  |
| H  | -5.97525700 | -4.00281500 | -0.25825700 |
| H  | -7.36485100 | -0.53118400 | 1.88212400  |
| H  | -7.78131200 | -2.80567100 | 0.96250400  |
| H  | -4.13010300 | 0.08932400  | -1.81662600 |
| H  | -3.79167900 | 1.56677700  | -0.78539000 |
| H  | -0.16619500 | 0.56960800  | -2.65274200 |
| C  | -0.80735500 | 5.06725900  | -0.62495100 |
| H  | 3.82335100  | 3.74365500  | -1.86738300 |
| H  | 3.81136600  | 1.96481600  | -1.86497600 |
| H  | 4.37933000  | 2.84424900  | -0.44390000 |
| H  | 3.71719100  | 2.97400400  | 1.59136300  |
| H  | 4.55261900  | 2.03532100  | 2.84641900  |
| H  | 2.77769700  | 2.13309000  | 2.82543800  |
| C  | -2.06470700 | 5.05705600  | -0.06058300 |
| H  | -0.45019500 | 5.92685000  | -1.18369900 |
| H  | -2.72228600 | 5.91256100  | -0.17854500 |
| C  | -2.49194700 | 3.94571500  | 0.70628300  |
| C  | -1.68767900 | 2.83337200  | 0.85742500  |
| H  | -3.46065400 | 3.97121200  | 1.19593700  |
| H  | -1.98605900 | 2.00518300  | 1.48220700  |
| C  | 5.15086900  | -3.64860200 | 0.17638000  |
| H  | 6.13339000  | -2.39721100 | 1.62471300  |
| H  | 5.85015000  | -4.47152900 | 0.28794600  |
| C  | 4.07072500  | -3.76959700 | -0.73428700 |
| C  | 3.15551700  | -2.74926600 | -0.90162500 |
| H  | 3.95596700  | -4.68415000 | -1.30807300 |
| H  | 2.31440800  | -2.83755000 | -1.57763500 |

File: p\_bp4\_R\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 6.62533000  | -1.51390700 | -1.71626000 |
| C  | 5.49550000  | -0.88629800 | -2.25447000 |
| C  | 4.29614000  | -0.86827800 | -1.54197000 |
| C  | 4.21999000  | -1.48225800 | -0.28242000 |
| C  | 5.35307000  | -2.11575800 | 0.25244000  |
| C  | 6.55008000  | -2.13334700 | -0.46310000 |
| C  | 2.96331000  | -1.47884800 | 0.51588000  |
| O  | 1.85648000  | -1.20038900 | -0.16383000 |
| Si | 0.19966000  | -1.03401900 | 0.43144000  |
| O  | -1.51016000 | -0.55957000 | 1.12432000  |
| N  | -2.53390000 | -0.33809000 | 0.27311000  |
| C  | -2.60265100 | 0.85820000  | -0.35904000 |
| C  | -3.62366100 | 1.11173000  | -1.30125000 |
| C  | -4.58243100 | 0.12818900  | -1.49509000 |
| C  | -4.55756000 | -1.08337100 | -0.78154000 |
| C  | -3.48200000 | -1.33050000 | 0.12700000  |
| C  | -1.59734100 | 1.88653000  | 0.00245000  |
| C  | -1.96227100 | 3.11812000  | 0.59490000  |
| C  | -0.96672200 | 4.06272000  | 0.78845000  |
| C  | 0.36747800  | 3.82376100  | 0.40080000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.70914900  | 2.55251100  | -0.15162000 |
| N  | -0.30511100 | 1.62624100  | -0.29646000 |
| O  | 0.00178900  | 0.41358100  | -0.79192000 |
| C  | 0.84403900  | 0.26205100  | 1.99002000  |
| C  | 2.09869900  | 0.24691100  | 2.11871000  |
| C  | 3.39135900  | -0.09844800 | 1.81925000  |
| Cl | -0.57938000 | -2.28914900 | -1.21234000 |
| Cl | 0.25970000  | -2.73448900 | 1.89070000  |
| C  | -3.38256100 | 3.3800      | 1.02473000  |
| H  | -1.21670200 | 5.01178000  | 1.25397000  |
| C  | -3.66852100 | 2.37790000  | -2.12069000 |
| H  | -5.37311100 | 0.29310900  | -2.22189000 |
| C  | -5.54500000 | -2.09241100 | -0.94346000 |
| H  | 2.87684000  | -2.29296800 | 1.24055000  |
| H  | 3.41241000  | -0.40254800 | -1.96535000 |
| H  | 5.29062000  | -2.59855800 | 1.22496000  |
| H  | 5.54797000  | -0.41737800 | -3.23324000 |
| H  | 7.42128000  | -2.63199700 | -0.04761000 |
| H  | 7.55765000  | -1.52736700 | -2.27412000 |
| H  | 3.94490000  | -0.69157800 | 2.54633000  |
| H  | 3.99180900  | 0.64357200  | 1.29255000  |
| H  | 0.05178900  | 0.77087100  | 2.51897000  |
| C  | 1.40375800  | 4.78240100  | 0.56087000  |
| H  | -4.54785100 | 2.97541900  | -1.85579000 |
| H  | -3.75640100 | 2.11531000  | -3.18010000 |
| H  | -2.77606100 | 2.99318000  | -1.99271000 |
| H  | -3.39778200 | 4.15470000  | 1.79591000  |
| H  | -3.85166100 | 2.47513000  | 1.42193000  |
| H  | -3.98816200 | 3.73050000  | 0.18198000  |
| C  | -5.45744000 | -3.26789100 | -0.23188000 |
| H  | -6.36221000 | -1.91282100 | -1.63535000 |
| H  | -6.21433900 | -4.03629100 | -0.35533000 |
| C  | -4.37932000 | -3.48711000 | 0.66395000  |
| C  | -3.39270000 | -2.53941000 | 0.84620000  |
| H  | -4.32415900 | -4.42154000 | 1.21401000  |
| H  | -2.55737000 | -2.70667000 | 1.51351000  |
| C  | 2.69392800  | 4.48014100  | 0.18283000  |
| H  | 1.15461800  | 5.75116100  | 0.98305000  |
| H  | 3.48198800  | 5.21693200  | 0.30327000  |
| C  | 3.00432900  | 3.20916200  | -0.36549000 |
| C  | 2.03091900  | 2.24514100  | -0.52937000 |
| H  | 4.02605900  | 2.98736200  | -0.65879000 |
| H  | 2.25400900  | 1.26699100  | -0.93293000 |

File: p\_bp5\_S\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.89745000 | -0.81284100 | 1.13545100  |
| C  | -5.84559000 | 0.03588900  | 1.50526100  |
| C  | -4.53851000 | -0.26176100 | 1.12318100  |
| C  | -4.27446000 | -1.40945100 | 0.36049100  |
| C  | -5.32709000 | -2.26274100 | -0.00043900 |
| C  | -6.63607000 | -0.38174100 | 0.38174100  |
| C  | -2.89323000 | -1.76307100 | -0.07148900 |
| O  | -2.08326000 | -0.72807100 | -0.28769900 |
| Si | -0.37558000 | -0.75348100 | -0.75203900 |
| O  | -0.06531000 | 0.52820900  | 0.60977100  |
| N  | 0.48205000  | 1.71707900  | 0.27524100  |
| C  | 1.82178000  | 1.78073900  | 0.10275100  |
| C  | 2.42966000  | 2.97604900  | -0.34087900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.62009000  | 4.09106900  | -0.50278900 |
| C  | 0.23864000  | 4.04848900  | -0.23968900 |
| C  | -0.35390000 | 2.80530900  | 0.14148100  |
| C  | 2.61364000  | 0.58113900  | 0.46540100  |
| C  | 3.56470000  | 0.62431900  | 1.51380100  |
| C  | 4.34833000  | -0.49755100 | 1.72588100  |
| C  | 4.22209000  | -1.65003100 | 0.92477100  |
| C  | 3.21832000  | -1.68148100 | -0.09155900 |
| N  | 2.42953000  | -0.55193100 | -0.25072900 |
| O  | 1.48100000  | -0.57921100 | -1.20370900 |
| C  | 0.06669000  | -2.09481100 | 0.81371100  |
| C  | -0.98142000 | -2.62368100 | 1.27774100  |
| C  | -2.32931000 | -2.83616100 | 1.42601100  |
| Cl | -0.75431000 | 0.74060900  | -2.34666900 |
| Cl | -0.50008000 | -2.47917100 | -2.17994900 |
| C  | 3.69827000  | 1.84273900  | 2.39067100  |
| H  | 5.07552000  | -0.49613100 | 2.53264100  |
| C  | 3.89652000  | 3.05195900  | -0.68422900 |
| H  | 2.06039000  | 5.02212900  | -0.84950900 |
| C  | -0.60947000 | 5.18058900  | -0.37667900 |
| H  | -2.84538000 | -2.55723100 | -0.82126900 |
| H  | -3.71912000 | 0.38716900  | 1.41418100  |
| H  | -5.11956000 | -3.15173100 | -0.59115900 |
| H  | -6.04708000 | 0.92779900  | 2.09234100  |
| H  | -7.44943000 | -2.61959100 | 0.08896100  |
| H  | -7.91554000 | -0.57843100 | 1.43408100  |
| H  | -2.80283000 | -2.38838100 | 2.30006100  |
| H  | -2.73018000 | -3.81104100 | 1.14840100  |
| H  | 1.10083000  | -2.22093100 | 1.09335100  |
| C  | 5.03011000  | -2.80334100 | 1.10466100  |
| H  | 4.19645000  | 1.57015900  | 3.32454100  |
| H  | 2.72042000  | 2.27468900  | 2.62367100  |
| H  | 4.29870000  | 2.61704900  | 1.90160100  |
| H  | 4.41374000  | 3.74734900  | -0.01410900 |
| H  | 4.00455000  | 3.43544900  | -1.70440900 |
| H  | 4.39163000  | 2.08040900  | -0.63150900 |
| C  | -1.96225000 | 5.06578900  | -0.14540900 |
| H  | -0.16677000 | 6.12761900  | -0.66964900 |
| H  | -2.60736000 | 5.93252900  | -0.25112900 |
| C  | -2.52596000 | 3.81623900  | 0.22170100  |
| C  | -1.74101000 | 2.69047900  | 0.36083100  |
| H  | -3.59636000 | 3.74067900  | 0.38738100  |
| H  | -2.16150000 | 1.72658900  | 0.61021100  |
| C  | 4.83887000  | -3.91528100 | 0.31308100  |
| H  | 5.79436000  | -2.78529100 | 1.87574100  |
| H  | 5.45972000  | -4.79487100 | 0.45216100  |
| C  | 3.83141000  | -3.92207100 | -0.68395900 |
| C  | 3.01916000  | -2.82397100 | -0.89206900 |
| H  | 3.69222000  | -4.80684100 | -1.29752900 |
| H  | 2.23938000  | -2.82455100 | -1.64294900 |

File: p\_bp5\_R\_B97D.xyz

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 1.88927000  | 2.65709000 | -0.18364000 |
| C | 0.49256000  | 2.78723000 | -0.06488000 |
| C | -0.10684000 | 4.04002000 | 0.27158000  |
| C | 0.74361000  | 5.16092000 | 0.46263000  |
| C | 2.10837000  | 5.03028000 | 0.32530000  |
| C | 2.67905000  | 3.77320000 | 0.00436000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -0.35248000 | 1.70998900  | -0.25668000 |
| C  | -1.69504000 | 1.80305900  | -0.17473000 |
| C  | -2.31621000 | 3.00589900  | 0.23438000  |
| C  | -1.50443000 | 4.10734900  | 0.44512000  |
| O  | 0.17692100  | 0.50594000  | -0.55360000 |
| Si | 0.33999100  | -0.80893000 | 0.83525000  |
| Cl | 0.32165100  | -2.52919000 | 2.27266000  |
| C  | -2.49726900 | 0.61506900  | -0.55003000 |
| C  | -3.36568900 | 0.63016900  | -1.66747000 |
| C  | -4.21797900 | -0.44769100 | -1.83664000 |
| C  | -4.22672900 | -1.53223100 | -0.93492000 |
| C  | -3.28302900 | -1.55037100 | 0.13797000  |
| N  | -2.42353900 | -0.46989100 | 0.25145000  |
| C  | -3.21343900 | -2.63079100 | 1.04019000  |
| C  | -4.09528900 | -3.68190100 | 0.87524000  |
| C  | -5.04514900 | -3.68723100 | -0.17649000 |
| C  | -5.10966900 | -2.63582100 | -1.06580000 |
| C  | -3.80070000 | 3.05787900  | 0.49287000  |
| C  | -3.29614000 | 1.74108900  | -2.68406000 |
| O  | -1.51073900 | -0.48329100 | 1.24153000  |
| O  | 2.06636100  | -0.99458000 | 0.46941000  |
| C  | 2.66467100  | -0.97392000 | -0.71748000 |
| C  | 4.13396100  | -1.20758000 | -0.69435000 |
| C  | 4.74300100  | -1.93895000 | 0.33705000  |
| C  | 6.12323100  | -2.13599000 | 0.32452000  |
| C  | 6.90176100  | -1.60968000 | -0.71458000 |
| C  | 6.29567100  | -0.87994000 | -1.74310000 |
| C  | 4.91398100  | -0.68260000 | -1.73577000 |
| C  | -0.17254900 | -2.17856000 | -0.65447000 |
| C  | 0.79184100  | -2.43079000 | -1.43307000 |
| C  | 2.09516100  | -2.43006000 | -1.85850000 |
| Cl | 0.79112000  | 0.66677000  | 2.42031000  |
| H  | -4.89393900 | -0.46522100 | -2.68665000 |
| H  | -1.95017000 | 5.04488900  | 0.76500000  |
| H  | 2.34474100  | -0.17992000 | -1.39884000 |
| H  | 4.13224100  | -2.13377500 | 1.14087000  |
| H  | 4.43776100  | -0.11283000 | -2.53037000 |
| H  | 6.59500100  | -2.69779000 | 1.12596000  |
| H  | 6.89779100  | -0.46385000 | -2.54599000 |
| H  | 7.97713100  | -1.76520000 | -0.71997000 |
| H  | 2.32796100  | -2.03675000 | -2.84774000 |
| H  | 2.70779100  | -3.27827000 | -1.55121000 |
| H  | -1.15442900 | -2.62471100 | -0.59522000 |
| H  | -4.15548000 | 1.68890900  | -3.35701000 |
| H  | -2.38121000 | 1.63433900  | -3.28044000 |
| H  | -3.26811000 | 2.73211900  | -2.22506000 |
| H  | -4.06829000 | 4.03110900  | 0.91117000  |
| H  | -4.09216000 | 2.27780900  | 1.20516000  |
| H  | -4.38509000 | 2.90438900  | -0.41983000 |
| H  | -5.82893900 | -2.63146100 | -1.87910000 |
| H  | -5.72316900 | -4.52862100 | -0.28026000 |
| H  | -4.05776900 | -4.51805100 | 1.56668000  |
| H  | -2.47434900 | -2.62072100 | 1.83155000  |
| H  | 0.29341000  | 6.11410000  | 0.72216000  |
| H  | 2.75491000  | 5.88990000  | 0.47191000  |
| H  | 3.75698000  | 3.68119000  | -0.08587000 |
| H  | 2.32229000  | 1.69246000  | -0.40032000 |

File: p\_bp1\_S\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 6.72773000  | -1.38351900 | -1.69734000 |
| C  | 5.49903000  | -1.74840900 | -2.26290000 |
| C  | 4.32188000  | -1.62397900 | -1.52558000 |
| C  | 4.36986000  | -1.12683900 | -0.21383000 |
| C  | 5.60175000  | -0.76550900 | -0.35271000 |
| C  | 6.77723000  | -0.88942900 | -0.38912000 |
| C  | 3.13858000  | -0.98003900 | 0.60830000  |
| O  | 2.01127000  | -0.83046900 | -0.08243000 |
| Si | 0.35179000  | -0.78731000 | 0.52163000  |
| O  | -1.43900000 | -0.61301000 | 1.19094000  |
| N  | -2.46320000 | -0.55506000 | 0.31229000  |
| C  | -2.64700000 | 0.58283000  | -0.39134000 |
| C  | -3.61567000 | 0.65278000  | -1.42003000 |
| C  | -4.42756000 | -0.45084100 | -1.61595000 |
| C  | -4.31722000 | -1.59993100 | -0.80731000 |
| C  | -3.29279000 | -1.65501000 | 0.18744000  |
| C  | -1.81954000 | 1.76571000  | -0.05131000 |
| C  | -2.38104100 | 2.94708000  | 0.48369000  |
| C  | -1.55269100 | 4.05093000  | 0.61025000  |
| C  | -0.19580100 | 4.00906000  | 0.22912000  |
| C  | 0.35376900  | 2.77720000  | -0.24130000 |
| N  | -0.50357000 | 1.70107000  | -0.33382000 |
| O  | -0.00937000 | 0.51555000  | -0.75088000 |
| C  | 0.62747000  | -2.36272000 | 1.82501000  |
| C  | 1.84812000  | -2.68270900 | 1.90522000  |
| C  | 3.18538000  | -2.63994900 | 1.60070000  |
| Cl | -0.28977000 | -2.27495000 | -1.05943000 |
| Cl | 0.84657000  | 0.67319000  | 2.19594000  |
| C  | -3.80244100 | 2.97176000  | 0.98345000  |
| H  | -1.95448100 | 4.97283000  | 1.02133000  |
| C  | -3.70352100 | 1.86579000  | -2.31098000 |
| H  | -5.16604000 | -0.43735100 | -2.41225000 |
| C  | -3.14043000 | -2.78688000 | 1.01045000  |
| H  | 3.24694000  | -0.32419900 | 1.47679000  |
| H  | 3.36470000  | -1.90094900 | -1.95618000 |
| H  | 5.63302000  | -0.38199900 | 1.36976000  |
| H  | 5.46103000  | -2.12880900 | -3.28002000 |
| H  | 7.72781000  | -0.60006800 | 0.05025000  |
| H  | 7.64250000  | -1.48249800 | -2.27542000 |
| H  | 3.55632000  | -3.39137900 | 0.90295000  |
| H  | 3.88734000  | -2.37124900 | 2.39017000  |
| H  | -0.26621000 | -2.76715000 | 2.74300000  |
| C  | 1.71429900  | 2.65947100  | -0.58722000 |
| C  | 0.66989900  | 5.13008000  | 0.32971000  |
| H  | -4.13211100 | 4.00321000  | 1.12972000  |
| H  | -3.85760100 | 2.44993000  | 1.94701000  |
| H  | -4.49674100 | 2.47139900  | 0.30441000  |
| H  | -4.39742000 | 1.67140900  | -3.13248000 |
| H  | -2.72041100 | 2.10574000  | -2.73024000 |
| H  | -4.05449100 | 2.74950000  | -1.76829000 |
| C  | 2.51712900  | 3.77712100  | -0.47904000 |
| H  | 2.10212000  | 1.70553100  | -0.91956000 |
| H  | 3.56693900  | 3.70447100  | -0.74622000 |
| C  | 1.99763900  | 5.01488100  | -0.02062000 |
| H  | 0.26276900  | 6.06987000  | 0.68980000  |
| H  | 2.65625900  | 5.87440100  | 0.05712000  |
| C  | -3.99733900 | -3.85533000 | 0.83855000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.37363000 | -2.79708000 | 1.77091000  |
| H | -3.89227900 | -4.72768000 | 1.47616000  |
| C | -5.00916900 | -3.83228100 | -0.15372000 |
| C | -5.16742000 | -2.72667100 | -0.96039000 |
| H | -5.66299900 | -4.69077100 | -0.27171000 |
| H | -5.94060000 | -2.69138100 | -1.72190000 |

File: p\_bp1\_R\_B97D.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.96166100 | -0.78309800 | 1.05204900  |
| C  | -6.17109000 | 0.10994200  | 0.31735900  |
| C  | -4.83651000 | -0.19188900 | 0.04774900  |
| C  | -4.28278100 | -1.39215900 | 0.52086900  |
| C  | -5.07734100 | -2.28758900 | 1.25322900  |
| C  | -6.41217100 | -1.98181800 | 1.52079900  |
| C  | -2.86264100 | -1.74846900 | 0.25922900  |
| O  | -2.06073100 | -0.72080900 | -0.00200100 |
| Si | -0.37547100 | -0.74770000 | -0.52690100 |
| O  | 1.40575900  | -0.58717000 | -1.18098100 |
| N  | 2.43265900  | -0.56875100 | -0.30582100 |
| C  | 2.66795000  | 0.56756900  | 0.39406900  |
| C  | 3.69254000  | 0.61043900  | 1.36645900  |
| C  | 4.48235900  | -0.51803100 | 1.52648900  |
| C  | 4.29404900  | -1.67023100 | 0.74242900  |
| C  | 3.22029900  | -1.69822100 | -0.20036100 |
| C  | 1.85462000  | 1.76752000  | 0.07647900  |
| C  | 2.43533000  | 2.95304900  | -0.42849100 |
| C  | 1.61474100  | 4.06085000  | -0.58117100 |
| C  | 0.25197100  | 4.03014000  | -0.23062100 |
| C  | -0.31307000 | 2.80446000  | 0.23772900  |
| N  | 0.52966000  | 1.71777000  | 0.33791900  |
| O  | 0.00336000  | 0.54153000  | 0.74518900  |
| C  | -0.67364100 | -2.24168000 | -1.91758100 |
| C  | -1.81072100 | -2.77596900 | -1.77648100 |
| C  | -3.07765100 | -2.92573900 | -1.27222100 |
| Cl | 0.23524900  | -2.26465000 | 1.04803900  |
| Cl | -0.86264000 | 0.73325000  | -2.19029100 |
| C  | 3.89132000  | 3.02079900  | -0.81366100 |
| H  | 2.03247100  | 4.97940000  | -0.98410100 |
| C  | 3.92015000  | 1.82013900  | 2.23795900  |
| H  | 5.26669900  | -0.51702100 | 2.27850900  |
| C  | 5.11282900  | -2.82484100 | 0.86720900  |
| H  | -2.44904100 | -2.50855900 | 0.92766900  |
| H  | -4.21636000 | 0.49399100  | -0.52062100 |
| H  | -4.64419100 | -3.21644900 | 1.61706900  |
| H  | -6.59743000 | 1.04168200  | -0.04451100 |
| H  | -7.02137100 | -2.67385800 | 2.09544900  |
| H  | -8.00128100 | -0.54452800 | 1.25947900  |
| H  | -3.33446100 | -3.85940900 | -0.77253100 |
| H  | -3.88862100 | -2.48469900 | -1.85250100 |
| H  | 0.11827900  | -2.36478000 | -2.64188100 |
| C  | -0.60249900 | 5.15867000  | -0.35181100 |
| H  | 4.80369000  | 2.37440900  | 1.90260900  |
| H  | 4.10505000  | 1.49404900  | 3.26597900  |
| H  | 3.06599000  | 2.50032900  | 2.23777900  |
| H  | 4.00438000  | 3.65413900  | -1.69839100 |
| H  | 4.30436000  | 2.03359900  | -1.03335100 |
| H  | 4.48255000  | 3.46768900  | -0.00665100 |
| C  | 4.87146900  | -3.93407100 | 0.08814900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.92618900  | -2.80650100 | 1.58613900  |
| H | 5.49948800  | -4.81438100 | 0.18350900  |
| C | 3.80122900  | -3.93632100 | -0.84286100 |
| C | 2.97650900  | -2.84001100 | -0.98944100 |
| H | 3.62280800  | -4.81861100 | -1.44982100 |
| H | 2.15367900  | -2.84413000 | -1.68949100 |
| C | -1.93451900 | 5.05841100  | -0.01651100 |
| H | -0.18125900 | 6.09194000  | -0.71264100 |
| H | -2.58487900 | 5.92280100  | -0.10858100 |
| C | -2.46919900 | 3.82834100  | 0.44658900  |
| C | -1.67897000 | 2.70402100  | 0.57098900  |
| H | -3.52250900 | 3.76671100  | 0.70287900  |
| H | -2.08272000 | 1.75696100  | 0.90276900  |

# ALLYLATION - wB97X-D/TZV(2d,2p)

File: a\_bp2\_S\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.29873200  | 1.33280800  | -1.99590600 |
| C  | 1.47337200  | 1.86202500  | -0.99252600 |
| C  | 1.92247100  | 2.89507100  | -0.14731600 |
| C  | 3.24224600  | 3.37311100  | -0.31721900 |
| C  | 4.04542500  | 2.84550400  | -1.28404700 |
| C  | 3.56478200  | 1.82674800  | -2.13244900 |
| N  | 0.20347500  | 1.38315300  | -0.79567200 |
| C  | -0.63377300 | 1.91172300  | 0.08796100  |
| C  | -0.21264200 | 2.90587300  | 0.99131100  |
| C  | 1.06643900  | 3.37558700  | 0.85736000  |
| C  | -2.03125400 | 1.41989300  | 0.09704700  |
| N  | -2.22239400 | 0.17207700  | 0.51299000  |
| C  | -3.45771600 | -0.34442800 | 0.79363900  |
| C  | -4.57558400 | 0.47283800  | 0.53367300  |
| C  | -4.37404700 | 1.74386700  | -0.02382100 |
| C  | -3.11488600 | 2.24271700  | -0.24733400 |
| C  | -3.59916200 | -1.63543000 | 1.32550500  |
| C  | -4.85706000 | -2.08952700 | 1.59783900  |
| C  | -5.99571200 | -1.29563300 | 1.33927600  |
| C  | -5.86139800 | -0.04450900 | 0.81692800  |
| O  | -1.14537400 | -0.60170600 | 0.68834500  |
| Si | -0.34002200 | -1.37609400 | -0.79899000 |
| Cl | -0.63799800 | -3.35863300 | 0.16235100  |
| C  | -2.90352300 | 3.57038400  | -0.91561400 |
| C  | -1.12257100 | 3.38691100  | 2.08440300  |
| O  | -0.22231100 | 0.36837400  | -1.54896000 |
| O  | 1.17282000  | -1.03727500 | 0.11922500  |
| C  | 2.11288600  | -1.87814000 | 0.38284300  |
| C  | 3.33601600  | -1.38527500 | 1.05288700  |
| C  | 3.58727500  | -0.02657400 | 1.19464400  |
| C  | 4.72593400  | 0.40306200  | 1.85377300  |
| C  | 5.61968800  | -0.52241000 | 2.37392400  |
| C  | 5.36697400  | -1.88169200 | 2.24275200  |
| C  | 4.22752300  | -2.31235500 | 1.58710400  |
| C  | 0.69423800  | -2.13378400 | -2.32468500 |
| Cl | -2.23754900 | -1.52245600 | -1.93520700 |
| H  | 1.43455200  | 4.12836200  | 1.54146000  |
| H  | -5.23746000 | 2.34454100  | -0.27779400 |
| H  | 1.82101800  | -2.89079900 | 0.64476800  |
| H  | 2.88105800  | 0.68808900  | 0.80500300  |
| H  | 4.02990200  | -3.37181300 | 1.48233000  |
| H  | 4.91303600  | 1.46209900  | 1.96616700  |
| H  | 6.05804500  | -2.60481200 | 2.65273300  |
| H  | 6.51001900  | -0.18549100 | 2.88678100  |
| H  | -0.55500800 | 3.97153300  | 2.80324700  |
| H  | -1.58056000 | 2.54994500  | 2.60928000  |
| H  | -1.92316900 | 4.01747500  | 1.69942800  |
| H  | -2.06563800 | 4.12633700  | -0.50292500 |
| H  | -3.79759800 | 4.18198000  | -0.82898400 |
| H  | -2.70025800 | 3.41375600  | -1.97542600 |
| H  | -6.72585900 | 0.57092200  | 0.61113100  |
| H  | -6.97793500 | -1.69026200 | 1.55603000  |
| H  | -4.98438400 | -3.07755100 | 2.01662100  |
| H  | -2.72272400 | -2.23854600 | 1.49885200  |
| H  | 3.59774400  | 4.15671500  | 0.33676300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.05408900  | 3.21118300  | -1.41027400 |
| H | 4.20936200  | 1.43046500  | -2.90401000 |
| H | 1.91897400  | 0.56560800  | -2.64844100 |
| H | -0.01818000 | -2.77282700 | -2.83489700 |
| C | 1.84509000  | -2.87432400 | -1.87189100 |
| H | 0.94847300  | -1.27795200 | -2.94340200 |
| C | 3.01645100  | -2.31361700 | -1.45671000 |
| H | 1.71594000  | -3.93817300 | -1.70762500 |
| H | 3.84212600  | -2.94556800 | -1.16510400 |
| H | 3.25312900  | -1.28567500 | -1.69751500 |

File: a\_bp2\_R\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.19535600 | -2.31361100 | 0.67834000  |
| C  | -3.28491200 | -0.92021400 | 0.53845200  |
| C  | -4.52901200 | -0.26216900 | 0.47460400  |
| C  | -5.70351200 | -1.04699000 | 0.54878300  |
| C  | -5.61434700 | -2.39922200 | 0.69236900  |
| C  | -4.35403800 | -3.03070400 | 0.76096900  |
| N  | -2.15994200 | -0.14404200 | 0.46344000  |
| C  | -2.19208000 | 1.18196700  | 0.41746700  |
| C  | -3.40364900 | 1.87627400  | 0.28235900  |
| C  | -4.55581700 | 1.13158300  | 0.30849800  |
| O  | -0.96280700 | -0.74033900 | 0.47788900  |
| Si | -0.02017500 | -0.92649200 | -1.09975800 |
| Cl | 0.11743800  | -3.10427200 | -0.64315300 |
| C  | -0.89635700 | 1.88746700  | 0.55200000  |
| C  | -0.57660100 | 2.63036600  | 1.70320300  |
| C  | 0.60621100  | 3.32141500  | 1.69486600  |
| C  | 1.44756500  | 3.32109800  | 0.56895500  |
| C  | 1.09971000  | 2.53221200  | -0.54351800 |
| N  | -0.04874600 | 1.78943700  | -0.46354900 |
| C  | 1.88997300  | 2.51450800  | -1.70288500 |
| C  | 3.03058000  | 3.26645700  | -1.72850500 |
| C  | 3.42117200  | 4.03595200  | -0.61319800 |
| C  | 2.64688200  | 4.06713900  | 0.50911100  |
| C  | -3.41355400 | 3.35819300  | 0.04360900  |
| C  | -1.46581800 | 2.58963400  | 2.91194600  |
| O  | -0.33672500 | 0.93284500  | -1.44555600 |
| O  | 1.35844100  | -0.45150700 | -0.04838400 |
| C  | 2.64551700  | -0.42701200 | -0.03625600 |
| C  | 3.41318800  | -1.36280800 | 0.81346600  |
| C  | 2.80268000  | -2.43215600 | 1.45878400  |
| C  | 3.54879900  | -3.25106200 | 2.29102900  |
| C  | 4.89932800  | -3.00415500 | 2.48881300  |
| C  | 5.50826900  | -1.92536100 | 1.85992300  |
| C  | 4.76652500  | -1.10686100 | 1.02874200  |
| C  | 1.16732000  | -1.12138200 | -2.68482200 |
| Cl | -1.83003500 | -1.20497300 | -2.34258000 |
| H  | 0.90341300  | 3.88482500  | 2.56916100  |
| H  | -5.51225500 | 1.62515100  | 0.19812400  |
| H  | 3.08575900  | 0.56774100  | -0.10750800 |
| H  | 1.75009100  | -2.61539700 | 1.30653700  |
| H  | 5.23996300  | -0.26244500 | 0.54291900  |
| H  | 3.07236900  | -4.08432000 | 2.78885800  |
| H  | 6.55798100  | -1.72382000 | 2.02114700  |
| H  | 5.47845400  | -3.64666900 | 3.13781200  |
| H  | -0.99160400 | 3.11241000  | 3.73811800  |
| H  | -1.64814000 | 1.56060200  | 3.22020300  |

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|---|-------------|--------------|-------------|
| H | -2.43246800 | 3.05677500   | 2.73061200  |
| H | -4.43525400 | 3.70949600   | -0.07180900 |
| H | -2.86586000 | 3.59776900   | -0.86772500 |
| H | -2.95633600 | 3.91549800   | 0.85913900  |
| H | 2.93017700  | 4.66429700   | 1.36428700  |
| H | 4.33505900  | 4.61041200   | -0.65779200 |
| H | 3.64108900  | 3.27424400   | -2.62038300 |
| H | 1.57250100  | 1.93514100   | -2.55378500 |
| H | -6.66315300 | -0.55331700  | 0.49087800  |
| H | -6.51241100 | -2.99711000  | 0.75244200  |
| H | -4.30394200 | -4.10400000  | 0.87663600  |
| H | -2.22671500 | -2.78640000  | 0.70824400  |
| H | 0.64814400  | -1.88757200  | -3.25121700 |
| C | 2.48197400  | -1.53707500  | -2.29105100 |
| H | 1.14294100  | -0.16408000  | -3.19867700 |
| C | 3.48465200  | -0.676116200 | -1.96311400 |
| H | 2.63129200  | -2.59227300  | -2.09101300 |
| H | 4.46012800  | -1.05394000  | -1.69729400 |
| H | 3.43319300  | 0.35536500   | -2.28231900 |

File: a\_bp3\_S\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.12333100 | -0.55237700 | 1.24217100  |
| C  | -5.78086000 | 0.68015700  | 0.77283500  |
| C  | -4.42715500 | 0.98622000  | 0.49933800  |
| C  | -3.46074000 | -0.01500800 | 0.71629200  |
| C  | -3.81891900 | -1.28514300 | 1.19439100  |
| C  | -5.13458500 | -1.53664900 | 1.45512300  |
| N  | -2.15397400 | 0.29802100  | 0.45047800  |
| C  | -1.76333000 | 1.50832100  | 0.06697800  |
| C  | -2.69509500 | 2.51574500  | -0.22862600 |
| C  | -4.01763900 | 2.23057600  | -0.00542500 |
| O  | -1.22952900 | -0.65071900 | 0.60312700  |
| Si | -0.43974100 | -1.48937900 | -0.91910000 |
| Cl | 0.61215900  | -2.34669000 | -2.66443400 |
| C  | -0.30409100 | 1.75239500  | -0.00875600 |
| C  | 0.35561000  | 2.59349000  | 0.90246200  |
| C  | 1.69217600  | 2.81901000  | 0.69012800  |
| C  | 2.37079600  | 2.25260200  | -0.40079300 |
| C  | 1.67585800  | 1.37856400  | -1.26041100 |
| N  | 0.35655000  | 1.13594800  | -0.98134300 |
| C  | 2.31142500  | 0.75680500  | -2.34494300 |
| C  | 3.63338200  | 1.02111000  | -2.55982300 |
| C  | 4.35619200  | 1.88470800  | -1.77092800 |
| C  | 3.74216000  | 2.48756500  | -0.65318100 |
| C  | -2.25236000 | 3.81415500  | -0.83789000 |
| C  | -0.36881200 | 3.14635200  | 2.09550100  |
| O  | -0.30667300 | 0.21367400  | -1.69435000 |
| O  | 1.16009400  | -1.18462200 | -0.15272100 |
| C  | 1.46606500  | -1.12760700 | 1.08860300  |
| C  | 2.89152800  | -0.96252200 | 1.41765800  |
| C  | 3.86892600  | -1.18328000 | 0.45148700  |
| C  | 5.19560800  | -0.93232400 | 0.74922500  |
| C  | 5.55061100  | -0.46240500 | 2.00740200  |
| C  | 4.57676900  | -0.24386800 | 2.97214900  |
| C  | 3.24733400  | -0.49398600 | 2.67864100  |
| C  | -0.57688200 | -3.21436000 | 0.07171400  |
| Cl | -2.38620400 | -1.64710600 | -1.92563700 |
| H  | 2.24570600  | 3.44241600  | 1.37956100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.76865100 | 2.97712800  | -0.22595700 |
| H | 0.75707400  | -0.68389800 | 1.78248800  |
| H | 3.57875700  | -1.53452800 | -0.52874600 |
| H | 2.48316400  | -0.31985300 | 3.42540000  |
| H | 5.95550300  | -1.09574800 | -0.00204400 |
| H | 4.85319500  | 0.12549600  | 3.94977300  |
| H | 6.58916600  | -0.26447400 | 2.23449000  |
| H | 0.33440300  | 3.64132500  | 2.75971700  |
| H | -0.86029000 | 2.34838900  | 2.65163600  |
| H | -1.13097300 | 3.87170100  | 1.81537800  |
| H | -3.11560000 | 4.44489800  | -1.03158000 |
| H | -1.74464200 | 3.63362400  | -1.78507600 |
| H | -1.56886200 | 4.36796600  | -0.19699400 |
| H | 4.28701000  | 3.14823100  | 0.00615900  |
| H | 5.40447000  | 2.06360400  | -1.90061100 |
| H | 4.13644300  | 0.55449100  | -3.39471100 |
| H | 1.75343900  | 0.08057900  | -2.97187700 |
| H | -3.05941600 | -2.03337500 | 1.34412900  |
| H | -5.42477600 | -2.50831000 | 1.82868300  |
| H | -6.52991500 | 1.44060200  | 0.60273400  |
| H | -7.15783200 | -0.78333400 | 1.45138100  |
| H | -1.63102600 | -3.47162700 | 0.02084500  |
| C | -0.10347200 | -3.08668500 | 1.43178400  |
| H | 0.01749000  | -3.90909300 | -0.51453800 |
| C | 1.20717600  | -3.14278600 | 1.79407000  |
| H | -0.81998300 | -2.78578100 | 2.18863400  |
| H | 1.49110700  | -3.05121600 | 2.83285300  |
| H | 1.94493000  | -3.55046800 | 1.11544500  |

File: a\_bp3\_R\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.59981800  | -1.27048600 | 0.86209300  |
| C  | 3.26176800  | -0.95825100 | 1.07502700  |
| C  | 2.91053600  | 0.02135500  | 1.99986800  |
| C  | 3.89727700  | 0.68426900  | 2.70566100  |
| C  | 5.23471400  | 0.37522500  | 2.48911000  |
| C  | 5.58583100  | -0.60135800 | 1.56814400  |
| C  | 2.23342100  | -1.60723600 | 0.24187700  |
| O  | 1.11288500  | -0.99988500 | 0.13409900  |
| Si | -0.39896100 | -1.52950600 | -0.67669100 |
| Cl | -2.33647800 | -1.90524400 | -1.64206900 |
| O  | -1.22037900 | -0.55752300 | 0.73200300  |
| N  | -2.22189700 | 0.28516200  | 0.47127000  |
| C  | -3.49520600 | -0.09519200 | 0.79564400  |
| C  | -4.54347400 | 0.79132500  | 0.47758400  |
| C  | -4.24076600 | 1.99654600  | -0.16649500 |
| C  | -2.94509400 | 2.36462500  | -0.43723400 |
| C  | -1.93183600 | 1.47442900  | -0.05750700 |
| C  | -5.86802000 | 0.41186100  | 0.80481000  |
| C  | -6.10617800 | -0.77848100 | 1.42080200  |
| C  | -5.03701400 | -1.64610100 | 1.73637000  |
| C  | -3.74785600 | -1.32381200 | 1.42858700  |
| C  | -0.49409900 | 1.81944800  | -0.16491700 |
| C  | 0.08028200  | 2.84017400  | 0.61229200  |
| C  | 1.41254500  | 3.10206000  | 0.42015300  |
| C  | 2.17002100  | 2.40670000  | -0.53452200 |
| C  | 1.55242500  | 1.38967000  | -1.28649600 |
| N  | 0.23603400  | 1.11678900  | -1.02246600 |
| C  | 2.26663400  | 0.65005400  | -2.24136400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.59310600  | 0.92139200  | -2.41549200 |
| C  | 4.24168300  | 1.92269800  | -1.66127500 |
| C  | 3.54668900  | 2.65364700  | -0.74539600 |
| C  | -2.65339100 | 3.65214000  | -1.15435700 |
| C  | -0.72907100 | 3.57354700  | 1.64110100  |
| O  | -0.34708300 | 0.07539100  | -1.63501600 |
| Cl | 0.68642900  | -2.52452800 | -2.34836600 |
| C  | -0.42712600 | -3.15368600 | 0.47132500  |
| C  | 0.89531400  | -3.71958900 | 0.61965500  |
| H  | 1.21796600  | -4.44011100 | -0.12281000 |
| H  | 1.89887000  | 3.85796400  | 1.02242500  |
| H  | -5.05036900 | 2.65475600  | -0.45363900 |
| H  | 2.59098100  | -2.19013600 | -0.60259100 |
| H  | 1.86701800  | 0.26042400  | 2.15115300  |
| H  | 4.86738600  | -2.02708600 | 0.13580300  |
| H  | 3.62692200  | 1.44578700  | 3.42387500  |
| H  | 6.62684700  | -0.83617800 | 1.39650900  |
| H  | 6.00492700  | 0.89880800  | 3.03878000  |
| H  | -1.10890200 | -3.83046000 | -0.03546000 |
| H  | -1.41353900 | 4.28225700  | 1.17638700  |
| H  | -0.06998500 | 4.13300600  | 2.29958100  |
| H  | -1.31829400 | 2.88726700  | 2.24746000  |
| H  | -3.14025100 | 3.63853000  | -2.12841400 |
| H  | -1.59185000 | 3.81412700  | -1.31808200 |
| H  | -3.05109400 | 4.49910400  | -0.59726400 |
| H  | 4.03067200  | 3.42563800  | -0.16396500 |
| H  | 5.29486000  | 2.10676300  | -1.81642400 |
| H  | 1.76615200  | -0.12689800 | -2.79636200 |
| H  | 4.15795400  | 0.35591100  | -3.14291200 |
| H  | -6.67558200 | 1.08598000  | 0.55648600  |
| H  | -7.11704200 | -1.06672300 | 1.67091500  |
| H  | -5.24418800 | -2.58651000 | 2.22678500  |
| H  | -2.93091000 | -1.98633900 | 1.65729700  |
| C  | 1.81658600  | -3.27518100 | 1.51742500  |
| H  | -0.83815000 | -2.82003000 | 1.42063900  |
| H  | 2.78469500  | -3.7500     | 1.58955700  |
| H  | 1.51175700  | -2.65491000 | 2.35020000  |

File: a\_bp4\_S\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.08950900 | 1.78905200  | 0.85449000  |
| C  | -1.66195700 | 1.55232500  | -0.03780300 |
| C  | -0.96342600 | 0.93355200  | -1.13450600 |
| Si | -0.84547200 | -0.97289400 | -0.72401500 |
| O  | -2.61234100 | -0.98395600 | -0.47911000 |
| C  | -3.22725500 | -0.29964100 | 0.44524100  |
| C  | -4.70990500 | -0.36650800 | 0.44518200  |
| C  | -5.39051900 | -0.10387300 | 1.62857700  |
| C  | -6.77184800 | -0.19710600 | 1.66789200  |
| C  | -7.47363700 | -0.54883500 | 0.52409100  |
| C  | -6.79325900 | -0.80958800 | -0.65877400 |
| C  | -5.41311000 | -0.71785000 | -0.70206900 |
| O  | 0.99608300  | -0.97362700 | -1.10458700 |
| N  | 1.98347900  | -1.21055500 | -0.22061800 |
| C  | 2.60424900  | -0.17704300 | 0.34462500  |
| C  | 3.62895200  | -0.37558700 | 1.28810400  |
| C  | 3.97617800  | -1.66342800 | 1.59191500  |
| C  | 3.36978900  | -2.75505900 | 0.94937600  |
| C  | 2.35853500  | -2.51663600 | -0.00038700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.74745900  | -4.09192700 | 1.20988200  |
| C  | 3.15239400  | -5.11855400 | 0.53894100  |
| C  | 2.16197100  | -4.85342000 | -0.42726100 |
| C  | 1.76085700  | -3.57566000 | -0.69939900 |
| C  | 2.28444700  | 1.18629900  | -0.13304800 |
| N  | 1.57844400  | 1.94973500  | 0.70521300  |
| C  | 1.31875600  | 3.27828300  | 0.38756400  |
| C  | 1.79043000  | 3.79396500  | -0.83174000 |
| C  | 2.52756600  | 2.96174900  | -1.69933000 |
| C  | 2.78524000  | 1.66471000  | -1.36342700 |
| C  | 0.58078700  | 4.06902400  | 1.28197900  |
| C  | 0.31885600  | 5.36970100  | 0.95331500  |
| C  | 0.78209900  | 5.91124000  | -0.26218400 |
| C  | 1.50080100  | 5.14406700  | -1.13311100 |
| O  | 1.11414000  | 1.45564800  | 1.79524100  |
| C  | 3.57519000  | 0.74809200  | -2.24923400 |
| C  | 4.29741800  | 0.80796200  | 1.91886200  |
| Cl | -1.11123400 | -2.23127600 | -2.36975300 |
| Cl | -0.52015400 | -1.69635500 | 1.22015200  |
| H  | -2.78321000 | -0.29810000 | 1.43844200  |
| H  | 0.05129800  | 1.28438100  | -1.27037400 |
| C  | -3.03022000 | 1.62121400  | 0.01439700  |
| H  | -1.51529800 | 0.96554100  | -2.07230700 |
| H  | 2.89530800  | 3.36483700  | -2.63281100 |
| H  | 4.74967300  | -1.85315000 | 2.32412200  |
| H  | -4.87690100 | -0.92662800 | -1.61733000 |
| H  | -4.83930100 | 0.16471500  | 2.52089700  |
| H  | -7.34080300 | -1.08844900 | -1.54834200 |
| H  | -7.29817700 | -0.00113600 | 2.59151400  |
| H  | -8.55181900 | -0.62584300 | 0.55487800  |
| H  | 3.94801900  | 1.28897300  | -3.11489500 |
| H  | 2.95550600  | -0.07688500 | -2.60172500 |
| H  | 4.42849200  | 0.32322700  | -1.71954600 |
| H  | 5.11093000  | 0.48481400  | 2.56278800  |
| H  | 3.58125700  | 1.37039600  | 2.51815500  |
| H  | 4.70382900  | 1.47930100  | 1.16235700  |
| H  | 1.86190900  | 5.55616600  | -2.06528200 |
| H  | 0.56789800  | 6.94339400  | -0.50081000 |
| H  | -0.24822400 | 5.99010800  | 1.63253400  |
| H  | 0.24149800  | 3.63418300  | 2.20842800  |
| H  | 4.51690600  | -4.27825700 | 1.94584900  |
| H  | 3.44221900  | -6.14004900 | 0.73876700  |
| H  | 1.70961900  | -5.67476500 | -0.96450200 |
| H  | 1.00857900  | -3.37462500 | -1.44320800 |
| H  | -3.50486800 | 2.10442300  | 0.85630700  |
| H  | -3.59218500 | 1.59703200  | -0.90950300 |

File: a\_bp4\_R\_wb97xd\_tzv2d2p.xyz

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 1.97058000  | 2.40358300 | -0.48631300 |
| C | 0.64183300  | 2.65383600 | -0.11008700 |
| C | 0.25053100  | 3.88423200 | 0.44865700  |
| C | 1.24041400  | 4.87926700 | 0.62119000  |
| C | 2.53025000  | 4.63656600 | 0.25077400  |
| C | 2.89479000  | 3.39258800 | -0.30705000 |
| N | -0.31880700 | 1.68691900 | -0.26010400 |
| C | -1.60072900 | 1.89043200 | 0.02056000  |
| C | -2.02613400 | 3.07609400 | 0.64814200  |
| C | -1.08600600 | 4.05382500 | 0.84825800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.55993600 | 0.83440700  | -0.38502200 |
| N  | -2.50207200 | -0.32658000 | 0.25911100  |
| C  | -3.43698300 | -1.31553900 | 0.11004400  |
| C  | -4.45633400 | -1.10612800 | -0.83885000 |
| C  | -4.44547000 | 0.07237000  | -1.60042200 |
| C  | -3.51313200 | 1.05692800  | -1.39248900 |
| C  | -3.37637300 | -2.49002600 | 0.87621600  |
| C  | -4.34409400 | -3.43495700 | 0.69093100  |
| C  | -5.37525100 | -3.25238800 | -0.25566900 |
| C  | -5.43093000 | -2.11694400 | -1.00705600 |
| O  | -1.48911300 | -0.52346100 | 1.10996300  |
| Si | 0.19444400  | -0.98253500 | 0.44011700  |
| Cl | 0.20627300  | -2.85460800 | 1.65283200  |
| C  | -3.4553900  | 2.28703200  | -2.25199700 |
| C  | -3.43451600 | 3.21589300  | 1.14840700  |
| O  | 0.04617200  | 0.50021300  | -0.74134500 |
| O  | 1.83809600  | -1.16586700 | -0.21446800 |
| C  | 2.88894900  | -1.62500800 | 0.37240700  |
| C  | 4.16995300  | -1.50844400 | -0.36319300 |
| C  | 4.25619900  | -0.74429200 | -1.52211900 |
| C  | 5.45736600  | -0.66101700 | -2.20569400 |
| C  | 6.57373800  | -1.34065200 | -1.73847900 |
| C  | 6.48555600  | -2.11626500 | -0.59019600 |
| C  | 5.28607600  | -2.20209000 | 0.09464500  |
| C  | 0.90188000  | 0.05871500  | 2.00451700  |
| Cl | -0.60171500 | -2.09825900 | -1.28266300 |
| H  | -1.37191100 | 4.97753100  | 1.33306700  |
| H  | -5.19310200 | 0.20107600  | -2.37158500 |
| H  | 2.77920000  | -2.50807100 | 0.99678400  |
| H  | 3.37781400  | -0.24154000 | -1.89993000 |
| H  | 5.21476200  | -2.80553000 | 0.99078300  |
| H  | 5.52062100  | -0.07300000 | -3.11086500 |
| H  | 7.35096700  | -2.65516200 | -0.23068600 |
| H  | 7.51124500  | -1.27285700 | -2.27305400 |
| H  | -4.23317000 | 2.24502900  | -3.00944300 |
| H  | -2.49210300 | 2.35176000  | -2.75750900 |
| H  | -3.59079600 | 3.20566100  | -1.68395000 |
| H  | -3.56214600 | 4.18022500  | 1.63246800  |
| H  | -3.65476200 | 2.43601300  | 1.87725700  |
| H  | -4.17309300 | 3.13877100  | 0.35306700  |
| H  | -6.21224500 | -1.96935100 | -1.73932200 |
| H  | -6.12211400 | -4.02291200 | -0.38235600 |
| H  | -4.31619000 | -4.34364800 | 1.27524100  |
| H  | -2.57348100 | -2.62590900 | 1.58277700  |
| H  | 0.95511600  | 5.82723300  | 1.05490700  |
| H  | 3.28397200  | 5.39906700  | 0.38418400  |
| H  | 3.92208100  | 3.21863600  | -0.59431600 |
| H  | 2.22668500  | 1.44494900  | -0.90705700 |
| H  | 0.11161500  | -0.02102400 | 2.74461600  |
| H  | 1.03102000  | 1.08938700  | 1.69146000  |
| C  | 2.13953300  | -0.50732100 | 2.47044400  |
| C  | 3.35003500  | -0.27770900 | 1.88249700  |
| H  | 2.08658800  | -1.27967100 | 3.22833000  |
| H  | 4.24498100  | -0.70751000 | 2.30785700  |
| H  | 3.48503000  | 0.57368400  | 1.22821300  |

File: a\_bp5\_S\_wb97xd\_tzv2d2p.xyz

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.96260400 | -2.79259600 | -0.93773000 |
|---|------------|-------------|-------------|

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.14777400  | -1.69544200 | -0.08024700 |
| C  | 4.09876700  | -1.72271700 | 0.95762400  |
| C  | 4.86893700  | -2.89707400 | 1.12722000  |
| C  | 4.68839400  | -3.96029400 | 0.29389700  |
| C  | 3.73288000  | -3.90309200 | -0.74319400 |
| N  | 2.39463600  | -0.55880000 | -0.22488900 |
| C  | 2.59278700  | 0.54161900  | 0.49740300  |
| C  | 3.49960800  | 0.54348500  | 1.57187000  |
| C  | 4.22682600  | -0.59966100 | 1.78846200  |
| C  | 1.84846100  | 1.76682000  | 0.11319100  |
| N  | 0.52490800  | 1.74377500  | 0.26496200  |
| C  | -0.26761700 | 2.84685900  | 0.12127300  |
| C  | 0.35299700  | 4.05162300  | -0.26236200 |
| C  | 1.72979500  | 4.05034100  | -0.51552000 |
| C  | 2.49878600  | 2.92508600  | -0.33514000 |
| C  | -1.65264200 | 2.77335000  | 0.34428400  |
| C  | -2.39451200 | 3.90835700  | 0.20032800  |
| C  | -1.79644900 | 5.13231400  | -0.17592000 |
| C  | -0.45663800 | 5.20467600  | -0.40744000 |
| O  | -0.04978700 | 0.58612600  | 0.59966300  |
| Si | -0.34359300 | -0.72413200 | -0.71364700 |
| Cl | -0.54077600 | -2.35044700 | -2.22136800 |
| C  | 3.96675700  | 2.94851300  | -0.65429100 |
| C  | 3.65018200  | 1.74592800  | 2.45733500  |
| O  | 1.46285900  | -0.53985100 | -1.18277600 |
| O  | -2.07202400 | -0.63725500 | -0.26951600 |
| C  | -2.91633200 | -1.60704900 | -0.19911300 |
| C  | -4.26694400 | -1.29891500 | 0.32238200  |
| C  | -4.48577100 | -0.22696900 | 1.18231700  |
| C  | -5.76517000 | 0.04888900  | 1.62868700  |
| C  | -6.83197000 | -0.74305800 | 1.22048800  |
| C  | -6.61584600 | -1.81157000 | 0.36317100  |
| C  | -5.33438000 | -2.09139100 | -0.08361700 |
| C  | -0.04717700 | -2.04859300 | 0.76914900  |
| Cl | -0.72067800 | 0.78048000  | -2.28131300 |
| H  | 4.92528000  | -0.63866700 | 2.61381000  |
| H  | 2.19862100  | 4.96147100  | -0.86377600 |
| H  | -2.87606500 | -2.37217800 | -0.97009500 |
| H  | -3.65153100 | 0.37971900  | 1.50528900  |
| H  | -5.16211300 | -2.92258900 | -0.75530800 |
| H  | -5.93405700 | 0.88037600  | 2.29898500  |
| H  | -7.44440900 | -2.42659600 | 0.04083600  |
| H  | -7.83131100 | -0.52590000 | 1.57197200  |
| H  | 2.69575700  | 2.23609000  | 2.63696100  |
| H  | 4.32785200  | 2.47642200  | 2.01658300  |
| H  | 4.06709800  | 1.44596900  | 3.41525400  |
| H  | 4.43684300  | 1.97527100  | -0.54556100 |
| H  | 4.48874600  | 3.65856300  | -0.01434800 |
| H  | 4.10460800  | 3.26904800  | -1.68576700 |
| H  | 0.01042400  | 6.13278200  | -0.70519900 |
| H  | -2.41313200 | 6.01275300  | -0.28563000 |
| H  | -3.46148300 | 3.86864600  | 0.36774400  |
| H  | -2.09682800 | 1.82655700  | 0.60143700  |
| H  | 5.59987300  | -2.92775900 | 1.92279000  |
| H  | 5.27761100  | -4.85669100 | 0.42314900  |
| H  | 3.60845400  | -4.75422400 | -1.39740500 |
| H  | 2.22077300  | -2.73992000 | -1.71898700 |
| H  | 0.89805800  | -2.53565400 | 0.55224100  |
| C  | -1.11627100 | -3.01125200 | 0.80214400  |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | 0.01474500  | -1.45994400 | 1.68012800 |
| C | -2.31933400 | -2.78599300 | 1.40457100 |
| H | -1.01628800 | -3.89659800 | 0.18582700 |
| H | -3.07437300 | -3.55866000 | 1.41582900 |
| H | -2.41434500 | -2.00114800 | 2.14309300 |

File: a\_bp5\_R\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.63172000 | 2.86002300  | 0.25049500  |
| C  | -0.23709300 | 2.86052000  | 0.08414300  |
| C  | 0.44728600  | 4.04149100  | -0.26914500 |
| C  | -0.30170300 | 5.23029400  | -0.44571700 |
| C  | -1.65115200 | 5.22246800  | -0.26973700 |
| C  | -2.31605200 | 4.02703000  | 0.08012300  |
| N  | 0.50440100  | 1.72256000  | 0.25380900  |
| C  | 1.83485300  | 1.70186900  | 0.15395600  |
| C  | 2.54736700  | 2.83727600  | -0.25676800 |
| C  | 1.83116900  | 3.99070500  | -0.46411300 |
| O  | -0.12198200 | 0.57916300  | 0.55544200  |
| Si | -0.37200800 | -0.74887500 | -0.78110500 |
| Cl | -0.53273600 | -2.35165200 | -2.30395700 |
| C  | 2.54094600  | 0.44856800  | 0.51706500  |
| C  | 3.42283500  | 0.38339900  | 1.60966700  |
| C  | 4.14987100  | -0.77022500 | 1.76633300  |
| C  | 4.03600200  | -1.84237000 | 0.86810900  |
| C  | 3.09696500  | -1.75547400 | -0.17794000 |
| N  | 2.35883700  | -0.60432200 | -0.27464500 |
| C  | 2.90023100  | -2.81014600 | -1.08293700 |
| C  | 3.66044100  | -3.93516000 | -0.93820400 |
| C  | 4.61380600  | -4.04769100 | 0.09628000  |
| C  | 4.79728600  | -3.02877400 | 0.98320500  |
| C  | 4.02812900  | 2.81218300  | -0.51145500 |
| C  | 3.54878200  | 1.52804500  | 2.57221600  |
| O  | 1.43274600  | -0.52698600 | -1.23273700 |
| O  | -2.12588700 | -0.81878300 | -0.45421400 |
| C  | -2.77062800 | -0.66781300 | 0.64516200  |
| C  | -4.21359200 | -0.98919600 | 0.62831000  |
| C  | -4.74264100 | -1.81570700 | -0.35828200 |
| C  | -6.09974000 | -2.08174100 | -0.37468600 |
| C  | -6.93187000 | -1.52389500 | 0.58823500  |
| C  | -6.40524000 | -0.69539600 | 1.56892000  |
| C  | -5.04601800 | -0.43003600 | 1.59164400  |
| C  | -0.06825900 | -2.08103400 | 0.69847800  |
| Cl | -0.76161200 | 0.78060000  | -2.31744100 |
| H  | 4.83483300  | -0.85897400 | 2.59912200  |
| H  | 2.34716100  | 4.88443000  | -0.78972100 |
| H  | -2.47395900 | 0.12990100  | 1.32149500  |
| H  | -4.08675000 | -2.23787600 | -1.10691800 |
| H  | -4.63035000 | 0.21559500  | 2.35508700  |
| H  | -6.51197700 | -2.72411500 | -1.14036600 |
| H  | -7.05354900 | -0.25636100 | 2.31430100  |
| H  | -7.99297200 | -1.73159300 | 0.57032700  |
| H  | 3.94308300  | 1.16859800  | 3.51930500  |
| H  | 2.58796700  | 2.00356700  | 2.75883300  |
| H  | 4.23526400  | 2.28576400  | 2.19619900  |
| H  | 4.44139500  | 1.80773200  | -0.50666400 |
| H  | 4.55738700  | 3.40787800  | 0.23139800  |
| H  | 4.22897000  | 3.25043300  | -1.48728100 |
| H  | 5.52150500  | -3.10608700 | 1.78179600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.19636200  | -4.95345900 | 0.18401100  |
| H | 3.52936800  | -4.75437800 | -1.63070300 |
| H | 2.15807300  | -2.71576100 | -1.85994100 |
| H | 0.22071700  | 6.13575600  | -0.72040400 |
| H | -2.22127500 | 6.13041100  | -0.40301500 |
| H | -3.38903700 | 4.03407800  | 0.20822000  |
| H | -2.14153400 | 1.94622900  | 0.49350600  |
| H | 0.97654800  | -2.01700000 | 0.98063900  |
| H | -0.28127000 | -3.04254800 | 0.24348100  |
| C | -0.90952400 | -1.80363000 | 1.83292700  |
| C | -2.20047900 | -2.22781500 | 1.93098500  |
| H | -0.54619500 | -1.09844700 | 2.57233100  |
| H | -2.78308100 | -2.00657100 | 2.81360700  |
| H | -2.55789900 | -3.02650700 | 1.29489800  |

File: a\_bp1\_S\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.00439700  | -2.92118200 | 0.87826000  |
| C  | 4.21827200  | -1.74954000 | 0.75656000  |
| C  | 3.16734800  | -1.74460000 | -0.18134500 |
| C  | 2.90275800  | -2.86480700 | -0.98700400 |
| C  | 3.68969700  | -3.96943600 | -0.84480600 |
| C  | 4.74425400  | -4.00357100 | 0.09456100  |
| N  | 2.41434900  | -0.60876200 | -0.28328000 |
| C  | 2.67050000  | 0.50563600  | 0.40248300  |
| C  | 3.67298000  | 0.52819500  | 1.38335900  |
| C  | 4.42484400  | -0.61128100 | 1.54403500  |
| O  | 1.39152100  | -0.60742900 | -1.14450300 |
| Si | -0.35074900 | -0.75623800 | -0.50700500 |
| Cl | -0.84460500 | 0.77887600  | -2.09615100 |
| C  | 1.88141500  | 1.71709400  | 0.06537000  |
| C  | 2.48080800  | 2.86425400  | -0.47968300 |
| C  | 1.69361500  | 3.97990200  | -0.62139300 |
| C  | 0.34830200  | 3.99014300  | -0.22373500 |
| C  | -0.22411700 | 2.80060500  | 0.26437200  |
| N  | 0.58120900  | 1.69798800  | 0.34297400  |
| C  | -1.57245400 | 2.73746000  | 0.65196900  |
| C  | -2.32782000 | 3.86955500  | 0.55470500  |
| C  | -1.78094900 | 5.07553800  | 0.06360500  |
| C  | -0.47484700 | 5.13730100  | -0.31906200 |
| C  | 3.90773500  | 1.72043100  | 2.26727300  |
| C  | 3.91866500  | 2.85587900  | -0.91026900 |
| O  | 0.03912300  | 0.54634500  | 0.74892300  |
| O  | -2.00974600 | -0.75070300 | 0.13403000  |
| C  | -3.12261200 | -0.74292600 | -0.51214200 |
| C  | -4.35341800 | -0.99453000 | 0.26646700  |
| C  | -4.30007600 | -1.63019800 | 1.50338200  |
| C  | -5.46499400 | -1.82756000 | 2.22317900  |
| C  | -6.68212100 | -1.39115000 | 1.71432400  |
| C  | -6.73496300 | -0.75285000 | 0.48339900  |
| C  | -5.57157200 | -0.55564500 | -0.24129100 |
| C  | -0.72502200 | -2.23241100 | -1.78455600 |
| Cl | 0.22694400  | -2.16349600 | 1.13693100  |
| H  | 2.11885800  | 4.87914500  | -1.04707100 |
| H  | 5.19921500  | -0.63196700 | 2.29970800  |
| H  | -3.22227000 | -0.05894800 | -1.35132800 |
| H  | -3.34758700 | -1.96267800 | 1.89244500  |
| H  | -5.60727100 | -0.05916600 | -1.20254800 |
| H  | -5.42568500 | -2.32112100 | 3.18426400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -7.68031000 | -0.40741100 | 0.08886700  |
| H | -7.59107600 | -1.54790000 | 2.27881600  |
| H | 4.09415100  | 3.66266100  | -1.61736200 |
| H | 4.18570800  | 1.91799300  | -1.39362800 |
| H | 4.58866200  | 3.00386000  | -0.06417300 |
| H | 3.90067300  | 1.40215900  | 3.30833300  |
| H | 3.14831400  | 2.48832300  | 2.15017800  |
| H | 4.88186400  | 2.16431100  | 2.06599100  |
| H | -1.97954800 | 1.80825100  | 1.01580900  |
| H | -3.36578400 | 3.84157600  | 0.85450900  |
| H | -0.04660800 | 6.05358600  | -0.70005600 |
| H | -2.40807100 | 5.95265600  | -0.00667700 |
| H | 2.09601600  | -2.83479100 | -1.69928100 |
| H | 3.50041400  | -4.83739100 | -1.46019200 |
| H | 5.34366700  | -4.89776200 | 0.18676000  |
| H | 5.80655400  | -2.93353000 | 1.60238000  |
| H | 0.02057200  | -2.11065300 | -2.56578000 |
| C | -2.06676800 | -2.13296800 | -2.30349300 |
| H | -0.56103100 | -3.14138700 | -1.21345200 |
| C | -3.17791200 | -2.52600700 | -1.61799200 |
| H | -2.21159300 | -1.58050200 | -3.22451100 |
| H | -4.15146400 | -2.45602200 | -2.08102200 |
| H | -3.08740900 | -3.18570200 | -0.76484600 |

File: a\_bp1\_R\_wb97xd\_tzv2d2p\_.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.72618900 | 2.65783800  | 0.59216400  |
| C  | -0.37684700 | 2.78741400  | 0.22679300  |
| C  | 0.15117100  | 4.00716200  | -0.23713600 |
| C  | -0.71783500 | 5.12053700  | -0.32049900 |
| C  | -2.02450800 | 4.99649300  | 0.04575500  |
| C  | -2.52730600 | 3.75916400  | 0.50463500  |
| N  | 0.47819200  | 1.72347600  | 0.30551900  |
| C  | 1.77502900  | 1.80105100  | 0.03505700  |
| C  | 2.32974600  | 2.97270900  | -0.50430600 |
| C  | 1.49822300  | 4.05776700  | -0.62931600 |
| C  | 2.60529700  | 0.62441000  | 0.39050000  |
| N  | 2.44468900  | -0.49227300 | -0.31166700 |
| C  | 3.27890200  | -1.57352600 | -0.19174300 |
| C  | 4.27270600  | -1.52261600 | 0.80453500  |
| C  | 4.35291400  | -0.39035200 | 1.63002100  |
| C  | 3.54150300  | 0.69700900  | 1.43700400  |
| C  | 3.15529200  | -2.68358100 | -1.04103900 |
| C  | 4.01925000  | -3.72834500 | -0.88129400 |
| C  | 5.01079400  | -3.71022500 | 0.12205600  |
| C  | 5.13650100  | -2.63312700 | 0.94713800  |
| O  | 1.43968400  | -0.55384300 | -1.19251200 |
| Si | -0.31634800 | -0.76854500 | -0.57099200 |
| Cl | -0.84508000 | 0.73765200  | -2.15314800 |
| C  | 3.58890800  | 1.89317200  | 2.34344100  |
| C  | 3.74799100  | 3.00240000  | -0.99510000 |
| O  | -0.00540900 | 0.54150400  | 0.69803400  |
| O  | -2.00676500 | -0.73251600 | -0.02260200 |
| C  | -2.75559400 | -1.69967200 | 0.37381200  |
| C  | -4.19539000 | -1.40281000 | 0.53323800  |
| C  | -4.76398000 | -0.29004100 | -0.08012800 |
| C  | -6.10427000 | -0.00859800 | 0.11649100  |
| C  | -6.87980500 | -0.83306900 | 0.92220400  |
| C  | -6.31275500 | -1.94180900 | 1.53467800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.97186100 | -2.22720200 | 1.34028000  |
| C  | -0.64892700 | -2.28859800 | -1.81210100 |
| Cl | 0.32183500  | -2.16519500 | 1.07283300  |
| H  | 1.88674500  | 4.97924800  | -1.04253900 |
| H  | 5.07839800  | -0.38111100 | 2.43225200  |
| H  | -2.33723400 | -2.41959800 | 1.07307400  |
| H  | -4.15053500 | 0.34670100  | -0.70278500 |
| H  | -4.52470300 | -3.09004000 | 1.81738500  |
| H  | -6.54733200 | 0.85646900  | -0.35724000 |
| H  | -6.91475300 | -2.58094300 | 2.16525200  |
| H  | -7.92699100 | -0.61043300 | 1.07438900  |
| H  | 2.61428000  | 2.06597000  | 2.79902800  |
| H  | 3.87530000  | 2.80266000  | 1.81803400  |
| H  | 4.31126100  | 1.72527300  | 3.13771200  |
| H  | 4.45358300  | 2.58811200  | -0.27851200 |
| H  | 4.04579400  | 4.02430000  | -1.21340100 |
| H  | 3.83223300  | 2.41848100  | -1.91202500 |
| H  | 5.89525800  | -2.60439600 | 1.71629000  |
| H  | 5.67617100  | -4.55494100 | 0.22770800  |
| H  | 3.94405900  | -4.58309300 | -1.53830700 |
| H  | 2.40469700  | -2.68480800 | -1.81232200 |
| H  | -0.32452400 | 6.06051300  | -0.68090900 |
| H  | -2.68774000 | 5.84732100  | -0.01636200 |
| H  | -3.56827700 | 3.68057700  | 0.78439000  |
| H  | -2.10079700 | 1.70262500  | 0.92275400  |
| H  | 0.32079000  | -2.75309700 | -1.95581800 |
| H  | -1.00463400 | -1.82940200 | -2.72862900 |
| C  | -1.60413800 | -3.20928000 | -1.24637700 |
| C  | -2.95164500 | -2.99917200 | -1.25382400 |
| H  | -1.22373400 | -4.03424700 | -0.65520700 |
| H  | -3.62045500 | -3.74538700 | -0.85011400 |
| H  | -3.38214200 | -2.26908700 | -1.92677900 |

# PROPARGYLATION - wB97X-D/TZV(2d,2p)

File: p\_bp1\_S\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 6.65345100  | -1.37162000 | -1.66697800 |
| C  | 5.43093300  | -1.66213300 | -2.25872300 |
| C  | 4.25978400  | -1.54577100 | -1.52997400 |
| C  | 4.31241100  | -1.13527000 | -0.20179000 |
| C  | 5.53664500  | -0.84114800 | 0.38949500  |
| C  | 6.70571900  | -0.95828200 | -0.34294800 |
| C  | 3.07243100  | -0.97894400 | 0.59281000  |
| O  | 1.97413100  | -0.84908100 | -0.08437700 |
| Si | 0.31344200  | -0.80315500 | 0.52368100  |
| O  | -1.43119900 | -0.61238300 | 1.16831000  |
| N  | -2.44542200 | -0.53930900 | 0.29673500  |
| C  | -2.61345100 | 0.58880100  | -0.38613500 |
| C  | -3.56280800 | 0.67874200  | -1.41860600 |
| C  | -4.37928200 | -0.40447600 | -1.61623600 |
| C  | -4.28924700 | -1.54960400 | -0.81055800 |
| C  | -3.28063500 | -1.61844600 | 0.16994200  |
| C  | -1.77697200 | 1.75952000  | -0.02445200 |
| C  | -2.32237800 | 2.92513600  | 0.53662100  |
| C  | -1.48590300 | 4.00602600  | 0.66803800  |
| C  | -0.14315600 | 3.95750600  | 0.26147800  |
| C  | 0.37618300  | 2.74327700  | -0.22635000 |
| N  | -0.48303600 | 1.68378500  | -0.31060900 |
| O  | -0.00709700 | 0.50509900  | -0.72533800 |
| C  | 0.62416400  | -2.32739900 | 1.74278700  |
| C  | 1.83600700  | -2.67511900 | 1.83344000  |
| C  | 3.16124300  | -2.73689800 | 1.60801200  |
| Cl | -0.31961600 | -2.21574400 | -1.06960700 |
| Cl | 0.83638400  | 0.64837800  | 2.14652900  |
| C  | -3.73490300 | 2.95286800  | 1.04367800  |
| H  | -1.86763300 | 4.92293300  | 1.09740500  |
| C  | -3.62061900 | 1.88750200  | -2.30771100 |
| H  | -5.11580000 | -0.38167900 | -2.40803000 |
| C  | -3.14355900 | -2.74538100 | 0.99451100  |
| H  | 3.16197400  | -0.38417100 | 1.49956800  |
| H  | 3.30315100  | -1.76358200 | -1.98347900 |
| H  | 5.57323100  | -0.51719600 | 1.42196500  |
| H  | 5.39119300  | -1.97858500 | -3.29186800 |
| H  | 7.65598700  | -0.72731100 | 0.11775800  |
| H  | 7.56672000  | -1.46467400 | -2.23858600 |
| H  | 3.52788200  | -3.46385700 | 0.89381400  |
| H  | 3.85198300  | -2.43733000 | 2.38614800  |
| H  | -0.21987700 | -2.79842300 | 2.21947300  |
| C  | 1.72023100  | 2.61527300  | -0.61079700 |
| C  | 0.73031400  | 5.06682800  | 0.35132700  |
| H  | -4.03040500 | 3.97392500  | 1.26881300  |
| H  | -3.80791400 | 2.36579500  | 1.95953000  |
| H  | -4.44854800 | 2.54050400  | 0.33413900  |
| H  | -4.34736900 | 1.72742300  | -3.09959800 |
| H  | -2.64995200 | 2.07059900  | -2.76740300 |
| H  | -3.90787500 | 2.78863100  | -1.76844400 |
| C  | 2.52578900  | 3.71288600  | -0.51613100 |
| H  | 2.08568400  | 1.66628400  | -0.96874400 |
| H  | 3.56222300  | 3.63665000  | -0.81261100 |
| C  | 2.03225000  | 4.94427500  | -0.03199900 |
| H  | 0.34412000  | 6.00265600  | 0.72968800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.69877900  | 5.79215100  | 0.03447000  |
| C | -4.01069400 | -3.78638900 | 0.82914000  |
| H | -2.37892300 | -2.76391300 | 1.75080100  |
| H | -3.92340300 | -4.65496900 | 1.46614500  |
| C | -5.01926900 | -3.74842600 | -0.15671900 |
| C | -5.15678700 | -2.65645800 | -0.95971900 |
| H | -5.68675000 | -4.59080200 | -0.26737500 |
| H | -5.92655400 | -2.61333100 | -1.71714900 |

File: p\_bp1\_R\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.87842000 | -0.80446000 | 0.98803200  |
| C  | -6.10459300 | 0.04079100  | 0.20248600  |
| C  | -4.77382300 | -0.25473300 | -0.03436400 |
| C  | -4.21397500 | -1.40432100 | 0.51539100  |
| C  | -4.98840600 | -2.24998400 | 1.30155000  |
| C  | -6.31921800 | -1.94847000 | 1.53936800  |
| C  | -2.78694500 | -1.72894400 | 0.29267600  |
| O  | -2.02262500 | -0.73010200 | -0.01865900 |
| Si | -0.33932100 | -0.74878200 | -0.55356900 |
| O  | 1.40464300  | -0.58341500 | -1.18059800 |
| N  | 2.41598900  | -0.55445200 | -0.30490600 |
| C  | 2.62844400  | 0.56448400  | 0.38408000  |
| C  | 3.60562500  | 0.61550500  | 1.39201900  |
| C  | 4.38533300  | -0.49916000 | 1.57147700  |
| C  | 4.23552700  | -1.63987200 | 0.77046100  |
| C  | 3.20670700  | -1.66658100 | -0.19076300 |
| C  | 1.81795300  | 1.76151000  | 0.04487200  |
| C  | 2.38824200  | 2.93143800  | -0.47469600 |
| C  | 1.56890800  | 4.02880600  | -0.60339300 |
| C  | 0.22152700  | 3.99552200  | -0.22428100 |
| C  | -0.32335800 | 2.78058500  | 0.23565000  |
| N  | 0.51462700  | 1.70587400  | 0.31302300  |
| O  | 0.00436400  | 0.53359400  | 0.70772400  |
| C  | -0.67774700 | -2.19205200 | -1.86125100 |
| C  | -1.79259100 | -2.76616100 | -1.70821600 |
| C  | -3.03220800 | -3.03442900 | -1.25818400 |
| Cl | 0.25548200  | -2.20123600 | 1.03340200  |
| Cl | -0.84262600 | 0.73128100  | -2.15182000 |
| C  | 3.82262600  | 2.99461300  | -0.91545200 |
| H  | 1.97617400  | 4.94617900  | -1.00864000 |
| C  | 3.76589300  | 1.83194400  | 2.25650000  |
| H  | 5.13974700  | -0.50262200 | 2.34671200  |
| C  | 5.05968500  | -2.78226300 | 0.90396700  |
| H  | -2.36109700 | -2.49108500 | 0.94200900  |
| H  | -4.16246600 | 0.39698500  | -0.64309900 |
| H  | -4.54759400 | -3.13991500 | 1.73228600  |
| H  | -6.54177500 | 0.93240100  | -0.22530900 |
| H  | -6.91895400 | -2.60287800 | 2.15631500  |
| H  | -7.91827800 | -0.57096500 | 1.17107600  |
| H  | -3.21618800 | -3.94681100 | -0.70479700 |
| H  | -3.87282600 | -2.62733500 | -1.80582800 |
| H  | 0.04883000  | -2.35764500 | -2.64104400 |
| C  | -0.63344200 | 5.12115200  | -0.31133500 |
| H  | 4.32525200  | 2.61370200  | 1.74461600  |
| H  | 4.31351900  | 1.57074900  | 3.15825500  |
| H  | 2.80234700  | 2.24359400  | 2.55087400  |
| H  | 3.86897800  | 3.37998500  | -1.93242400 |
| H  | 4.30751300  | 2.02241400  | -0.90479600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.39323900  | 3.67190700  | -0.28135700 |
| C | 4.85691900  | -3.86915200 | 0.10843400  |
| H | 5.84650800  | -2.76952700 | 1.64482400  |
| H | 5.48839200  | -4.74021500 | 0.20783100  |
| C | 3.82207500  | -3.86839000 | -0.85157700 |
| C | 2.99829500  | -2.79160300 | -1.00423200 |
| H | 3.67711500  | -4.73873500 | -1.47548900 |
| H | 2.20512000  | -2.78777000 | -1.73133800 |
| C | -1.94215200 | 5.01363400  | 0.04862800  |
| H | -0.22566100 | 6.05600600  | -0.66877900 |
| H | -2.59457000 | 5.87258300  | -0.01548200 |
| C | -2.46223700 | 3.78140900  | 0.50541600  |
| C | -1.67705900 | 2.66981800  | 0.59598100  |
| H | -3.50523800 | 3.71631500  | 0.78112600  |
| H | -2.06700200 | 1.72049300  | 0.92551100  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.56029400  | -0.57772100 | 2.43415000  |
| C  | 4.65097400  | 0.35311500  | 1.95160300  |
| C  | 3.53538300  | -0.06632400 | 1.24787100  |
| C  | 3.32543300  | -1.42015600 | 1.01830400  |
| C  | 4.23243700  | -2.35321200 | 1.51391500  |
| C  | 5.34606800  | -1.93280700 | 2.21947200  |
| C  | 2.13712800  | -1.90239900 | 0.27689400  |
| O  | 1.15530100  | -1.07052700 | 0.10993900  |
| Si | -0.35834600 | -1.38193400 | -0.79173900 |
| O  | -1.15847300 | -0.63412800 | 0.69596500  |
| N  | -2.22180200 | 0.16061800  | 0.52492300  |
| C  | -2.00925200 | 1.41191900  | 0.13271300  |
| C  | -3.07808000 | 2.25517700  | -0.21048800 |
| C  | -4.34603100 | 1.76663900  | -0.01835400 |
| C  | -4.57095500 | 0.48898000  | 0.51675900  |
| C  | -3.46717400 | -0.34504600 | 0.78211400  |
| C  | -0.60365700 | 1.88191200  | 0.11134600  |
| C  | -0.14479400 | 2.86725800  | 1.00345800  |
| C  | 1.13368900  | 3.32806800  | 0.82496100  |
| C  | 1.96099700  | 2.82833900  | -0.19350900 |
| C  | 1.48168000  | 1.78977100  | -1.01601900 |
| N  | 0.20527100  | 1.34499100  | -0.79498900 |
| O  | -0.26552800 | 0.34388700  | -1.54372000 |
| C  | 0.68190200  | -2.04225500 | -2.35817800 |
| C  | 1.89902800  | -2.28263900 | -2.11976500 |
| C  | 3.07875000  | -2.34458700 | -1.47722700 |
| Cl | -2.23766300 | -1.56356600 | -1.93787300 |
| Cl | -0.61776900 | -3.38214700 | 0.09820700  |
| C  | -0.98483400 | 3.31547700  | 2.16381700  |
| H  | 1.52641300  | 4.08261100  | 1.49337800  |
| C  | -2.82842500 | 3.60851700  | -0.81103500 |
| H  | -5.19856700 | 2.37855900  | -0.28199000 |
| C  | -5.86660600 | -0.01866200 | 0.76988600  |
| H  | 1.86595200  | -2.93908800 | 0.45989700  |
| H  | 2.81676200  | 0.65200200  | 0.88864500  |
| H  | 4.06563600  | -3.41000500 | 1.34786400  |
| H  | 4.80924500  | 1.40861400  | 2.12586700  |
| H  | 6.04694900  | -2.66125800 | 2.60251500  |
| H  | 6.43215400  | -0.24879400 | 2.98272300  |
| H  | 3.78976000  | -1.54040500 | -1.62501000 |
| H  | 3.49365700  | -3.30862800 | -1.21231400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.16783800  | -2.13375400 | -3.30164900 |
| C | 3.28702300  | 3.27852100  | -0.39112100 |
| H | -0.54970900 | 4.20028700  | 2.62033700  |
| H | -1.01981200 | 2.52608300  | 2.91537300  |
| H | -2.01039500 | 3.54435600  | 1.88633300  |
| H | -3.75478700 | 4.01034200  | -1.21270600 |
| H | -2.10384300 | 3.54814300  | -1.62182400 |
| H | -2.44815000 | 4.31863700  | -0.07739500 |
| C | -6.02289400 | -1.27613000 | 1.27098300  |
| H | -6.72066100 | 0.60956300  | 0.55977600  |
| H | -7.01273300 | -1.66285500 | 1.46619500  |
| C | -4.89779900 | -2.08691100 | 1.53494000  |
| C | -3.63053000 | -1.64306200 | 1.28956900  |
| H | -5.04261700 | -3.08008200 | 1.93544100  |
| H | -2.76408700 | -2.25973600 | 1.46647400  |
| C | 4.06681300  | 2.71207100  | -1.35464900 |
| H | 3.66696300  | 4.06828600  | 0.24132600  |
| H | 5.08168900  | 3.05291300  | -1.49964800 |
| C | 3.55840900  | 1.68018300  | -2.17174200 |
| C | 2.28391800  | 1.21565000  | -2.01425400 |
| H | 4.18969400  | 1.24964600  | -2.93604300 |
| H | 1.88378000  | 0.42752300  | -2.63039000 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.89570500  | -2.84328600 | 2.63773900  |
| C  | 3.59388100  | -3.22596200 | 2.34470700  |
| C  | 2.83483500  | -2.48878600 | 1.45149700  |
| C  | 3.38425200  | -1.36457200 | 0.84545200  |
| C  | 4.68732600  | -0.97563000 | 1.14658500  |
| C  | 5.44133700  | -1.71383000 | 2.04130400  |
| C  | 2.59190900  | -0.54269300 | -0.09502500 |
| O  | 1.30505500  | -0.65222300 | -0.07063700 |
| Si | -0.10024100 | -0.99621800 | -1.11463200 |
| N  | -1.01815200 | -0.77665100 | 0.46143700  |
| O  | -2.16917700 | -0.09601800 | 0.47272100  |
| C  | -2.11532100 | 1.23308300  | 0.46178500  |
| C  | -3.28757600 | 2.00209000  | 0.40624400  |
| C  | -4.48342700 | 1.32899300  | 0.44226200  |
| C  | -4.54101100 | -0.06749300 | 0.55009400  |
| C  | -3.33869300 | -0.80177300 | 0.55598600  |
| C  | -0.77532700 | 1.86571900  | 0.53335500  |
| C  | -0.36164600 | 2.63773300  | 1.63032200  |
| C  | 0.85786000  | 3.26256400  | 1.53666100  |
| C  | 1.64567400  | 3.17503000  | 0.38023900  |
| C  | 1.20037700  | 2.36746900  | -0.68423700 |
| N  | 0.02057500  | 1.69719600  | -0.52019500 |
| O  | -0.36522300 | 0.83917000  | -1.46949800 |
| C  | 1.06481200  | -1.17666900 | -2.70232400 |
| C  | 2.30833600  | -1.16025900 | -2.48326000 |
| C  | 3.49962200  | -1.12459200 | -1.86794800 |
| Cl | -1.91167600 | -1.24364700 | -2.35382600 |
| Cl | -0.00547400 | -3.16881000 | -0.70183900 |
| C  | -1.18320400 | 2.74436900  | 2.88280000  |
| H  | 1.22107500  | 3.84354900  | 2.37403900  |
| C  | -3.23074900 | 3.49742200  | 0.29034700  |
| H  | -5.40955000 | 1.88596700  | 0.39113700  |
| C  | -5.76049200 | -0.78021000 | 0.63305600  |
| H  | 2.97604700  | 0.46356700  | -0.25315200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.81939900  | -2.77520600 | 1.21822400  |
| H | 5.11056000  | -0.09520900 | 0.67905600  |
| H | 3.16812700  | -4.10151800 | 2.81491400  |
| H | 6.45291400  | -1.41134400 | 2.27354400  |
| H | 5.48608700  | -3.42373200 | 3.33342300  |
| H | 4.14713700  | -0.26744500 | -2.00537100 |
| H | 3.98464000  | -2.06238300 | -1.62993000 |
| H | 0.57426800  | -1.34608900 | -3.64811500 |
| C | 2.88758900  | 3.83967400  | 0.23806100  |
| H | -0.54443100 | 2.57910600  | 3.74832600  |
| H | -1.98759900 | 2.01469400  | 2.91589300  |
| H | -1.61541600 | 3.73978500  | 2.97826600  |
| H | -3.08377200 | 3.96334100  | 1.26400000  |
| H | -4.16717900 | 3.87011100  | -0.11677200 |
| H | -2.42419200 | 3.81959400  | -0.36539100 |
| C | 3.60759500  | 3.70908200  | -0.91158900 |
| H | 3.24414300  | 4.45355400  | 1.05320900  |
| H | 4.55370800  | 4.21936600  | -1.01934300 |
| C | 3.12345100  | 2.91592200  | -1.97476300 |
| C | 1.93907800  | 2.24459700  | -1.87340000 |
| H | 3.69873900  | 2.84012800  | -2.88645500 |
| H | 1.56163600  | 1.62973600  | -2.67349800 |
| C | -5.75225100 | -2.13898900 | 0.72962300  |
| H | -6.68861400 | -0.22625500 | 0.62157100  |
| H | -6.68389700 | -2.68194300 | 0.79807300  |
| C | -4.53189100 | -2.84934700 | 0.73959100  |
| C | -3.33358900 | -2.20312400 | 0.64776400  |
| H | -4.54719600 | -3.92718200 | 0.81699300  |
| H | -2.39569000 | -2.73517700 | 0.63283600  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.50021100  | -0.47070900 | 2.10113600  |
| C  | 5.16743200  | -0.83280400 | 0.80236600  |
| C  | 3.85314400  | -1.11589200 | 0.47613700  |
| C  | 2.86686600  | -1.03399000 | 1.45382700  |
| C  | 3.19987800  | -0.67039900 | 2.75493200  |
| C  | 4.51640600  | -0.38801800 | 3.07697800  |
| C  | 1.44907800  | -1.26093000 | 1.10818200  |
| O  | 1.15508100  | -1.19105100 | -0.14663800 |
| Si | -0.42436600 | -1.46934200 | -0.93376500 |
| O  | -1.19321900 | -0.65383300 | 0.58802200  |
| N  | -2.14108500 | 0.27358400  | 0.44637700  |
| C  | -1.78238000 | 1.50053300  | 0.06684400  |
| C  | -2.74577400 | 2.48773700  | -0.17652500 |
| C  | -4.05865900 | 2.16132800  | 0.06749800  |
| C  | -4.42793600 | 0.90124600  | 0.55226100  |
| C  | -3.42999200 | -0.07624900 | 0.73639800  |
| C  | -0.32731700 | 1.77244800  | -0.02728300 |
| C  | 0.31711700  | 2.65948800  | 0.85072800  |
| C  | 1.65433200  | 2.88943100  | 0.64311900  |
| C  | 2.34907400  | 2.29281000  | -0.41948500 |
| C  | 1.66711800  | 1.39119300  | -1.25985400 |
| N  | 0.34914300  | 1.14291700  | -0.98273000 |
| O  | -0.29895000 | 0.21220900  | -1.70038400 |
| C  | -0.58677500 | -3.21341100 | -0.00912800 |
| C  | 0.20952400  | -3.38157100 | 0.96093100  |
| C  | 1.22992300  | -3.19976700 | 1.81567500  |
| Cl | -2.37839200 | -1.65589900 | -1.91288900 |

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|----|-------------|-------------|-------------|
| Cl | 0.60660400  | -2.37460700 | -2.65142300 |
| C  | -0.42742900 | 3.30165700  | 1.98434900  |
| H  | 2.19296700  | 3.54745000  | 1.31198600  |
| C  | -2.38607500 | 3.83982300  | -0.72362800 |
| H  | -4.82930700 | 2.89825400  | -0.11607000 |
| C  | -5.76865000 | 0.55448900  | 0.84904900  |
| C  | -3.74157600 | -1.36269300 | 1.20884500  |
| H  | 0.71714100  | -0.88164100 | 1.81748500  |
| H  | 3.58099300  | -1.38356900 | -0.53484300 |
| H  | 2.42887500  | -0.60337400 | 3.51201500  |
| H  | 5.93380500  | -0.88815900 | 0.04200100  |
| H  | 4.77458200  | -0.10308400 | 4.08737300  |
| H  | 6.52876600  | -0.24987700 | 2.35161500  |
| H  | 2.18146200  | -3.66379400 | 1.58788800  |
| H  | 1.03293000  | -2.98886800 | 2.85912900  |
| H  | -1.30520700 | -3.92077800 | -0.39399100 |
| C  | 3.71883600  | 2.53876500  | -0.67215000 |
| H  | -1.11129200 | 2.60226700  | 2.46194700  |
| H  | -1.00743900 | 4.15683600  | 1.63908600  |
| H  | 0.27577600  | 3.65773100  | 2.73261600  |
| H  | -1.32027400 | 3.95275500  | -0.90107300 |
| H  | -2.71040700 | 4.62585100  | -0.04321900 |
| H  | -2.89733700 | 3.99118500  | -1.67311900 |
| C  | 4.34294000  | 1.92240900  | -1.71468900 |
| H  | 4.25252700  | 3.22097100  | -0.02575400 |
| H  | 5.38922400  | 2.11057400  | -1.90736000 |
| C  | 3.63214000  | 1.03318100  | -2.54865700 |
| C  | 2.31340100  | 0.75620000  | -2.33104900 |
| H  | 4.14244100  | 0.55705100  | -3.37374900 |
| H  | 1.76653300  | 0.06163800  | -2.94765100 |
| C  | -5.04420100 | -1.65130100 | 1.49228200  |
| H  | -2.95628900 | -2.09028500 | 1.33293100  |
| H  | -5.30078600 | -2.63436600 | 1.86073400  |
| C  | -6.06535500 | -0.69182400 | 1.30943400  |
| H  | -6.54129600 | 1.29655200  | 0.70487300  |
| H  | -7.08838100 | -0.95511700 | 1.53648600  |

File: p\_bp3\_R\_wb97xd\_tzv2d2p.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.27664400  | 0.21214700  | 2.40796500  |
| C  | 3.95408500  | 0.58731900  | 2.60969300  |
| C  | 2.93844400  | -0.06214600 | 1.93223600  |
| C  | 3.24570400  | -1.09491900 | 1.05147100  |
| C  | 4.56811700  | -1.47554600 | 0.85552600  |
| C  | 5.58336800  | -0.81863400 | 1.53148000  |
| C  | 2.18416900  | -1.74652100 | 0.25611100  |
| O  | 1.11934800  | -1.04465600 | 0.06576100  |
| Si | -0.39183100 | -1.49345500 | -0.75595700 |
| O  | -1.19168500 | -0.59065200 | 0.69616900  |
| N  | -2.20151500 | 0.25456000  | 0.47075200  |
| C  | -1.92341600 | 1.45547800  | -0.03581200 |
| C  | -2.94689900 | 2.34217500  | -0.39699500 |
| C  | -4.23713500 | 1.95899400  | -0.12197200 |
| C  | -4.52517300 | 0.74072000  | 0.50641400  |
| C  | -3.46750000 | -0.14149800 | 0.80232500  |
| C  | -0.48822000 | 1.81739100  | -0.12853100 |
| C  | 0.07349100  | 2.81421400  | 0.68788800  |
| C  | 1.40604000  | 3.08875800  | 0.51428600  |
| C  | 2.17761600  | 2.42242200  | -0.44990300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.57405000  | 1.42253900  | -1.23585600 |
| N  | 0.25412400  | 1.14444000  | -0.99852200 |
| O  | -0.32342100 | 0.12501600  | -1.65433100 |
| C  | -0.49931800 | -3.14963800 | 0.33320200  |
| C  | 0.55916700  | -3.44563100 | 0.96160900  |
| C  | 1.80131800  | -3.37500600 | 1.46961700  |
| Cl | -2.33214500 | -1.84110700 | -1.71518000 |
| Cl | 0.67075300  | -2.48108500 | -2.42567200 |
| C  | -0.74729100 | 3.50022400  | 1.74057100  |
| H  | 1.88288100  | 3.82849600  | 1.14344500  |
| C  | -2.66350900 | 3.62556200  | -1.12340000 |
| H  | -5.05418200 | 2.61476600  | -0.39267900 |
| C  | -5.84267300 | 0.34233700  | 0.83815400  |
| H  | 2.51414000  | -2.37907000 | -0.56482900 |
| H  | 1.90640700  | 0.22678600  | 2.07545600  |
| H  | 4.80253000  | -2.27351200 | 0.16275200  |
| H  | 3.71719800  | 1.38965600  | 3.29472100  |
| H  | 6.61290600  | -1.10586800 | 1.37023000  |
| H  | 6.06975100  | 0.72532000  | 2.93436400  |
| H  | 2.57215400  | -4.03881200 | 1.09816000  |
| H  | 1.92922600  | -3.00232500 | 2.47818400  |
| H  | -1.42999300 | -3.69616400 | 0.33542000  |
| C  | 2.30335900  | 0.70531700  | -2.19619100 |
| C  | 3.55635900  | 2.67765000  | -0.63519600 |
| H  | -0.10165300 | 4.08727800  | 2.38816700  |
| H  | -1.28280100 | 2.77733400  | 2.35467400  |
| H  | -1.48245500 | 4.17454600  | 1.30241800  |
| H  | -3.32331600 | 4.41474300  | -0.76987200 |
| H  | -2.84809400 | 3.48225100  | -2.18813100 |
| H  | -1.63512900 | 3.95808100  | -1.01355400 |
| C  | 4.26596300  | 1.96896200  | -1.55737700 |
| H  | 4.03034200  | 3.43589300  | -0.02794200 |
| H  | 5.32088100  | 2.15842600  | -1.69307900 |
| C  | 3.63143800  | 0.98360700  | -2.34396900 |
| H  | 1.81314400  | -0.05982200 | -2.77641400 |
| H  | 4.20903200  | 0.43539700  | -3.07453000 |
| C  | -6.06303600 | -0.86032100 | 1.43745200  |
| H  | -6.65976200 | 1.01092900  | 0.60669900  |
| H  | -7.06900500 | -1.16335600 | 1.68990500  |
| C  | -4.98282100 | -1.72043800 | 1.73566600  |
| C  | -3.69927400 | -1.38033100 | 1.42275900  |
| H  | -5.17689900 | -2.66760800 | 2.21832800  |
| H  | -2.86861000 | -2.02949300 | 1.64425300  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.71937700 | -2.34803600 | 0.81345200  |
| C  | -5.69009500 | -3.02388900 | 0.17024900  |
| C  | -4.46418600 | -2.40963800 | -0.01541700 |
| C  | -4.26894700 | -1.11092400 | 0.44214000  |
| C  | -5.29792900 | -0.43408300 | 1.08773100  |
| C  | -6.52189600 | -1.05459700 | 1.27570300  |
| C  | -2.96084000 | -0.43847000 | 0.26387300  |
| O  | -1.93431800 | -1.21391300 | 0.12645600  |
| Si | -0.28071200 | -0.94621200 | -0.41511100 |
| O  | 1.41655400  | -0.62088800 | -1.10765200 |
| N  | 2.45668500  | -0.48538000 | -0.28003800 |
| C  | 2.60073600  | 0.68171600  | 0.33061600  |
| C  | 3.60055400  | 0.88378000  | 1.29343000  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.48252800  | -0.14715700 | 1.49837400  |
| C  | 4.39348700  | -1.34880300 | 0.77801500  |
| C  | 3.33176500  | -1.52686200 | -0.13133500 |
| C  | 1.68072600  | 1.77117600  | -0.07073800 |
| C  | 2.13470500  | 2.87515500  | -0.81299700 |
| C  | 1.24450700  | 3.89515300  | -1.03108900 |
| C  | -0.03589700 | 3.88170000  | -0.45388200 |
| C  | -0.44272300 | 2.74893100  | 0.27590100  |
| N  | 0.41621500  | 1.68094900  | 0.32941900  |
| O  | -0.02289000 | 0.51509800  | 0.81996500  |
| C  | -0.90179300 | 0.29914800  | -1.84640300 |
| C  | -2.12044400 | 0.61810100  | -1.77834700 |
| C  | -3.41284700 | 0.62063900  | -1.40192900 |
| Cl | 0.43906300  | -2.19258300 | 1.21589600  |
| Cl | -0.42903100 | -2.63713100 | -1.83534300 |
| C  | 3.52009100  | 2.88449600  | -1.39165100 |
| H  | 1.53835900  | 4.74333800  | -1.63501000 |
| C  | 3.64212300  | 2.14792100  | 2.10176100  |
| H  | 5.26602000  | -0.03887200 | 2.23639900  |
| C  | 5.31112200  | -2.41160000 | 0.94720400  |
| H  | -2.82343200 | 0.46038100  | 0.85300200  |
| H  | -3.65279500 | -2.92794200 | -0.50743700 |
| H  | -5.13949900 | 0.57419300  | 1.45063400  |
| H  | -5.84444200 | -4.03349600 | -0.18447900 |
| H  | -7.32011300 | -0.53161900 | 1.78379500  |
| H  | -7.67531100 | -2.83223000 | 0.95847900  |
| H  | -4.09833500 | -0.01551700 | -1.94737500 |
| H  | -3.83754900 | 1.50934300  | -0.95148200 |
| H  | -0.18801600 | 0.57542600  | -2.60690500 |
| C  | -0.94055900 | 4.96377800  | -0.56372700 |
| H  | 3.61705100  | 3.69790800  | -2.10562200 |
| H  | 3.73441600  | 1.94982200  | -1.90802900 |
| H  | 4.28053700  | 3.02086800  | -0.62351300 |
| H  | 3.81485500  | 3.03011500  | 1.48726400  |
| H  | 4.43773700  | 2.09196700  | 2.83966000  |
| H  | 2.69900400  | 2.29193000  | 2.82862300  |
| C  | -2.14715600 | 4.91886100  | 0.06935800  |
| H  | -0.64721500 | 5.82847200  | -1.14203200 |
| H  | -2.83297600 | 5.74990800  | -0.00899500 |
| C  | -2.49510800 | 3.80529900  | 0.86207600  |
| C  | -1.66286700 | 2.72758800  | 0.96542200  |
| H  | -3.42733800 | 3.81191000  | 1.40888000  |
| H  | -1.88756900 | 1.89933900  | 1.61477800  |
| C  | 5.15947200  | -3.56524400 | 0.23797000  |
| H  | 6.12534200  | -2.28962000 | 1.64757100  |
| H  | 5.86303800  | -4.37526700 | 0.36611500  |
| C  | 4.08589400  | -3.71528100 | -0.66650100 |
| C  | 3.17126400  | -2.71910600 | -0.85393700 |
| H  | 3.98061000  | -4.64102400 | -1.21398600 |
| H  | 2.33411800  | -2.82709000 | -1.52593700 |

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|   |            |             |             |
|---|------------|-------------|-------------|
| C | 6.55934300 | -1.52948600 | -1.69133900 |
| C | 5.43741600 | -0.91957700 | -2.23544600 |
| C | 4.24514700 | -0.90186800 | -1.53123800 |
| C | 4.17377900 | -1.49216200 | -0.27414400 |
| C | 5.29577800 | -2.11501700 | 0.26388400  |
| C | 6.48506700 | -2.13336600 | -0.44349600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.90941100  | -1.48729900 | 0.50205800  |
| O  | 1.83243000  | -1.19681000 | -0.16118000 |
| Si | 0.18422900  | -0.99447300 | 0.44836900  |
| O  | -1.49622200 | -0.53242500 | 1.11249100  |
| N  | -2.50998300 | -0.32761800 | 0.26417800  |
| C  | -2.57390800 | 0.84225600  | -0.37381900 |
| C  | -3.56527300 | 1.08172600  | -1.33506000 |
| C  | -4.50432900 | 0.09685700  | -1.53071200 |
| C  | -4.49223200 | -1.09204900 | -0.79319300 |
| C  | -3.45009000 | -1.31058700 | 0.13013500  |
| C  | -1.57739600 | 1.87481600  | 0.00322200  |
| C  | -1.94983900 | 3.08297300  | 0.61580700  |
| C  | -0.96464700 | 4.01747700  | 0.81789600  |
| C  | 0.36052800  | 3.79155700  | 0.41578300  |
| C  | 0.69589300  | 2.54786100  | -0.15099900 |
| N  | -0.30382800 | 1.62349700  | -0.28984600 |
| O  | 0.00379100  | 0.41843000  | -0.77617600 |
| C  | 0.85179900  | 0.21804900  | 1.91395700  |
| C  | 2.10442000  | 0.21302700  | 2.05710300  |
| C  | 3.40517000  | -0.05718600 | 1.83572400  |
| Cl | -0.58481500 | -2.22783800 | -1.17986900 |
| Cl | 0.24130100  | -2.70752100 | 1.83972600  |
| C  | -3.36559800 | 3.32548500  | 1.05003700  |
| H  | -1.21061400 | 4.95551400  | 1.29742200  |
| C  | -3.59888300 | 2.33730500  | -2.15961600 |
| H  | -5.27689900 | 0.24334800  | -2.27421800 |
| C  | -5.47232900 | -2.10179200 | -0.94945000 |
| H  | 2.81892100  | -2.25885000 | 1.26399200  |
| H  | 3.36296100  | -0.45163900 | -1.96320400 |
| H  | 5.23625000  | -2.58888300 | 1.23563700  |
| H  | 5.49060700  | -0.46207300 | -3.21358600 |
| H  | 7.35389700  | -2.62015300 | -0.02305400 |
| H  | 7.48943400  | -1.54242800 | -2.24275800 |
| H  | 3.94501400  | -0.67557500 | 2.54125800  |
| H  | 3.99413000  | 0.67295700  | 1.29359600  |
| H  | 0.12780700  | 0.76769900  | 2.49537700  |
| C  | 1.38920100  | 4.75025200  | 0.57679700  |
| H  | -4.46395100 | 2.94541800  | -1.89817000 |
| H  | -3.68895000 | 2.07498200  | -3.21181400 |
| H  | -2.70369100 | 2.94111600  | -2.04195900 |
| H  | -3.38979800 | 4.10147300  | 1.81070500  |
| H  | -3.81654600 | 2.42619800  | 1.46502100  |
| H  | -3.98126400 | 3.65870300  | 0.21555200  |
| C  | -5.40119000 | -3.24248800 | -0.20977300 |
| H  | -6.26960800 | -1.94594700 | -1.66248300 |
| H  | -6.15101000 | -4.01175100 | -0.32589900 |
| C  | -4.34944300 | -3.43292500 | 0.71458600  |
| C  | -3.37673400 | -2.49201100 | 0.88712400  |
| H  | -4.31083800 | -4.34627300 | 1.29097800  |
| H  | -2.56025900 | -2.63453700 | 1.57684900  |
| C  | 2.66088400  | 4.46382100  | 0.17966900  |
| H  | 1.14496100  | 5.70674500  | 1.01686600  |
| H  | 3.44358600  | 5.19890200  | 0.29912100  |
| C  | 2.96777900  | 3.20968000  | -0.39310300 |
| C  | 2.00806300  | 2.25376000  | -0.55515400 |
| H  | 3.98172000  | 3.00239700  | -0.70536800 |
| H  | 2.22463700  | 1.28715000  | -0.97943500 |

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|----|-------------|-------------|-------------|
| C  | -6.89706200 | -0.75285400 | 1.03157000  |
| C  | -5.87833600 | 0.12405500  | 1.38321400  |
| C  | -4.56891400 | -0.15763300 | 1.03654400  |
| C  | -4.27330000 | -1.32012600 | 0.33282800  |
| C  | -5.29283400 | -2.19900500 | -0.01479500 |
| C  | -6.60348100 | -1.91393200 | 0.32040000  |
| C  | -2.88746100 | -1.64303300 | -0.08378700 |
| O  | -2.08143900 | -0.63798700 | -0.25351500 |
| Si | -0.36856200 | -0.70717600 | -0.71001000 |
| O  | -0.02698800 | 0.56477700  | 0.61453500  |
| N  | 0.56108400  | 1.71850300  | 0.27748200  |
| C  | 1.88100100  | 1.72535800  | 0.09089100  |
| C  | 2.53246100  | 2.87695400  | -0.37218700 |
| C  | 1.77333600  | 4.01310900  | -0.52534600 |
| C  | 0.40548800  | 4.03215800  | -0.22954600 |
| C  | -0.21978000 | 2.83319500  | 0.16509300  |
| C  | 2.62101100  | 0.49231400  | 0.45612400  |
| C  | 3.55854600  | 0.48586400  | 1.50449600  |
| C  | 4.27076900  | -0.66876900 | 1.70950300  |
| C  | 4.08740300  | -1.80211700 | 0.90260800  |
| C  | 3.10288500  | -1.76783100 | -0.10422700 |
| N  | 2.38194000  | -0.60963300 | -0.25073200 |
| O  | 1.43230700  | -0.57905500 | -1.18968300 |
| C  | -0.03060500 | -2.00345800 | 0.78830600  |
| C  | -1.07733300 | -2.52551100 | 1.26354600  |
| C  | -2.37877000 | -2.77995100 | 1.49732800  |
| Cl | -0.73849000 | 0.79532800  | -2.25970700 |
| Cl | -0.58688200 | -2.35729200 | -2.16270900 |
| C  | 3.75278000  | 1.69157900  | 2.37691900  |
| H  | 4.99522100  | -0.71183700 | 2.51197400  |
| C  | 3.98983700  | 2.88255900  | -0.73720000 |
| H  | 2.24346700  | 4.91906200  | -0.88509600 |
| C  | -0.39196100 | 5.19723300  | -0.34177900 |
| H  | -2.79916300 | -2.45937000 | -0.79699400 |
| H  | -3.77392800 | 0.51999300  | 1.31190200  |
| H  | -5.06164400 | -3.10189900 | -0.56574600 |
| H  | -6.10749900 | 1.03036100  | 1.92654700  |
| H  | -7.39411600 | -2.59590900 | 0.05201800  |
| H  | -7.92038400 | -0.52887600 | 1.29977800  |
| H  | -2.84802100 | -2.30140300 | 2.34778500  |
| H  | -2.80144100 | -3.72804300 | 1.18924300  |
| H  | 0.96465900  | -2.19374100 | 1.15781200  |
| C  | 4.82544600  | -2.99621700 | 1.07427300  |
| H  | 4.22206300  | 1.39675900  | 3.31173400  |
| H  | 2.80609300  | 2.17681800  | 2.60597900  |
| H  | 4.40048600  | 2.42474000  | 1.89774200  |
| H  | 4.54260900  | 3.57961400  | -0.10897200 |
| H  | 4.09886100  | 3.21087900  | -1.76969800 |
| H  | 4.44957100  | 1.90199900  | -0.65228300 |
| C  | -1.72490300 | 5.14184000  | -0.06959000 |
| H  | 0.07868800  | 6.12088100  | -0.64762900 |
| H  | -2.33215100 | 6.03155700  | -0.15385200 |
| C  | -2.32809700 | 3.92372300  | 0.31725300  |
| C  | -1.59804000 | 2.77773700  | 0.43050900  |
| H  | -3.38972500 | 3.89809800  | 0.51814200  |
| H  | -2.04551600 | 1.83596700  | 0.69960700  |
| C  | 4.57807800  | -4.07418400 | 0.27736300  |
| H  | 5.58170200  | -3.03255100 | 1.84537900  |

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|---|------------|-------------|-------------|
| H | 5.14047800 | -4.98710800 | 0.41023900  |
| C | 3.58554800 | -4.01186300 | -0.72351700 |
| C | 2.84715500 | -2.88031200 | -0.92180900 |
| H | 3.40406600 | -4.87701500 | -1.34511400 |
| H | 2.07939400 | -2.82440000 | -1.67698200 |

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|---|-------------|-------------|-------------|
| H | -3.30112500 | 2.68453900  | -2.27349700 |
| H | -4.05664500 | 3.96154000  | 0.93884300  |
| H | -4.07673000 | 2.21586800  | 1.18074900  |
| H | -4.36354900 | 2.88786300  | -0.42037900 |
| H | -5.71832900 | -2.66414900 | -1.90552900 |
| H | -5.65222900 | -4.50482000 | -0.27218100 |
| H | -4.04185400 | -4.45203000 | 1.60338600  |
| H | -2.47186300 | -2.56425800 | 1.85951700  |
| H | 0.26800900  | 6.08706200  | 0.68189100  |
| H | 2.70751500  | 5.88506500  | 0.39735700  |
| H | 3.71652500  | 3.69383600  | -0.15597400 |
| H | 2.31341700  | 1.70397800  | -0.42747000 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.87276600  | 2.66037500  | -0.21034400 |
| C  | 0.48157900  | 2.77845900  | -0.06992700 |
| C  | -0.11577800 | 4.01133500  | 0.25910500  |
| C  | 0.72122800  | 5.13936700  | 0.42799100  |
| C  | 2.06937800  | 5.02239500  | 0.27115800  |
| C  | 2.64452300  | 3.77384800  | -0.04657700 |
| N  | -0.34821500 | 1.70237700  | -0.24499500 |
| C  | -1.67132700 | 1.78829600  | -0.17065800 |
| C  | -2.30438200 | 2.97287500  | 0.23900700  |
| C  | -1.50558700 | 4.06843100  | 0.44466800  |
| O  | 0.18030400  | 0.50702800  | -0.52594700 |
| Si | 0.30210900  | -0.79647900 | 0.83790500  |
| Cl | 0.31899300  | -2.43681900 | 2.30547800  |
| C  | -2.45847300 | 0.59392700  | -0.55905400 |
| C  | -3.28507500 | 0.59465900  | -1.69628900 |
| C  | -4.11469800 | -0.48326700 | -1.86959400 |
| C  | -4.14250400 | -1.54703400 | -0.95302900 |
| C  | -3.23823600 | -1.54136700 | 0.12734000  |
| N  | -2.39412000 | -0.46587000 | 0.24026100  |
| C  | -3.18856000 | -2.59518300 | 1.05378100  |
| C  | -4.05832900 | -3.63682700 | 0.89423600  |
| C  | -4.97748300 | -3.66651300 | -0.17534600 |
| C  | -5.01888700 | -2.64874500 | -1.08161500 |
| C  | -3.78387800 | 3.00879300  | 0.49343600  |
| C  | -3.19237600 | 1.69561400  | -2.71280000 |
| O  | -1.49898300 | -0.46028900 | 1.23383700  |
| O  | 2.03143900  | -0.97737200 | 0.48038100  |
| C  | 2.61110700  | -0.96765300 | -0.67980200 |
| C  | 4.07313200  | -1.21009500 | -0.68181300 |
| C  | 4.69155400  | -1.82598700 | 0.40102200  |
| C  | 6.06138200  | -2.02300600 | 0.38757500  |
| C  | 6.81586500  | -1.60711300 | -0.70189200 |
| C  | 6.19939800  | -0.98830400 | -1.78035000 |
| C  | 4.82887200  | -0.79088900 | -1.77196500 |
| C  | -0.13778500 | -2.13406900 | -0.57874800 |
| C  | 0.82065300  | -2.43629700 | -1.34537100 |
| C  | 2.06754200  | -2.53633700 | -1.83948600 |
| Cl | 0.76625000  | 0.68374500  | 2.37427900  |
| H  | -4.76723700 | -0.52078100 | -2.73161500 |
| H  | -1.95177100 | 5.00116600  | 0.76290400  |
| H  | 2.25648900  | -0.23692600 | -1.40503500 |
| H  | 4.09716800  | -2.13914900 | 1.24766200  |
| H  | 4.34592500  | -0.30817900 | -2.61252700 |
| H  | 6.54338700  | -2.49851800 | 1.23041000  |
| H  | 6.78638800  | -0.65781500 | -2.62590700 |
| H  | 7.88610800  | -1.76187800 | -0.70821000 |
| H  | 2.29495000  | -2.14038000 | -2.82096000 |
| H  | 2.68966700  | -3.35229800 | -1.49291300 |
| H  | -1.09603900 | -2.63086700 | -0.58184500 |
| H  | -3.96449200 | 1.57341500  | -3.46752800 |
| H  | -2.22179800 | 1.66206800  | -3.20867800 |

# ALLYLATION - M06-2X/6-31+G(d,p)

File: a\_bp1\_S\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.95201600  | -3.02104800 | 0.83934900  |
| C  | 4.19067200  | -1.82406500 | 0.73915900  |
| C  | 3.12829800  | -1.78247500 | -0.19584200 |
| C  | 2.82204700  | -2.88932400 | -1.01694500 |
| C  | 3.58629300  | -4.02154300 | -0.89260000 |
| C  | 4.65594000  | -4.09254800 | 0.03927400  |
| N  | 2.40407900  | -0.62164600 | -0.28205000 |
| C  | 2.68540700  | 0.48201200  | 0.42072400  |
| C  | 3.69834200  | 0.46899000  | 1.40282800  |
| C  | 4.43187300  | -0.69423700 | 1.54196700  |
| O  | 1.38579000  | -0.58417500 | -1.15508500 |
| Si | -0.35847400 | -0.72758200 | -0.52349300 |
| Cl | -0.84593000 | 0.82374500  | -2.08448800 |
| C  | 1.91811200  | 1.71476400  | 0.09432300  |
| C  | 2.54505600  | 2.87139800  | -0.42145500 |
| C  | 1.76401700  | 3.99861500  | -0.57634500 |
| C  | 0.39971200  | 4.01125500  | -0.21676700 |
| C  | -0.19381300 | 2.81564000  | 0.25141000  |
| N  | 0.60785800  | 1.70540100  | 0.34173300  |
| C  | -1.55741700 | 2.74658200  | 0.60668100  |
| C  | -2.31161000 | 3.88771300  | 0.49480000  |
| C  | -1.74580500 | 5.10176700  | 0.02318400  |
| C  | -0.42227300 | 5.16515200  | -0.32776500 |
| C  | 3.94907300  | 1.63839400  | 2.32030700  |
| C  | 4.00018900  | 2.85062900  | -0.80636300 |
| O  | 0.04697700  | 0.55527600  | 0.74068700  |
| O  | -2.02048500 | -0.70880300 | 0.12351200  |
| C  | -3.14624700 | -0.68560900 | -0.51051800 |
| C  | -4.36336700 | -0.96572600 | 0.28247600  |
| C  | -4.27205400 | -1.60237800 | 1.52511500  |
| C  | -5.42660000 | -1.82552400 | 2.26757700  |
| C  | -6.66780800 | -1.41470000 | 1.77475300  |
| C  | -6.75644900 | -0.77650500 | 0.53688000  |
| C  | -5.60443500 | -0.55243800 | -0.21139600 |
| C  | -0.75012300 | -2.18560100 | -1.82249300 |
| Cl | 0.20940000  | -2.15422500 | 1.10260000  |
| H  | 2.20784900  | 4.90407200  | -0.98160300 |
| H  | 5.21611600  | -0.74114500 | 2.29361500  |
| H  | -3.25324800 | 0.00489100  | -1.35047800 |
| H  | -3.29826900 | -1.90988900 | 1.89501600  |
| H  | -5.66538600 | -0.05606800 | -1.17682300 |
| H  | -5.36088800 | -2.31765800 | 3.23245500  |
| H  | -7.71972300 | -0.45216500 | 0.15747400  |
| H  | -7.56627200 | -1.59132400 | 2.35755700  |
| H  | 4.22712300  | 3.71896800  | -1.42573500 |
| H  | 4.24797100  | 1.94978000  | -1.37329300 |
| H  | 4.64938900  | 2.88838900  | 0.07309100  |
| H  | 3.74040500  | 1.33459900  | 3.34947800  |
| H  | 3.31854400  | 2.49889400  | 2.09502300  |
| H  | 4.99614100  | 1.94764100  | 2.27005100  |
| H  | -1.97127200 | 1.80701800  | 0.95147300  |
| H  | -3.36087200 | 3.86166300  | 0.76878100  |
| H  | 0.01903200  | 6.08705800  | -0.69217000 |
| H  | -2.37176200 | 5.98367700  | -0.05732700 |
| H  | 2.00173200  | -2.82671300 | -1.71916300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.36718100  | -4.88091300 | -1.51700100 |
| H | 5.23760900  | -5.00475100 | 0.11280900  |
| H | 5.76508400  | -3.06151900 | 1.55669800  |
| H | -0.00525700 | -2.04568500 | -2.60863500 |
| C | -2.10180100 | -2.07293200 | -2.33447200 |
| H | -0.58496400 | -3.11183100 | -1.26948400 |
| C | -3.21042700 | -2.48331500 | -1.64287300 |
| H | -2.25511700 | -1.49808600 | -3.24673900 |
| H | -4.19616700 | -2.40211200 | -2.08888500 |
| H | -3.10807400 | -3.14481900 | -0.78569700 |

File: a\_bp1\_R\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.72605400 | 2.59580500  | 0.59819100  |
| C  | -0.37240100 | 2.76564300  | 0.23517100  |
| C  | 0.13451000  | 4.00924600  | -0.21294300 |
| C  | -0.76279600 | 5.11016400  | -0.28321900 |
| C  | -2.07391400 | 4.95021100  | 0.08080800  |
| C  | -2.55367500 | 3.68738300  | 0.52261200  |
| N  | 0.50401500  | 1.71589800  | 0.29657300  |
| C  | 1.80637700  | 1.81171200  | 0.01754500  |
| C  | 2.34477700  | 3.01291600  | -0.48755600 |
| C  | 1.48664700  | 4.09201200  | -0.59650600 |
| C  | 2.64574100  | 0.63038800  | 0.35346800  |
| N  | 2.44621700  | -0.50364600 | -0.32217800 |
| C  | 3.25609400  | -1.60776300 | -0.19149400 |
| C  | 4.27601600  | -1.56113200 | 0.78894700  |
| C  | 4.41537600  | -0.40043200 | 1.57644300  |
| C  | 3.62738300  | 0.71141600  | 1.36794500  |
| C  | 3.07865000  | -2.73833200 | -1.01463200 |
| C  | 3.91317500  | -3.81376900 | -0.83724600 |
| C  | 4.92850600  | -3.80238300 | 0.15372100  |
| C  | 5.10915900  | -2.70055300 | 0.94852700  |
| O  | 1.43615500  | -0.56053700 | -1.20530400 |
| Si | -0.31474000 | -0.76207200 | -0.58180800 |
| Cl | -0.84646900 | 0.76754400  | -2.13097800 |
| C  | 3.76721200  | 1.95210800  | 2.20906000  |
| C  | 3.77717300  | 3.12109400  | -0.94198900 |
| O  | 0.03420700  | 0.52376800  | 0.69106900  |
| O  | -2.00177700 | -0.72287800 | -0.00438000 |
| C  | -2.75405800 | -1.68404100 | 0.41913200  |
| C  | -4.19561600 | -1.37773800 | 0.55920900  |
| C  | -4.74653200 | -0.26126900 | -0.07947200 |
| C  | -6.09521700 | 0.03191300  | 0.09306100  |
| C  | -6.89245700 | -0.78495500 | 0.89907100  |
| C  | -6.34079200 | -1.89696900 | 1.53639300  |
| C  | -4.99155500 | -2.19500000 | 1.36725000  |
| C  | -0.69146400 | -2.26462100 | -1.84080600 |
| Cl | 0.32228100  | -2.18363200 | 1.03539600  |
| H  | 1.86492800  | 5.03321000  | -0.98768900 |
| H  | 5.16621900  | -0.38624100 | 2.36184900  |
| H  | -2.32867900 | -2.40308000 | 1.12201300  |
| H  | -4.11079500 | 0.36449000  | -0.70003800 |
| H  | -4.55338700 | -3.05841000 | 1.86162500  |
| H  | -6.52784400 | 0.89735900  | -0.39830500 |
| H  | -6.95972100 | -2.52765700 | 2.16579500  |
| H  | -7.94436500 | -0.55289500 | 1.03187100  |
| H  | 2.79232200  | 2.32112900  | 2.53739900  |
| H  | 4.27023800  | 2.75567200  | 1.66422400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.36354200  | 1.72583700  | 3.09367800  |
| H | 4.33563800  | 2.19543300  | -0.79696000 |
| H | 4.28994800  | 3.92766000  | -0.41227300 |
| H | 3.79706500  | 3.35782200  | -2.00878600 |
| H | 5.88730500  | -2.67203500 | 1.70460100  |
| H | 5.56723300  | -4.67063900 | 0.27271400  |
| H | 3.79548800  | -4.68755900 | -1.46910700 |
| H | 2.30931600  | -2.73154000 | -1.77364200 |
| H | -0.38692400 | 6.06749200  | -0.62888700 |
| H | -2.75788900 | 5.79015400  | 0.02939800  |
| H | -3.59734200 | 3.58364500  | 0.80034300  |
| H | -2.07686300 | 1.61944400  | 0.91001300  |
| H | 0.28441200  | -2.70852500 | -2.03748600 |
| H | -1.09998300 | -1.79758700 | -2.73679700 |
| C | -1.60892200 | -3.20996900 | -1.23785200 |
| C | -2.96590700 | -3.01988100 | -1.20590300 |
| H | -1.19167900 | -4.02776900 | -0.65223900 |
| H | -3.61671500 | -3.77012800 | -0.76881700 |
| H | -3.42683000 | -2.29059100 | -1.86772500 |

File: a\_bp2\_S\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.30301800  | 1.26368400  | -1.97792200 |
| C  | 1.47255700  | 1.83767800  | -0.99391900 |
| C  | 1.92321300  | 2.89999400  | -0.17351500 |
| C  | 3.25766600  | 3.35671400  | -0.34092100 |
| C  | 4.07100500  | 2.78295400  | -1.28468500 |
| C  | 3.58530200  | 1.73902400  | -2.11251000 |
| N  | 0.19327300  | 1.37367800  | -0.79335400 |
| C  | -0.65535000 | 1.93539500  | 0.06729400  |
| C  | -0.24088300 | 2.97562700  | 0.93372200  |
| C  | 1.05144800  | 3.43278000  | 0.80013400  |
| C  | -2.05389900 | 1.43522300  | 0.09129400  |
| N  | -2.23195600 | 0.17566200  | 0.50209100  |
| C  | -3.46145400 | -0.36451400 | 0.77902600  |
| C  | -4.59910800 | 0.44294200  | 0.53168400  |
| C  | -4.41560500 | 1.73216600  | -0.00196800 |
| C  | -3.15589700 | 2.25596900  | -0.22316600 |
| C  | -3.57769800 | -1.67297600 | 1.29400100  |
| C  | -4.83535300 | -2.15276200 | 1.56142600  |
| C  | -5.99453000 | -1.36916100 | 1.31767800  |
| C  | -5.88253900 | -0.10092200 | 0.81198600  |
| O  | -1.14326900 | -0.58807900 | 0.68826000  |
| Si | -0.33709600 | -1.37541100 | -0.78395500 |
| Cl | -0.61502400 | -3.34100500 | 0.20894300  |
| C  | -2.99168900 | 3.62575600  | -0.82987100 |
| C  | -1.17470500 | 3.52652200  | 1.97797900  |
| O  | -0.23554000 | 0.34991300  | -1.54311800 |
| O  | 1.18966800  | -1.01618300 | 0.11470100  |
| C  | 2.12235100  | -1.86083500 | 0.42139800  |
| C  | 3.35953300  | -1.35486700 | 1.05847100  |
| C  | 3.64241300  | 0.01140700  | 1.11779300  |
| C  | 4.80094000  | 0.45452800  | 1.74814000  |
| C  | 5.67795200  | -0.46496000 | 2.32536400  |
| C  | 5.39031100  | -1.83061800 | 2.27906100  |
| C  | 4.23309700  | -2.27572500 | 1.64887800  |
| C  | 0.69148700  | -2.17196400 | -2.30145500 |
| Cl | -2.24047700 | -1.54449700 | -1.90635600 |
| H  | 1.41467700  | 4.21894800  | 1.45635500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.29023100 | 2.33167900  | -0.24145000 |
| H | 1.81882400  | -2.86533200 | 0.71743800  |
| H | 2.94300400  | 0.71638200  | 0.68695900  |
| H | 4.00523700  | -3.33827700 | 1.61186800  |
| H | 5.01625700  | 1.51768600  | 1.79320400  |
| H | 6.06623200  | -2.54599000 | 2.73551500  |
| H | 6.58143300  | -0.11831900 | 2.81678000  |
| H | -0.60483200 | 4.09583300  | 2.71294700  |
| H | -1.70551300 | 2.72604400  | 2.49935500  |
| H | -1.91765100 | 4.19790700  | 1.53860600  |
| H | -1.94759200 | 3.92904600  | -0.91513900 |
| H | -3.52667000 | 4.37427000  | -0.24030100 |
| H | -3.41982500 | 3.62433300  | -1.83577500 |
| H | -6.75908500 | 0.50870100  | 0.61760700  |
| H | -6.97291200 | -1.78415900 | 1.53373700  |
| H | -4.94658400 | -3.15361100 | 1.96435400  |
| H | -2.68599600 | -2.26470600 | 1.45694300  |
| H | 3.61463200  | 4.16100300  | 0.29424500  |
| H | 5.09103100  | 3.13011100  | -1.40658600 |
| H | 4.23753200  | 1.30823600  | -2.86488500 |
| H | 1.91439700  | 0.47675300  | -2.60905000 |
| H | -0.03387400 | -2.81404300 | -2.80005200 |
| C | 1.83484700  | -2.92631400 | -1.82840800 |
| H | 0.95635100  | -1.32731400 | -2.94025600 |
| C | 3.02164900  | -2.37292300 | -1.42442200 |
| H | 1.68535900  | -3.98819500 | -1.63661700 |
| H | 3.83992100  | -3.01080200 | -1.10771600 |
| H | 3.27218100  | -1.34644100 | -1.68200800 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.07880500 | -2.37531200 | 0.61606300  |
| C  | -3.22989200 | -0.97841000 | 0.49771600  |
| C  | -4.50491400 | -0.36538700 | 0.43230200  |
| C  | -5.65183400 | -1.20172400 | 0.48635100  |
| C  | -5.50700200 | -2.55931000 | 0.60896100  |
| C  | -4.21528600 | -3.14377500 | 0.67664200  |
| N  | -2.13326000 | -0.15386600 | 0.44111900  |
| C  | -2.21401900 | 1.17538700  | 0.40315900  |
| C  | -3.45741500 | 1.82890800  | 0.2700      |
| C  | -4.58621000 | 1.03529000  | 0.28375800  |
| O  | -0.91096900 | -0.70886700 | 0.46061500  |
| Si | 0.02917900  | -0.86506600 | -1.12275900 |
| Cl | 0.24524000  | -3.02901100 | -0.66697800 |
| C  | -0.93910800 | 1.92273800  | 0.55331600  |
| C  | -0.65823700 | 2.68302700  | 1.71362300  |
| C  | 0.52241900  | 3.39248200  | 1.72914500  |
| C  | 1.40191400  | 3.38185000  | 0.62352500  |
| C  | 1.09113600  | 2.57386500  | -0.49598800 |
| N  | -0.06387200 | 1.83023100  | -0.44478000 |
| C  | 1.92087900  | 2.53938800  | -1.63510900 |
| C  | 3.06746100  | 3.29816400  | -1.63322200 |
| C  | 3.41971800  | 4.09125100  | -0.51171000 |
| C  | 2.60386200  | 4.13681200  | 0.59061500  |
| C  | -3.52096100 | 3.31425000  | 0.03203500  |
| C  | -1.57959400 | 2.62923700  | 2.90334000  |
| O  | -0.33217200 | 0.97863400  | -1.44421700 |
| O  | 1.40927300  | -0.32915100 | -0.08920300 |
| C  | 2.69691000  | -0.38651800 | -0.03085400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.37392700  | -1.39055600 | 0.82023500  |
| C  | 2.63194400  | -2.29662500 | 1.58412800  |
| C  | 3.28737800  | -3.17208600 | 2.44683000  |
| C  | 4.67694900  | -3.14144600 | 2.55676000  |
| C  | 5.41817900  | -2.21823800 | 1.81468600  |
| C  | 4.76807900  | -1.34088300 | 0.95608200  |
| C  | 1.21530500  | -1.03607200 | -2.71660800 |
| Cl | -1.78454400 | -1.18856400 | -2.34361500 |
| H  | 0.78960400  | 3.97393500  | 2.60712500  |
| H  | -5.56472700 | 1.49502000  | 0.17449300  |
| H  | 3.20226600  | 0.58279500  | -0.09877000 |
| H  | 1.55138200  | -2.29923600 | 1.50493800  |
| H  | 5.34378800  | -0.61225400 | 0.39040700  |
| H  | 2.71010200  | -3.87433100 | 3.03927500  |
| H  | 6.49816700  | -2.18052400 | 1.91166800  |
| H  | 5.18312800  | -3.82700400 | 3.22906000  |
| H  | -1.16841200 | 3.23079700  | 3.71437000  |
| H  | -1.68408100 | 1.59976100  | 3.25877700  |
| H  | -2.57986000 | 3.00589300  | 2.67629000  |
| H  | -4.55841500 | 3.64894100  | 0.05057800  |
| H  | -3.10055600 | 3.55193800  | -0.94996600 |
| H  | -2.96379100 | 3.88685800  | 0.77664700  |
| H  | 2.85678100  | 4.74987700  | 1.44938600  |
| H  | 4.33398400  | 4.67358600  | -0.53535500 |
| H  | 3.70937700  | 3.29505400  | -2.50790900 |
| H  | 1.62554800  | 1.94740000  | -2.49149100 |
| H  | -6.63363500 | -0.74321000 | 0.42882200  |
| H  | -6.38304500 | -3.19700100 | 0.65121200  |
| H  | -4.12351600 | -4.22041400 | 0.77161200  |
| H  | -2.08505900 | -2.80563000 | 0.64461300  |
| H  | 0.68613500  | -1.78924400 | -3.30073200 |
| C  | 2.53236000  | -1.47964500 | -2.32668100 |
| H  | 1.20147100  | -0.06591400 | -3.21834300 |
| C  | 3.55707700  | -0.63516900 | -2.00060800 |
| H  | 2.66437700  | -2.54354400 | -2.13274300 |
| H  | 4.52918700  | -1.03095900 | -1.73004400 |
| H  | 3.51700900  | 0.40866800  | -2.29809500 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.12632600 | -0.61404100 | 1.23764100  |
| C  | -5.79775500 | 0.63667700  | 0.78317600  |
| C  | -4.44226800 | 0.96310100  | 0.50913700  |
| C  | -3.46007000 | -0.03656400 | 0.71242300  |
| C  | -3.80034600 | -1.32467800 | 1.17446500  |
| C  | -5.12059000 | -1.59592700 | 1.43420400  |
| N  | -2.15356400 | 0.29724300  | 0.44792800  |
| C  | -1.77360400 | 1.51866900  | 0.07106400  |
| C  | -2.71977900 | 2.52813000  | -0.20890900 |
| C  | -4.04609100 | 2.22526900  | 0.01907500  |
| O  | -1.21425000 | -0.64518200 | 0.60092200  |
| Si | -0.44458600 | -1.48341000 | -0.92308500 |
| Cl | 0.58444600  | -2.32609400 | -2.68044900 |
| C  | -0.31229200 | 1.77184300  | -0.00750500 |
| C  | 0.34542800  | 2.63310200  | 0.89973800  |
| C  | 1.68932100  | 2.86083600  | 0.68655600  |
| C  | 2.37667900  | 2.27070400  | -0.39689500 |
| C  | 1.68314700  | 1.37430200  | -1.24727800 |
| N  | 0.35626700  | 1.14028000  | -0.97096800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.32198900  | 0.72175800  | -2.32087600 |
| C  | 3.65272200  | 0.98600100  | -2.53797900 |
| C  | 4.37459000  | 1.87597900  | -1.70198000 |
| C  | 3.75447600  | 2.50335200  | -0.65180500 |
| C  | -2.29244900 | 3.83462200  | -0.82364100 |
| C  | -0.39194300 | 3.19463800  | 2.08674800  |
| O  | -0.30864100 | 0.21952100  | -1.69172400 |
| O  | 1.16751300  | -1.17410700 | -0.16459900 |
| C  | 1.47772000  | -1.08584900 | 1.07818100  |
| C  | 2.90805400  | -0.95009100 | 1.40333000  |
| C  | 3.87763300  | -1.18420400 | 0.42080700  |
| C  | 5.21834200  | -0.96451300 | 0.71602000  |
| C  | 5.59059000  | -0.51262000 | 1.98449000  |
| C  | 4.62267000  | -0.28056000 | 2.96388200  |
| C  | 3.27925900  | -0.49866200 | 2.67469100  |
| C  | -0.56183700 | -3.21230900 | 0.06613200  |
| Cl | -2.40493700 | -1.61988000 | -1.90138600 |
| H  | 2.24102500  | 3.50123800  | 1.36984100  |
| H  | -4.80890800 | 2.97074900  | -0.18749200 |
| H  | 0.75945400  | -0.64484100 | 1.77277300  |
| H  | 3.56565200  | -1.52057000 | -0.56385200 |
| H  | 2.51755700  | -0.31683200 | 3.42901100  |
| H  | 5.97425500  | -1.13623400 | -0.04335700 |
| H  | 4.91594100  | 0.07150300  | 3.94721900  |
| H  | 6.63807300  | -0.33917600 | 2.20980800  |
| H  | 0.30561400  | 3.72207700  | 2.73799600  |
| H  | -0.86049500 | 2.39105500  | 2.66289900  |
| H  | -1.17789300 | 3.89677200  | 1.79647500  |
| H  | -3.13632700 | 4.52446700  | -0.84935200 |
| H  | -1.95421100 | 3.66797200  | -1.85118100 |
| H  | -1.47481100 | 4.31516800  | -0.28254600 |
| H  | 4.29722300  | 3.18251300  | -0.00220300 |
| H  | 5.42642300  | 2.05513500  | -1.89650800 |
| H  | 4.16225100  | 0.49826200  | -3.36210300 |
| H  | 1.76052100  | 0.02753400  | -2.93353300 |
| H  | -3.02625000 | -2.06816700 | 1.30763800  |
| H  | -5.40113900 | -2.58079900 | 1.79152500  |
| H  | -6.55758800 | 1.39517600  | 0.62565300  |
| H  | -7.16087000 | -0.86167700 | 1.44811800  |
| H  | -1.61509700 | -3.49223700 | -0.00014500 |
| C  | -0.10697800 | -3.07246700 | 1.44158300  |
| H  | 0.05459800  | -3.90617200 | -0.50759500 |
| C  | 1.20394000  | -3.13974200 | 1.81869500  |
| H  | -0.83317400 | -2.75734800 | 2.19107200  |
| H  | 1.48906400  | -3.03039600 | 2.86020800  |
| H  | 1.95037400  | -3.54093500 | 1.13750500  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.63581100  | -1.21685800 | 0.83174300  |
| C  | 3.29069300  | -0.89399000 | 1.03600100  |
| C  | 2.93246800  | 0.10560000  | 1.94798800  |
| C  | 3.92309700  | 0.77775500  | 2.65481200  |
| C  | 5.26770900  | 0.45643000  | 2.45079600  |
| C  | 5.62416400  | -0.53923100 | 1.54029200  |
| C  | 2.26283800  | -1.55378300 | 0.20818800  |
| O  | 1.12006100  | -0.97506300 | 0.13253900  |
| Si | -0.41139200 | -1.53304800 | -0.64309300 |
| Cl | -2.36014300 | -1.93353400 | -1.57031800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.21442400 | -0.52911300 | 0.73937400  |
| N  | -2.23074800 | 0.29929100  | 0.46072500  |
| C  | -3.50072800 | -0.09705500 | 0.79602600  |
| C  | -4.56707700 | 0.77687600  | 0.47043600  |
| C  | -4.28058900 | 1.98774900  | -0.18660500 |
| C  | -2.98367800 | 2.37099500  | -0.46967100 |
| C  | -1.95401600 | 1.48772700  | -0.08780500 |
| C  | -5.88967000 | 0.37961200  | 0.81017400  |
| C  | -6.10717400 | -0.81364100 | 1.44612500  |
| C  | -5.01829200 | -1.66782500 | 1.76661100  |
| C  | -3.72817100 | -1.32939700 | 1.44566200  |
| C  | -0.51461300 | 1.83642800  | -0.20660400 |
| C  | 0.06323100  | 2.87993000  | 0.55201100  |
| C  | 1.41101500  | 3.11475400  | 0.37695600  |
| C  | 2.17794500  | 2.37071300  | -0.54448800 |
| C  | 1.54895300  | 1.34852200  | -1.29366200 |
| N  | 0.22028100  | 1.10245600  | -1.04036200 |
| C  | 2.26094300  | 0.56726500  | -2.22722800 |
| C  | 3.60776800  | 0.79500400  | -2.37053500 |
| C  | 4.27298200  | 1.78987100  | -1.60728200 |
| C  | 3.57405100  | 2.56947500  | -0.72254100 |
| C  | -2.70502200 | 3.65713700  | -1.20399500 |
| C  | -0.75966400 | 3.64986100  | 1.54968800  |
| O  | -0.36912500 | 0.04936400  | -1.63707300 |
| Cl | 0.65569200  | -2.55512600 | -2.30346900 |
| C  | -0.39920400 | -3.12798600 | 0.54589700  |
| C  | 0.93383900  | -3.70247600 | 0.65309400  |
| H  | 1.23154500  | -4.43043500 | -0.10013200 |
| H  | 1.90184000  | 3.88248000  | 0.96938700  |
| H  | -5.10429000 | 2.63627100  | -0.47433800 |
| H  | 2.60750800  | -2.14972400 | -0.63954800 |
| H  | 1.88231800  | 0.34973300  | 2.08590600  |
| H  | 4.90323400  | -1.98922900 | 0.11466900  |
| H  | 3.65146700  | 1.55492100  | 3.36203300  |
| H  | 6.66911200  | -0.78277800 | 1.38009800  |
| H  | 6.03937600  | 0.98488500  | 3.00151800  |
| H  | -1.10865800 | -3.81773900 | 0.08470600  |
| H  | -1.44240800 | 4.34533000  | 1.05369400  |
| H  | -0.10211500 | 4.23093300  | 2.19711100  |
| H  | -1.35520500 | 2.97903800  | 2.17478000  |
| H  | -3.17419300 | 3.61611300  | -2.19038400 |
| H  | -1.63955200 | 3.83698400  | -1.35180900 |
| H  | -3.13254400 | 4.50687300  | -0.66570000 |
| H  | 4.06847300  | 3.34001700  | -0.13964600 |
| H  | 5.34027200  | 1.93486900  | -1.73433600 |
| H  | 1.74266500  | -0.20265600 | -2.78511700 |
| H  | 4.17479300  | 0.19945500  | -3.07828200 |
| H  | -6.71166600 | 1.04138200  | 0.55767000  |
| H  | -7.11538500 | -1.11484900 | 1.70820000  |
| H  | -5.21124900 | -2.60935100 | 2.26926800  |
| H  | -2.89189600 | -1.97743200 | 1.66968700  |
| C  | 1.88503800  | -3.25662800 | -3.25662300 |
| H  | -0.76807200 | -2.76891500 | 1.50948600  |
| H  | 2.86503000  | -3.72176400 | 1.56555200  |
| H  | 1.60804500  | -2.61525400 | 2.35972200  |

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|   |             |            |            |
|---|-------------|------------|------------|
| H | -1.02425400 | 1.68206700 | 0.93401900 |
|---|-------------|------------|------------|

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|----|-------------|-------------|-------------|
| C  | -1.63235400 | 1.48163400  | 0.04861900  |
| C  | -0.98008200 | 0.91779100  | -1.10989900 |
| Si | -0.80114900 | -0.99630500 | -0.71696500 |
| O  | -2.55982600 | -1.05534000 | -0.43971900 |
| C  | -3.19322500 | -0.40439900 | 0.51034600  |
| C  | -4.67843300 | -0.48890400 | 0.47376000  |
| C  | -5.40256800 | -0.20508100 | 1.63494200  |
| C  | -6.79172800 | -0.29728500 | 1.62449600  |
| C  | -7.45508300 | -0.67252100 | 0.45583400  |
| C  | -6.72899200 | -0.95886200 | -0.70231400 |
| C  | -5.34058900 | -0.86703300 | -0.69769000 |
| O  | 1.03156300  | -0.95930400 | -1.12729600 |
| N  | 2.02390400  | -1.16696300 | -0.23639500 |
| C  | 2.59466300  | -0.11250300 | 0.35152900  |
| C  | 3.61329300  | -0.28136400 | 1.31783200  |
| C  | 4.00297700  | -1.56644600 | 1.61886300  |
| C  | 3.44088500  | -2.67877500 | 0.95499600  |
| C  | 2.43237300  | -2.46646300 | -0.01520600 |
| C  | 3.85574900  | -4.01107700 | 1.21503500  |
| C  | 3.29566100  | -5.05653700 | 0.52638700  |
| C  | 2.30297100  | -4.81435200 | -0.45482800 |
| C  | 1.86543200  | -3.54039000 | -0.73008600 |
| C  | 2.22960800  | 1.23864700  | -0.13760900 |
| N  | 1.52182800  | 2.00226800  | 0.70497900  |
| C  | 1.21527300  | 3.32036300  | 0.36583000  |
| C  | 1.63604300  | 3.82279000  | -0.88638300 |
| C  | 2.37392500  | 2.98819900  | -1.76301600 |
| C  | 2.68444500  | 1.70164700  | -1.40008800 |
| C  | 0.48251500  | 4.11148900  | 1.27477000  |
| C  | 0.17524000  | 5.40523900  | 0.92432700  |
| C  | 0.58305300  | 5.93389000  | -0.32458300 |
| C  | 1.29652100  | 5.16282200  | -1.20922200 |
| O  | 1.09267400  | 1.51813100  | 1.82211000  |
| C  | 3.48453200  | 0.78010800  | -2.27921900 |
| C  | 4.23021400  | 0.93071100  | 1.95658000  |
| Cl | -1.06157600 | -2.26991600 | -2.34645300 |
| Cl | -0.41509400 | -1.67912500 | 1.22903900  |
| H  | -2.75645600 | -0.44176500 | 1.51162500  |
| H  | 0.02595800  | 1.28711500  | -1.29851500 |
| C  | -3.00939000 | 1.51867600  | 0.15586000  |
| H  | -1.59300200 | 0.95249300  | -2.01442100 |
| H  | 2.70172100  | 3.37980200  | -2.72134400 |
| H  | 4.77542400  | -1.73615800 | 2.36401700  |
| H  | -4.76377800 | -1.09527400 | -1.58853700 |
| H  | -4.88051100 | 0.08372900  | 2.54407300  |
| H  | -7.24684600 | -1.25723500 | -1.60800800 |
| H  | -7.35426800 | -0.08091400 | 2.52657000  |
| H  | -8.53786200 | -0.74551200 | 0.44762400  |
| H  | 3.81470900  | 1.30941000  | -3.17362400 |
| H  | 2.88467200  | -0.08182200 | -2.58783000 |
| H  | 4.36988200  | 0.40817200  | -1.75317000 |
| H  | 4.99993800  | 0.63043000  | 2.68811200  |
| H  | 3.46564300  | 1.50760700  | 2.48521300  |
| H  | 4.69067200  | 1.57670000  | 1.20225300  |
| H  | 1.61578200  | 5.56232700  | -2.16671600 |
| H  | 0.33007400  | 6.95747100  | -0.57958500 |
| H  | -0.38477900 | 6.02886000  | 1.61282300  |
| H  | 0.18680700  | 3.68463300  | 2.22486100  |
| H  | 4.62347500  | -4.17757500 | 1.96358900  |

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|---|-------------|-------------|-------------|
| H | 3.61476700  | -6.07373000 | 0.72507600  |
| H | 1.87905900  | -5.64897600 | -1.00290900 |
| H | 1.11417600  | -3.35370600 | -1.48530500 |
| H | -3.46207800 | 1.96026900  | 1.03808000  |
| H | -3.60241900 | 1.53643300  | -0.75445800 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.94453700 | 2.37401700  | 0.45484100  |
| C  | -0.60902500 | 2.65139300  | 0.09180600  |
| C  | -0.21920800 | 3.91233600  | -0.41866500 |
| C  | -1.21908900 | 4.91370100  | -0.55765900 |
| C  | -2.51534000 | 4.64662100  | -0.20064500 |
| C  | -2.87704900 | 3.37076300  | 0.30746000  |
| N  | 0.35747100  | 1.68424600  | 0.21505600  |
| C  | 1.65050000  | 1.89602100  | -0.05293900 |
| C  | 2.07768500  | 3.11882900  | -0.61638800 |
| C  | 1.12614900  | 4.10607700  | -0.78892200 |
| C  | 2.60158800  | 0.82218000  | 0.33950700  |
| N  | 2.49946600  | -0.35884000 | -0.27481400 |
| C  | 3.39924800  | -1.38259500 | -0.10423100 |
| C  | 4.44099100  | -1.18507300 | 0.83407300  |
| C  | 4.49214400  | 0.02550500  | 1.55345600  |
| C  | 3.59289400  | 1.04574200  | 1.32037000  |
| C  | 3.27717800  | -2.58142000 | -0.83769800 |
| C  | 4.21012200  | -3.56637800 | -0.62574400 |
| C  | 5.26376300  | -3.39762300 | 0.31029800  |
| C  | 5.37744300  | -2.23573500 | 1.02813300  |
| O  | 1.48073600  | -0.54427700 | -1.12912800 |
| Si | -0.20175800 | -0.97428300 | -0.45264800 |
| Cl | -0.25572800 | -2.84607500 | -1.65592400 |
| C  | 3.64296700  | 2.33517000  | 2.09638700  |
| C  | 3.49951800  | 3.34282500  | -1.06284400 |
| O  | -0.00758600 | 0.49469500  | 0.70656100  |
| O  | -1.85093800 | -1.12703300 | 0.21294800  |
| C  | -2.90720400 | -1.61253700 | -0.35685400 |
| C  | -4.18708400 | -1.47315300 | 0.37993300  |
| C  | -4.26117600 | -0.68639800 | 1.53343400  |
| C  | -5.46501100 | -0.58498500 | 2.22493800  |
| C  | -6.59286300 | -1.27012200 | 1.77118400  |
| C  | -6.51453000 | -2.06923800 | 0.62908100  |
| C  | -5.31342900 | -2.17321800 | -0.06521500 |
| C  | -0.91551600 | 0.06030900  | -2.02858400 |
| Cl | 0.58520700  | -2.09915200 | 1.26533500  |
| H  | 1.42118300  | 5.05856100  | -1.22223000 |
| H  | 5.26150900  | 0.15516000  | 2.30965100  |
| H  | -2.79389700 | -2.50749000 | -0.97179400 |
| H  | -3.37079200 | -0.18538800 | 1.89881700  |
| H  | -5.24866400 | -2.79617600 | -0.95413100 |
| H  | -5.51988600 | 0.01966800  | 3.12434000  |
| H  | -7.38722800 | -2.61389900 | 0.28423700  |
| H  | -7.52996800 | -1.19077600 | 2.31288200  |
| H  | 4.19283400  | 2.17821400  | 3.02520500  |
| H  | 2.64164600  | 2.69162700  | 2.34909200  |
| H  | 4.15572200  | 3.12151800  | 1.53518000  |
| H  | 3.93532200  | 4.19938700  | -0.54239400 |
| H  | 3.50789500  | 3.56410900  | -2.13298500 |
| H  | 4.13521600  | 2.47209900  | -0.89848100 |
| H  | 6.17528000  | -2.09578600 | 1.75008600  |

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| H | 5.98038600  | -4.19824200 | 0.45625600  |
| H | 4.13699400  | -4.49516700 | -1.18122300 |
| H | 2.45457900  | -2.70412400 | -1.53114300 |
| H | -0.93311600 | 5.88394800  | -0.95048900 |
| H | -3.27623500 | 5.41162000  | -0.30759100 |
| H | -3.90896100 | 3.17927900  | 0.58354400  |
| H | -2.19301600 | 1.39043800  | 0.83506500  |
| H | -0.11977100 | -0.03206800 | -2.76936400 |
| H | -1.04492200 | 1.10039100  | -1.72789900 |
| C | -2.15903400 | -0.51609600 | -2.49029600 |
| C | -3.37499800 | -0.27455800 | -1.90225300 |
| H | -2.10481100 | -1.30647500 | -3.23714200 |
| H | -4.27721200 | -0.71427000 | -2.31409800 |
| H | -3.50543700 | 0.58359200  | -1.24681400 |

File: a\_bp5\_S\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.93196100  | -2.79650200 | -0.96434800 |
| C  | 3.14127200  | -1.70741800 | -0.09156300 |
| C  | 4.10934500  | -1.74955200 | 0.93962400  |
| C  | 4.87643300  | -2.93564700 | 1.08746000  |
| C  | 4.67626800  | -3.99477900 | 0.23933300  |
| C  | 3.70250900  | -3.92027700 | -0.79005600 |
| N  | 2.39271800  | -0.55941100 | -0.21811600 |
| C  | 2.60756000  | 0.54007900  | 0.50884500  |
| C  | 3.52781300  | 0.52683300  | 1.58352100  |
| C  | 4.25477300  | -0.62831000 | 1.78388000  |
| C  | 1.86877600  | 1.77616500  | 0.13294900  |
| N  | 0.53819700  | 1.74853800  | 0.26053400  |
| C  | -0.26489500 | 2.84687000  | 0.10146000  |
| C  | 0.35804100  | 4.06727500  | -0.25396000 |
| C  | 1.74864800  | 4.08032000  | -0.46891600 |
| C  | 2.52601400  | 2.95130300  | -0.28801600 |
| C  | -1.66165000 | 2.74673400  | 0.27850900  |
| C  | -2.41604500 | 3.88115500  | 0.12018300  |
| C  | -1.81749100 | 5.12387100  | -0.22217100 |
| C  | -0.46409000 | 5.21719300  | -0.41185500 |
| O  | -0.03879900 | 0.58738700  | 0.59967200  |
| Si | -0.34097800 | -0.71396300 | -0.70622000 |
| Cl | -0.54391600 | -2.33716100 | -2.20657600 |
| C  | 4.00204500  | 2.98764700  | -0.59129600 |
| C  | 3.67422400  | 1.72309900  | 2.48543200  |
| O  | 1.45943400  | -0.52746500 | -1.18059000 |
| O  | -2.07363800 | -0.62877100 | -0.25458800 |
| C  | -2.93112600 | -1.59708100 | -0.21561800 |
| C  | -4.27728200 | -1.29279900 | 0.32329700  |
| C  | -4.48569100 | -0.20887500 | 1.18209700  |
| C  | -5.76727600 | 0.06932900  | 1.64334400  |
| C  | -6.84220500 | -0.73283900 | 1.25054700  |
| C  | -6.63402700 | -1.81467900 | 0.39565600  |
| C  | -5.35133800 | -2.09707600 | -0.06755300 |
| C  | -0.05385400 | -2.04263300 | 0.78341600  |
| Cl | -0.72119300 | 0.79238000  | -2.26514700 |
| H  | 4.96224000  | -0.68009400 | 2.60721800  |
| H  | 2.22179400  | 5.00420700  | -0.79267000 |
| H  | -2.88625100 | -2.35331000 | -1.00186000 |
| H  | -3.64163800 | 0.40226500  | 1.48670100  |
| H  | -5.18218600 | -2.93682600 | -0.73678000 |
| H  | -5.93188500 | 0.90964300  | 2.30997200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -7.46921900 | -2.43497100 | 0.08790900  |
| H | -7.84162900 | -0.51286600 | 1.61209000  |
| H | 2.69882200  | 2.11473500  | 2.78520200  |
| H | 4.23003800  | 2.52972900  | 1.99969500  |
| H | 4.22127400  | 1.43709500  | 3.38426200  |
| H | 4.50046200  | 2.03828800  | -0.39372700 |
| H | 4.49466600  | 3.77087400  | -0.00970900 |
| H | 4.14228900  | 3.22066800  | -1.64996600 |
| H | 0.00305700  | 6.15738000  | -0.68638600 |
| H | -2.44458500 | 6.00055100  | -0.34219100 |
| H | -3.49202000 | 3.82692700  | 0.24752700  |
| H | -2.09815700 | 1.78157600  | 0.50185400  |
| H | 5.61840000  | -2.98023400 | 1.87807500  |
| H | 5.26472300  | -4.89892000 | 0.35038900  |
| H | 3.56327400  | -4.76671700 | -1.45394500 |
| H | 2.17657600  | -2.72427000 | -1.73815500 |
| H | 0.90614500  | -2.52107200 | 0.58488500  |
| C | -1.11726000 | -3.02350400 | 0.78890200  |
| H | -0.01924500 | -1.45233200 | 1.70132700  |
| C | -2.33309200 | -2.81639900 | 1.38734300  |
| H | -1.00251100 | -3.90046100 | 0.15417300  |
| H | -3.09163600 | -3.59254200 | 1.37300500  |
| H | -2.44479600 | -2.03267000 | 2.13192600  |

File: a\_bp5\_R\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.68206300  | 2.79716500  | -0.15634200 |
| C  | 0.27533100  | 2.84400300  | -0.05706900 |
| C  | -0.39553000 | 4.05614500  | 0.24124900  |
| C  | 0.38023700  | 5.23576700  | 0.41437700  |
| C  | 1.74323300  | 5.18693100  | 0.29626400  |
| C  | 2.39382000  | 3.95685300  | 0.01481400  |
| N  | -0.49119800 | 1.71875300  | -0.23634800 |
| C  | -1.82849500 | 1.72357000  | -0.16406500 |
| C  | -2.53235000 | 2.89008400  | 0.20277200  |
| C  | -1.79313300 | 4.04170200  | 0.39143100  |
| O  | 0.12200600  | 0.56049000  | -0.53580000 |
| Si | 0.35322900  | -0.75846200 | 0.79926500  |
| Cl | 0.50896300  | -2.34335600 | 2.32940300  |
| C  | -2.54744600 | 0.47016100  | -0.51788700 |
| C  | -3.43949100 | 0.40654900  | -1.61415100 |
| C  | -4.17717000 | -0.74927600 | -1.76630700 |
| C  | -4.05932000 | -1.82748900 | -0.86256900 |
| C  | -3.11044100 | -1.74078300 | 0.18442300  |
| N  | -2.36828000 | -0.58554100 | 0.27705800  |
| C  | -2.89967600 | -2.79834400 | 1.09310700  |
| C  | -3.66232700 | -3.93206300 | 0.94947200  |
| C  | -4.62789600 | -4.04572500 | -0.08353200 |
| C  | -4.82222900 | -3.01987800 | -0.97355000 |
| C  | -4.02052700 | 2.90043100  | 0.44540800  |
| C  | -3.54960000 | 1.55609700  | -2.57965300 |
| O  | -1.44509400 | -0.51107100 | 1.24461500  |
| O  | 2.11417000  | -0.83681800 | 0.46121500  |
| C  | 2.75292300  | -0.66964800 | -0.64474800 |
| C  | 4.19478500  | -0.99999900 | -0.64655600 |
| C  | 4.73679600  | -1.80240900 | 0.36300200  |
| C  | 6.09983500  | -2.07745400 | 0.36169300  |
| C  | 6.92025500  | -1.55128000 | -0.63921800 |
| C  | 6.37871600  | -0.74567900 | -1.64171200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.01420700  | -0.47028200 | -1.64768500 |
| C  | 0.04619000  | -2.09813200 | -0.67663600 |
| Cl | 0.75634400  | 0.77820400  | 2.32135900  |
| H  | -4.86815700 | -0.83751800 | -2.60036400 |
| H  | -2.30176400 | 4.96053200  | 0.67257900  |
| H  | 2.43039900  | 0.12051100  | -1.32631800 |
| H  | 4.08560300  | -2.19518700 | 1.13805600  |
| H  | 4.58406600  | 0.15677700  | -2.42500300 |
| H  | 6.52598200  | -2.69886100 | 1.14242700  |
| H  | 7.01841900  | -0.33243500 | -2.41435400 |
| H  | 7.98379400  | -1.76754200 | -0.63542800 |
| H  | -4.06656600 | 1.22787300  | -3.48201200 |
| H  | -2.56266800 | 1.93057800  | -2.86320700 |
| H  | -4.11781100 | 2.38718800  | -2.15259800 |
| H  | -4.49025300 | 1.93303000  | 0.26861200  |
| H  | -4.50700900 | 3.64719800  | -0.18718200 |
| H  | -4.20804100 | 3.17334600  | 1.48711300  |
| H  | -5.55269600 | -3.09909400 | -1.77202500 |
| H  | -5.21203800 | -4.95555100 | -0.16743500 |
| H  | -3.52229400 | -4.75595600 | 1.64084000  |
| H  | -2.14891500 | -2.69729700 | 1.86772600  |
| H  | -0.13247600 | 6.16415500  | 0.64367500  |
| H  | 2.33489400  | 6.08596800  | 0.42886700  |
| H  | 3.47581000  | 3.92957700  | -0.05442800 |
| H  | 2.17585900  | 1.85430200  | -0.33219100 |
| H  | -1.00459900 | -2.04435600 | -0.96064800 |
| H  | 0.26631700  | -3.06699300 | -0.22712600 |
| C  | 0.88268100  | -1.82270900 | -1.82789700 |
| C  | 2.17061900  | -2.26741700 | -1.94266200 |
| H  | 0.51591500  | -1.10857500 | -2.56481700 |
| H  | 2.75862400  | -2.04319700 | -2.82653800 |
| H  | 2.53549800  | -3.05706400 | -1.29073900 |

# PROPARGYLATION - M06-2X/6-31+G(d,p)

File: p\_bp1\_S\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 6.62401700  | -1.40780300 | -1.72894400 |
| C  | 5.38196500  | -1.77175300 | -2.25433400 |
| C  | 4.22719500  | -1.60499300 | -1.49678100 |
| C  | 4.31934800  | -1.07463400 | -0.20578300 |
| C  | 5.56120100  | -0.70918300 | 0.32154200  |
| C  | 6.71308000  | -0.87346400 | -0.44308700 |
| C  | 3.09869000  | -0.87791000 | 0.61327700  |
| O  | 1.98038100  | -0.79239400 | -0.05228900 |
| Si | 0.31597500  | -0.77822200 | 0.55754200  |
| O  | -1.42919600 | -0.62575100 | 1.18168700  |
| N  | -2.44169800 | -0.57054600 | 0.29916500  |
| C  | -2.66560000 | 0.57627800  | -0.34930600 |
| C  | -3.67459100 | 0.66985500  | -1.33451900 |
| C  | -4.45952400 | -0.44473600 | -1.54500600 |
| C  | -4.28273900 | -1.62462500 | -0.79609400 |
| C  | -3.23415100 | -1.68450100 | 0.15336800  |
| C  | -1.82223000 | 1.75633200  | -0.01656700 |
| C  | -2.35106900 | 2.95184800  | 0.51093700  |
| C  | -1.49237300 | 4.03148900  | 0.61306400  |
| C  | -0.14844000 | 3.95554700  | 0.20111700  |
| C  | 0.35137900  | 2.71704500  | -0.26918300 |
| N  | -0.52430700 | 1.66680300  | -0.32276700 |
| O  | -0.05773800 | 0.47415800  | -0.72669900 |
| C  | 0.67126200  | -2.25244400 | 1.83262200  |
| C  | 1.90187600  | -2.56584700 | 1.92849000  |
| C  | 3.23647900  | -2.59856500 | 1.70678600  |
| Cl | -0.26759300 | -2.24865700 | -0.99972400 |
| Cl | 0.80772900  | 0.73151500  | 2.12692700  |
| C  | -3.77315100 | 3.05427200  | 0.99751000  |
| H  | -1.86451200 | 4.96790700  | 1.02135000  |
| C  | -3.86026700 | 1.92849800  | -2.13951800 |
| H  | -5.23570900 | -0.41683400 | -2.30505100 |
| C  | -3.01139600 | -2.84066600 | 0.92873900  |
| H  | 3.19624300  | -0.24128600 | 1.49666500  |
| H  | 3.25296400  | -1.87719400 | -1.89186200 |
| H  | 5.62492600  | -0.29156600 | 1.32336100  |
| H  | 5.31508700  | -2.18357300 | -3.25605300 |
| H  | 7.67703800  | -0.58373000 | -0.03792500 |
| H  | 7.52271900  | -1.53827100 | -2.32350100 |
| H  | 3.62912600  | -3.33898900 | 1.01394600  |
| H  | 3.91664600  | -2.24357400 | 2.47746000  |
| H  | -0.15936800 | -2.70679600 | 2.35982700  |
| C  | 1.69784100  | 2.55319500  | -0.66029900 |
| C  | 0.74889500  | 5.05670000  | 0.26617700  |
| H  | -4.29924300 | 3.86091600  | 0.48119600  |
| H  | -3.76956600 | 3.28839100  | 2.06503900  |
| H  | -4.33154200 | 2.12703500  | 0.86257900  |
| H  | -4.44049500 | 1.70357300  | -3.03514200 |
| H  | -2.90158800 | 2.35117700  | -2.44918100 |
| H  | -4.40326400 | 2.69081400  | -1.57382600 |
| C  | 2.52578900  | 3.64494100  | -0.58844900 |
| H  | 2.04187800  | 1.58278300  | -0.99688100 |
| H  | 3.56320600  | 3.54659600  | -0.88987200 |
| C  | 2.05323200  | 4.90212100  | -0.12354800 |
| H  | 0.37862800  | 6.00995500  | 0.62858700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.73716500  | 5.74230800  | -0.07629300 |
| C | -3.83478900 | -3.92247800 | 0.74241800  |
| H | -2.20622600 | -2.85452200 | 1.64824900  |
| H | -3.67690800 | -4.81779000 | 1.33400700  |
| C | -4.88551900 | -3.89321200 | -0.21095300 |
| C | -5.10581100 | -2.77052700 | -0.96498200 |
| H | -5.51533200 | -4.76692300 | -0.33727300 |
| H | -5.90696800 | -2.73048600 | -1.69597700 |

File: p\_bp1\_R\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.89860500 | -0.77034500 | 0.94138700  |
| C  | -6.09034300 | 0.09148900  | 0.19624200  |
| C  | -4.74907000 | -0.21464200 | -0.01126400 |
| C  | -4.21699400 | -1.38980100 | 0.52991600  |
| C  | -5.02430900 | -2.25343700 | 1.27572800  |
| C  | -6.36504000 | -1.94066200 | 1.48270600  |
| C  | -2.78669800 | -1.72339600 | 0.33094600  |
| O  | -2.01549200 | -0.72358700 | 0.00963600  |
| Si | -0.33669300 | -0.74063700 | -0.54756000 |
| O  | 1.40128700  | -0.58126700 | -1.18091300 |
| N  | 2.41842800  | -0.55954300 | -0.30493800 |
| C  | 2.66522000  | 0.57238600  | 0.36054400  |
| C  | 3.68456600  | 0.62922500  | 1.33782500  |
| C  | 4.45487900  | -0.50169700 | 1.51684600  |
| C  | 4.24984900  | -1.66601500 | 0.74993200  |
| C  | 3.18711600  | -1.69178500 | -0.18453900 |
| C  | 1.84404100  | 1.77101000  | 0.03690700  |
| C  | 2.40028600  | 2.96066300  | -0.47635800 |
| C  | 1.56127100  | 4.05482500  | -0.58905900 |
| C  | 0.20896200  | 3.99942700  | -0.20359300 |
| C  | -0.31864600 | 2.76759000  | 0.25308900  |
| N  | 0.53903000  | 1.70273300  | 0.32009400  |
| O  | 0.03980600  | 0.52292500  | 0.72050100  |
| C  | -0.68773500 | -2.16985900 | -1.88050400 |
| C  | -1.80350300 | -2.75638000 | -1.70628300 |
| C  | -3.03540400 | -3.04642900 | -1.22641300 |
| Cl | 0.25676300  | -2.21034300 | 1.01545200  |
| Cl | -0.84697900 | 0.76387100  | -2.11170300 |
| C  | 3.83031600  | 3.04505000  | -0.94304700 |
| H  | 1.95594700  | 4.98621300  | -0.98767000 |
| C  | 3.89890100  | 1.86894400  | 2.16464700  |
| H  | 5.24129200  | -0.49954300 | 2.26716200  |
| C  | 5.05289700  | -2.83034300 | 0.88692800  |
| H  | -2.35875600 | -2.48932300 | 0.98170500  |
| H  | -4.10574400 | 0.44433700  | -0.58758600 |
| H  | -4.60310200 | -3.16300500 | 1.69646400  |
| H  | -6.50729700 | 1.00231500  | -0.22108000 |
| H  | -6.99159100 | -2.60586100 | 2.06758800  |
| H  | -7.94421000 | -0.52828500 | 1.10284200  |
| H  | -3.19276300 | -3.96418400 | -0.66459900 |
| H  | -3.89708500 | -2.64343800 | -1.75276900 |
| H  | 0.03157500  | -2.30758700 | -2.67987600 |
| C  | -0.66952500 | 5.11496600  | -0.28282200 |
| H  | 4.46443500  | 2.62560700  | 1.61372000  |
| H  | 4.46894500  | 1.61473000  | 3.05891700  |
| H  | 2.95008100  | 2.31150500  | 2.47672700  |
| H  | 3.84371900  | 3.29413800  | -2.00705900 |
| H  | 4.37184000  | 2.10717200  | -0.81474200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.36305000  | 3.83605200  | -0.40945000 |
| C | 4.79617800  | -3.93685800 | 0.12035300  |
| H | 5.86727300  | -2.81837100 | 1.60395900  |
| H | 5.41088400  | -4.82446700 | 0.22167200  |
| C | 3.72501000  | -3.93386000 | -0.81100200 |
| C | 2.92054200  | -2.83358700 | -0.96870800 |
| H | 3.53522000  | -4.81989700 | -1.40709000 |
| H | 2.09401000  | -2.82445800 | -1.66552900 |
| C | -1.98330000 | 4.97959800  | 0.08088700  |
| H | -0.27743200 | 6.06294800  | -0.63602200 |
| H | -2.65339300 | 5.83018600  | 0.02265100  |
| C | -2.48429300 | 3.72811600  | 0.53170700  |
| C | -1.67540200 | 2.62334200  | 0.61648500  |
| H | -3.52979800 | 3.64402600  | 0.80913400  |
| H | -2.04372500 | 1.65602200  | 0.93624800  |

File: p\_bp2\_S\_631+g\_M06-2X.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.52845200  | -0.28042900 | 2.42021900  |
| C  | 4.47223300  | 0.54714800  | 2.04367300  |
| C  | 3.36997700  | 0.01438000  | 1.37744200  |
| C  | 3.32294600  | -1.34720900 | 1.07668600  |
| C  | 4.37556200  | -2.18078900 | 1.47376100  |
| C  | 5.47371700  | -1.64843700 | 2.14062800  |
| C  | 2.14753300  | -1.93402300 | 0.36951100  |
| O  | 1.14242900  | -1.09733900 | 0.14537200  |
| Si | -0.36933700 | -1.42537400 | -0.68690100 |
| O  | -1.17237700 | -0.59721100 | 0.73942900  |
| N  | -2.22756400 | 0.20181200  | 0.51068800  |
| C  | -1.99742200 | 1.44421400  | 0.07787000  |
| C  | -3.06665000 | 2.29813400  | -0.26855900 |
| C  | -4.34692100 | 1.82320300  | -0.06297400 |
| C  | -4.58445400 | 0.54804700  | 0.48828700  |
| C  | -3.48068600 | -0.29267300 | 0.77235800  |
| C  | -0.58203600 | 1.89629400  | 0.02539800  |
| C  | -0.10762300 | 2.96427600  | 0.81774900  |
| C  | 1.19712900  | 3.37168900  | 0.61526000  |
| C  | 2.02971400  | 2.74859200  | -0.33298800 |
| C  | 1.52492100  | 1.64757600  | -1.06957700 |
| N  | 0.23034000  | 1.26414800  | -0.82963200 |
| O  | -0.27109200 | 0.23374400  | -1.53139400 |
| C  | 0.62004600  | -2.22646900 | -2.34366700 |
| C  | 1.81202700  | -2.47626900 | -2.03128900 |
| C  | 2.97782100  | -2.51962800 | -1.30311400 |
| Cl | -2.24746500 | -1.65377700 | -1.82646300 |
| Cl | -0.62779600 | -3.38052100 | 0.26291700  |
| C  | -0.94847700 | 3.61804800  | 1.88407800  |
| H  | 1.59777700  | 4.18701500  | 1.21211200  |
| C  | -2.81382000 | 3.66222600  | -0.85341100 |
| H  | -5.19670300 | 2.44688000  | -0.32747500 |
| C  | -5.88986500 | 0.05017200  | 0.74858300  |
| H  | 1.85563700  | -2.92794200 | 0.71383500  |
| H  | 2.52871400  | 0.64254700  | 1.11296900  |
| H  | 4.33586400  | -3.24639500 | 1.26148200  |
| H  | 4.49914800  | 1.60792600  | 2.27421000  |
| H  | 6.28625800  | -2.29940600 | 2.44594100  |
| H  | 6.38677400  | 0.13339500  | 2.93943300  |
| H  | 3.72756600  | -1.76409300 | -1.53220500 |
| H  | 3.36767300  | -3.49729200 | -1.02906700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.01862600  | -2.31837600 | -3.23521200 |
| C | 3.37996200  | 3.13935300  | -0.54826000 |
| H | -1.10895800 | 4.67396900  | 1.65201200  |
| H | -0.41882800 | 3.56478500  | 2.83813900  |
| H | -1.91766200 | 3.13614100  | 2.01407900  |
| H | -3.68025700 | 3.97309600  | -1.43850300 |
| H | -1.94004800 | 3.66550300  | -1.50847600 |
| H | -2.65818300 | 4.40794700  | -0.06869800 |
| C | -6.05392100 | -1.20735500 | 1.26766300  |
| H | -6.74191100 | 0.68488700  | 0.52934700  |
| H | -7.04964000 | -1.58669300 | 1.46860300  |
| C | -4.92737200 | -2.02676300 | 1.54338600  |
| C | -3.64906000 | -1.59112900 | 1.29808000  |
| H | -5.08029900 | -3.02001300 | 1.95109900  |
| H | -2.78101800 | -2.21130900 | 1.48313100  |
| C | 4.15679800  | 2.46039500  | -1.44943500 |
| H | 3.77630800  | 3.97505200  | 0.01932300  |
| H | 5.18836000  | 2.75384100  | -1.60876500 |
| C | 3.62019600  | 1.37051600  | -2.18484500 |
| C | 2.32236500  | 0.95871600  | -2.00831000 |
| H | 4.24850000  | 0.85566200  | -2.90391700 |
| H | 1.89680300  | 0.13507200  | -2.56635500 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.65697800  | -3.03236600 | 2.69300400  |
| C  | 3.27130600  | -3.10113800 | 2.55353200  |
| C  | 2.61769300  | -2.29030800 | 1.62814800  |
| C  | 3.36092800  | -1.41075000 | 0.83564600  |
| C  | 4.75178500  | -1.33065400 | 0.98828600  |
| C  | 5.39848800  | -2.14129200 | 1.91188700  |
| C  | 2.68966500  | -0.48438200 | -0.10300200 |
| O  | 1.39571000  | -0.43735800 | -0.13310200 |
| Si | -0.00430700 | -0.89035100 | -1.14865100 |
| O  | -0.92274200 | -0.73224400 | 0.43614900  |
| N  | -2.12731600 | -0.13945000 | 0.43589100  |
| C  | -2.17585900 | 1.19396400  | 0.43163200  |
| C  | -3.40999200 | 1.87490600  | 0.36108800  |
| C  | -4.55621000 | 1.10588500  | 0.37335000  |
| C  | -4.50411500 | -0.29959700 | 0.47293700  |
| C  | -3.24150200 | -0.93995600 | 0.49539500  |
| C  | -0.88219700 | 1.91901600  | 0.54139100  |
| C  | -0.55726700 | 2.72636900  | 1.65348000  |
| C  | 0.64358700  | 3.40678400  | 1.60981400  |
| C  | 1.50349000  | 3.32326400  | 0.49725000  |
| C  | 1.14670000  | 2.47861300  | -0.58202700 |
| N  | -0.02983000 | 1.78194800  | -0.47840400 |
| O  | -0.35601800 | 0.92845100  | -1.46121000 |
| C  | 1.14099300  | -0.98609900 | -2.77096900 |
| C  | 2.39191100  | -1.05128100 | -2.54235900 |
| C  | 3.58821600  | -1.11206200 | -1.92588800 |
| Cl | -1.81261300 | -1.22555100 | -2.36255000 |
| Cl | 0.23824500  | -3.04505700 | -0.74997100 |
| C  | -1.43433600 | 2.81170200  | 2.87603200  |
| H  | 0.93581300  | 4.02366100  | 2.45579000  |
| C  | -3.45443600 | 3.37558400  | 0.25306100  |
| H  | -5.52624500 | 1.59146900  | 0.30709700  |
| C  | -5.66790600 | -1.11288100 | 0.52962000  |
| H  | 3.18503400  | 0.47942300  | -0.25028200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.53965500  | -2.32374400 | 1.51805000  |
| H | 5.32550700  | -0.63783400 | 0.37647100  |
| H | 2.69584900  | -3.78361700 | 3.17038300  |
| H | 6.47563000  | -2.08075600 | 2.02648600  |
| H | 5.16096300  | -3.66680600 | 3.41519300  |
| H | 4.28826700  | -0.28563400 | -2.02249500 |
| H | 4.00820700  | -2.08995800 | -1.70295900 |
| H | 0.63496000  | -1.07028200 | -3.72595900 |
| C | 2.73025100  | 4.03669900  | 0.41327900  |
| H | -2.30951300 | 2.16421000  | 2.81687800  |
| H | -1.76954400 | 3.83982100  | 3.03525300  |
| H | -0.85594900 | 2.51223100  | 3.75334800  |
| H | -3.26397600 | 3.85230000  | 1.21869900  |
| H | -4.44315500 | 3.68937600  | -0.08353600 |
| H | -2.71542400 | 3.74515300  | -0.46208000 |
| C | 3.52528600  | 3.91191800  | -0.69624900 |
| H | 3.01507800  | 4.67887400  | 1.24023900  |
| H | 4.45875800  | 4.45995900  | -0.76069100 |
| C | 3.13243600  | 3.07420500  | -1.77336900 |
| C | 1.96196000  | 2.35621400  | -1.72907100 |
| H | 3.76677000  | 3.00309400  | -2.65066400 |
| H | 1.64814100  | 1.71448000  | -2.54243600 |
| C | -5.54956300 | -2.47553700 | 0.61578500  |
| H | -6.64048300 | -0.63224900 | 0.50603900  |
| H | -6.43776700 | -3.09594200 | 0.66144000  |
| C | -4.26924800 | -3.08830700 | 0.64157100  |
| C | -3.11821600 | -2.34286400 | 0.57618400  |
| H | -4.19865800 | -4.16862900 | 0.70791800  |
| H | -2.13390200 | -2.79550500 | 0.57204200  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.53711200  | -0.45922100 | 2.05652900  |
| C  | 5.18613500  | -0.87768200 | 0.77104300  |
| C  | 3.85664900  | -1.14755200 | 0.46425800  |
| C  | 2.87683500  | -0.99928100 | 1.45203200  |
| C  | 3.22604800  | -0.58215900 | 2.74052600  |
| C  | 4.55791100  | -0.31082000 | 3.04076000  |
| C  | 1.45180900  | -1.21345900 | 1.12181100  |
| O  | 1.15582600  | -1.18998800 | -0.14086700 |
| Si | -0.43267700 | -1.47832400 | -0.91182100 |
| O  | -1.17985900 | -0.63334900 | 0.59599000  |
| N  | -2.14053700 | 0.28641100  | 0.43943200  |
| C  | -1.79053200 | 1.51755600  | 0.04798700  |
| C  | -2.76827100 | 2.50339800  | -0.19358100 |
| C  | -4.08431600 | 2.16329100  | 0.05840900  |
| C  | -4.44222900 | 0.89257300  | 0.54476400  |
| C  | -3.42898800 | -0.07965400 | 0.73180300  |
| C  | -0.33291700 | 1.79423100  | -0.05347900 |
| C  | 0.31178400  | 2.71405600  | 0.80441900  |
| C  | 1.65917000  | 2.93145200  | 0.59952900  |
| C  | 2.36399700  | 2.28664600  | -0.43871600 |
| C  | 1.68003500  | 1.35554300  | -1.25775500 |
| N  | 0.35156500  | 1.12943900  | -0.98575100 |
| O  | -0.30131500 | 0.19293500  | -1.69943600 |
| C  | -0.59505200 | -3.21573000 | 0.04397500  |
| C  | 0.20551300  | -3.35855600 | 1.02813500  |
| C  | 1.22644300  | -3.15583400 | 1.88869000  |
| Cl | -2.39725300 | -1.66386400 | -1.86241800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Cl | 0.57541100  | -2.40024100 | -2.62720100 |
| C  | -0.44562100 | 3.39700700  | 1.91175400  |
| H  | 2.19697400  | 3.61471300  | 1.25186700  |
| C  | -2.42212000 | 3.85792800  | -0.75546300 |
| H  | -4.86581800 | 2.89650700  | -0.12294400 |
| C  | -5.78483700 | 0.52848100  | 0.84123000  |
| C  | -3.72261600 | -1.37702700 | 1.20519000  |
| H  | 0.71289600  | -0.81829200 | 1.82279000  |
| H  | 3.56170100  | -1.45829500 | -0.53370400 |
| H  | 2.45748600  | -0.46319200 | 3.50034500  |
| H  | 5.94917100  | -0.98675500 | 0.00703900  |
| H  | 4.83243600  | 0.01757700  | 4.03769300  |
| H  | 6.57519500  | -0.24630200 | 2.29140000  |
| H  | 2.18725500  | -3.61548200 | 1.66986800  |
| H  | 1.02494900  | -2.90887600 | 2.92793900  |
| H  | -1.31210800 | -3.93421200 | -0.33871000 |
| C  | 3.74302800  | 2.51638300  | -0.69119400 |
| H  | -1.11974800 | 2.70521000  | 2.42298300  |
| H  | -1.04039500 | 4.23204200  | 1.53038100  |
| H  | 0.25681700  | 3.79650400  | 2.64405700  |
| H  | -1.34938200 | 3.99583300  | -0.89496400 |
| H  | -2.79705200 | 4.65052900  | -0.10300400 |
| H  | -2.90056600 | 3.97430400  | -1.73124900 |
| C  | 4.37360300  | 1.85503600  | -1.71327000 |
| H  | 4.27610700  | 3.22422000  | -0.06473200 |
| H  | 5.42554300  | 2.03314400  | -1.90805600 |
| C  | 3.66087900  | 0.93209300  | -2.52130000 |
| C  | 2.33038800  | 0.66864100  | -2.30353300 |
| H  | 4.17780600  | 0.41855100  | -3.32491100 |
| H  | 1.77858000  | -0.04986900 | -2.89653500 |
| C  | -5.03026900 | -1.68230400 | 1.48619100  |
| H  | -2.92223500 | -2.09597600 | 1.32788400  |
| H  | -5.27802700 | -2.67308400 | 1.85167400  |
| C  | -6.06845800 | -0.72965700 | 1.30200300  |
| H  | -6.56812200 | 1.26505400  | 0.69511100  |
| H  | -7.09178000 | -1.00755000 | 1.52904800  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.30984300  | 0.22470700  | 2.40194800  |
| C  | 3.98416700  | 0.63532100  | 2.56014300  |
| C  | 2.96784000  | -0.00898500 | 1.86231900  |
| C  | 3.28116000  | -1.07121800 | 1.00747500  |
| C  | 4.60703800  | -1.48567300 | 0.85073300  |
| C  | 5.62132900  | -0.83381600 | 1.54707600  |
| C  | 2.22112000  | -1.72283000 | 0.20618500  |
| O  | 1.13656300  | -1.03175400 | 0.04489000  |
| Si | -0.39056700 | -1.48466700 | -0.75262700 |
| O  | -1.16759100 | -0.56881300 | 0.69327300  |
| N  | -2.20185800 | 0.25522800  | 0.46731200  |
| C  | -1.95459500 | 1.46412400  | -0.05134500 |
| C  | -3.00838700 | 2.33155600  | -0.40186600 |
| C  | -4.29380500 | 1.91152600  | -0.11569100 |
| C  | -4.54604000 | 0.68139400  | 0.52024300  |
| C  | -3.45629700 | -0.17379100 | 0.81581400  |
| C  | -0.52314900 | 1.85116300  | -0.15508200 |
| C  | 0.02303900  | 2.88767600  | 0.63543700  |
| C  | 1.36663800  | 3.15949800  | 0.47777700  |
| C  | 2.16326300  | 2.44874400  | -0.44404300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.56966900  | 1.42077400  | -1.21476200 |
| N  | 0.23943900  | 1.15420400  | -0.99616800 |
| O  | -0.33114300 | 0.12802200  | -1.65627300 |
| C  | -0.47850100 | -3.15033400 | 0.33964300  |
| C  | 0.60577600  | -3.44666000 | 0.94384200  |
| C  | 1.86725000  | -3.38150400 | 1.42374600  |
| Cl | -2.34590000 | -1.83971000 | -1.67534400 |
| Cl | 0.64900500  | -2.46687200 | -2.43226600 |
| C  | -0.82583600 | 3.61777500  | 1.64121300  |
| H  | 1.83042100  | 3.92962800  | 1.08865000  |
| C  | -2.76460300 | 3.63843200  | -1.11132000 |
| H  | -5.13456600 | 2.54682700  | -0.38291300 |
| C  | -5.85418400 | 0.24370200  | 0.86591300  |
| H  | 2.54236000  | -2.35258400 | -0.62697400 |
| H  | 1.93238200  | 0.30444500  | 1.96541900  |
| H  | 4.84200000  | -2.30659400 | 0.17751100  |
| H  | 3.74630600  | 1.46148400  | 3.22277600  |
| H  | 6.65210300  | -1.14808600 | 1.42128400  |
| H  | 6.10180300  | 0.73221800  | 2.94344800  |
| H  | 2.63355300  | -4.03856300 | 1.01943800  |
| H  | 2.02297800  | -3.00957500 | 2.43350200  |
| H  | -1.40965100 | -3.70676000 | 0.34939200  |
| C  | 2.31511200  | 0.66193600  | -2.14097300 |
| C  | 3.55559400  | 2.68652400  | -0.60291300 |
| H  | -0.18683600 | 4.19893000  | 2.30680500  |
| H  | -1.41190200 | 2.92102600  | 2.24629200  |
| H  | -1.51885700 | 4.30910100  | 1.15410000  |
| H  | -3.21021900 | 4.46740800  | -0.55572800 |
| H  | -3.23685300 | 3.60479100  | -2.09661200 |
| H  | -1.70410000 | 3.84588800  | -1.26000400 |
| C  | 4.28584900  | 1.93232700  | -1.48417600 |
| H  | 4.02245200  | 3.46443000  | -0.00712600 |
| H  | 5.35038200  | 2.10640700  | -1.59677200 |
| C  | 3.65792600  | 0.92266000  | -2.25972700 |
| H  | 1.82547500  | -0.11644400 | -2.71322600 |
| H  | 4.25114700  | 0.34306300  | -2.95909800 |
| C  | -6.03385400 | -0.96686700 | 1.48098600  |
| H  | -6.69589800 | 0.88815800  | 0.63463800  |
| H  | -7.03121400 | -1.29909700 | 1.74701900  |
| C  | -4.92021100 | -1.79740100 | 1.77872500  |
| C  | -3.64254100 | -1.42120200 | 1.44980200  |
| H  | -5.08410100 | -2.74938100 | 2.27196000  |
| H  | -2.78337200 | -2.04250900 | 1.66649600  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.78111600 | -2.29160000 | 0.45618600  |
| C  | -5.59654800 | -2.87926600 | 0.00788000  |
| C  | -4.40948100 | -2.15244500 | 0.01225200  |
| C  | -4.41543000 | -0.82939200 | 0.46382200  |
| C  | -5.59996300 | -0.23866200 | 0.91477700  |
| C  | -6.78238200 | -0.97248000 | 0.91330300  |
| C  | -3.15772600 | -0.04449000 | 0.48667300  |
| O  | -2.05220300 | -0.72510200 | 0.47441600  |
| Si | -0.44279100 | -0.72921600 | -0.23844200 |
| O  | 1.22332800  | -0.65061800 | -1.06346900 |
| N  | 2.33248100  | -0.70861000 | -0.31087300 |
| C  | 2.73803400  | 0.41588900  | 0.28587300  |
| C  | 3.86426400  | 0.42067200  | 1.13269700  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.56098300  | -0.76688600 | 1.25826800  |
| C  | 4.17741800  | -1.93015800 | 0.56589200  |
| C  | 3.01291900  | -1.89652500 | -0.24123800 |
| C  | 1.98121600  | 1.65256500  | -0.04230700 |
| C  | 2.58230600  | 2.71695600  | -0.75287300 |
| C  | 1.83190900  | 3.85910900  | -0.93872400 |
| C  | 0.53801500  | 3.98651000  | -0.39093500 |
| C  | -0.02370900 | 2.88776800  | 0.30060700  |
| N  | 0.71387400  | 1.72962800  | 0.37094900  |
| O  | 0.14730000  | 0.64448100  | 0.92186600  |
| C  | -0.99274100 | 0.58894500  | -1.64056200 |
| C  | -2.20098000 | 0.97935500  | -1.57651800 |
| C  | -3.49807100 | 1.09217500  | -1.21492800 |
| Cl | 0.20574800  | -2.08556200 | 1.32748800  |
| Cl | -0.95695900 | -2.38258600 | -1.62624400 |
| C  | 3.97362700  | 2.57708400  | -1.31039300 |
| H  | 2.24796300  | 4.68831700  | -1.50434800 |
| C  | 4.28014300  | 1.64034800  | 1.91412300  |
| H  | 5.43264500  | -0.80447200 | 1.90674600  |
| C  | 4.89822500  | -3.15285400 | 0.65231000  |
| H  | -3.17190700 | 0.85640700  | 1.10343800  |
| H  | -3.47661100 | -2.59440900 | -0.32563000 |
| H  | -5.59434600 | 0.78938400  | 1.26912400  |
| H  | -5.59810700 | -3.90703000 | -0.34014400 |
| H  | -7.70169700 | -0.51983300 | 1.26998600  |
| H  | -7.70333100 | -2.86381600 | 0.45415100  |
| H  | -4.23393100 | 0.50748200  | -1.76068200 |
| H  | -3.85105200 | 2.01120000  | -1.75174800 |
| H  | -0.25644200 | 0.82834800  | -2.40156600 |
| C  | -0.23754100 | 5.17226900  | -0.50301300 |
| H  | 4.14517400  | 3.34745200  | -2.06302700 |
| H  | 4.11864000  | 1.60013900  | -1.77809500 |
| H  | 4.73073100  | 2.69710100  | -0.53028100 |
| H  | 3.64900900  | 2.50661800  | 1.71322200  |
| H  | 5.31696500  | 1.90361300  | 1.68974500  |
| H  | 4.21514000  | 1.42171700  | 2.98306500  |
| C  | -1.47887300 | 5.24201300  | 0.07470200  |
| H  | 0.17919600  | 6.01636500  | -1.04291100 |
| H  | -2.06628900 | 6.14987500  | -0.00591900 |
| C  | -1.99619800 | 4.14034000  | 0.80500600  |
| C  | -1.28717000 | 2.97040100  | 0.91939000  |
| H  | -2.96328700 | 4.22865400  | 1.28917100  |
| H  | -1.63885100 | 2.12958200  | 1.50157000  |
| C  | 4.46742600  | -4.25286200 | -0.04070500 |
| H  | 5.78791800  | -3.18951400 | 1.27224800  |
| H  | 5.01770200  | -5.18519300 | 0.02225900  |
| C  | 3.29839700  | -4.18725100 | -0.84514000 |
| C  | 2.56589100  | -3.03145900 | -0.95130900 |
| H  | 2.97521900  | -5.07130100 | -1.38422300 |
| H  | 1.66024400  | -2.97278200 | -1.54284500 |

File: p\_bp4\_R\_631+g\_M06-2X.xyz

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 6.53101900 | -1.52332900 | -1.76020700 |
| C | 5.37135100 | -0.97453700 | -2.30861200 |
| C | 4.18808800 | -0.96400000 | -1.57438300 |
| C | 4.16791100 | -1.50125400 | -0.28394000 |
| C | 5.32736000 | -2.06397500 | 0.26053300  |
| C | 6.50679900 | -2.07333200 | -0.47704900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.90977900  | -1.51377700 | 0.50578600  |
| O  | 1.82702800  | -1.20013700 | -0.14873600 |
| Si | 0.17676500  | -0.99176200 | 0.46265000  |
| O  | -1.49771800 | -0.51900100 | 1.12435100  |
| N  | -2.51086500 | -0.31998300 | 0.26571300  |
| C  | -2.58146000 | 0.85610600  | -0.37100900 |
| C  | -3.58844300 | 1.09808000  | -1.32745700 |
| C  | -4.53301000 | 0.10569600  | -1.51441000 |
| C  | -4.50339100 | -1.09528200 | -0.78358600 |
| C  | -3.44339700 | -1.31592700 | 0.12997800  |
| C  | -1.57941500 | 1.89025700  | 0.00075700  |
| C  | -1.95116100 | 3.12215300  | 0.58470300  |
| C  | -0.95429000 | 4.05779400  | 0.77633100  |
| C  | 0.38201900  | 3.80554200  | 0.39950800  |
| C  | 0.71484200  | 2.53609900  | -0.12868800 |
| N  | -0.30013200 | 1.62209900  | -0.27062000 |
| O  | 0.00048300  | 0.41059000  | -0.75855900 |
| C  | 0.85451300  | 0.23480300  | 1.92847500  |
| C  | 2.11625700  | 0.20871200  | 2.08087600  |
| C  | 3.42227300  | -0.08261600 | 1.87179400  |
| Cl | -0.60773600 | -2.22426800 | -1.15252700 |
| Cl | 0.24173300  | -2.69328800 | 1.85413900  |
| C  | -3.37620100 | 3.37703500  | 0.99658900  |
| H  | -1.19954300 | 5.01566700  | 1.22724600  |
| C  | -3.62712700 | 2.34968800  | -2.16685700 |
| H  | -5.32086500 | 0.25484700  | -2.24834100 |
| C  | -5.48216800 | -2.11546300 | -0.93696900 |
| H  | 2.81447400  | -2.28820400 | 1.27057300  |
| H  | 3.27315000  | -0.56815900 | -2.00328300 |
| H  | 5.30519900  | -2.49500500 | 1.25858400  |
| H  | 5.38628900  | -0.56419800 | -3.31306600 |
| H  | 7.40474200  | -2.51223400 | -0.05494000 |
| H  | 7.45093300  | -1.53185100 | -2.33588600 |
| H  | 3.94490400  | -0.72322400 | 2.57787700  |
| H  | 4.03084800  | 0.63781600  | 1.32824700  |
| H  | 0.12446200  | 0.79341700  | 2.50536300  |
| C  | 1.42462800  | 4.76030800  | 0.54816500  |
| H  | -4.57237500 | 2.87907800  | -2.02155100 |
| H  | -3.55983300 | 2.07294400  | -3.22200500 |
| H  | -2.80591500 | 3.03317800  | -1.94954600 |
| H  | -3.41238500 | 4.21152400  | 1.69773700  |
| H  | -3.81187900 | 2.49992400  | 1.48136900  |
| H  | -4.00001300 | 3.63547600  | 0.13657400  |
| C  | -5.38997200 | -3.26897600 | -0.20461800 |
| H  | -6.29324500 | -1.95703200 | -1.64012000 |
| H  | -6.13715900 | -4.04642400 | -0.31906100 |
| C  | -4.31702700 | -3.46145500 | 0.70641700  |
| C  | -3.34409400 | -2.50891300 | 0.87877400  |
| H  | -4.26236100 | -4.38411300 | 1.27404600  |
| H  | -2.50896200 | -2.65080300 | 1.55390100  |
| C  | 2.70591300  | 4.44277200  | 0.17800600  |
| H  | 1.18314400  | 5.73744800  | 0.95377200  |
| H  | 3.49880300  | 5.17426100  | 0.28749000  |
| C  | 3.00957900  | 3.15910800  | -0.34832700 |
| C  | 2.03538700  | 2.20401200  | -0.49950000 |
| H  | 4.03091300  | 2.92811700  | -0.63380500 |
| H  | 2.24329600  | 1.21225200  | -0.88425700 |

|    |             |             |              |
|----|-------------|-------------|--------------|
| C  | -6.85615800 | -0.74538800 | 1.17902900   |
| C  | -5.79955100 | 0.09346900  | 1.54248000   |
| C  | -4.50577600 | -0.19218500 | 1.11984100   |
| C  | -4.26728000 | -1.32075500 | 0.33019900   |
| C  | -5.32241200 | -2.16318100 | -0.02945400  |
| C  | -6.61737300 | -1.87225400 | 0.39304300   |
| C  | -2.90102100 | -1.64522100 | -0.15154300  |
| O  | -2.07396800 | -0.63935600 | -0.26429400  |
| Si | -0.36103800 | -0.69163700 | -0.72794100  |
| O  | -0.02829200 | 0.56302100  | 0.60252600   |
| N  | 0.55953200  | 1.72461700  | 0.27209600   |
| C  | 1.88873500  | 1.74203700  | 0.12383700   |
| C  | 2.54893700  | 2.91426700  | -0.29955600  |
| C  | 1.77840400  | 4.05130300  | -0.46004700  |
| C  | 0.39199600  | 4.04916800  | -0.22076500  |
| C  | -0.23601000 | 2.83142400  | 0.13606200   |
| C  | 2.62266700  | 0.49856600  | 0.48271600   |
| C  | 3.56130300  | 0.47375000  | 1.54145700   |
| C  | 4.27309700  | -0.69235700 | 1.73307700   |
| C  | 4.08352800  | -1.82044100 | 0.90655000   |
| C  | 3.09356100  | -1.76860000 | -0.10440900  |
| N  | 2.37907900  | -0.59898400 | -0.23805400  |
| O  | 1.43859100  | -0.55336800 | -1.19234000  |
| C  | -0.01677800 | -2.01451600 | 0.76468000   |
| C  | -1.07140300 | -2.59168300 | 1.17903000   |
| C  | -2.37950500 | -2.89908500 | 1.35319900   |
| Cl | -0.72757600 | 0.82292800  | -2.25990700  |
| Cl | -0.57547600 | -2.32252100 | -2.19281800  |
| C  | 3.74004400  | 1.66826900  | 2.43985600   |
| H  | 4.99704600  | -0.75099700 | 2.54164500   |
| C  | 4.01969000  | 2.93944000  | -0.62874600  |
| H  | 2.25395700  | 4.97287600  | -0.78689400  |
| C  | -0.42230400 | 5.20732400  | -0.35783600  |
| H  | -2.83579200 | -2.41941400 | -0.91869100  |
| H  | -3.67567200 | 0.44741300  | 1.40161700   |
| H  | -5.13045000 | -3.03799900 | -0.64548700  |
| H  | -5.98800400 | 0.96963500  | 2.15450000   |
| H  | -7.43832500 | -2.52100300 | 0.10625200   |
| H  | -7.86516400 | -0.51856200 | 1.50819900   |
| H  | -2.89021200 | -2.48327900 | 2.21816900   |
| H  | -2.76474900 | -3.84117300 | 0.96974400   |
| H  | 0.97767000  | -2.17848400 | 1.16377500   |
| C  | 4.81740200  | -3.02598400 | 1.06166000   |
| H  | 4.29113600  | 1.37292200  | 3.33310900   |
| H  | 2.77519700  | 2.07763100  | 2.74957600   |
| H  | 4.30508200  | 2.46426500  | 1.94770300   |
| H  | 4.53433500  | 3.69972300  | -0.103583100 |
| H  | 4.14317600  | 3.19965100  | -1.68315700  |
| H  | 4.50805700  | 1.97807900  | -0.46694000  |
| C  | -1.77333500 | 5.12461500  | -0.14764600  |
| H  | 0.04885100  | 6.14522200  | -0.63330900  |
| H  | -2.39440200 | 6.00756900  | -0.25150400  |
| C  | -2.37726900 | 3.88487500  | 0.19589900   |
| C  | -1.63054900 | 2.74291600  | 0.33470400   |
| H  | -3.45144300 | 3.83917600  | 0.34059400   |
| H  | -2.07201800 | 1.78086900  | 0.56056600   |
| C  | 4.56008400  | -4.09781300 | 0.24522100   |
| H  | 5.57742900  | -3.07727900 | 1.83438500   |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 5.12138100 | -5.01812100 | 0.36345400  |
| C | 3.55896100 | -4.01694300 | -0.75644600 |
| C | 2.82191100 | -2.87202100 | -0.94021300 |
| H | 3.36925700 | -4.87616800 | -1.39067300 |
| H | 2.04755900 | -2.79636200 | -1.69401400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.68570600 | 2.49200500  | -2.46297300 |
| H | -4.09095900 | 3.97908200  | 0.85438000  |
| H | -4.20147400 | 2.21335500  | 0.87607200  |
| H | -4.33202900 | 3.09670100  | -0.65431800 |
| H | -5.71822400 | -2.76785600 | -1.82466400 |
| H | -5.55977100 | -4.60947100 | -0.17514700 |
| H | -3.90579000 | -4.49818300 | 1.67314700  |
| H | -2.37629900 | -2.55247100 | 1.88992900  |
| H | 0.27582200  | 6.10783000  | 0.67705900  |
| H | 2.73546100  | 5.86727000  | 0.49887500  |
| H | 3.74117400  | 3.64752900  | 0.01154000  |
| H | 2.31100200  | 1.65825400  | -0.29927400 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.87901900  | 2.63209000  | -0.11841700 |
| C  | 0.47836600  | 2.77552100  | -0.03689600 |
| C  | -0.11967000 | 4.02500500  | 0.25627400  |
| C  | 0.72866900  | 5.14824200  | 0.45044000  |
| C  | 2.08826700  | 5.00967100  | 0.35186300  |
| C  | 2.66235800  | 3.74305400  | 0.06947900  |
| N  | -0.35846000 | 1.70314000  | -0.23343600 |
| C  | -1.68891900 | 1.79499900  | -0.20007800 |
| C  | -2.32784300 | 3.00349900  | 0.15567900  |
| C  | -1.52224500 | 4.10119300  | 0.37647800  |
| O  | 0.18080400  | 0.50726200  | -0.51530800 |
| Si | 0.30878600  | -0.78623400 | 0.84094600  |
| Cl | 0.34139200  | -2.41719400 | 2.31078800  |
| C  | -2.47736300 | 0.58986900  | -0.57106000 |
| C  | -3.35413600 | 0.57529900  | -1.67717200 |
| C  | -4.17062300 | -0.52982600 | -1.82512900 |
| C  | -4.14572600 | -1.59869900 | -0.90871400 |
| C  | -3.21046000 | -1.56469600 | 0.15535200  |
| N  | -2.38167100 | -0.47217500 | 0.23749300  |
| C  | -3.11192500 | -2.61273100 | 1.09641500  |
| C  | -3.96049300 | -3.68393200 | 0.95857900  |
| C  | -4.90722700 | -3.74689700 | -0.09748400 |
| C  | -4.99987600 | -2.73030700 | -1.01212300 |
| C  | -3.82343600 | 3.07084500  | 0.31340500  |
| C  | -3.37803900 | 1.68322900  | -2.69852200 |
| O  | -1.48096900 | -0.44210500 | 1.23277500  |
| O  | 2.03994300  | -0.96372300 | 0.46658400  |
| C  | 2.61080000  | -0.93754600 | -0.70500700 |
| C  | 4.07433900  | -1.18146000 | -0.71847200 |
| C  | 4.69790000  | -1.79065500 | 0.37472000  |
| C  | 6.07321700  | -1.99981600 | 0.35074800  |
| C  | 6.82483300  | -1.59772600 | -0.75552400 |
| C  | 6.20149600  | -0.98248900 | -1.84225300 |
| C  | 4.82502000  | -0.77518500 | -1.82607700 |
| C  | -0.13890400 | -2.13569400 | -0.57760700 |
| C  | 0.82399800  | -2.43485300 | -1.35683200 |
| C  | 2.07137000  | -2.52717100 | -1.87002300 |
| Cl | 0.77744300  | 0.69702600  | 2.36849600  |
| H  | -4.85420600 | -0.57625400 | -2.66938700 |
| H  | -1.97487900 | 5.04938700  | 0.65445500  |
| H  | 2.22992900  | -0.20950300 | -1.42657200 |
| H  | 4.10094800  | -2.08678400 | 1.23145600  |
| H  | 4.33415100  | -0.29564700 | -2.66984400 |
| H  | 6.56167400  | -2.47214100 | 1.19667700  |
| H  | 6.78673400  | -0.66447500 | -2.69868900 |
| H  | 7.89768600  | -1.76100500 | -0.76896000 |
| H  | 2.28906800  | -2.12326400 | -2.85557200 |
| H  | 2.71128300  | -3.33386700 | -1.51979500 |
| H  | -1.09396000 | -2.65079900 | -0.56759700 |
| H  | -4.38420800 | 2.09890900  | -2.79222600 |
| H  | -3.09453600 | 1.27628700  | -3.67269700 |

# ALLYLATION - B3LYP/6-31G(d)

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|    |             |             |             |
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| C  | 5.08958700  | -2.88670900 | 0.94442200  |
| C  | 4.27399700  | -1.73198700 | 0.80517500  |
| C  | 3.21814700  | -1.76127500 | -0.15054500 |
| C  | 2.99330000  | -2.89822400 | -0.95351300 |
| C  | 3.81742100  | -3.99123100 | -0.79618700 |
| C  | 4.86592300  | -3.99190700 | 0.15788000  |
| N  | 2.43675300  | -0.63031800 | -0.27241800 |
| C  | 2.68114500  | 0.51538800  | 0.39262200  |
| C  | 3.68496300  | 0.56361300  | 1.39137400  |
| C  | 4.45307400  | -0.57174200 | 1.58421700  |
| O  | 1.40761600  | -0.66241800 | -1.14650600 |
| Si | -0.37007800 | -0.78986800 | -0.51077800 |
| Cl | -0.83890900 | 0.70408500  | -2.15254400 |
| C  | 1.89341300  | 1.72610100  | 0.02941100  |
| C  | 2.49181000  | 2.88965200  | -0.50639700 |
| C  | 1.69618800  | 4.01852300  | -0.63601600 |
| C  | 0.34660500  | 4.03059000  | -0.23678100 |
| C  | -0.23764900 | 2.81981000  | 0.23599700  |
| N  | 0.57303500  | 1.70990800  | 0.30108400  |
| C  | -1.58999500 | 2.76140500  | 0.63289400  |
| C  | -2.34343500 | 3.91237700  | 0.56286300  |
| C  | -1.78887900 | 5.12994300  | 0.09004700  |
| C  | -0.47412700 | 5.18931000  | -0.30581100 |
| C  | 3.89351300  | 1.79276200  | 2.24251700  |
| C  | 3.92871000  | 2.92204100  | -0.97106500 |
| O  | 0.02900700  | 0.54779900  | 0.72523300  |
| O  | -2.04440400 | -0.77671200 | 0.11277500  |
| C  | -3.18005300 | -0.79191600 | -0.54095500 |
| C  | -4.40676500 | -1.01133300 | 0.26178900  |
| C  | -4.34890000 | -1.59677100 | 1.53643100  |
| C  | -5.51659200 | -1.76321400 | 2.27691900  |
| C  | -6.74688300 | -1.35023700 | 1.75442600  |
| C  | -6.80803400 | -0.76452200 | 0.48697800  |
| C  | -5.64267100 | -0.59639700 | -0.25840200 |
| C  | -0.72712000 | -2.33528900 | -1.78757000 |
| Cl | 0.20306200  | -2.17082200 | 1.16809300  |
| H  | 2.12799500  | 4.92531600  | -1.05052600 |
| H  | 5.22103300  | -0.57075100 | 2.35203000  |
| H  | -3.28060500 | -0.10037000 | -1.37876400 |
| H  | -3.38991600 | -1.90732600 | 1.93787300  |
| H  | -5.68778800 | -0.13846200 | -1.24338100 |
| H  | -5.46896700 | -2.21313300 | 3.26432300  |
| H  | -7.76078800 | -0.43701800 | 0.08157500  |
| H  | -7.65503900 | -1.48229100 | 2.33557100  |
| H  | 3.96602500  | 3.25811100  | -2.01217600 |
| H  | 4.41309700  | 1.94594100  | -0.92024500 |
| H  | 4.51752800  | 3.63079300  | -0.37946200 |
| H  | 4.46129100  | 1.52729300  | 3.13733200  |
| H  | 2.94362700  | 2.23064200  | 2.56131600  |
| H  | 4.45934400  | 2.56576000  | 1.71238400  |
| H  | -2.00429200 | 1.82568100  | 0.98235300  |
| H  | -3.38280900 | 3.88669300  | 0.87418000  |
| H  | -0.03928400 | 6.11435100  | -0.67065600 |
| H  | -2.41204900 | 6.01697600  | 0.04225500  |
| H  | 2.19501300  | -2.89324500 | -1.68144600 |

|   |             |             |             |
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| H | 3.65957800  | -4.86833200 | -1.41550900 |
| H | 5.49375100  | -4.87077400 | 0.26189900  |
| H | 5.89085600  | -2.87138500 | 1.67639200  |
| H | 0.05084700  | -2.24435500 | -2.54715900 |
| C | -2.05533700 | -2.22017700 | -2.33791200 |
| H | -0.59004100 | -3.22368800 | -1.17034300 |
| C | -3.20419900 | -2.53714700 | -1.63778000 |
| H | -2.16945900 | -1.68257500 | -3.27712100 |
| H | -4.16855000 | -2.47316900 | -2.13217500 |
| H | -3.14911000 | -3.21312000 | -0.78879100 |

File: a\_bp1\_R\_631g\_B3LYP.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.67052200 | 2.75938500  | 0.55107200  |
| C  | -0.30709400 | 2.84401100  | 0.19904500  |
| C  | 0.27314200  | 4.07008300  | -0.23878700 |
| C  | -0.56200500 | 5.21788800  | -0.31614500 |
| C  | -1.88720200 | 5.13347500  | 0.03789400  |
| C  | -2.43809800 | 3.90054500  | 0.47373100  |
| N  | 0.51957600  | 1.74680500  | 0.27619900  |
| C  | 1.84523200  | 1.78501400  | 0.03871000  |
| C  | 2.44199500  | 2.96450400  | -0.46213100 |
| C  | 1.63401400  | 4.08390100  | -0.59734000 |
| C  | 2.64076700  | 0.57811300  | 0.39798500  |
| N  | 2.43818000  | -0.55516500 | -0.30213400 |
| C  | 3.25434600  | -1.66391700 | -0.19855100 |
| C  | 4.27455200  | -1.64175700 | 0.79519700  |
| C  | 4.39753700  | -0.50408100 | 1.61727500  |
| C  | 3.61377200  | 0.62071300  | 1.42730100  |
| C  | 3.10222100  | -2.76923300 | -1.05977800 |
| C  | 3.95253000  | -3.84388700 | -0.91523900 |
| C  | 4.95729700  | -3.85710000 | 0.08440000  |
| C  | 5.11627700  | -2.77890000 | 0.92265400  |
| O  | 1.42172600  | -0.59350700 | -1.19135600 |
| Si | -0.36927500 | -0.75970900 | -0.57608400 |
| Cl | -0.83283100 | 0.72230900  | -2.20444100 |
| C  | 3.77343900  | 1.83337500  | 2.31180400  |
| C  | 3.89187700  | 3.02470300  | -0.88074700 |
| O  | -0.01566300 | 0.57169200  | 0.67522200  |
| O  | -2.07822500 | -0.69782900 | -0.05200100 |
| C  | -2.85001900 | -1.65705900 | 0.39652700  |
| C  | -4.29040700 | -1.33859400 | 0.54376100  |
| C  | -4.87195500 | -0.25869600 | -0.13918000 |
| C  | -6.22188400 | 0.03175700  | 0.04278200  |
| C  | -7.00083200 | -0.75046500 | 0.90213400  |
| C  | -6.42527500 | -1.82622100 | 1.58376500  |
| C  | -5.07509700 | -2.12135400 | 1.40474600  |
| C  | -0.72606000 | -2.32844500 | -1.83352200 |
| Cl | 0.23188200  | -2.14723500 | 1.10728100  |
| H  | 2.06467500  | 5.00319800  | -0.98475400 |
| H  | 5.13775500  | -0.51013900 | 2.41174800  |
| H  | -2.43028600 | -2.31723900 | 1.15637400  |
| H  | -4.25985100 | 0.34643300  | -0.79990500 |
| H  | -4.62534500 | -2.95682600 | 1.93552200  |
| H  | -6.66886700 | 0.86959800  | -0.48446900 |
| H  | -7.02631400 | -2.43198600 | 2.25538400  |
| H  | -8.05329900 | -0.52048500 | 1.04113600  |
| H  | 2.80685200  | 2.24807300  | 2.61092400  |
| H  | 4.34164600  | 2.62706000  | 1.81569700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.31917700  | 1.55785300  | 3.21723100  |
| H | 4.45724200  | 3.71296200  | -0.24361400 |
| H | 3.95863300  | 3.40191900  | -1.90605800 |
| H | 4.38142900  | 2.05015100  | -0.85315400 |
| H | 5.88821300  | -2.77021300 | 1.68566000  |
| H | 5.60641600  | -4.72141100 | 0.17919000  |
| H | 3.85193100  | -4.69394000 | -1.58235200 |
| H | 2.34599700  | -2.74680100 | -1.83078900 |
| H | -0.12993200 | 6.15426900  | -0.65428100 |
| H | -2.52185500 | 6.01197900  | -0.01634800 |
| H | -3.48694500 | 3.85447300  | 0.74883900  |
| H | -2.08445000 | 1.81142900  | 0.86609200  |
| H | 0.25483000  | -2.75848700 | -2.03325500 |
| H | -1.14544700 | -1.86499100 | -2.72598500 |
| C | -1.62497900 | -3.25759500 | -1.19555000 |
| C | -2.98978400 | -3.05307500 | -1.10914000 |
| H | -1.19230500 | -4.05556400 | -0.59571300 |
| H | -3.61909200 | -3.81111600 | -0.65315100 |
| H | -3.47851100 | -2.39738200 | -1.82447500 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.23826500  | 1.56948600  | -2.11465500 |
| C  | 1.47207200  | 1.97935800  | -1.00460900 |
| C  | 1.94131100  | 2.99222100  | -0.11932100 |
| C  | 3.22179900  | 3.55632500  | -0.36315300 |
| C  | 3.96915500  | 3.14529000  | -1.44313900 |
| C  | 3.46846900  | 2.15619500  | -2.32506000 |
| N  | 0.22725400  | 1.43516900  | -0.75308600 |
| C  | -0.59558600 | 1.90465700  | 0.20096300  |
| C  | -0.13774500 | 2.85542600  | 1.14916100  |
| C  | 1.13210500  | 3.37232600  | 0.97302000  |
| C  | -2.00499600 | 1.42928600  | 0.19977700  |
| N  | -2.22601600 | 0.14364500  | 0.51946400  |
| C  | -3.47773300 | -0.37490400 | 0.77637700  |
| C  | -4.59255000 | 0.49404000  | 0.59245000  |
| C  | -4.36532700 | 1.80405500  | 0.12188300  |
| C  | -3.08766900 | 2.29838300  | -0.07720600 |
| C  | -3.64504600 | -1.70277200 | 1.21753900  |
| C  | -4.92224400 | -2.14908200 | 1.48121700  |
| C  | -6.04932000 | -1.30819900 | 1.30224600  |
| C  | -5.89050800 | -0.01483600 | 0.86220600  |
| O  | -1.15071100 | -0.66490600 | 0.64645100  |
| Si | -0.32379800 | -1.36040800 | -0.87973300 |
| Cl | -0.66537700 | -3.40606500 | -0.02741900 |
| C  | -2.85792700 | 3.68173900  | -0.63693400 |
| C  | -0.97677800 | 3.22944300  | 2.34773500  |
| O  | -0.20950200 | 0.43849300  | -1.54774600 |
| O  | 1.18987500  | -1.07871100 | 0.06279600  |
| C  | 2.11265900  | -1.96367200 | 0.35649400  |
| C  | 3.32245400  | -1.51308000 | 1.08417400  |
| C  | 3.73231900  | -0.17216100 | 1.10364600  |
| C  | 4.86027700  | 0.20345900  | 1.82871600  |
| C  | 5.59056600  | -0.75378000 | 2.54014700  |
| C  | 5.18632600  | -2.09144700 | 2.52651500  |
| C  | 4.05875200  | -2.47058200 | 1.80123800  |
| C  | 0.75967400  | -2.06370000 | -2.46382600 |
| Cl | -2.20797000 | -1.42808600 | -2.07877300 |
| H  | 1.52026600  | 4.09363100  | 1.68591800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.22069900 | 2.44015900  | -0.08592800 |
| H | 1.76295400  | -2.95862500 | 0.62834700  |
| H | 3.16315100  | 0.56863400  | 0.55692700  |
| H | 3.74256700  | -3.51061300 | 1.79289000  |
| H | 5.16941900  | 1.24461800  | 1.84024500  |
| H | 5.74638600  | -2.83730800 | 3.08252900  |
| H | 6.46963000  | -0.45734100 | 3.10509200  |
| H | -0.40572700 | 3.88464700  | 3.00893900  |
| H | -1.26214100 | 2.33860700  | 2.91729400  |
| H | -1.89739400 | 3.75337900  | 2.07549500  |
| H | -2.37446800 | 4.35544500  | 0.07694800  |
| H | -3.81331400 | 4.12950100  | -0.91903600 |
| H | -2.22675600 | 3.63939300  | -1.53038900 |
| H | -6.74564200 | 0.63778700  | 0.71798900  |
| H | -7.04182200 | -1.69281500 | 1.51328900  |
| H | -5.06665300 | -3.16645000 | 1.83042000  |
| H | -2.78021000 | -2.34129400 | 1.33604300  |
| H | 3.58910100  | 4.32197500  | 0.31270600  |
| H | 4.94342900  | 3.58490500  | -1.62964000 |
| H | 4.05915700  | 1.85860200  | -3.18541900 |
| H | 1.83972300  | 0.83260900  | -2.79680600 |
| H | 0.02940300  | -2.59486100 | -3.07229400 |
| C | 1.82134100  | -2.92058300 | -1.99578300 |
| H | 1.11110600  | -1.16435300 | -2.97083800 |
| C | 3.00066300  | -2.46177400 | -1.44151800 |
| H | 1.60022000  | -3.98196400 | -1.90056600 |
| H | 3.76464000  | -3.17176400 | -1.14052400 |
| H | 3.34911900  | -1.45764500 | -1.66654500 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.12258600 | -2.40768600 | 0.60666100  |
| C  | -3.25304400 | -1.00745300 | 0.50060700  |
| C  | -4.53427900 | -0.38075300 | 0.48723800  |
| C  | -5.68797600 | -1.20688500 | 0.57285900  |
| C  | -5.55530700 | -2.57034700 | 0.68064700  |
| C  | -4.26837900 | -3.16696900 | 0.70069500  |
| N  | -2.14906900 | -0.18770300 | 0.42238500  |
| C  | -2.21439000 | 1.15869000  | 0.41807200  |
| C  | -3.46481200 | 1.81176500  | 0.34255300  |
| C  | -4.60283600 | 1.01939700  | 0.37051300  |
| O  | -0.92475900 | -0.76167500 | 0.42937900  |
| Si | 0.04634100  | -0.91285300 | -1.14570600 |
| Cl | 0.20089200  | -3.11725300 | -0.74687000 |
| C  | -0.93325400 | 1.90241400  | 0.56206800  |
| C  | -0.65517000 | 2.69741700  | 1.70251200  |
| C  | 0.51013200  | 3.44321800  | 1.69574600  |
| C  | 1.37105700  | 3.46114400  | 0.57880700  |
| C  | 1.07273200  | 2.62131300  | -0.53226300 |
| N  | -0.04919700 | 1.82180200  | -0.44933300 |
| C  | 1.87558200  | 2.63409200  | -1.69197500 |
| C  | 2.97914200  | 3.46092300  | -1.72588500 |
| C  | 3.31884100  | 4.27565500  | -0.61714900 |
| C  | 2.53121300  | 4.27821700  | 0.51063700  |
| C  | -3.59262300 | 3.30951300  | 0.19327200  |
| C  | -1.57831500 | 2.71248400  | 2.89649700  |
| O  | -0.30228500 | 0.95648800  | -1.45248200 |
| O  | 1.41581500  | -0.44865900 | -0.08791600 |
| C  | 2.72407300  | -0.46777700 | -0.02646200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.42880600  | -1.41854300 | 0.86924400  |
| C  | 2.75647700  | -2.44724100 | 1.54521000  |
| C  | 3.45095900  | -3.26842400 | 2.43318600  |
| C  | 4.81544300  | -3.07163700 | 2.65817600  |
| C  | 5.48857000  | -2.03771500 | 1.99902000  |
| C  | 4.79863600  | -1.21395900 | 1.11481700  |
| C  | 1.26598500  | -1.07254600 | -2.78528700 |
| Cl | -1.75222900 | -1.17577000 | -2.44840300 |
| H  | 0.76419200  | 4.04512500  | 2.56326700  |
| H  | -5.57883700 | 1.49265200  | 0.30875600  |
| H  | 3.17557900  | 0.52775300  | -0.04395900 |
| H  | 1.69692100  | -2.59269600 | 1.37773800  |
| H  | 5.32310600  | -0.40446300 | 0.61219900  |
| H  | 2.92281400  | -4.06186400 | 2.95414500  |
| H  | 6.54663000  | -1.87193100 | 2.17911900  |
| H  | 5.35174000  | -3.71477600 | 3.35007900  |
| H  | -1.02956200 | 3.04162600  | 3.78208300  |
| H  | -1.99566900 | 1.72368100  | 3.10384800  |
| H  | -2.41294500 | 3.40702700  | 2.75225800  |
| H  | -4.11504900 | 3.74502700  | 1.05136600  |
| H  | -4.18609800 | 3.53637600  | -0.69839100 |
| H  | -2.62937100 | 3.80982300  | 0.08566500  |
| H  | 2.77182200  | 4.91089100  | 1.35895200  |
| H  | 4.19820200  | 4.90917500  | -0.66830100 |
| H  | 3.59230300  | 3.49336500  | -2.62080000 |
| H  | 1.59415200  | 2.02907700  | -2.54231300 |
| H  | -6.66627300 | -0.73730400 | 0.55712600  |
| H  | -6.43680400 | -3.19925100 | 0.75079700  |
| H  | -4.18340100 | -4.24536400 | 0.78869200  |
| H  | -2.13850200 | -2.85635400 | 0.60612900  |
| H  | 0.71855400  | -1.78854300 | -3.39583900 |
| C  | 2.55849700  | -1.54562700 | -2.38486200 |
| H  | 1.26299000  | -0.07726400 | -3.23311000 |
| C  | 3.56334100  | -0.72385300 | -1.91252900 |
| H  | 2.68068800  | -2.62018200 | -2.26255600 |
| H  | 4.52957100  | -1.14554400 | -1.65876000 |
| H  | 3.56579500  | 0.32435500  | -2.19762100 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.10320400 | -1.00743400 | 1.21414400  |
| C  | -5.83119000 | 0.30307100  | 0.89910800  |
| C  | -4.49555400 | 0.71936300  | 0.65323000  |
| C  | -3.46001200 | -0.25653200 | 0.72668000  |
| C  | -3.74682200 | -1.59933200 | 1.04408000  |
| C  | -5.05453100 | -1.95755200 | 1.28984100  |
| N  | -2.16689900 | 0.16804100  | 0.49219800  |
| C  | -1.84144400 | 1.45704700  | 0.28303200  |
| C  | -2.84790900 | 2.44073300  | 0.12277300  |
| C  | -4.16050700 | 2.04546100  | 0.31069000  |
| O  | -1.18091700 | -0.75132500 | 0.50400400  |
| Si | -0.34748900 | -1.31371100 | -1.14272500 |
| Cl | 0.74989900  | -1.84585400 | -3.00900800 |
| C  | -0.39647300 | 1.80865000  | 0.25779500  |
| C  | 0.19841800  | 2.62511600  | 1.25068300  |
| C  | 1.50604400  | 3.02888000  | 1.04089900  |
| C  | 2.22645600  | 2.65351400  | -0.11230600 |
| C  | 1.61808300  | 1.76455700  | -1.04656300 |
| N  | 0.32795600  | 1.35646900  | -0.78004500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.29986900  | 1.33073800  | -2.20124000 |
| C  | 3.57918400  | 1.79627300  | -2.41922900 |
| C  | 4.20919200  | 2.67834600  | -1.50576200 |
| C  | 3.55031600  | 3.09579700  | -0.37285400 |
| C  | -2.51121800 | 3.84366200  | -0.32276100 |
| C  | -0.54340900 | 2.99026700  | 2.51461200  |
| O  | -0.27191400 | 0.49180900  | -1.63255200 |
| O  | 1.23876000  | -1.12883000 | -0.29105300 |
| C  | 1.55487000  | -1.36799200 | 0.95314400  |
| C  | 2.98814400  | -1.30484500 | 1.31651500  |
| C  | 3.99118100  | -1.34773000 | 0.33519300  |
| C  | 5.32997400  | -1.25800300 | 0.70840300  |
| C  | 5.67810400  | -1.12820700 | 2.05704800  |
| C  | 4.68188900  | -1.08387300 | 3.03684100  |
| C  | 3.34120300  | -1.17298300 | 2.66919900  |
| C  | -0.49968200 | -3.24357600 | -0.49222200 |
| Cl | -2.30735000 | -1.35645100 | -2.19769800 |
| H  | 1.99600400  | 3.65369600  | 1.78175200  |
| H  | -4.95814300 | 2.77244000  | 0.19099000  |
| H  | 0.85424300  | -1.03728300 | 1.72067300  |
| H  | 3.71162000  | -1.44118300 | -0.70869900 |
| H  | 2.56460600  | -1.14279700 | 3.42978900  |
| H  | 6.10454600  | -1.28809000 | -0.05227600 |
| H  | 4.94980400  | -0.97940900 | 0.48398500  |
| H  | 6.72368900  | -1.06020800 | 2.34331500  |
| H  | 0.14154500  | 3.46391000  | 3.22142800  |
| H  | -0.96603500 | 2.10232600  | 2.99567500  |
| H  | -1.36653300 | 3.68853700  | 2.33475600  |
| H  | -3.42731200 | 4.43015100  | -0.42032100 |
| H  | -2.01491400 | 3.82834800  | -1.29916400 |
| H  | -1.85108100 | 4.36916600  | 0.37241200  |
| H  | 4.02275500  | 3.76900800  | 0.33523800  |
| H  | 5.21846500  | 3.02323500  | -1.70556400 |
| H  | 4.11386200  | 1.48000100  | -3.30913700 |
| H  | 1.81448400  | 0.64771100  | -2.88510700 |
| H  | -2.94598400 | -2.32173100 | 1.09680500  |
| H  | -5.28426700 | -2.98749000 | 1.54318000  |
| H  | -6.62507500 | 1.04034700  | 0.83529800  |
| H  | -7.12407500 | -1.32124400 | 1.40564800  |
| H  | -1.55348600 | -3.48906600 | -0.62265300 |
| C  | -0.05160900 | -3.36636000 | 0.87332300  |
| H  | 0.12086600  | -3.79518400 | -1.19950800 |
| C  | 1.27673700  | -3.42602000 | 1.23820300  |
| H  | -0.78306900 | -3.22700900 | 1.66844200  |
| H  | 1.54976100  | -3.54804400 | 2.28153900  |
| H  | 2.02379100  | -3.73004700 | 0.51039100  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.64431100  | -1.52288700 | 0.97166300  |
| C  | 3.29340000  | -1.17140500 | 1.11948800  |
| C  | 2.90569800  | -0.32558900 | 2.17101500  |
| C  | 3.86065400  | 0.15903300  | 3.06101400  |
| C  | 5.20608400  | -0.19445000 | 2.91101700  |
| C  | 5.59647300  | -1.03366200 | 1.86400600  |
| C  | 2.30863000  | -1.67762300 | 0.13650600  |
| O  | 1.17931800  | -1.02902500 | 0.03759100  |
| Si | -0.32439000 | -1.44950200 | -0.86577200 |
| Cl | -2.27372000 | -1.74930000 | -1.89719000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.17741700 | -0.66337800 | 0.65615900  |
| N  | -2.21167500 | 0.18768900  | 0.50435500  |
| C  | -3.47776400 | -0.26334800 | 0.81239700  |
| C  | -4.56537300 | 0.63699300  | 0.61596000  |
| C  | -4.30049300 | 1.91988900  | 0.10197900  |
| C  | -3.00869100 | 2.35598000  | -0.14626500 |
| C  | -1.95205300 | 1.45290600  | 0.11389500  |
| C  | -5.87714400 | 0.18874300  | 0.93099400  |
| C  | -6.07675400 | -1.07664500 | 1.42808300  |
| C  | -4.97681700 | -1.94953500 | 1.62688900  |
| C  | -3.69124800 | -1.56146400 | 1.32102700  |
| C  | -0.52413600 | 1.86000300  | 0.02133000  |
| C  | 0.02921600  | 2.86135100  | 0.85634700  |
| C  | 1.32990900  | 3.26156600  | 0.59950500  |
| C  | 2.07959200  | 2.72053000  | -0.46414600 |
| C  | 1.50719500  | 1.67585800  | -1.24651000 |
| N  | 0.22994600  | 1.26982600  | -0.92366600 |
| C  | 2.21352600  | 1.08959000  | -2.31666400 |
| C  | 3.48175000  | 1.55173100  | -2.59694100 |
| C  | 4.07790200  | 2.58357800  | -1.82909700 |
| C  | 3.39389400  | 3.15565000  | -0.78227100 |
| C  | -2.77538600 | 3.73687800  | -0.71268200 |
| C  | -0.75158100 | 3.45874600  | 2.00212300  |
| O  | -0.32318200 | 0.25640100  | -1.63235400 |
| Cl | 0.80388600  | -2.22553400 | -2.64220500 |
| C  | -0.39685200 | -3.25328200 | 0.08179000  |
| C  | 0.91748600  | -3.84447700 | 0.13210800  |
| H  | 1.23176700  | -4.45152000 | -0.71456200 |
| H  | 1.78723800  | 4.01999200  | 1.22808800  |
| H  | -5.13425900 | 2.58685500  | -0.09925600 |
| H  | 2.72065600  | -2.10534100 | -0.77757800 |
| H  | 1.86137300  | -0.05041200 | 2.27553400  |
| H  | 4.94684400  | -2.17445000 | 0.15560500  |
| H  | 3.55855300  | 0.81444300  | 3.87280900  |
| H  | 6.64084500  | -1.30486700 | 1.74183200  |
| H  | 5.94794800  | 0.18530400  | 3.60760900  |
| H  | -1.10541200 | -3.83375900 | -0.50892200 |
| H  | -1.37317700 | 4.29856200  | 1.67326700  |
| H  | -0.06125800 | 3.84149500  | 2.75796500  |
| H  | -1.40412000 | 2.72403600  | 2.48053100  |
| H  | -3.44092200 | 3.89651900  | -1.56645600 |
| H  | -1.75089200 | 3.88645900  | -1.05701200 |
| H  | -3.00629400 | 4.51011500  | 0.02787100  |
| H  | 3.83759200  | 3.94817800  | -0.18798000 |
| H  | 5.07956100  | 2.92153000  | -2.07384200 |
| H  | 1.75423400  | 0.29757200  | -2.89238800 |
| H  | 4.03351000  | 1.11661000  | -3.42405300 |
| H  | -6.70914000 | 0.86792400  | 0.77543700  |
| H  | -7.07857600 | -1.41457900 | 1.67221300  |
| H  | -5.15046200 | -2.94370400 | 2.02598000  |
| H  | -2.85157300 | -2.22441100 | 1.46820100  |
| C  | 1.86824700  | -3.49567200 | 1.06890500  |
| H  | -0.79348000 | -3.01734700 | 1.07061600  |
| H  | 2.83509400  | -3.98932000 | 1.07301900  |
| H  | 1.55729300  | -3.04919300 | 2.00923100  |

File: a\_bp4\_R\_631g\_B3LYP\_ts.xyz

|   |             |            |            |
|---|-------------|------------|------------|
| C | -1.83415700 | 2.63506200 | 0.52736000 |
|---|-------------|------------|------------|

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.49487600 | 2.77535900  | 0.10955100  |
| C  | -0.01439100 | 3.99436800  | -0.44851900 |
| C  | -0.92683900 | 5.07422900  | -0.58085700 |
| C  | -2.23177500 | 4.93591500  | -0.16661900 |
| C  | -2.68277400 | 3.71365200  | 0.39064300  |
| N  | 0.40131300  | 1.72969600  | 0.23541700  |
| C  | 1.71171400  | 1.84872200  | -0.04533600 |
| C  | 2.20965200  | 3.01386700  | -0.68285400 |
| C  | 1.32969100  | 4.06416500  | -0.87405900 |
| C  | 2.61346300  | 0.74545100  | 0.38313600  |
| N  | 2.49107700  | -0.43822000 | -0.24225000 |
| C  | 3.38768800  | -1.47579100 | -0.09466300 |
| C  | 4.44753900  | -1.29382300 | 0.84070600  |
| C  | 4.49934900  | -0.09870800 | 1.58756100  |
| C  | 3.60129200  | 0.93413300  | 1.38022300  |
| C  | 3.26765600  | -2.66003400 | -0.84940300 |
| C  | 4.21146500  | -3.64871400 | -0.67093400 |
| C  | 5.27322100  | -3.49605200 | 0.25572500  |
| C  | 5.38850800  | -2.34535100 | 1.00017000  |
| O  | 1.45398800  | -0.59561500 | -1.09476300 |
| Si | -0.27257400 | -0.96708100 | -0.41607100 |
| Cl | -0.33587600 | -2.86437000 | -1.62333200 |
| C  | 3.62527300  | 2.17619900  | 2.23904300  |
| C  | 3.62635300  | 3.07584700  | -1.20223300 |
| O  | -0.04884300 | 0.56135300  | 0.72968400  |
| O  | -1.94255300 | -1.06746800 | 0.21315000  |
| C  | -3.00837500 | -1.53975200 | -0.38892900 |
| C  | -4.29871500 | -1.42571500 | 0.33621500  |
| C  | -4.43461500 | -0.60723500 | 1.46747900  |
| C  | -5.65241100 | -0.54716100 | 2.14193500  |
| C  | -6.74239500 | -1.29991800 | 1.69468400  |
| C  | -6.60966200 | -2.12270600 | 0.57243000  |
| C  | -5.39350600 | -2.18675000 | -0.10380500 |
| C  | -0.92959500 | 0.10846800  | -2.03766600 |
| Cl | 0.45220200  | -2.07579000 | 1.34916000  |
| H  | 1.67752000  | 4.96932200  | -1.33627300 |
| H  | 5.26827200  | 0.01046500  | 2.34640700  |
| H  | -2.88076000 | -2.45246800 | -0.97154500 |
| H  | -3.57991900 | -0.04463700 | 1.82686800  |
| H  | -5.28887100 | -2.82998100 | -0.97403000 |
| H  | -5.75005200 | 0.08134900  | 3.02237500  |
| H  | -7.45073600 | -2.71723200 | 0.22836200  |
| H  | -7.68992900 | -1.25125500 | 2.22347300  |
| H  | 4.43527900  | 2.10641100  | 2.96834200  |
| H  | 2.68420100  | 2.28255300  | 2.78929300  |
| H  | 3.77288900  | 3.09407200  | 1.66336800  |
| H  | 3.78512300  | 4.01772200  | -1.73163200 |
| H  | 3.81890700  | 2.25656800  | -1.90330600 |
| H  | 4.37546000  | 3.00993200  | -0.40828400 |
| H  | 6.19548700  | -2.21873300 | 1.71494700  |
| H  | 5.99625800  | -4.29618700 | 0.37630600  |
| H  | 4.13729200  | -4.56360900 | -1.24998000 |
| H  | 2.44517000  | -2.77323900 | -1.54267000 |
| H  | -0.57205700 | 6.00589200  | -1.00977400 |
| H  | -2.92384400 | 5.76581000  | -0.26478600 |
| H  | -3.71311500 | 3.62481500  | 0.71964100  |
| H  | -2.16159000 | 1.69669300  | 0.95339100  |
| H  | -0.10563600 | 0.03710900  | -2.74823200 |
| H  | -1.06625900 | 1.13344100  | -1.69358100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.15282300 | -0.46485200 | -2.53680600 |
| C | -3.38805000 | -0.26928900 | -1.94390500 |
| H | -2.07483800 | -1.24092200 | -3.29511100 |
| H | -4.27348300 | -0.70100400 | -2.40008200 |
| H | -3.55716600 | 0.61095100  | -1.32946700 |

File: a\_bp5\_S\_631g\_B3LYP.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.00119500  | -2.80456200 | -0.97214900 |
| C  | 3.18349200  | -1.70930400 | -0.10079800 |
| C  | 4.18227200  | -1.72853500 | 0.91604400  |
| C  | 4.99423200  | -2.88835100 | 1.03857400  |
| C  | 4.81707200  | -3.95091200 | 0.18426400  |
| C  | 3.81957500  | -3.90395200 | -0.82265800 |
| N  | 2.40334500  | -0.57565300 | -0.20953900 |
| C  | 2.60473500  | 0.53945100  | 0.52564500  |
| C  | 3.53912400  | 0.52995500  | 1.58892600  |
| C  | 4.30405000  | -0.61277200 | 1.76528400  |
| C  | 1.86892000  | 1.77158400  | 0.12799000  |
| N  | 0.52823100  | 1.76924000  | 0.24854000  |
| C  | -0.25391600 | 2.89297200  | 0.08638500  |
| C  | 0.39910200  | 4.09805200  | -0.30152700 |
| C  | 1.78870600  | 4.07195500  | -0.53402600 |
| C  | 2.54539600  | 2.93159300  | -0.32268200 |
| C  | -1.64603000 | 2.85044400  | 0.30499000  |
| C  | -2.37163600 | 4.01104500  | 0.14926800  |
| C  | -1.74623100 | 5.22439700  | -0.23534300 |
| C  | -0.39089200 | 5.26787000  | -0.46274700 |
| O  | -0.07412300 | 0.61434100  | 0.60035100  |
| Si | -0.38459600 | -0.73717300 | -0.68961100 |
| Cl | -0.55863700 | -2.42938100 | -2.15031400 |
| C  | 4.03098900  | 2.92956900  | -0.59131200 |
| C  | 3.69127000  | 1.68923700  | 2.54571200  |
| O  | 1.44862000  | -0.56012000 | -1.16347200 |
| O  | -2.12207800 | -0.65590900 | -0.24071100 |
| C  | -2.98609300 | -1.63713200 | -0.15370000 |
| C  | -4.34650400 | -1.30470800 | 0.33631400  |
| C  | -4.58980300 | -0.18554700 | 1.14728800  |
| C  | -5.88727600 | 0.10852100  | 1.55796100  |
| C  | -6.95197100 | -0.71070400 | 1.16673000  |
| C  | -6.71458700 | -1.82729500 | 0.36173600  |
| C  | -5.41655800 | -2.12581600 | -0.05015800 |
| C  | -0.07898200 | -2.02824100 | 0.88481900  |
| Cl | -0.75719100 | 0.72876200  | -2.30035500 |
| H  | 5.02639300  | -0.64825100 | 2.57597900  |
| H  | 2.27802200  | 4.97516400  | -0.88641700 |
| H  | -2.94551500 | -2.40158300 | -0.93021800 |
| H  | -3.76212800 | 0.44609300  | 1.45306300  |
| H  | -5.23130000 | -2.99140300 | -0.68103400 |
| H  | -6.07132300 | 0.97763400  | 2.18286600  |
| H  | -7.53868900 | -2.46306600 | 0.05204300  |
| H  | -7.96292400 | -0.47759800 | 1.48833800  |
| H  | 4.70450700  | 2.10171000  | 2.50303200  |
| H  | 3.52541600  | 1.33939100  | 3.56994200  |
| H  | 2.98241000  | 2.49505400  | 2.35266700  |
| H  | 4.28500900  | 3.76674400  | -1.24558800 |
| H  | 4.35544200  | 2.00702800  | -1.08040800 |
| H  | 4.61259000  | 3.04524500  | 0.32924400  |
| H  | 0.09803400  | 6.18893300  | -0.76353200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.34682500 | 6.12023200  | -0.35477100 |
| H | -3.44357900 | 3.99441200  | 0.31785100  |
| H | -2.11386100 | 1.91420000  | 0.57427000  |
| H | 5.75394600  | -2.91106200 | 1.81340400  |
| H | 5.44222100  | -4.83303500 | 0.27608700  |
| H | 3.69803900  | -4.74945100 | -1.49210600 |
| H | 2.23476700  | -2.76115000 | -1.73474800 |
| H | 0.90514100  | -2.46950800 | 0.72710300  |
| C | -1.11499100 | -3.02815500 | 0.89796900  |
| H | -0.08980700 | -1.38454700 | 1.76550300  |
| C | -2.37524100 | -2.80701200 | 1.42047600  |
| H | -0.96007800 | -3.92665500 | 0.30471200  |
| H | -3.10670900 | -3.60943700 | 1.42414900  |
| H | -2.51267400 | -2.03763800 | 2.17485200  |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.64871000  | 2.87869600  | -0.27480500 |
| C  | 0.25394800  | 2.87528200  | -0.07087600 |
| C  | -0.42880300 | 4.07121400  | 0.30140700  |
| C  | 0.32846500  | 5.26365900  | 0.46214200  |
| C  | 1.68569900  | 5.25745900  | 0.25077800  |
| C  | 2.34345100  | 4.05772800  | -0.12041400 |
| N  | -0.50155300 | 1.73163100  | -0.23058700 |
| C  | -1.84745000 | 1.71441000  | -0.12032700 |
| C  | -2.54797300 | 2.86240600  | 0.31637300  |
| C  | -1.81593900 | 4.02050500  | 0.52299000  |
| O  | 0.12303500  | 0.57538100  | -0.55653500 |
| Si | 0.39649600  | -0.78356600 | 0.76756800  |
| Cl | 0.52804100  | -2.44143500 | 2.25622600  |
| C  | -2.56859100 | 0.47085400  | -0.50708800 |
| C  | -3.48097200 | 0.43811000  | -1.59113200 |
| C  | -4.24085400 | -0.70775600 | -1.75608800 |
| C  | -4.13724900 | -1.80396600 | -0.87491800 |
| C  | -3.16019600 | -1.76076700 | 0.16185000  |
| N  | -2.38500200 | -0.62043500 | 0.26008800  |
| C  | -2.98388400 | -2.83795800 | 1.05430700  |
| C  | -3.79483700 | -3.94423300 | 0.91172800  |
| C  | -4.77479300 | -4.01372300 | -0.11000500 |
| C  | -4.94117600 | -2.96880700 | -0.98930000 |
| C  | -4.03204800 | 2.85365700  | 0.60064500  |
| C  | -3.60475900 | 1.59602400  | -2.55144000 |
| O  | -1.43953000 | -0.58008700 | 1.21956500  |
| O  | 2.16139300  | -0.86075700 | 0.48502000  |
| C  | 2.84215200  | -0.69203600 | -0.66202100 |
| C  | 4.28886200  | -1.00974700 | -0.61679500 |
| C  | 4.82134100  | -1.83535100 | 0.38564400  |
| C  | 6.19044500  | -2.08759700 | 0.42056900  |
| C  | 7.03589100  | -1.52205400 | -0.53993300 |
| C  | 6.50914900  | -0.69740800 | -1.53778900 |
| C  | 5.13980700  | -0.44257900 | -1.57802100 |
| C  | 0.08312500  | -2.11270400 | -0.77592600 |
| Cl | 0.78005300  | 0.71859900  | 2.33840500  |
| H  | -4.94293000 | -0.76624800 | -2.58248700 |
| H  | -2.32575000 | 4.91671400  | 0.86473900  |
| H  | 2.56865300  | 0.14488500  | -1.30546100 |
| H  | 4.16069000  | -2.26260700 | 1.13270900  |
| H  | 4.72816200  | 0.20239600  | -2.35059800 |
| H  | 6.60113200  | -2.72287800 | 1.19982700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 7.16407700  | -0.25127200 | -2.28028300 |
| H | 8.10323100  | -1.72096600 | -0.50786500 |
| H | -4.08150600 | 1.25818700  | -3.47464300 |
| H | -2.62831100 | 2.01699000  | -2.80718800 |
| H | -4.22171500 | 2.40232500  | -2.14192500 |
| H | -4.45452500 | 1.84836200  | 0.62319100  |
| H | -4.58022300 | 3.44194200  | -0.14324700 |
| H | -4.21599400 | 3.31348800  | 1.57638400  |
| H | -5.68546500 | -3.01203700 | -1.77811800 |
| H | -5.39431700 | -4.90039500 | -0.19638000 |
| H | -3.67917500 | -4.77783800 | 1.59690300  |
| H | -2.22586700 | -2.77806000 | 1.82423900  |
| H | -0.19043600 | 6.17216700  | 0.75075600  |
| H | 2.26164600  | 6.16913400  | 0.37034600  |
| H | 3.41655400  | 4.06517900  | -0.28142200 |
| H | 2.15417200  | 1.96541100  | -0.54365100 |
| H | -0.97341700 | -2.05513500 | -1.03176900 |
| H | 0.32162100  | -3.07940700 | -0.33338600 |
| C | 0.91662100  | -1.79030900 | -1.90546300 |
| C | 2.24131200  | -2.16553000 | -1.99562100 |
| H | 0.53917100  | -1.06735500 | -2.62708200 |
| H | 2.81866900  | -1.91969300 | -2.88146600 |
| H | 2.60329700  | -3.00467100 | -1.40839500 |

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| H  | -0.86605200 | 1.87923400  | 1.00610400  |
| C  | -1.50323800 | 1.74404300  | 0.13110900  |
| C  | -0.91908400 | 1.11163100  | -1.02360900 |
| Si | -1.06891200 | -0.84605300 | -0.68103100 |
| O  | -2.81968200 | -0.63801400 | -0.44455000 |
| C  | -3.38826300 | 0.08693500  | 0.51528800  |
| C  | -4.87328700 | 0.18624500  | 0.45239700  |
| C  | -5.58403500 | 0.47095600  | 1.62739700  |
| C  | -6.97590200 | 0.54608000  | 1.60177100  |
| C  | -7.66359200 | 0.34153200  | 0.40300700  |
| C  | -6.95663600 | 0.05771900  | -0.77040300 |
| C  | -5.56602600 | -0.01723400 | -0.75020200 |
| O  | 0.77945300  | -1.06854300 | -1.08510400 |
| N  | 1.74844900  | -1.45031000 | -0.20712600 |
| C  | 2.52793500  | -0.50197800 | 0.35384300  |
| C  | 3.50144600  | -0.86267100 | 1.32034800  |
| C  | 3.65491800  | -2.20151500 | 1.62262100  |
| C  | 2.91478200  | -3.20053800 | 0.95697700  |
| C  | 1.94134400  | -2.80902100 | -0.00567600 |
| C  | 3.11303700  | -4.58617600 | 1.19527200  |
| C  | 2.39391900  | -5.52328000 | 0.49064400  |
| C  | 1.45357900  | -5.11084800 | -0.48328000 |
| C  | 1.21796400  | -3.77458400 | -0.73303900 |
| C  | 2.45939300  | 0.88724900  | -0.17109000 |
| N  | 1.96373300  | 1.81391200  | 0.68299800  |
| C  | 2.01596300  | 3.17511500  | 0.36165400  |
| C  | 2.55410500  | 3.56702500  | -0.89347000 |
| C  | 3.03353700  | 2.57417300  | -1.78291900 |
| C  | 3.00306600  | 1.23987500  | -1.43710900 |
| C  | 1.53145300  | 4.12231800  | 1.28576700  |
| C  | 1.58520600  | 5.46108400  | 0.95778500  |
| C  | 2.11172000  | 5.87896700  | -0.28818600 |
| C  | 2.58520400  | 4.95455500  | -1.19340700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | 1.42530400  | 1.44131300  | 1.79996700  |
| C  | 3.53563600  | 0.17282000  | -2.36066500 |
| C  | 4.34217300  | 0.19536800  | 1.98643400  |
| Cl | -1.47685800 | -2.01036800 | -2.38606000 |
| Cl | -0.82777600 | -1.66215600 | 1.25586800  |
| H  | -2.99667100 | -0.06590100 | 1.52298100  |
| H  | 0.13756700  | 1.31373800  | -1.17292000 |
| C  | -2.88051400 | 1.92492800  | 0.24703200  |
| H  | -1.48890600 | 1.25125100  | -1.94630500 |
| H  | 3.44486800  | 2.87593400  | -2.74115000 |
| H  | 4.38824500  | -2.50040500 | 3.26583000  |
| H  | -5.01321100 | -0.24582900 | -1.65547300 |
| H  | -5.04797100 | 0.62353100  | 2.56079900  |
| H  | -7.49155900 | -0.10856600 | -1.70085700 |
| H  | -7.52189200 | 0.75906800  | 2.51594000  |
| H  | -8.74802900 | 0.39939100  | 0.38255400  |
| H  | 3.97426500  | 0.62941200  | -3.25088200 |
| H  | 2.73680400  | -0.50399000 | -2.68228900 |
| H  | 4.30995700  | -0.43245500 | -1.87560100 |
| H  | 5.05842400  | -0.26652300 | 2.66933100  |
| H  | 3.70462700  | 0.87986900  | 2.55537900  |
| H  | 4.90267100  | 0.78545600  | 1.25334100  |
| H  | 2.99302000  | 5.27038600  | -2.14902400 |
| H  | 2.14291100  | 6.93723700  | -0.52840700 |
| H  | 1.22156100  | 6.20197100  | 1.66285700  |
| H  | 1.13843200  | 3.77543700  | 2.23234100  |
| H  | 3.84899600  | -4.88499800 | 1.93516100  |
| H  | 2.55137800  | -6.58156200 | 0.67126200  |
| H  | 0.90759100  | -5.85828300 | -1.05003400 |
| H  | 0.50780600  | -3.46610600 | -1.48629100 |
| H  | -3.26559000 | 2.43138300  | 1.12759200  |
| H  | -3.44640600 | 2.09108200  | -0.66589100 |

# PROPARGYLATION - B3LYP/6-31G(d)

File: p\_bp1\_S\_B3LYP\_ts.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 6.73072400  | -1.34732800 | -1.70096600 |
| C  | 5.49993000  | -1.68155600 | -2.27560100 |
| C  | 4.32682300  | -1.57657300 | -1.53164300 |
| C  | 4.38019800  | -1.13254800 | -0.20153100 |
| C  | 5.61640100  | -0.79822400 | 0.37191800  |
| C  | 6.78710900  | -0.90324900 | -0.37717100 |
| C  | 3.14491600  | -0.99156600 | 0.61348200  |
| O  | 2.02299400  | -0.84868600 | -0.07203200 |
| Si | 0.35079800  | -0.81091000 | 0.52226900  |
| O  | -1.42849700 | -0.63489700 | 1.16387100  |
| N  | -2.45285300 | -0.57023500 | 0.28211200  |
| C  | -2.63074000 | 0.57161500  | -0.40775000 |
| C  | -3.59077000 | 0.64343000  | -1.44720000 |
| C  | -4.40560700 | -0.45817200 | -1.64072500 |
| C  | -4.31309200 | -1.60323000 | -0.82350200 |
| C  | -3.29062600 | -1.66119100 | 0.16709100  |
| C  | -1.81348700 | 1.75744400  | -0.02963400 |
| C  | -2.38843100 | 2.92810500  | 0.52092800  |
| C  | -1.56752300 | 4.03523100  | 0.66003500  |
| C  | -0.21181900 | 4.01422900  | 0.27156000  |
| C  | 0.34752100  | 2.79246100  | -0.20176500 |
| N  | -0.49591600 | 1.70720100  | -0.28903100 |
| O  | 0.01403200  | 0.52946000  | -0.71445800 |
| C  | 0.63189200  | -2.37767800 | 1.75668500  |
| C  | 1.85494300  | -2.70712900 | 1.86016200  |
| C  | 3.19819000  | -2.69752000 | 1.62307700  |
| Cl | -0.27027600 | -2.21121000 | -1.09877300 |
| Cl | 0.84125700  | 0.61126700  | 2.18807800  |
| C  | -3.81309900 | 2.94690600  | 1.01968100  |
| H  | -1.97704700 | 4.94982200  | 1.07896900  |
| C  | -3.67501500 | 1.84794300  | -2.35421800 |
| H  | -5.14189800 | -0.44344400 | -2.43861400 |
| C  | -3.15748900 | -2.78188700 | 1.01055300  |
| H  | 3.23888500  | -0.36310300 | 1.50149900  |
| H  | 3.36761500  | -1.82745400 | -1.97208300 |
| H  | 5.65835700  | -0.44929100 | 1.40065000  |
| H  | 5.45572800  | -2.02213600 | -3.30601600 |
| H  | 7.74021000  | -0.63624700 | 0.06970500  |
| H  | 7.64288800  | -1.43022900 | -2.28495100 |
| H  | 3.59523100  | -3.43687200 | 0.92896300  |
| H  | 3.87552900  | -2.41966200 | 2.42945700  |
| H  | -0.23746100 | -2.83776700 | 2.20607400  |
| C  | 1.70307700  | 2.69692500  | -0.57680100 |
| C  | 0.63783300  | 5.14914800  | 0.35784500  |
| H  | -4.11286900 | 3.96954400  | 1.25832300  |
| H  | -3.89866400 | 2.34739800  | 1.93339400  |
| H  | -4.52833900 | 2.54325500  | 0.29943400  |
| H  | -4.36081100 | 1.64096100  | -3.17872600 |
| H  | -2.69575500 | 2.08801600  | -2.78052200 |
| H  | -4.03892100 | 2.74148500  | -1.83783500 |
| C  | 2.48679200  | 3.82703400  | -0.48805700 |
| H  | 2.09755900  | 1.75119800  | -0.92294000 |
| H  | 3.53026900  | 3.77440200  | -0.78156600 |
| C  | 1.95728500  | 5.05600400  | -0.01877900 |
| H  | 0.22363800  | 6.08365600  | 0.72245800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.60282200  | 5.92598900  | 0.04351800  |
| C | -4.03281000 | -3.83495900 | 0.85665000  |
| H | -2.39577300 | -2.78847100 | 1.77591000  |
| H | -3.94666100 | -4.69695000 | 1.51025800  |
| C | -5.04345100 | -3.81091300 | -0.13655100 |
| C | -5.18154900 | -2.71863400 | -0.96040900 |
| H | -5.71251900 | -4.65888500 | -0.23946000 |
| H | -5.95545400 | -2.68393000 | -1.72062000 |

File: p\_bp1\_R\_B3LYP\_ts.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.96763600 | -0.77202800 | 1.05231300  |
| C  | -6.19968600 | 0.08092500  | 0.25258200  |
| C  | -4.86684400 | -0.22146800 | -0.01679600 |
| C  | -4.29167300 | -1.38465500 | 0.51784100  |
| C  | -5.06489200 | -2.23826300 | 1.31901500  |
| C  | -6.39788600 | -1.93071000 | 1.58658200  |
| C  | -2.86741200 | -1.72641400 | 0.26693400  |
| O  | -2.08247100 | -0.71149200 | -0.05311200 |
| Si | -0.38359300 | -0.74457000 | -0.56814700 |
| O  | 1.40023800  | -0.60393700 | -1.17802800 |
| N  | 2.41535900  | -0.59525200 | -0.28508300 |
| C  | 2.64264400  | 0.53489100  | 0.41754000  |
| C  | 3.63133300  | 0.55782300  | 1.42933700  |
| C  | 4.40671100  | -0.57884800 | 1.59660700  |
| C  | 4.24810100  | -1.71433700 | 0.78140200  |
| C  | 3.20213900  | -1.72286300 | -0.18680400 |
| C  | 1.86042200  | 1.75175500  | 0.06140000  |
| C  | 2.47413000  | 2.92393400  | -0.43950200 |
| C  | 1.67826300  | 4.04924200  | -0.59099700 |
| C  | 0.31385800  | 4.05226300  | -0.24373800 |
| C  | -0.28214300 | 2.83621400  | 0.19945200  |
| N  | 0.53268500  | 1.73032300  | 0.28848200  |
| O  | -0.02397100 | 0.56327100  | 0.68616100  |
| C  | -0.69859200 | -2.22203600 | -1.90083600 |
| C  | -1.82331300 | -2.79025000 | -1.73803600 |
| C  | -3.07526400 | -3.00767300 | -1.24115800 |
| Cl | 0.18643000  | -2.19480700 | 1.04567400  |
| Cl | -0.82894400 | 0.71356200  | -2.20824900 |
| C  | 3.93469800  | 2.96646600  | -0.82038800 |
| H  | 2.12064700  | 4.96112300  | -0.98178300 |
| C  | 3.83700500  | 1.75110400  | 2.33187100  |
| H  | 5.16550900  | -0.59418400 | 2.37381200  |
| C  | 5.07170100  | -2.86705500 | 0.89614500  |
| H  | -2.43502900 | -2.46193100 | 0.94765100  |
| H  | -4.26371200 | 0.43731100  | -0.63279200 |
| H  | -4.61914600 | -3.13626000 | 1.73939000  |
| H  | -6.64173100 | 0.98332100  | -0.15991500 |
| H  | -6.98916500 | -2.59140300 | 2.21362100  |
| H  | -8.00653700 | -0.53237800 | 1.26012800  |
| H  | -3.28015000 | -3.93158100 | -0.70217600 |
| H  | -3.91564600 | -2.61706400 | -1.81306200 |
| H  | 0.05070200  | -2.37422500 | -2.66685200 |
| C  | -0.50846300 | 5.20756100  | -0.33779100 |
| H  | 4.71316600  | 2.33329200  | 2.02637300  |
| H  | 4.01697500  | 1.40710500  | 3.35419600  |
| H  | 2.97352100  | 2.41819000  | 2.35004300  |
| H  | 4.06829300  | 3.62342600  | -1.68407800 |
| H  | 4.32658200  | 1.98147000  | -1.08226900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.54614500  | 3.37101800  | -0.00648000 |
| C | 4.86447800  | -3.95044400 | 0.07664400  |
| H | 5.86492500  | -2.86617600 | 1.63693500  |
| H | 5.49779900  | -4.82738400 | 0.16142400  |
| C | 3.82375500  | -3.93064300 | -0.88669200 |
| C | 2.99331000  | -2.84007100 | -1.02142300 |
| H | 3.67720200  | -4.79168600 | -1.53074400 |
| H | 2.19929400  | -2.82233600 | -1.75305800 |
| C | -1.83726300 | 5.13981800  | 0.00704900  |
| H | -0.06429400 | 6.13646800  | -0.68084900 |
| H | -2.46238000 | 6.02424400  | -0.05973700 |
| C | -2.40383300 | 3.91675000  | 0.44966400  |
| C | -1.64872100 | 2.76818100  | 0.54231200  |
| H | -3.45494500 | 3.88387500  | 0.71788300  |
| H | -2.07522700 | 1.82764500  | 0.86304100  |

File: p\_bp2\_S\_ts\_B3LYP.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.50748400  | -0.79717000 | 2.67305400  |
| C  | 4.66254700  | 0.18479600  | 2.14777700  |
| C  | 3.58194100  | -0.17511000 | 1.34510500  |
| C  | 3.33604300  | -1.52561200 | 1.06207900  |
| C  | 4.18396600  | -2.50913800 | 1.59736000  |
| C  | 5.26381500  | -2.14595700 | 2.39886700  |
| C  | 2.18281800  | -1.96222300 | 0.23247600  |
| O  | 1.19371100  | -1.09921200 | 0.06454800  |
| Si | -0.31091000 | -1.37198100 | -0.87166900 |
| O  | -1.14690700 | -0.70109500 | 0.64467100  |
| N  | -2.22329600 | 0.10701400  | 0.51637800  |
| C  | -2.01075100 | 1.40387000  | 0.22172600  |
| C  | -3.10491200 | 2.27018400  | -0.01508600 |
| C  | -4.37850700 | 1.75603700  | 0.16662400  |
| C  | -4.59457400 | 0.43134800  | 0.59351800  |
| C  | -3.47002300 | -0.42837800 | 0.76035900  |
| C  | -0.60417000 | 1.89009600  | 0.19706600  |
| C  | -0.13465000 | 2.88347500  | 1.08975800  |
| C  | 1.13551700  | 3.39293400  | 0.87239100  |
| C  | 1.93882700  | 2.95766400  | -0.19894400 |
| C  | 1.45919400  | 1.90525400  | -1.03291200 |
| N  | 0.20983800  | 1.39344800  | -0.75700900 |
| O  | -0.25868700 | 0.39844700  | -1.54029100 |
| C  | 0.76603800  | -1.95846700 | -2.49470400 |
| C  | 1.97554300  | -2.23870400 | -2.22183200 |
| C  | 3.11635500  | -2.34786000 | -1.48379700 |
| Cl | -2.17552700 | -1.51860800 | -2.08571900 |
| Cl | -0.57712500 | -3.43763400 | -0.08998900 |
| C  | -0.94626300 | 3.36392700  | 2.27013400  |
| H  | 1.52436200  | 4.15462300  | 1.54231000  |
| C  | -2.90701500 | 3.69378900  | -0.47697600 |
| H  | -5.23881300 | 2.39270000  | -0.01761200 |
| C  | -5.88875100 | -0.09859300 | 0.84329600  |
| H  | 1.87569500  | -2.99551300 | 0.39479100  |
| H  | 2.91719600  | 0.58256600  | 0.94989800  |
| H  | 3.99183300  | -3.55915800 | 1.39077800  |
| H  | 4.84420400  | 1.23294800  | 2.36727300  |
| H  | 5.91081600  | -2.91347100 | 2.81293200  |
| H  | 6.34876500  | -0.51292200 | 3.29850900  |
| H  | 3.86351900  | -1.56218300 | -1.58598400 |
| H  | 3.51884500  | -3.33704200 | -1.27296900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.24922700  | -1.98314900 | -3.44504300 |
| C | 3.22258100  | 3.50235500  | -0.47460400 |
| H | -1.22685500 | 4.41574500  | 2.15188300  |
| H | -0.34227600 | 3.29002100  | 3.17991200  |
| H | -1.85466500 | 2.78058800  | 2.42634400  |
| H | -3.80313800 | 4.03636800  | -1.00011000 |
| H | -2.05976200 | 3.78883400  | -1.16105300 |
| H | -2.74091000 | 4.37400800  | 0.36508400  |
| C | -6.03475300 | -1.40368200 | 1.25019800  |
| H | -6.75024500 | 0.54830700  | 0.71149700  |
| H | -7.02358000 | -1.80526400 | 1.44621600  |
| C | -4.89813800 | -2.23529500 | 1.41568900  |
| C | -3.62500800 | -1.76840900 | 1.17045200  |
| H | -5.03241600 | -3.26243300 | 1.73936800  |
| H | -2.75446100 | -2.40068400 | 1.27975600  |
| C | 3.96422700  | 3.02838500  | -1.53064800 |
| H | 3.59530700  | 4.30012500  | 0.15981000  |
| H | 4.94089900  | 3.45078900  | -1.74269700 |
| C | 3.45882700  | 1.98951200  | -2.35326500 |
| C | 2.22513600  | 1.42269800  | -2.11498300 |
| H | 4.05297500  | 1.63640600  | -3.19007000 |
| H | 1.83049300  | 0.63291300  | -2.73849600 |

File: p\_bp2\_R\_ts\_B3LYP.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.89808300  | -2.83548300 | 2.77092700  |
| C  | 3.58963300  | -3.22538700 | 2.46899100  |
| C  | 2.85418600  | -2.53563100 | 1.50714000  |
| C  | 3.43063300  | -1.44511700 | 0.83811700  |
| C  | 4.74469900  | -1.05522100 | 1.14527400  |
| C  | 5.47436100  | -1.74721700 | 2.10900700  |
| C  | 2.67151600  | -0.66227400 | -0.16973100 |
| O  | 1.35697900  | -0.70847300 | -0.11890900 |
| Si | -0.06299800 | -0.99757400 | -1.15122300 |
| O  | -0.98333300 | -0.78745600 | 0.44356200  |
| N  | -2.15899900 | -0.12125900 | 0.46159800  |
| C  | -2.12567100 | 1.22440800  | 0.45604300  |
| C  | -3.32825900 | 1.96900700  | 0.40424100  |
| C  | -4.51936100 | 1.26352400  | 0.45340000  |
| C  | -4.55092300 | -0.13998000 | 0.57116000  |
| C  | -3.31998600 | -0.85830400 | 0.56260500  |
| C  | -0.79485300 | 1.88594400  | 0.54680400  |
| C  | -0.42559200 | 2.70261100  | 1.64213400  |
| C  | 0.76883600  | 3.39925100  | 1.54989700  |
| C  | 1.58292400  | 3.33179400  | 0.40307300  |
| C  | 1.20609200  | 2.45260200  | -0.65375400 |
| N  | 0.04566700  | 1.72696300  | -0.49593300 |
| O  | -0.30504800 | 0.85971500  | -1.47081300 |
| C  | 1.07409200  | -1.17068000 | -2.81189900 |
| C  | 2.31803300  | -1.28160400 | -2.57688100 |
| C  | 3.48134200  | -1.38357200 | -1.88174700 |
| Cl | -1.89498500 | -1.18971100 | -2.41222200 |
| Cl | 0.00019700  | -3.19813300 | -0.78022800 |
| C  | -1.25660800 | 2.80043600  | 2.89976300  |
| H  | 1.08177300  | 4.02636700  | 2.37984700  |
| C  | -3.32370400 | 3.47289800  | 0.27473900  |
| H  | -5.45934400 | 1.80558800  | 0.40693300  |
| C  | -5.75940100 | -0.87940000 | 0.67612200  |
| H  | 3.07983000  | 0.33094300  | -0.37111800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.83838300  | -2.83022800 | 1.26848600  |
| H | 5.19107400  | -0.20599900 | 0.63352400  |
| H | 3.14075000  | -4.06789300 | 2.98708000  |
| H | 6.48775400  | -1.43728300 | 2.34633500  |
| H | 5.46633100  | -3.37588600 | 3.52260200  |
| H | 4.25436100  | -0.63084500 | -2.02268500 |
| H | 3.84917800  | -2.38191900 | -1.65036600 |
| H | 0.54404600  | -1.25611800 | -3.75156000 |
| C | 2.77615100  | 4.08948500  | 0.25332500  |
| H | -0.63145200 | 2.56552000  | 3.76714800  |
| H | -2.10307800 | 2.11275100  | 2.90491800  |
| H | -1.63695400 | 3.81774500  | 3.03960700  |
| H | -3.16444100 | 3.96314500  | 1.24092600  |
| H | -4.28943600 | 3.81076000  | -0.10842600 |
| H | -2.54700900 | 3.82065200  | -0.41179300 |
| C | 3.52471000  | 3.98509000  | -0.89527900 |
| H | 3.07412400  | 4.75411300  | 1.05798700  |
| H | 4.42984800  | 4.57229400  | -1.01018200 |
| C | 3.11801800  | 3.11729600  | -1.94072400 |
| C | 1.97825100  | 2.34905400  | -1.83107600 |
| H | 3.71225700  | 3.05970500  | -2.84704900 |
| H | 1.65859900  | 1.68658500  | -2.62371700 |
| C | -5.72467500 | -2.24974900 | 0.78192900  |
| H | -6.70125800 | -0.34004800 | 0.67589000  |
| H | -6.64859400 | -2.81240800 | 0.86722600  |
| C | -4.48532000 | -2.93871100 | 0.77911000  |
| C | -3.28907000 | -2.26413700 | 0.66506900  |
| H | -4.47720100 | -4.02057700 | 0.86443500  |
| H | -2.34043300 | -2.78341000 | 0.64568100  |

File: p\_bp3\_S\_ts\_B3LYP.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.62228600  | -1.13923400 | 2.14395200  |
| C  | 5.30129100  | -1.22797400 | 0.78551800  |
| C  | 3.97273300  | -1.35220000 | 0.38495600  |
| C  | 2.95294400  | -1.38589000 | 1.34823500  |
| C  | 3.27824100  | -1.29615800 | 2.71072800  |
| C  | 4.60874100  | -1.17136900 | 3.10591800  |
| C  | 1.52550600  | -1.49918800 | 0.95367700  |
| O  | 1.23904300  | -1.16056100 | -0.28978100 |
| Si | -0.32390000 | -1.28868200 | -1.15815800 |
| O  | -1.11779900 | -0.72512800 | 0.48290700  |
| N  | -2.13948500 | 0.15286900  | 0.47643300  |
| C  | -1.86802600 | 1.45610200  | 0.24949000  |
| C  | -2.92149400 | 2.39112900  | 0.12838900  |
| C  | -4.21296600 | 1.93515500  | 0.34679200  |
| C  | -4.48311500 | 0.59906600  | 0.69508200  |
| C  | -3.40156500 | -0.32767600 | 0.74716200  |
| C  | -0.43384200 | 1.85521500  | 0.20894700  |
| C  | 0.12640400  | 2.72985800  | 1.17243500  |
| C  | 1.43978000  | 3.12940700  | 0.98790300  |
| C  | 2.20085900  | 2.70343000  | -0.11876800 |
| C  | 1.62131200  | 1.77900700  | -1.03611000 |
| N  | 0.32561400  | 1.37512600  | -0.79369200 |
| O  | -0.24218300 | 0.49571700  | -1.65381400 |
| C  | -0.54372400 | -3.21163200 | -0.58305500 |
| C  | 0.22006800  | -3.54462700 | 0.37732800  |
| C  | 1.23880500  | -3.45552300 | 1.27727700  |
| Cl | -2.29561900 | -1.34481000 | -2.18840600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Cl | 0.74312800  | -1.88396200 | -3.00391300 |
| C  | -0.66199200 | 3.19245200  | 2.37386800  |
| H  | 1.89968200  | 3.79421900  | 1.71321000  |
| C  | -2.69107300 | 3.82930400  | -0.27245900 |
| H  | -5.04218800 | 2.63070000  | 0.25298700  |
| C  | -5.79247800 | 0.12064400  | 0.97437500  |
| C  | -3.61265700 | -1.68251500 | 1.07895600  |
| H  | 0.80193900  | -1.18975900 | 1.71010700  |
| H  | 3.71437900  | -1.41454400 | -0.66658400 |
| H  | 2.48943400  | -1.32080300 | 3.45899200  |
| H  | 6.08872700  | -1.19913800 | 0.03801700  |
| H  | 4.85438300  | -1.09751800 | 4.16115700  |
| H  | 6.65956500  | -1.04322700 | 2.45169400  |
| H  | 2.18866900  | -3.91382700 | 1.00693400  |
| H  | 1.01528500  | -3.45935200 | 2.34270700  |
| H  | -1.25797400 | -3.80605300 | -1.13783800 |
| C  | 3.53221200  | 3.13862200  | -0.35446400 |
| H  | -1.28281000 | 2.39276400  | 2.78684700  |
| H  | -1.31779900 | 4.03418200  | 2.12827500  |
| H  | 0.02201400  | 3.52876300  | 3.15665800  |
| H  | -1.64695600 | 4.04554400  | -0.50179500 |
| H  | -3.02283600 | 4.51378200  | 0.51535800  |
| H  | -3.27967000 | 4.05454000  | -1.16776200 |
| C  | 4.22506800  | 2.68240100  | -1.45101100 |
| H  | 3.98181900  | 3.83878800  | 0.34219000  |
| H  | 5.23965800  | 3.02152900  | -1.63286600 |
| C  | 3.62211100  | 1.76844500  | -2.35182300 |
| C  | 2.33738600  | 1.30874600  | -2.15593800 |
| H  | 4.18276200  | 1.42263100  | -3.21435100 |
| H  | 1.87389400  | 0.60361500  | -2.83237100 |
| C  | -4.89613100 | -2.09888300 | 1.35574500  |
| H  | -2.77292600 | -2.36272300 | 1.11460400  |
| H  | -5.07241900 | -3.13671000 | 1.61979200  |
| C  | -5.99193600 | -1.19943200 | 1.29996000  |
| H  | -6.62212100 | 0.81878900  | 0.92876700  |
| H  | -6.99144100 | -1.56183100 | 1.51683600  |

File: p\_bp3\_R\_ts\_B3LYP.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.24484000  | -0.35137100 | 2.79661800  |
| C  | 3.92584300  | 0.09900400  | 2.91544900  |
| C  | 2.93927200  | -0.38742700 | 2.06091200  |
| C  | 3.26865000  | -1.33154400 | 1.07627800  |
| C  | 4.59241800  | -1.78168000 | 0.96031700  |
| C  | 5.57675900  | -1.29024700 | 1.81650000  |
| C  | 2.24039600  | -1.85552800 | 0.13913000  |
| O  | 1.18355100  | -1.08564400 | -0.04036600 |
| Si | -0.31803900 | -1.40847900 | -0.94916100 |
| O  | -1.14359400 | -0.69005700 | 0.60539000  |
| N  | -2.18529000 | 0.16017700  | 0.49213700  |
| C  | -1.93752900 | 1.43700100  | 0.13063400  |
| C  | -3.00599500 | 2.33461200  | -0.09703500 |
| C  | -4.29149900 | 1.87888500  | 0.15232200  |
| C  | -4.53978400 | 0.58305400  | 0.64147700  |
| C  | -3.44122900 | -0.30956800 | 0.80745200  |
| C  | -0.51219000 | 1.85936900  | 0.05241000  |
| C  | 0.02679500  | 2.84446800  | 0.91558100  |
| C  | 1.33214400  | 3.24964000  | 0.68860800  |
| C  | 2.10315900  | 2.72540600  | -0.36761100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.54389800  | 1.69761600  | -1.18136000 |
| N  | 0.25865100  | 1.29267100  | -0.89404200 |
| O  | -0.28776800 | 0.30841100  | -1.64916100 |
| C  | -0.50946900 | -3.23662400 | -0.09961800 |
| C  | 0.52989700  | -3.61485900 | 0.52594700  |
| C  | 1.78143300  | -3.56160500 | 1.06213900  |
| Cl | -2.26885400 | -1.65156300 | -1.98688100 |
| Cl | 0.78642900  | -2.18670900 | -2.71871900 |
| C  | -0.77218800 | 3.42508400  | 2.05765100  |
| H  | 1.77685100  | 3.99765800  | 1.33848800  |
| C  | -2.79354700 | 3.73137800  | -0.63134800 |
| H  | -5.13322400 | 2.54243800  | -0.02554800 |
| C  | -5.84266100 | 0.11315700  | 0.96197800  |
| H  | 2.62334800  | -2.34683500 | -0.75737900 |
| H  | 1.91510900  | -0.03906300 | 2.14285700  |
| H  | 4.85275900  | -2.50876500 | 0.19535100  |
| H  | 3.66827900  | 0.83113400  | 3.67543000  |
| H  | 6.60092800  | -1.63726400 | 1.71684200  |
| H  | 6.01141900  | 0.03015100  | 3.46494000  |
| H  | 2.55572700  | -4.21188000 | 0.65812400  |
| H  | 1.87016900  | -3.35291800 | 2.12711700  |
| H  | -1.45328100 | -3.74702500 | -0.23968900 |
| C  | 2.27081500  | 1.12682200  | -2.24620400 |
| C  | 3.42557400  | 3.16110200  | -0.65012900 |
| H  | -0.09588200 | 3.75459300  | 2.85039200  |
| H  | -1.46722400 | 2.69872600  | 2.48581200  |
| H  | -1.35095400 | 4.29867000  | 1.73871200  |
| H  | -3.06516900 | 4.48322800  | 0.11726000  |
| H  | -3.43945400 | 3.89000800  | -1.50050200 |
| H  | -1.76464800 | 3.91380700  | -0.94463700 |
| C  | 4.12927200  | 2.60500800  | -1.69226700 |
| H  | 3.85968100  | 3.94111000  | -0.03279700 |
| H  | 5.13720100  | 2.94312300  | -1.90971000 |
| C  | 3.54625400  | 1.58865700  | -2.49076300 |
| H  | 1.82153600  | 0.34623400  | -2.84497900 |
| H  | 4.11496800  | 1.16485600  | -3.31222900 |
| C  | -6.02081500 | -1.16389200 | 1.43723200  |
| H  | -6.68455900 | 0.78494900  | 0.82913500  |
| H  | -7.01563800 | -1.51848600 | 1.68623800  |
| C  | -4.90835500 | -2.02720300 | 1.60950300  |
| C  | -3.63075600 | -1.61916900 | 1.29607600  |
| H  | -5.06649300 | -3.02905300 | 1.99562700  |
| H  | -2.77715000 | -2.26894200 | 1.42776800  |

File: p\_bp4\_S\_B3LYP.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -6.86021900 | -2.25431000 | 0.84433200  |
| C  | -5.77841200 | -2.95772900 | 0.30450900  |
| C  | -4.56011200 | -2.31649700 | 0.09251900  |
| C  | -4.41876500 | -0.96028000 | 0.42271700  |
| C  | -5.50558900 | -0.25648600 | 0.96305800  |
| C  | -6.72171000 | -0.90367300 | 1.17516000  |
| C  | -3.12307500 | -0.25609600 | 0.22544700  |
| O  | -2.05400400 | -1.02583400 | 0.19923500  |
| Si | -0.39169500 | -0.87762400 | -0.37610500 |
| O  | 1.33784000  | -0.65441700 | -1.09382000 |
| N  | 2.40726400  | -0.61830600 | -0.27018900 |
| C  | 2.65471900  | 0.53604800  | 0.36787000  |
| C  | 3.69193700  | 0.62261200  | 1.32618800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.50199900  | -0.48981700 | 1.48337900  |
| C  | 4.31295800  | -1.66449200 | 0.72597000  |
| C  | 3.20709200  | -1.73627900 | -0.17072500 |
| C  | 1.84322100  | 1.71681600  | -0.03247200 |
| C  | 2.42730800  | 2.80446300  | -0.72924000 |
| C  | 1.64486800  | 3.92573300  | -0.93933700 |
| C  | 0.33791300  | 4.02070800  | -0.41787000 |
| C  | -0.22188000 | 2.89178700  | 0.24601400  |
| N  | 0.54197800  | 1.74053700  | 0.31426000  |
| O  | -0.02410200 | 0.61584300  | 0.80640400  |
| C  | -0.93868600 | 0.35888200  | -1.88755800 |
| C  | -2.16836600 | 0.67466900  | -1.87435700 |
| C  | -3.47955800 | 0.65897100  | -1.50121400 |
| Cl | 0.26738600  | -2.12451400 | 1.29512500  |
| Cl | -0.63580700 | -2.60758900 | -1.77084100 |
| C  | 3.83047400  | 2.71513300  | -1.28048900 |
| H  | 2.05082400  | 4.76437500  | -1.49689100 |
| C  | 3.86078400  | 1.84531600  | 2.19481800  |
| H  | 5.30956500  | -0.46061900 | 2.20886500  |
| C  | 5.16079200  | -2.79852500 | 0.83511000  |
| H  | -3.02355700 | 0.67450300  | 0.78426000  |
| H  | -3.71307800 | -2.85613900 | -0.31784200 |
| H  | -5.39716700 | 0.79328200  | 1.22547200  |
| H  | -5.88458600 | -4.00889700 | 0.05278300  |
| H  | -7.55755600 | -0.35699300 | 1.60158000  |
| H  | -7.80766900 | -2.75907300 | 1.01007700  |
| H  | -4.14478500 | -0.00934000 | -2.04580100 |
| H  | -3.94549800 | 1.57845600  | -1.15138400 |
| H  | -0.17897600 | 0.58148100  | -2.62659100 |
| C  | -0.45052600 | 5.19784000  | -0.52158500 |
| H  | 4.01193900  | 3.54990000  | -1.96111800 |
| H  | 3.98111600  | 1.78476500  | -1.83657400 |
| H  | 4.59193800  | 2.75835300  | -0.49526400 |
| H  | 4.75463900  | 1.74209200  | 2.81360800  |
| H  | 2.99959500  | 1.96077900  | 2.86278400  |
| H  | 3.95372500  | 2.77024300  | 1.61953300  |
| C  | -1.70106300 | 5.25081400  | 0.04902600  |
| H  | -0.03637300 | 6.05541800  | -1.04221100 |
| H  | -2.29496500 | 6.15590800  | -0.02317900 |
| C  | -2.20983100 | 4.13549700  | 0.75931200  |
| C  | -1.48894800 | 2.96394500  | 0.85664200  |
| H  | -3.17629500 | 4.20768100  | 1.24767900  |
| H  | -1.84469900 | 2.12486900  | 1.43653400  |
| C  | 4.91225000  | -3.92275900 | 0.08275500  |
| H  | 6.00306500  | -2.75470500 | 1.51825600  |
| H  | 5.56361600  | -4.78674800 | 0.16499700  |
| C  | 3.80559600  | -3.96535300 | -0.80250400 |
| C  | 2.94983600  | -2.89283300 | -0.93377000 |
| H  | 3.62580700  | -4.86168900 | -1.38739500 |
| H  | 2.09363700  | -2.92038700 | -1.59482200 |

File: p\_bp5\_S\_B3LYP\_ts.xyz

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -6.98069900 | -0.76194400 | 1.03270700  |
| C | -5.95041500 | 0.11074000  | 1.39903600  |
| C | -4.63101200 | -0.18348400 | 1.06427000  |
| C | -4.33119800 | -1.35633600 | 0.35597000  |
| C | -5.36605400 | -2.23162700 | -0.00438100 |
| C | -6.68661100 | -1.93232200 | 0.32973200  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.93752600 | -1.70199700 | -0.03886400 |
| O  | -2.11928400 | -0.67950400 | -0.24442600 |
| Si | -0.40035600 | -0.73314700 | -0.70407200 |
| O  | -0.06302300 | 0.57804500  | 0.60166700  |
| N  | 0.53681100  | 1.73969000  | 0.25314300  |
| C  | 1.87650600  | 1.74474000  | 0.10645100  |
| C  | 2.54005600  | 2.90866600  | -0.34865000 |
| C  | 1.77592100  | 4.05025200  | -0.53350800 |
| C  | 0.39318400  | 4.07274700  | -0.27096000 |
| C  | -0.25004700 | 2.86205800  | 0.11812000  |
| C  | 2.61824000  | 0.51297400  | 0.49140300  |
| C  | 3.56562700  | 0.50602200  | 1.54432400  |
| C  | 4.31734700  | -0.64388800 | 1.72747800  |
| C  | 4.17191600  | -1.76983200 | 0.89443500  |
| C  | 3.16284600  | -1.75155400 | -0.11281500 |
| N  | 2.39778100  | -0.60649200 | -0.23032000 |
| O  | 1.43440600  | -0.59385100 | -1.17443600 |
| C  | -0.01785600 | -2.01099700 | 0.85172000  |
| C  | -1.06857300 | -2.53799400 | 1.33011700  |
| C  | -2.40043300 | -2.77690600 | 1.51154600  |
| Cl | -0.76546800 | 0.72845400  | -2.30191000 |
| Cl | -0.57735500 | -2.44661000 | -2.11145500 |
| C  | 3.74884400  | 1.68354200  | 2.47199200  |
| H  | 5.04534500  | -0.67944800 | 2.53297200  |
| C  | 4.01840700  | 2.92360700  | -0.65708700 |
| H  | 2.25647500  | 4.95726900  | -0.88851400 |
| C  | -0.40202900 | 5.24296100  | -0.40566500 |
| H  | -2.85950300 | -2.51443800 | -0.76334400 |
| H  | -3.83021700 | 0.48960500  | 1.35147800  |
| H  | -5.13804700 | -3.13916200 | -0.55781400 |
| H  | -6.17801000 | 1.02173000  | 1.94501100  |
| H  | -7.48355700 | -2.61001400 | 0.03830600  |
| H  | -8.00883100 | -0.52843900 | 1.29395400  |
| H  | -2.88201400 | -2.31082500 | 2.36994100  |
| H  | -2.80210600 | -3.75254500 | 1.24162200  |
| H  | 0.99827300  | -2.16203800 | 1.18892100  |
| C  | 4.96649700  | -2.93993300 | 1.02782600  |
| H  | 3.88092800  | 1.32292700  | 3.49593400  |
| H  | 2.89402800  | 2.36201300  | 2.46282600  |
| H  | 4.64492300  | 2.25771300  | 2.21298700  |
| H  | 4.59941600  | 3.31112000  | 0.18666200  |
| H  | 4.20572000  | 3.58236700  | -1.50938200 |
| H  | 4.40222300  | 1.93253400  | -0.90805500 |
| C  | -1.75226200 | 5.19449800  | -0.15322300 |
| H  | 0.07957600  | 6.16751400  | -0.70773100 |
| H  | -2.35700600 | 6.08993500  | -0.25266100 |
| C  | -2.36786400 | 3.97583600  | 0.23203100  |
| C  | -1.63782300 | 2.81526700  | 0.36289000  |
| H  | -3.43625800 | 3.95572500  | 0.42146400  |
| H  | -2.09801100 | 1.87582900  | 0.63373800  |
| C  | 4.76222100  | -4.01404300 | 0.19383600  |
| H  | 5.73437300  | -2.96172300 | 1.79450000  |
| H  | 5.37411100  | -4.90450300 | 0.29396000  |
| C  | 3.75327900  | -3.96869900 | -0.80122000 |
| C  | 2.95099900  | -2.85873400 | -0.96096800 |
| H  | 3.60862200  | -4.82439800 | -1.45280300 |
| H  | 2.17465800  | -2.81766000 | -1.71324200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 6.70708800  | -1.49720200 | -1.67113200 |
| C  | 5.59597600  | -0.84477000 | -2.21330400 |
| C  | 4.39388200  | -0.80350700 | -1.50909800 |
| C  | 4.29557500  | -1.41874300 | -0.25255700 |
| C  | 5.41174400  | -2.07922700 | 0.28477700  |
| C  | 6.61151800  | -2.11782900 | -0.42222600 |
| C  | 3.02126000  | -1.41593800 | 0.51637500  |
| O  | 1.93404500  | -1.09647500 | -0.16722800 |
| Si | 0.26397300  | -0.97314000 | 0.42436600  |
| O  | -1.45568300 | -0.59164400 | 1.10263000  |
| N  | -2.49503300 | -0.42981300 | 0.25380000  |
| C  | -2.62482200 | 0.75666800  | -0.37605600 |
| C  | -3.64797600 | 0.94568400  | -1.33287900 |
| C  | -4.55176500 | -0.09005600 | -1.51765300 |
| C  | -4.47780300 | -1.28602300 | -0.78080500 |
| C  | -3.39506000 | -1.46491000 | 0.12962600  |
| C  | -1.69064800 | 1.84714000  | 0.01680100  |
| C  | -2.14266100 | 3.04673900  | 0.62015600  |
| C  | -1.21520100 | 4.05742100  | 0.81334200  |
| C  | 0.12879400  | 3.92239900  | 0.41001900  |
| C  | 0.55839000  | 2.67852000  | -0.13495000 |
| N  | -0.38217900 | 1.67671000  | -0.25877300 |
| O  | 0.01528700  | 0.48679900  | -0.75677700 |
| C  | 0.86906000  | 0.24170100  | 1.96639600  |
| C  | 2.12636200  | 0.23422100  | 2.13818200  |
| C  | 3.43631700  | -0.06990700 | 1.90218400  |
| Cl | -0.44508000 | -2.18674700 | -1.26028000 |
| Cl | 0.36160600  | -2.72844300 | 1.79286100  |
| C  | -3.57614200 | 3.21914700  | 1.06097100  |
| H  | -1.53067100 | 4.98509100  | 1.28144400  |
| C  | -3.75706500 | 2.19631400  | -2.17332400 |
| H  | -5.34549500 | 0.02566500  | -2.25028600 |
| C  | -5.42197200 | -2.33977700 | -0.91812600 |
| H  | 2.90501800  | -2.23996200 | 1.22273500  |
| H  | 3.52272200  | -0.31981300 | -1.93741900 |
| H  | 5.33740000  | -2.56891300 | 1.25274900  |
| H  | 5.66417300  | -0.37402400 | -3.18975200 |
| H  | 7.46869500  | -2.63611100 | -0.00276500 |
| H  | 7.64193100  | -1.52883100 | -2.22330000 |
| H  | 3.96487200  | -0.69257000 | 2.62204400  |
| H  | 4.05262200  | 0.68772900  | 1.41982000  |
| H  | 0.09878800  | 0.74838700  | 2.53366600  |
| C  | 1.08682800  | 4.96387800  | 0.53856400  |
| H  | -4.66245100 | 2.76011700  | -1.92418000 |
| H  | -3.82864400 | 1.91786100  | -3.22929700 |
| H  | -2.89740500 | 2.85878000  | -2.06274100 |
| H  | -3.63435400 | 3.99634200  | 1.62680100  |
| H  | -3.98874200 | 2.29791100  | 1.48066700  |
| H  | -4.21933100 | 3.52896100  | 0.23065200  |
| C  | -5.28803000 | -3.48843500 | -0.17574700 |
| H  | -6.24541800 | -2.21366200 | -1.61387600 |
| H  | -6.01211500 | -4.29012700 | -0.27812100 |
| C  | -4.20460800 | -3.63769600 | 0.72796500  |
| C  | -3.25838100 | -2.64864600 | 0.88450800  |
| H  | -4.11664600 | -4.55172600 | 1.30647900  |
| H  | -2.42154500 | -2.75986900 | 1.56082600  |
| C  | 2.38425300  | 4.76648700  | 0.12752100  |
| H  | 0.77072800  | 5.91395900  | 0.95728300  |

|   |            |            |             |
|---|------------|------------|-------------|
| H | 3.11124700 | 5.56676300 | 0.21950900  |
| C | 2.78286100 | 3.52135500 | -0.42202900 |
| C | 1.89088100 | 2.47867200 | -0.55016600 |
| H | 3.80869400 | 3.38714600 | -0.75004000 |
| H | 2.17870500 | 1.52328800 | -0.96608200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.45752500 | -2.62407600 | 1.84807500  |
| H | -2.36120400 | 1.66379200  | -3.25461000 |
| H | -3.40264600 | 2.69062900  | -2.27130100 |
| H | -4.11934000 | 1.56878400  | -3.43357000 |
| H | 2.30118400  | 1.77604600  | -0.45034900 |
| H | 3.68575000  | 3.80028200  | -0.16910700 |
| H | 2.64242800  | 5.97840000  | 0.42136500  |
| H | 0.18592800  | 6.13821300  | 0.72839400  |
| H | -2.02801300 | 5.01235100  | 0.80761900  |
| H | -4.10440600 | 3.94962300  | 1.02495000  |
| H | -4.44413700 | 2.93628500  | -0.37825100 |
| H | -4.14508800 | 2.18931900  | 1.19473300  |

File: p\_bp5\_R\_B3LYP\_ts.xyz

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.35951700 | 2.97270700  | 0.26340400  |
| C  | -1.71392000 | 1.78592100  | -0.16094800 |
| N  | -0.37210900 | 1.72078000  | -0.23206500 |
| C  | 0.45005000  | 2.81597600  | -0.05468500 |
| C  | -0.17045700 | 4.05266900  | 0.28870300  |
| C  | -1.56655700 | 4.08599800  | 0.47890700  |
| C  | 0.65420800  | 5.19615600  | 0.46176600  |
| C  | 2.01529800  | 5.10247700  | 0.29196600  |
| C  | 2.60940300  | 3.86102600  | -0.04521400 |
| C  | 1.84733700  | 2.72518800  | -0.21171800 |
| C  | -2.49385500 | 0.58395000  | -0.56160200 |
| C  | -3.36022100 | 0.58701400  | -1.68357300 |
| C  | -4.19884300 | -0.50217500 | -1.84586900 |
| C  | -4.20514500 | -1.58041300 | -0.93557500 |
| C  | -3.25889900 | -1.58498800 | 0.13021500  |
| N  | -2.40663700 | -0.50142200 | 0.22918300  |
| C  | -3.19147400 | -2.64938400 | 1.05312800  |
| C  | -4.07734300 | -3.69713900 | 0.90882600  |
| C  | -5.02750300 | -3.71876100 | -0.14207200 |
| C  | -5.08995900 | -2.68501800 | -1.04819800 |
| C  | -3.31163300 | 1.69401500  | -2.70921300 |
| O  | -1.48742800 | -0.50462500 | 1.21835200  |
| Si | 0.34330100  | -0.81431200 | 0.81251000  |
| Cl | 0.35309700  | -2.50712300 | 2.24674100  |
| O  | 0.18385900  | 0.52552400  | -0.53487900 |
| C  | -3.84489200 | 3.00902800  | 0.53442900  |
| O  | 2.07871200  | -0.98072500 | 0.44522300  |
| C  | 2.69005100  | -0.95528000 | -0.72635600 |
| C  | 4.15888600  | -1.19116600 | -0.68983700 |
| C  | 4.75625500  | -1.87410900 | 0.38033400  |
| C  | 6.13612300  | -2.06352100 | 0.39826300  |
| C  | 6.92786900  | -1.57557600 | -0.64658100 |
| C  | 6.33612700  | -0.89242700 | -1.71217800 |
| C  | 4.95535300  | -0.70223600 | -1.73631000 |
| C  | -0.11660100 | -2.14409100 | -0.65286800 |
| C  | 0.84836000  | -2.40793000 | -1.43732200 |
| C  | 2.12927100  | -2.44072800 | -1.90204900 |
| Cl | 0.78815100  | 0.64079300  | 2.38970000  |
| H  | -1.08503700 | -2.62769200 | -0.63758000 |
| H  | 2.36227600  | -0.17594100 | -1.41823900 |
| H  | 2.35546300  | -2.03685400 | -2.88754000 |
| H  | 2.74958600  | -3.28340500 | -1.59971700 |
| H  | 4.13674600  | -2.24115600 | 1.19168000  |
| H  | 6.59654300  | -2.58869500 | 1.22998300  |
| H  | 8.00370600  | -1.72408900 | -0.62759000 |
| H  | 6.94886700  | -0.50507000 | -2.52079100 |
| H  | 4.49592300  | -0.16541300 | -2.56275800 |
| H  | -4.87493900 | -0.53127200 | -2.69505100 |
| H  | -5.81235900 | -2.69367000 | -1.85818400 |
| H  | -5.70822300 | -4.55919600 | -0.22936700 |
| H  | -4.04548900 | -4.51922800 | 1.61651900  |

# ALLYLATION - B97D/6-31G\*

File: a\_bp1\_S\_B97D\_631g.xyz

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.0543950  | -2.9579330 | -0.9234950 |
| C  | 4.2751390  | -1.7739860 | -0.7733480 |
| C  | 3.1978550  | -1.7866350 | 0.1741370  |
| C  | 2.9137090  | -2.9355220 | 0.9487700  |
| C  | 3.7040280  | -4.0621090 | 0.7776160  |
| C  | 4.7745300  | -4.0786210 | -0.1608000 |
| N  | 2.4455140  | -0.6294920 | 0.3041340  |
| C  | 2.7149500  | 0.5157960  | -0.3748030 |
| C  | 3.7472270  | 0.5482950  | -1.3502620 |
| C  | 4.5040270  | -0.6050480 | -1.5358630 |
| O  | 1.4168650  | -0.6372770 | 1.1757300  |
| Si | -0.3711660 | -0.7667880 | 0.5119100  |
| Cl | -0.8279620 | 0.7602160  | 2.1562470  |
| C  | 1.9245890  | 1.7328430  | -0.0516170 |
| C  | 2.5199160  | 2.9156310  | 0.4561550  |
| C  | 1.7173130  | 4.0496390  | 0.5726340  |
| C  | 0.3563070  | 4.0426540  | 0.1923070  |
| C  | -0.2281390 | 2.8153810  | -0.2674420 |
| N  | 0.5972170  | 1.7085230  | -0.3400620 |
| C  | -1.5945880 | 2.7329810  | -0.6259580 |
| C  | -2.3677200 | 3.8802900  | -0.5358600 |
| C  | -1.8141060 | 5.1133580  | -0.0849520 |
| C  | -0.4804390 | 5.1944230  | 0.2754710  |
| C  | 3.9983050  | 1.7857570  | -2.1824680 |
| C  | 3.9634430  | 2.9607300  | 0.9068830  |
| O  | 0.0626350  | 0.5430650  | -0.7615080 |
| O  | -2.0429750 | -0.7449090 | -0.1271260 |
| C  | -3.1880870 | -0.7571000 | 0.5329840  |
| C  | -4.4106620 | -0.9842750 | -0.2771840 |
| C  | -4.3516240 | -1.6079320 | -1.5415010 |
| C  | -5.5264440 | -1.7939910 | -2.2794880 |
| C  | -6.7633140 | -1.3668280 | -1.7617670 |
| C  | -6.8240920 | -0.7474300 | -0.5011700 |
| C  | -5.6515900 | -0.5591030 | 0.2415410  |
| C  | -0.7421810 | -2.3294880 | 1.8369300  |
| Cl | 0.2109570  | -2.2031550 | -1.1478530 |
| H  | 2.1493360  | 4.9693810  | 0.9700810  |
| H  | 5.2913530  | -0.6117790 | -2.2907410 |
| H  | -3.2932340 | -0.0437850 | 1.3601040  |
| H  | -3.3866470 | -1.9303810 | -1.9327340 |
| H  | -5.6898940 | -0.0787320 | 1.2216630  |
| H  | -5.4806110 | -2.2714790 | -3.2596490 |
| H  | -7.7814550 | -0.4111800 | -0.1001000 |
| H  | -7.6766860 | -1.5156310 | -2.3402700 |
| H  | 4.0077520  | 3.3302300  | 1.9422420  |
| H  | 4.4463540  | 1.9766450  | 0.8733370  |
| H  | 4.5420450  | 3.6584560  | 0.2827580  |
| H  | 4.5189560  | 1.5075870  | -3.1086240 |
| H  | 3.0591870  | 2.2925010  | -2.4448060 |
| H  | 4.6327730  | 2.5052190  | -1.6432290 |
| H  | -2.0088780 | 1.7838450  | -0.9534540 |
| H  | -3.4213530 | 3.8351830  | -0.8121970 |
| H  | -0.0454850 | 6.1300600  | 0.6273320  |
| H  | -2.4507870 | 5.9959230  | -0.0220900 |
| H  | 2.0921260  | -2.9193020 | 1.6579630  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 3.4974390  | -4.9523370 | 1.3719190  |
| H | 5.3740540  | -4.9816600 | -0.2762200 |
| H | 5.8699000  | -2.9552460 | -1.6469670 |
| H | 0.0420470  | -2.2225850 | 2.5954750  |
| C | -2.0733160 | -2.1782950 | 2.3682820  |
| H | -0.6140720 | -3.2247420 | 1.2185440  |
| C | -3.2217860 | -2.4746620 | 1.6358650  |
| H | -2.1939070 | -1.6093470 | 3.2933560  |
| H | -4.1983750 | -2.3940380 | 2.1154250  |
| H | -3.1537370 | -3.1709590 | 0.7965970  |

File: a\_bp1\_R\_B97D\_631G.xyz

|    |            |            |            |
|----|------------|------------|------------|
| C  | -1.7422420 | 2.6629320  | -0.5709630 |
| C  | -0.3762140 | 2.8053170  | -0.2304790 |
| C  | 0.1615090  | 4.0568150  | 0.2219010  |
| C  | -0.7224760 | 5.1720980  | 0.3134060  |
| C  | -2.0559340 | 5.0331340  | -0.0301530 |
| C  | -2.5623710 | 3.7763820  | -0.4711410 |
| N  | 0.4968290  | 1.7370490  | -0.3134840 |
| C  | 1.8221240  | 1.8174510  | -0.0359100 |
| C  | 2.3740800  | 3.0229820  | 0.4655670  |
| C  | 1.5250140  | 4.1222030  | 0.5885640  |
| C  | 2.6584570  | 0.6340100  | -0.3679920 |
| N  | 2.4701470  | -0.5140120 | 0.3329200  |
| C  | 3.3053960  | -1.6161450 | 0.2134210  |
| C  | 4.3455860  | -1.5584540 | -0.7731230 |
| C  | 4.4713010  | -0.3982060 | -1.5724120 |
| C  | 3.6558150  | 0.7115360  | -1.3768430 |
| C  | 3.1465560  | -2.7499380 | 1.0425880  |
| C  | 4.0097000  | -3.8229850 | 0.8770770  |
| C  | 5.0341160  | -3.8002500 | -0.1105220 |
| C  | 5.2006220  | -2.6891150 | -0.9192890 |
| O  | 1.4482140  | -0.5793310 | 1.2112360  |
| Si | -0.3479730 | -0.7787210 | 0.5489040  |
| Cl | -0.8558450 | 0.7172590  | 2.1870070  |
| C  | 3.7962240  | 1.9490950  | -2.2344010 |
| C  | 3.8195070  | 3.1252030  | 0.9014050  |
| O  | 0.0135330  | 0.5458940  | -0.7262070 |
| O  | -2.0520860 | -0.7277090 | 0.0060820  |
| C  | -2.8333160 | -1.7051930 | -0.4163420 |
| C  | -4.2737230 | -1.3716280 | -0.5531900 |
| C  | -4.8368910 | -0.2659420 | 0.1192500  |
| C  | -6.1953050 | 0.0294390  | -0.0456020 |
| C  | -6.9998880 | -0.7764720 | -0.8721870 |
| C  | -6.4411530 | -1.8808270 | -1.5390930 |
| C  | -5.0821500 | -2.1802330 | -1.3786650 |
| C  | -0.6957450 | -2.3787010 | 1.8451040  |
| Cl | 0.3157750  | -2.1956670 | -1.1090700 |
| H  | 1.9210070  | 5.0601590  | 0.9808560  |
| H  | 5.2288840  | -0.3763350 | -2.3564630 |
| H  | -2.4215690 | -2.3768490 | -1.1798230 |
| H  | -4.2024160 | 0.3521520  | 0.7546180  |
| H  | -4.6403800 | -3.0355990 | -1.8945370 |
| H  | -6.6295410 | 0.8878210  | 0.4697800  |
| H  | -7.0624760 | -2.5043420 | -2.1837270 |
| H  | -8.0588030 | -0.5436100 | -0.9966560 |
| H  | 2.8137200  | 2.3279780  | -2.5506210 |
| H  | 4.3097990  | 2.7571000  | -1.6925780 |

|   |            |            |            |
|---|------------|------------|------------|
| H | 4.3876300  | 1.7138970  | -3.1292980 |
| H | 4.3447990  | 2.1640740  | 0.8448730  |
| H | 4.3604960  | 3.8582870  | 0.2838670  |
| H | 3.8594630  | 3.4774150  | 1.9430100  |
| H | 5.9866830  | -2.6511650 | -1.6739070 |
| H | 5.6928930  | -4.6614710 | -0.2221960 |
| H | 3.9005630  | -4.6975140 | 1.5186670  |
| H | 2.3742630  | -2.7549990 | 1.8042820  |
| H | -0.3234480 | 6.1260740  | 0.6585740  |
| H | -2.7289210 | 5.8878280  | 0.0399110  |
| H | -3.6173370 | 3.6846340  | -0.7306620 |
| H | -2.1219380 | 1.6952310  | -0.8854800 |
| H | 0.2978700  | -2.7990440 | 2.0276060  |
| H | -1.1187030 | -1.9056090 | 2.7373360  |
| C | -1.5960140 | -3.2977680 | 1.1972860  |
| C | -2.9670010 | -3.0626160 | 1.0977350  |
| H | -1.1667950 | -4.0910680 | 0.5805760  |
| H | -3.6099580 | -3.8186150 | 0.6444220  |
| H | -3.4425880 | -2.3982400 | 1.8230480  |

File: a\_BP2\_S\_B97D\_631g

|    |            |            |            |
|----|------------|------------|------------|
| C  | 2.3083940  | 1.2208330  | 2.0883220  |
| C  | 1.5056950  | 1.8060800  | 1.0819650  |
| C  | 1.9989300  | 2.8876330  | 0.2771790  |
| C  | 3.3345350  | 3.3369610  | 0.4972390  |
| C  | 4.1208940  | 2.7449230  | 1.4702410  |
| C  | 3.6000600  | 1.6913700  | 2.2723750  |
| N  | 0.2211220  | 1.3483780  | 0.8318820  |
| C  | -0.6018060 | 1.9260640  | -0.0828460 |
| C  | -0.1332350 | 2.9722010  | -0.9216380 |
| C  | 1.1675290  | 3.4280470  | -0.7298720 |
| C  | -2.0130850 | 1.4663770  | -0.1269830 |
| N  | -2.2504520 | 0.1926510  | -0.5270420 |
| C  | -3.5188540 | -0.3047650 | -0.7798820 |
| C  | -4.6301910 | 0.5688100  | -0.5285840 |
| C  | -4.3838210 | 1.8660360  | -0.0223460 |
| C  | -3.0898860 | 2.3404600  | 0.1741450  |
| C  | -3.7088340 | -1.6178030 | -1.2682750 |
| C  | -5.0045260 | -2.0511770 | -1.5078200 |
| C  | -6.1255220 | -1.2087770 | -1.2616230 |
| C  | -5.9436460 | 0.0755790  | -0.7784880 |
| O  | -1.1885630 | -0.6178230 | -0.7291540 |
| Si | -0.3687160 | -1.4480330 | 0.7484140  |
| Cl | -0.6844720 | -3.4417930 | -0.2397590 |
| C  | -2.8429310 | 3.7338400  | 0.7068470  |
| C  | -0.9808720 | 3.5610770  | -2.0287680 |
| O  | -0.2454870 | 0.3196800  | 0.3196800  |
| O  | 1.1569280  | -1.0769940 | -0.1574220 |
| C  | 2.1388230  | -1.9129120 | -0.4475990 |
| C  | 3.3441500  | -1.3681690 | -1.1221280 |
| C  | 3.6296680  | 0.0105740  | -1.1555770 |
| C  | 4.7723990  | 0.4750020  | -1.8168160 |
| C  | 5.6425690  | -0.4328540 | -2.4458600 |
| C  | 5.3607420  | -1.8104550 | -2.4173510 |
| C  | 4.2175940  | -2.2772090 | -1.7577670 |
| C  | 0.7096400  | -2.2707310 | 2.3435950  |
| Cl | -2.2670280 | -1.5915280 | 1.9554970  |
| H  | 1.5600690  | 4.2167150  | -1.3729360 |

|   |            |            |            |
|---|------------|------------|------------|
| H | -5.2315610 | 2.5100030  | 0.2151870  |
| H | 1.8480120  | -2.9170850 | -0.7758960 |
| H | 2.9470990  | 0.7059550  | -0.6791960 |
| H | 3.9932510  | -3.3457440 | -1.7339590 |
| H | 4.9827360  | 1.5453540  | -1.8435810 |
| H | 6.0289760  | -2.5174320 | -2.9112410 |
| H | 6.5336360  | -0.0690190 | -2.9601470 |
| H | -0.4115290 | 3.5414900  | -2.9698660 |
| H | -1.9178680 | 3.0129110  | -2.1823360 |
| H | -1.2216020 | 4.6126680  | -1.8110080 |
| H | -1.9533470 | 3.7710120  | 1.3503240  |
| H | -2.6986740 | 4.4510390  | -0.1155460 |
| H | -3.7127380 | 4.0646390  | 1.2904210  |
| H | -6.7915390 | 0.7323790  | -0.5833100 |
| H | -7.1312880 | -1.5821290 | -1.4548610 |
| H | -5.1649640 | -3.0597740 | -1.8891310 |
| H | -2.8493310 | -2.2593350 | -1.4376460 |
| H | 3.7169650  | 4.1505970  | -0.1193140 |
| H | 5.1428510  | 3.0880250  | 1.6302730  |
| H | 4.2242390  | 1.2455340  | 3.0467800  |
| H | 1.9006420  | 0.4288120  | 2.7057060  |
| H | -0.0230620 | -2.9068870 | 2.8489470  |
| C | 1.8382360  | -3.0101560 | 1.8400500  |
| H | 0.9677980  | -1.3949450 | 2.9484320  |
| C | 2.9955120  | -2.4199540 | 1.3372460  |
| H | 1.6901380  | -4.0747140 | 1.6399870  |
| H | 3.8223940  | -3.0542600 | 1.0158450  |
| H | 3.2595320  | -1.4044090 | 1.6404350  |

File: A\_BP2\_R\_B97D\_631G.xyz

|    |            |            |            |
|----|------------|------------|------------|
| C  | -3.2475100 | -2.3171150 | -0.6177720 |
| C  | -3.3227270 | -0.9079890 | -0.5225520 |
| C  | -4.5861060 | -0.2242480 | -0.5058860 |
| C  | -5.7758860 | -1.0069480 | -0.5790120 |
| C  | -5.6979040 | -2.3850790 | -0.6745170 |
| C  | -4.4310580 | -3.0357440 | -0.6961980 |
| N  | -2.1811180 | -0.1290820 | -0.4475540 |
| C  | -2.1980160 | 1.2282230  | -0.4148080 |
| C  | -3.4266680 | 1.9313330  | -0.3603850 |
| C  | -4.6024970 | 1.1840190  | -0.3976820 |
| O  | -0.9804080 | -0.7482480 | -0.4747040 |
| Si | -0.0108760 | -0.9734840 | 1.1102630  |
| Cl | 0.1599160  | -3.1654930 | 0.6319130  |
| C  | -0.8892270 | 1.9245450  | -0.5105640 |
| C  | -0.5495230 | 2.7246150  | -1.6341180 |
| C  | 0.6709970  | 3.3911150  | -0.6112550 |
| C  | 1.5273680  | 3.3245820  | -0.4856270 |
| C  | 1.1525840  | 2.5007750  | 0.6268840  |
| N  | -0.0321060 | 1.7870380  | 0.5306200  |
| C  | 1.9540540  | 2.4293340  | 1.7894380  |
| C  | 3.1390240  | 3.1508950  | 1.8286690  |
| C  | 3.5540850  | 3.9430990  | 0.7220380  |
| C  | 2.7621960  | 4.0324970  | -0.4109320 |
| C  | -3.4864500 | 3.4379100  | -0.2331690 |
| C  | -1.4711870 | 2.8179910  | -2.8285660 |
| O  | -0.3484750 | 0.9162320  | 1.5064090  |
| O  | 1.3605890  | -0.4460710 | 0.0775410  |

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|----|------------|------------|------------|
| C  | 2.6773880  | -0.4349300 | 0.0304520  |
| C  | 3.3933520  | -1.3507460 | -0.8949810 |
| C  | 2.7164470  | -2.3369230 | -1.6407330 |
| C  | 3.4256390  | -3.1357480 | -2.5483190 |
| C  | 4.8083510  | -2.9567180 | -2.7225370 |
| C  | 5.4849130  | -1.9617600 | -1.9931480 |
| C  | 4.7803350  | -1.1610340 | -1.0881000 |
| C  | 1.2304560  | -1.1811520 | 2.7905070  |
| Cl | -1.8282670 | -1.2631820 | 2.4060500  |
| H  | 0.9751540  | 3.9852090  | -2.4736670 |
| H  | -5.5630540 | 1.6984010  | -0.3440440 |
| H  | 3.1036350  | 0.5784170  | 0.0751810  |
| H  | 1.6433700  | -2.4581050 | -1.5145720 |
| H  | 5.3020140  | -0.3835410 | -0.5251150 |
| H  | 2.8963070  | -3.8961830 | -3.1250380 |
| H  | 6.5562770  | -1.8103240 | -2.1339000 |
| H  | 5.3560860  | -3.5824810 | -3.4293330 |
| H  | -0.8963210 | 3.1051960  | -3.7191530 |
| H  | -1.9746290 | 1.8615630  | -3.0269010 |
| H  | -2.2471500 | 3.5820290  | -2.6678540 |
| H  | -3.8986550 | 3.8866860  | -1.1500040 |
| H  | -4.1568040 | 3.7071080  | 0.5964190  |
| H  | -2.5026430 | 3.8821520  | -0.0391190 |
| H  | 3.0588820  | 4.6502320  | -1.2587550 |
| H  | 4.4945890  | 4.4912200  | 0.7756740  |
| H  | 3.7579660  | 3.1112800  | 2.7252780  |
| H  | 1.6207920  | 1.8354750  | 2.6344960  |
| H  | -6.7378450 | -0.4942950 | -0.5612580 |
| H  | -6.6088010 | -2.9809590 | -0.7329350 |
| H  | -4.3878770 | -4.1223830 | -0.7719910 |
| H  | -2.2781310 | -2.8071280 | -0.6189910 |
| H  | 0.6788790  | -1.9293440 | 3.3675620  |
| C  | 2.5201070  | -1.6274120 | 2.3566460  |
| H  | 1.2121920  | -0.1902310 | 3.2583440  |
| C  | 3.5078460  | -0.7634060 | 1.8919140  |
| H  | 2.6483880  | -2.6978200 | 2.1773690  |
| H  | 4.4814020  | -1.1638980 | 1.6107700  |
| H  | 3.4968240  | 0.2731040  | 2.2329080  |

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|----|------------|------------|------------|
| C  | -6.1875870 | -0.5715970 | -1.2476300 |
| C  | -5.8515730 | 0.6782440  | -0.7580770 |
| C  | -4.4906920 | 0.9974200  | -0.4743370 |
| C  | -3.4962220 | -0.0126700 | -0.7009550 |
| C  | -3.8462600 | -1.2892180 | -1.1997840 |
| C  | -5.1801340 | -1.5533870 | -1.4700880 |
| N  | -2.1786750 | 0.3125840  | -0.4214390 |
| C  | -1.7902400 | 1.5432550  | 0.0062710  |
| C  | -2.7501120 | 2.5509560  | 0.2751220  |
| C  | -4.0896190 | 2.2527400  | 0.0351630  |
| O  | -1.2406600 | -0.6279440 | -0.6205110 |
| Si | -0.4184780 | -1.5548490 | 0.8841100  |
| Cl | 0.6438040  | -2.5390040 | 2.5888690  |
| C  | -0.3302760 | 1.7924740  | 0.1080450  |
| C  | 0.3274970  | 2.7330370  | -0.7281630 |
| C  | 1.6882370  | 2.9411180  | -0.5229450 |
| C  | 2.3954110  | 2.2701110  | 0.5018670  |
| C  | 1.7008820  | 1.3179070  | 1.3220810  |

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|----|------------|------------|------------|
| N  | 0.3585760  | 1.1003050  | 1.0488920  |
| C  | 2.3645820  | 0.6098850  | 2.3489730  |
| C  | 3.7161530  | 0.8494570  | 2.5493610  |
| C  | 4.4323780  | 1.7766960  | 1.7418090  |
| C  | 3.7854530  | 2.4751040  | 0.7373700  |
| C  | -2.3617810 | 3.9006440  | 0.8386200  |
| C  | -0.4174970 | 3.4489450  | -1.8317980 |
| O  | -0.3056100 | 0.1409000  | 1.7388680  |
| O  | 1.1918870  | -1.2262250 | 0.1241470  |
| C  | 1.5046190  | -1.0765090 | -1.1409400 |
| C  | 2.9365760  | -0.8874420 | -1.4507080 |
| C  | 3.9380920  | -1.2055160 | -0.5083570 |
| C  | 5.2792700  | -0.9425540 | -0.8062650 |
| C  | 5.6305600  | -0.3696320 | -2.0424910 |
| C  | 4.6346120  | -0.0562690 | -2.9845690 |
| C  | 3.2904240  | -0.3160220 | -2.6915330 |
| C  | -0.5795980 | -3.2981230 | -0.2573380 |
| Cl | -2.4080620 | -1.7939740 | 1.8798800  |
| H  | 2.2279910  | 3.6323710  | -1.1714930 |
| H  | -4.8504050 | 3.0053930  | 0.2455170  |
| H  | 0.7976060  | -0.5374100 | -1.7818780 |
| H  | 3.6497530  | -1.6304730 | 0.4521580  |
| H  | 2.5096050  | -0.0695200 | -3.4143850 |
| H  | 6.0527500  | -1.1774730 | -0.0735440 |
| H  | 4.9062760  | 0.3918310  | -3.9415110 |
| H  | 6.6781440  | -0.1653050 | -2.2698910 |
| H  | -1.1428070 | 2.7865800  | -2.3252050 |
| H  | -0.9665320 | 4.3185920  | -1.4402310 |
| H  | 0.2952040  | 3.8128150  | -2.5840670 |
| H  | -1.3035610 | 3.9492830  | 1.1225120  |
| H  | -2.5661710 | 4.6973300  | 0.1069960  |
| H  | -2.9679080 | 4.1103270  | 1.7323480  |
| H  | 4.3189090  | 3.1894850  | 0.1102560  |
| H  | 5.4964610  | 1.9337860  | 1.9179100  |
| H  | 4.2387940  | 0.3105180  | 3.3397580  |
| H  | 1.8159630  | -0.1112370 | 2.9466370  |
| H  | -3.0740900 | -2.0351410 | -1.3563640 |
| H  | -5.4612060 | -2.5333600 | -1.8561090 |
| H  | -6.6116490 | 1.4398140  | -0.5824400 |
| H  | -7.2284490 | -0.8114090 | -1.4649480 |
| H  | -1.6370110 | -3.5728250 | -0.1737760 |
| C  | -0.1527480 | -3.0383570 | -1.6139930 |
| H  | 0.0681360  | -4.0038990 | 0.2757640  |
| C  | 1.1823300  | -2.9776380 | -1.9934110 |
| H  | -0.9000390 | -2.6769240 | -2.3257640 |
| H  | 1.4475690  | -2.7936020 | -3.0354380 |
| H  | 1.9371090  | -3.4734490 | -1.3790590 |

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|   |           |            |            |
|---|-----------|------------|------------|
| C | 4.6388620 | -1.2628630 | -0.9509030 |
| C | 3.2781120 | -0.9284240 | -1.1096060 |
| C | 2.9034680 | 0.1015860  | -1.9989340 |
| C | 3.8869430 | 0.7966500  | -2.7107040 |
| C | 5.2450740 | 0.4669730  | -2.5454830 |
| C | 5.6195380 | -0.5633830 | -1.6653740 |
| C | 2.2743380 | -1.6269830 | -0.2777610 |

|    |            |            |            |
|----|------------|------------|------------|
| O  | 1.1266310  | -1.0150090 | -0.1196930 |
| Si | -0.3826170 | -1.5577650 | 0.7032210  |
| Cl | -2.3727260 | -1.9696770 | 1.6386470  |
| O  | -1.2128450 | -0.5398230 | -0.7308020 |
| N  | -2.2309890 | 0.2960560  | -0.4622670 |
| C  | -3.5133760 | -0.0939800 | -0.8136560 |
| C  | -4.5888340 | 0.8058840  | -0.5064490 |
| C  | -4.2997870 | 2.0212690  | 0.1536570  |
| C  | -2.9929620 | 2.3926620  | 0.4615330  |
| C  | -1.9513190 | 1.5004680  | 0.1054280  |
| C  | -5.9139400 | 0.4186650  | -0.8645420 |
| C  | -6.1403840 | -0.7898380 | -1.4992490 |
| C  | -5.0546880 | -1.6626220 | -1.7959800 |
| C  | -3.7519130 | -1.3314100 | -1.4565430 |
| C  | -0.5158010 | 1.8556390  | 0.2366140  |
| C  | 0.0599710  | 2.9156420  | -0.5132830 |
| C  | 1.4187050  | 3.1635850  | -0.3455490 |
| C  | 2.2021390  | 2.4191340  | 0.5670620  |
| C  | 1.5815410  | 1.3721410  | 1.3266050  |
| N  | 0.2399210  | 1.1185600  | 1.0850030  |
| C  | 2.3194100  | 0.5966720  | 2.2490030  |
| C  | 3.6770440  | 0.8457120  | 2.3856900  |
| C  | 4.3243640  | 1.8587890  | 1.6239600  |
| C  | 3.6001900  | 2.6368530  | 0.7379280  |
| C  | -2.7225240 | 3.6926330  | 1.1876450  |
| C  | -0.7660780 | 3.7102970  | -1.4988850 |
| O  | -0.3483910 | 0.0616990  | 1.6972500  |
| Cl | 0.7019150  | -2.6204330 | 2.3645400  |
| C  | -0.4481420 | -3.2194620 | -0.5510920 |
| C  | 0.8756760  | -3.7868440 | -0.6748340 |
| H  | 1.1841820  | -4.5238990 | 0.0708880  |
| H  | 1.8977070  | 3.9403700  | -0.9427820 |
| H  | -5.1235810 | 2.6827510  | 0.4253610  |
| H  | 2.6630510  | -2.2035630 | 0.5690400  |
| H  | 1.8490660  | 0.3544000  | -2.1076930 |
| H  | 4.9204390  | -2.0588080 | -0.2581630 |
| H  | 3.5988340  | 1.5989380  | -3.3920460 |
| H  | 6.6725300  | -0.8165380 | -1.5338840 |
| H  | 6.0094930  | 1.0134890  | -3.1003870 |
| H  | -1.1652400 | -3.8882560 | -0.0622970 |
| H  | -1.3533310 | 4.4863540  | -0.9848670 |
| H  | -0.1050680 | 4.2089590  | -2.2203210 |
| H  | -1.4680160 | 3.0666020  | -2.0476660 |
| H  | -3.2933250 | 3.7100620  | 2.1283610  |
| H  | -1.6613980 | 3.8269510  | 1.4304050  |
| H  | -3.0567770 | 4.5483890  | 0.5815040  |
| H  | 4.0798080  | 3.4207300  | 0.1516720  |
| H  | 5.3953000  | 2.0214530  | 1.7448770  |
| H  | 1.8224150  | -0.1860590 | 2.8136770  |
| H  | 4.2580080  | 0.2490040  | 3.0891620  |
| H  | -6.7345320 | 1.0965180  | -0.6283570 |
| H  | -7.1543090 | -1.0811090 | -1.7738830 |
| H  | -5.2501330 | -2.6119380 | -2.2949850 |
| H  | -2.9205320 | -1.9964360 | -1.6667150 |
| C  | 1.8490830  | -3.2659520 | -1.5182790 |
| H  | -0.8332860 | -2.8134250 | -1.4943300 |
| H  | 2.8278170  | -3.7432600 | -1.5849080 |
| H  | 1.5473530  | -2.6553180 | -2.3722730 |

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| H  | -0.9773050 | 1.6524680  | -0.9880490 |
| C  | -1.6051950 | 1.4486050  | -0.1162560 |
| C  | -0.9832090 | 0.9319110  | 1.0711150  |
| Si | -0.8245260 | -1.0641940 | 0.6903200  |
| O  | -2.5885480 | -1.1161530 | 0.4511930  |
| C  | -3.2426380 | -0.4534490 | -0.5232380 |
| C  | -4.7328640 | -0.5696370 | -0.4747920 |
| C  | -5.4588420 | -0.4070260 | -1.6713680 |
| C  | -6.8565160 | -0.5123510 | -1.6629110 |
| C  | -7.5329670 | -0.7706230 | -0.4587190 |
| C  | -6.8084120 | -0.9255490 | 0.7376240  |
| C  | -5.4122480 | -0.8192610 | 0.7342800  |
| O  | 1.0562240  | -0.9498660 | 1.1154790  |
| N  | 2.0768440  | -1.1305560 | 0.2352140  |
| C  | 2.6456750  | -0.0391990 | -0.3407070 |
| C  | 3.7024640  | -0.1884780 | -1.2784700 |
| C  | 4.1409540  | -1.4719000 | -1.5773620 |
| C  | 3.5916460  | -2.6070730 | -0.9338140 |
| C  | 2.5368050  | -2.4276360 | 0.0222110  |
| C  | 4.0559730  | -3.9296550 | -1.1886130 |
| C  | 3.5073270  | -5.0072350 | -0.5139550 |
| C  | 2.4806080  | -4.8003790 | 0.4469830  |
| C  | 1.9916600  | -3.5295120 | 0.7184190  |
| C  | 2.2336970  | 1.2973620  | 0.1482730  |
| N  | 1.5392570  | 2.0657880  | -0.7440340 |
| C  | 1.1660180  | 3.3806440  | -0.3943680 |
| C  | 1.5005910  | 3.8756710  | 0.9061970  |
| C  | 2.2204150  | 3.0472420  | 1.8091250  |
| C  | 2.5999800  | 1.7654610  | 1.4408380  |
| C  | 0.4543700  | 4.1709270  | -1.3258540 |
| C  | 0.0710010  | 5.4555290  | -0.9628370 |
| C  | 0.3856700  | 5.9704030  | 0.3238580  |
| C  | 1.0864930  | 5.1982080  | 1.2380260  |
| O  | 1.1885380  | 1.5782870  | -1.8870860 |
| C  | 3.3781900  | 0.8630550  | 2.3699560  |
| C  | 4.3227000  | 1.0374650  | -1.9034510 |
| Cl | -1.0345490 | -2.2853310 | 2.3980520  |
| Cl | -0.4238210 | -1.8418610 | -1.2449180 |
| H  | -2.8276740 | -0.5788690 | -1.5324870 |
| H  | 0.0298950  | 1.2790720  | 1.2747370  |
| C  | -3.0057570 | 1.3891250  | -0.2714800 |
| H  | -1.6236410 | 0.9604430  | 1.9628590  |
| H  | 2.4848670  | 3.4323230  | 2.7942900  |
| H  | 4.9441850  | -1.6127580 | -2.3017930 |
| H  | -4.8414920 | -0.9415000 | 1.6549170  |
| H  | -4.9270670 | -0.2101100 | -2.6047980 |
| H  | -7.3335650 | -1.1301110 | 1.6719900  |
| H  | -7.4149960 | -0.3963500 | -2.5929640 |
| H  | -8.6211740 | -0.8518060 | -0.4511500 |
| H  | 3.6926190  | 1.4182440  | 3.2637730  |
| H  | 2.7608880  | 0.0077960  | 2.6859430  |
| H  | 4.2750540  | 0.4619530  | 1.8716510  |
| H  | 5.1391480  | 0.7501220  | -2.5788250 |
| H  | 3.5620760  | 1.5921250  | -2.4731690 |
| H  | 4.7252820  | 1.7107090  | -1.1302130 |
| H  | 1.3349260  | 5.5872920  | 2.2263980  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 0.0743270  | 6.9809480  | 0.5907990  |
| H | -0.4756230 | 6.0749830  | -1.6744970 |
| H | 0.2285580  | 3.7575690  | -2.3058260 |
| H | 4.8530820  | -4.0670750 | -1.9197010 |
| H | 3.8667520  | -6.0172840 | -0.7111110 |
| H | 2.0677140  | -5.6530560 | 0.9864020  |
| H | 1.2156120  | -3.3740170 | 1.4599280  |
| H | -3.4396690 | 1.8318620  | -1.1708900 |
| H | -3.6010800 | 1.5154000  | 0.6368290  |

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|    |            |            |            |
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| C  | -2.0092590 | 2.3245470  | -0.4775340 |
| C  | -0.6757410 | 2.6237140  | -0.1109690 |
| C  | -0.3133020 | 3.9012100  | 0.4298780  |
| C  | -1.3402940 | 4.8794500  | 0.5793390  |
| C  | -2.6429000 | 4.5871750  | 0.2112080  |
| C  | -2.9752770 | 3.3068140  | -0.3163540 |
| N  | 0.3244630  | 1.6715810  | -0.2430590 |
| C  | 1.6281620  | 1.9128740  | 0.0581720  |
| C  | 2.0114540  | 3.1490270  | 0.6430410  |
| C  | 1.0280910  | 4.1199450  | 0.8215010  |
| C  | 2.6167170  | 0.8734880  | -0.3300820 |
| N  | 2.5415500  | -0.3406330 | 0.2747960  |
| C  | 3.4834190  | -1.3418650 | 0.0958440  |
| C  | 4.5535090  | -1.0850090 | -0.8261220 |
| C  | 4.5821590  | 0.1479220  | -1.5172880 |
| C  | 3.6352560  | 1.1411080  | -1.2822300 |
| C  | 3.3919150  | -2.5667140 | 0.7970340  |
| C  | 4.3701100  | -3.5257430 | 0.5794010  |
| C  | 5.4403110  | -3.2992870 | -0.3318370 |
| C  | 5.5302560  | -2.1040670 | -1.0240880 |
| O  | 1.5174350  | -0.5704330 | 1.1231580  |
| Si | -0.1944940 | -1.0541890 | 0.4205150  |
| Cl | -0.2135800 | -2.9301770 | 1.6744610  |
| C  | 3.6823610  | 2.4492030  | -2.0403540 |
| C  | 3.4294130  | 3.4152940  | 1.0999280  |
| O  | -0.0073620 | 0.4748810  | -0.7494460 |
| O  | -1.8613560 | -1.1815470 | -0.2327730 |
| C  | -2.9513780 | -1.6268650 | 0.3660740  |
| C  | -4.2263610 | -1.4853350 | -0.3858030 |
| C  | -4.3208280 | -0.6812610 | -1.5408790 |
| C  | -5.5417290 | -0.5731760 | -2.2188850 |
| C  | -6.6744100 | -1.2626470 | -1.7511080 |
| C  | -6.5810900 | -2.0722210 | -0.6050700 |
| C  | -5.3628370 | -2.1827480 | 0.0758280  |
| C  | -0.9034680 | 0.0549470  | 2.0725020  |
| Cl | 0.6019630  | -2.1596490 | -1.3320630 |
| H  | 1.2965150  | 5.0732630  | 1.2784510  |
| H  | 5.3662050  | 0.3220800  | -2.2552510 |
| H  | -2.8506240 | -2.5420690 | 0.9620710  |
| H  | -3.4332150 | -0.1748280 | -1.9179980 |
| H  | -5.2850540 | -2.8083330 | 0.9677410  |
| H  | -5.6083300 | 0.0417970  | -3.1178930 |
| H  | -7.4551610 | -2.6175450 | -0.2459440 |
| H  | -7.6239170 | -1.1759450 | -2.2819310 |
| H  | 4.1619500  | 2.2906310  | -3.0157430 |
| H  | 2.6781210  | 2.8622270  | -2.2069660 |
| H  | 4.2739700  | 3.1998650  | -1.4946330 |

|   |            |            |            |
|---|------------|------------|------------|
| H | 3.8971920  | 4.1913580  | 0.4750930  |
| H | 3.4132530  | 3.7909870  | 2.1337030  |
| H | 4.0566130  | 2.5161240  | 1.0686270  |
| H | 6.3430180  | -1.9175020 | -1.7263230 |
| H | 6.1903570  | -4.0756300 | -0.4835080 |
| H | 4.3133130  | -4.4734120 | 1.1152000  |
| H | 2.5635250  | -2.7386630 | 1.4780100  |
| H | -1.0758550 | 5.8540420  | 0.9901200  |
| H | -3.4236570 | 5.3387080  | 0.3274950  |
| H | -4.0059380 | 3.0908210  | -0.5989460 |
| H | -2.2458070 | 1.3395930  | -0.8676870 |
| H | -0.0848620 | -0.0285250 | 2.7953000  |
| H | -1.0361790 | 1.0816420  | 1.7216560  |
| C | -2.1327990 | -0.5300160 | 2.5346050  |
| C | -3.3534870 | -0.3356060 | 1.8899460  |
| H | -2.0723290 | -1.3275660 | 3.2788850  |
| H | -4.2601340 | -0.7678770 | 2.3151190  |
| H | -3.4922360 | 0.5556570  | 1.2735240  |

File: a\_bp5\_s\_B97D\_631g

|    |            |            |            |
|----|------------|------------|------------|
| C  | 3.0788450  | -2.7622900 | 0.9331930  |
| C  | 3.2319620  | -1.6418050 | 0.0820520  |
| C  | 4.2060570  | -1.6282050 | -0.9709610 |
| C  | 5.0239960  | -2.7822130 | -1.1447160 |
| C  | 4.8751450  | -3.8756080 | -0.3081590 |
| C  | 3.9018440  | -3.8614830 | 0.7303610  |
| N  | 2.4316250  | -0.5165930 | 0.2341000  |
| C  | 2.5906950  | 0.6126860  | -0.5064630 |
| C  | 3.5135700  | 0.6396590  | -1.5870250 |
| C  | 4.2973440  | -0.4896860 | -1.8054600 |
| C  | 1.8149630  | 1.8211220  | -0.1238430 |
| N  | 0.4634840  | 1.7557160  | -0.2423220 |
| C  | -0.3730140 | 2.8451930  | -0.0751600 |
| C  | 0.2352820  | 4.1003710  | 0.2615660  |
| C  | 1.6341830  | 4.1508350  | 0.4565670  |
| C  | 2.4421530  | 3.0297440  | 0.2739770  |
| C  | -1.7737300 | 2.7183480  | -0.2277800 |
| C  | -2.5591760 | 3.8492240  | -0.0675590 |
| C  | -1.9814650 | 5.1117230  | 0.2524110  |
| C  | -0.6132620 | 5.2355910  | 0.4208710  |
| O  | -0.0856600 | 0.5722310  | -0.5719630 |
| Si | -0.3487890 | -0.7686440 | 0.7746160  |
| Cl | -0.4690680 | -2.4732500 | 2.2431360  |
| C  | 3.9296930  | 3.1168260  | 0.5382840  |
| C  | 3.6287520  | 1.8485490  | -2.4884290 |
| O  | 1.5089320  | -0.5295820 | 1.2144470  |
| O  | -2.0883510 | -0.7130410 | 0.3149860  |
| C  | -2.9391310 | -1.7116310 | 0.1801560  |
| C  | -4.2799320 | -1.3730320 | -0.3603500 |
| C  | -4.4785480 | -0.2607230 | -1.2053130 |
| C  | -5.7618690 | 0.0371270  | -1.6764870 |
| C  | -6.8535180 | -0.7750560 | -1.3157370 |
| C  | -6.6567330 | -1.8892690 | -0.4827080 |
| C  | -5.3725410 | -2.1918350 | -0.0097610 |
| C  | 0.0257860  | -2.1048410 | -0.8108080 |
| Cl | -0.7380110 | 0.7236610  | 2.3759130  |
| H  | 5.0027760  | -0.5000980 | -2.6372250 |
| H  | 2.0905870  | 5.0929400  | 0.7639520  |

|   |            |            |            |
|---|------------|------------|------------|
| H | -2.9181100 | -2.4915490 | 0.9510190  |
| H | -3.6255750 | 0.3553380  | -1.4899810 |
| H | -5.2125970 | -3.0540300 | 0.6409760  |
| H | -5.9145430 | 0.9005500  | -2.3261640 |
| H | -7.5013690 | -2.5194500 | -0.2002530 |
| H | -7.8531220 | -0.5399680 | -1.6850860 |
| H | 2.6639690  | 2.3598990  | -2.6086210 |
| H | 4.3492770  | 2.5754950  | -2.0841690 |
| H | 3.9887380  | 1.5368220  | -3.4782900 |
| H | 4.4197330  | 2.1358510  | 0.5130590  |
| H | 4.4177040  | 3.7723920  | -0.1989770 |
| H | 4.0957770  | 3.5576890  | 1.5324390  |
| H | -0.1596190 | 6.1925310  | 0.6796830  |
| H | -2.6269010 | 5.9817440  | 0.3742890  |
| H | -3.6404670 | 3.7664680  | -0.1798850 |
| H | -2.2029880 | 1.7434730  | -0.4363060 |
| H | 5.7645570  | -2.7784990 | -1.9449060 |
| H | 5.5048940  | -4.7551180 | -0.4424750 |
| H | 3.7989890  | -4.7293180 | 1.3819910  |
| H | 2.3249160  | -2.7443300 | 1.7159580  |
| H | 0.9982120  | -2.5503780 | -0.5813190 |
| C | -1.0228550 | -3.0905230 | -0.8475210 |
| H | 0.0608750  | -1.4677540 | -1.7020250 |
| C | -2.2753850 | -2.8409400 | -1.4004090 |
| H | -0.9029630 | -3.9863910 | -0.2337680 |
| H | -3.0228140 | -3.6350420 | -1.4329660 |
| H | -2.3763300 | -2.0531180 | -2.1503490 |

File: a\_bp5\_R\_B97D\_631g.xyz

|    |            |            |            |
|----|------------|------------|------------|
| C  | 1.7270600  | 2.8374080  | 0.0811350  |
| C  | 0.3155900  | 2.8748630  | 0.0136020  |
| C  | -0.3766790 | 4.0980830  | -0.2807310 |
| C  | 0.3938980  | 5.2805620  | -0.4817610 |
| C  | 1.7742460  | 5.2390360  | -0.3926000 |
| C  | 2.4381970  | 4.0113600  | -0.1153390 |
| N  | -0.4530640 | 1.7377770  | 0.2228020  |
| C  | -1.8101710 | 1.7441130  | 0.1797670  |
| C  | -2.5214400 | 2.9226440  | -0.1684000 |
| C  | -1.7858230 | 4.0819450  | -0.3926780 |
| O  | 0.1638050  | 0.5769280  | 0.5227330  |
| Si | 0.3887740  | -0.7884200 | -0.8335130 |
| Cl | 0.4708270  | -2.4707530 | -2.3177940 |
| C  | -2.5358080 | 0.4995680  | 0.5409700  |
| C  | -3.4337900 | 0.4432590  | 1.6388960  |
| C  | -4.2193640 | -0.6988060 | 1.7809060  |
| C  | -4.1423760 | -1.7722690 | 0.8646460  |
| C  | -3.1799060 | -1.7110940 | -0.1993860 |
| N  | -2.3929240 | -0.5704490 | -0.2870510 |
| C  | -3.0191260 | -2.7778140 | -1.1140130 |
| C  | -3.8333390 | -3.8928350 | -0.9736810 |
| C  | -4.8024470 | -3.9772090 | 0.0659650  |
| C  | -4.9530750 | -2.9400520 | 0.9705590  |
| C  | -4.0273730 | 2.9190310  | -0.3087530 |
| C  | -3.5239010 | 1.5555020  | 2.6615230  |
| O  | -1.4700640 | -0.5121040 | -1.2633290 |
| O  | 2.1543480  | -0.9093290 | -0.4831910 |
| C  | 2.8014410  | -0.7224100 | 0.6476950  |
| C  | 4.2487430  | -1.0418690 | 0.6547730  |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 4.8167350  | -1.9109480 | -0.3005700 |
| C  | 6.1908560  | -2.1748720 | -0.2677260 |
| C  | 7.0030900  | -1.5812400 | 0.7163400  |
| C  | 6.4379830  | -0.7168140 | 1.6701950  |
| C  | 5.0634430  | -0.4496570 | 1.6424660  |
| C  | 0.0120190  | -2.1422480 | 0.7459010  |
| Cl | 0.7983340  | 0.7195850  | -2.4110120 |
| H  | -4.9132470 | -0.7701680 | 2.6196690  |
| H  | -2.3056360 | 5.0001870  | -0.6685750 |
| H  | 2.5013690  | 0.1292990  | 1.2693700  |
| H  | 4.1778240  | -2.3607260 | -1.0605850 |
| H  | 4.6157190  | 0.2220650  | 2.3784080  |
| H  | 6.6318240  | -2.8422490 | -1.0098200 |
| H  | 7.0672760  | -0.2516940 | 2.4304940  |
| H  | 8.0738360  | -1.7908060 | 0.7379260  |
| H  | -4.5332060 | 1.9938730  | 2.6687100  |
| H  | -3.3374700 | 1.1416220  | 3.6641100  |
| H  | -2.7957900 | 2.3552400  | 2.4809360  |
| H  | -4.5164770 | 3.0741800  | 0.6648360  |
| H  | -4.3360800 | 3.7372970  | -0.9729630 |
| H  | -4.3943630 | 1.9704940  | -0.7244200 |
| H  | -5.6859310 | -2.9931040 | 1.7760300  |
| H  | -5.4251410 | -4.8680470 | 0.1486480  |
| H  | -3.7261980 | -4.7198690 | -1.6757210 |
| H  | -2.2685800 | -2.7086970 | -1.8965260 |
| H  | -0.1301450 | 6.2097060  | -0.7067180 |
| H  | 2.3600200  | 6.1455050  | -0.5451470 |
| H  | 3.5268080  | 3.9869190  | -0.0659430 |
| H  | 2.2344610  | 1.8975330  | 0.2570040  |
| H  | -1.0525750 | -2.0662110 | 0.9793000  |
| H  | 0.2583770  | -3.1139180 | 0.3056720  |
| C  | 0.8326580  | -1.8095560 | 1.8815470  |
| C  | 2.1692510  | -2.1809530 | 1.9729090  |
| H  | 0.4532200  | -1.0671400 | 2.5888910  |
| H  | 2.7481080  | -1.9279300 | 2.8621360  |
| H  | 2.5270740  | -3.0312350 | 1.3882490  |

# PROPARGYLATION- B97D/6-31G\*

File:P\_BP1\_S\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 6.7542630  | -1.3347690 | 1.6948120  |
| C  | 5.5239190  | -1.6696610 | 2.2897520  |
| C  | 4.3354080  | -1.5690860 | 1.5559540  |
| C  | 4.3749730  | -1.1228650 | 0.2188090  |
| C  | 5.6090740  | -0.7924950 | -0.3778320 |
| C  | 6.7952700  | -0.8944160 | 0.3604760  |
| C  | 3.1354500  | -0.9992220 | -0.5986310 |
| O  | 2.0068860  | -0.8528490 | 0.0999220  |
| Si | 0.3373140  | -0.8225610 | -0.5162470 |
| O  | -1.4548100 | -0.6276380 | -1.1832170 |
| N  | -2.4803310 | -0.5473600 | -0.3079890 |
| C  | -2.6723510 | 0.6169250  | 0.3665700  |
| C  | -3.6871700 | 0.7212950  | 1.3546610  |
| C  | -4.5083240 | -0.3827860 | 1.5630320  |
| C  | -4.3709070 | -1.5633400 | 0.7976640  |
| C  | -3.3163970 | -1.6460360 | -0.1723530 |
| C  | -1.8150010 | 1.7837050  | 0.0296810  |
| C  | -2.3395200 | 2.9928980  | -0.4919300 |
| C  | -1.4688480 | 4.0744520  | -0.6219790 |
| C  | -0.1103210 | 3.9896270  | -0.2414730 |
| C  | 0.3993710  | 2.7355620  | 0.2354000  |
| N  | -0.4936900 | 1.6847650  | 0.3225660  |
| O  | -0.0357360 | 0.4896770  | 0.7553430  |
| C  | 0.6165960  | -2.3984330 | -1.8015600 |
| C  | 1.8471660  | -2.7266330 | -1.8788730 |
| C  | 3.1892910  | -2.6801530 | -1.5692710 |
| Cl | -0.3077300 | -2.2800040 | 1.0701430  |
| Cl | 0.8306070  | 0.6245920  | -2.1904210 |
| C  | -3.7789380 | 3.1174450  | -0.9407260 |
| H  | -1.8436210 | 5.0136900  | -1.0314540 |
| C  | -3.8537140 | 1.9800030  | 2.1762210  |
| H  | -5.2796800 | -0.3392720 | 2.3326220  |
| C  | -3.1458640 | -2.8021120 | -0.9678300 |
| H  | 3.2278310  | -0.3530780 | -1.4820440 |
| H  | 3.3756550  | -1.8225420 | 2.0061020  |
| H  | 5.6318540  | -0.4510690 | -1.4150340 |
| H  | 5.4932550  | -2.0086430 | 3.3265490  |
| H  | 7.7476220  | -0.6295900 | -0.1015170 |
| H  | 7.6779830  | -1.4159620 | 2.2703140  |
| H  | 3.5609170  | -3.4232810 | -0.8549980 |
| H  | 3.9011370  | -2.4236250 | -2.3612650 |
| H  | -0.2695510 | -2.8255110 | -2.2584770 |
| C  | 1.7585830  | 2.5727630  | 0.5930700  |
| C  | 0.7953570  | 5.0865670  | -0.3410400 |
| H  | -4.3121740 | 3.8599030  | -0.3278260 |
| H  | -3.8043110 | 3.4692090  | -1.9828680 |
| H  | -4.3198030 | 2.1648150  | -0.8874440 |
| H  | -4.3823290 | 1.7435400  | 3.1094540  |
| H  | -2.8834840 | 2.4313220  | 2.4258990  |
| H  | -4.4480080 | 2.7314280  | 1.6346470  |
| C  | 2.6005810  | 3.6690880  | 0.4845030  |
| H  | 2.1144640  | 1.6039530  | 0.9320100  |
| H  | 3.6504090  | 3.5628910  | 0.7585700  |
| C  | 2.1225210  | 4.9277520  | 0.0180900  |
| H  | 0.4178200  | 6.0425460  | -0.7043450 |

|   |            |            |            |
|---|------------|------------|------------|
| H | 2.8122500  | 5.7684240  | -0.0580150 |
| C | -4.0114560 | -3.8702160 | -0.7866520 |
| H | -2.3597990 | -2.8304600 | -1.7140540 |
| H | -3.8913510 | -4.7624610 | -1.4012330 |
| C | -5.0508820 | -3.8214150 | 0.1845240  |
| C | -5.2288730 | -2.6897390 | 0.9611950  |
| H | -5.7109140 | -4.6798320 | 0.3093060  |
| H | -6.0255960 | -2.6321210 | 1.7032600  |

File: P\_BP1\_R\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -6.9648260 | -0.7949530 | -1.0511800 |
| C  | -6.1648860 | 0.1115250  | -0.3314510 |
| C  | -4.8259860 | -0.1937350 | -0.0573310 |
| C  | -4.2779420 | -1.4107130 | -0.5140680 |
| C  | -5.0820970 | -2.3204580 | -1.2306620 |
| C  | -6.4213840 | -2.0108160 | -1.5011450 |
| C  | -2.8563700 | -1.7694150 | -0.2496570 |
| O  | -2.0534770 | -0.7366990 | 0.0135920  |
| Si | -0.3568550 | -0.7729260 | 0.5426630  |
| O  | 1.4370430  | -0.6016440 | 1.1908150  |
| N  | 2.4559570  | -0.5580500 | 0.3075220  |
| C  | 2.6774690  | 0.5978310  | -0.3721070 |
| C  | 3.7041320  | 0.6733990  | -1.3506490 |
| C  | 4.5069280  | -0.4481110 | -1.5388900 |
| C  | 4.3298950  | -1.6246330 | -0.7750930 |
| C  | 3.2563520  | -1.6826280 | 0.1754030  |
| C  | 1.8424750  | 1.7837400  | -0.0450400 |
| C  | 2.3930910  | 2.9866880  | 0.4646040  |
| C  | 1.5461790  | 4.0877430  | 0.5879030  |
| C  | 0.1846020  | 4.0281930  | 0.2149680  |
| C  | -0.3538950 | 2.7798760  | -0.2452170 |
| N  | 0.5165450  | 1.7097180  | -0.3289090 |
| O  | 0.0236510  | 0.5204280  | -0.7416590 |
| C  | -0.6467380 | -2.2645850 | 1.9209670  |
| C  | -1.7957490 | -2.8027900 | 1.7884670  |
| C  | -3.0727240 | -2.9443570 | 1.2901260  |
| Cl | 0.2525740  | -2.2648870 | -1.0386890 |
| Cl | -0.8325760 | 0.7032830  | 2.1913940  |
| C  | 3.8343600  | 3.0858280  | 0.9138490  |
| H  | 1.9430190  | 5.0223450  | 0.9872420  |
| C  | 3.9059880  | 1.9219770  | -2.1797410 |
| H  | 5.2917380  | -0.4234930 | -2.2957190 |
| C  | 5.1609930  | -2.7727550 | -0.9259980 |
| H  | -2.4359240 | -2.5337870 | -0.9167680 |
| H  | -4.1962610 | 0.5006050  | 0.4988710  |
| H  | -4.6521800 | -3.2621900 | -1.5792050 |
| H  | -6.5872330 | 1.0560740  | 0.0157090  |
| H  | -7.0386160 | -2.7131130 | -2.0634820 |
| H  | -8.0081950 | -0.5536250 | -1.2612860 |
| H  | -3.3457510 | -3.8808160 | 0.7926210  |
| H  | -3.8811890 | -2.4939380 | 1.8765700  |
| H  | 0.1448450  | -2.4058330 | 2.6507650  |
| C  | -0.6971870 | 5.1449190  | 0.3096870  |
| H  | 4.5167300  | 2.6618070  | -1.6405710 |
| H  | 4.4326070  | 1.6662390  | -3.1089950 |
| H  | 2.9483260  | 2.3957020  | -2.4362030 |
| H  | 3.8643750  | 3.4406510  | 1.9548780  |
| H  | 4.3579240  | 2.1234500  | 0.8651710  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 4.3819860  | 3.8166060  | 0.2997150  |
| C | 4.9324270  | -3.9041590 | -0.1622290 |
| H | 5.9748520  | -2.7333190 | -1.6503950 |
| H | 5.5712220  | -4.7798270 | -0.2775420 |
| C | 3.8632870  | -3.9342730 | 0.7773480  |
| C | 3.0249000  | -2.8432070 | 0.9495810  |
| H | 3.6961150  | -4.8325770 | 1.3718270  |
| H | 2.2030540  | -2.8646430 | 1.6574970  |
| C | -2.0298800 | 5.0103750  | -0.0381670 |
| H | -0.2971330 | 6.0960560  | 0.6613090  |
| H | -2.7015190 | 5.8658560  | 0.0345890  |
| C | -2.5372640 | 3.7568120  | -0.4872240 |
| C | -1.7194070 | 2.6419930  | -0.5903590 |
| H | -3.5915230 | 3.6686530  | -0.7508460 |
| H | -2.1009710 | 1.6771350  | -0.9114540 |

File: P\_BP2\_S\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.0543950  | -2.9579330 | -0.9234950 |
| C  | 4.2751390  | -1.7739860 | -0.7733480 |
| C  | 3.1978550  | -1.7866350 | 0.1741370  |
| C  | 2.9137090  | -2.9355220 | 0.9487700  |
| C  | 3.7040280  | -4.0621090 | 0.7776160  |
| C  | 4.7745300  | -4.0786210 | -0.1608000 |
| N  | 2.4455140  | -0.6294920 | 0.3041340  |
| C  | 2.7149500  | 0.5157960  | -0.3748030 |
| C  | 3.7472270  | 0.5482950  | -1.3502620 |
| C  | 4.5040270  | -0.6050480 | -1.5358630 |
| O  | 1.4168650  | -0.6372770 | 1.1757300  |
| Si | -0.3711660 | -0.7667880 | 0.5119100  |
| Cl | -0.8279620 | 0.7602160  | 2.1562470  |
| C  | 1.9245890  | 1.7328430  | -0.0516170 |
| C  | 2.5199160  | 2.9156310  | 0.4561550  |
| C  | 1.7173130  | 4.0496390  | 0.5726340  |
| C  | 0.3563070  | 4.0426540  | 0.1923070  |
| C  | -0.2281390 | 2.8153810  | -0.2674420 |
| N  | 0.5972170  | 1.7085230  | -0.3400620 |
| C  | -1.5945880 | 2.7329810  | -0.6259580 |
| C  | -2.3677200 | 3.8802900  | -0.5358600 |
| C  | -1.8141060 | 5.1133580  | -0.0849520 |
| C  | -0.4804390 | 5.1944230  | 0.2754710  |
| C  | 3.9983050  | 1.7857570  | -2.1824680 |
| C  | 3.9634430  | 2.9607300  | 0.9068830  |
| O  | 0.0626350  | 0.5430650  | -0.7615080 |
| O  | -2.0429750 | -0.7449090 | -0.1271260 |
| C  | -3.1880870 | -0.7571000 | 0.5329840  |
| C  | -4.4106620 | -0.9842750 | -0.2771840 |
| C  | -4.3516240 | -1.6079320 | -1.5415010 |
| C  | -5.5264440 | -1.7939910 | -2.2794880 |
| C  | -6.7633140 | -1.3668280 | -1.7617670 |
| C  | -6.8240920 | -0.7474300 | -0.5011700 |
| C  | -5.6515900 | -0.5591030 | 0.2415410  |
| C  | -0.7421810 | -2.3294880 | 1.8369300  |
| Cl | 0.2109570  | -2.2031550 | -1.1478530 |
| H  | 2.1493360  | 4.9693810  | 0.9700810  |
| H  | 5.2913530  | -0.6117790 | -2.2907410 |
| H  | -3.2932340 | -0.0437850 | 1.3601040  |
| H  | -3.3866470 | -1.9303810 | -1.9327340 |
| H  | -5.6898940 | -0.0787320 | 1.2216630  |

|   |            |            |            |
|---|------------|------------|------------|
| H | -5.4806110 | -2.2714790 | -3.2596490 |
| H | -7.7814550 | -0.4111800 | -0.1001000 |
| H | -7.6766860 | -1.5156310 | -2.3402700 |
| H | 4.0077520  | 3.3302300  | 1.9422420  |
| H | 4.4463540  | 1.9766450  | 0.8733370  |
| H | 4.5420450  | 3.6584560  | 0.2827580  |
| H | 4.5189560  | 1.5075870  | -3.1086240 |
| H | 3.0591870  | 2.2925010  | -2.4448060 |
| H | 4.6327730  | 2.5052190  | -1.6432290 |
| H | -2.0088780 | 1.7838450  | -0.9534540 |
| H | -3.4213530 | 3.8351830  | -0.8121970 |
| H | -0.0454850 | 6.1300600  | 0.6273320  |
| H | -2.4507870 | 5.9959230  | -0.0220900 |
| H | 2.0921260  | -2.9193020 | 1.6579630  |
| H | 3.4974390  | -4.9523370 | 1.3719190  |
| H | 5.3740540  | -4.9816600 | -0.2762200 |
| H | 5.8699000  | -2.9552460 | -1.6469670 |
| H | 0.0420470  | -2.2225850 | 2.5954750  |
| C | -2.0733160 | -2.1782950 | 2.3682820  |
| H | -0.6140720 | -3.2247420 | 1.2185440  |
| C | -3.2217860 | -2.4746620 | 1.6358650  |
| H | -2.1939070 | -1.6093470 | 3.2933560  |
| H | -4.1983750 | -2.3940380 | 2.1154250  |
| H | -3.1537370 | -3.1709590 | 0.7965970  |

File: P\_BP2\_R\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 4.8720770  | -2.7029480 | -2.8561980 |
| C  | 3.5418500  | -3.0827710 | -2.6023470 |
| C  | 2.7912390  | -2.4178440 | -1.6241990 |
| C  | 3.3750820  | -1.3615850 | -0.8956870 |
| C  | 4.7102260  | -0.9813600 | -1.1511880 |
| C  | 5.4554610  | -1.6487710 | -2.1303510 |
| C  | 2.6163950  | -0.6116090 | 0.1415490  |
| O  | 1.2929950  | -0.6741930 | 0.0942940  |
| Si | -0.1178800 | -1.0438300 | 1.1220870  |
| O  | -1.0435600 | -0.7835890 | -0.4812200 |
| N  | -2.1883760 | -0.0684170 | -0.4883910 |
| C  | -2.1024020 | 1.2859670  | -0.4735470 |
| C  | -3.2769510 | 2.0815360  | -0.4607550 |
| C  | -4.5044170 | 1.4262060  | -0.5186750 |
| C  | -4.5927660 | 0.0175030  | -0.6032680 |
| C  | -3.3857080 | -0.7592720 | -0.5787650 |
| C  | -0.7466530 | 1.8952530  | -0.5017360 |
| C  | -0.2911380 | 2.7041920  | -1.5745630 |
| C  | 0.9609680  | 3.3025980  | -1.4505260 |
| C  | 1.7435060  | 3.1544100  | -0.2820420 |
| C  | 1.2571970  | 2.3177140  | 0.7769480  |
| N  | 0.0421060  | 1.6857870  | 0.5838640  |
| O  | -0.3901610 | 0.8191380  | 1.5229980  |
| C  | 1.0417470  | -1.2324030 | 2.8189210  |
| C  | 2.2887370  | -1.3079740 | 2.5615220  |
| C  | 3.4268810  | -1.3521740 | 1.7969100  |
| Cl | -1.9648130 | -1.2917720 | 2.3801030  |
| Cl | -0.0020810 | -3.2360570 | 0.6833270  |
| C  | -1.0977590 | 2.8861890  | -2.8414020 |
| H  | 1.3496760  | 3.9040250  | -2.2732500 |
| C  | -3.2008430 | 3.5886040  | -0.3656690 |
| H  | -5.4237910 | 2.0123100  | -0.4963800 |

|   |            |            |            |
|---|------------|------------|------------|
| C | -5.8359300 | -0.6745640 | -0.6883930 |
| H | 3.0058480  | 0.3966110  | 0.3402990  |
| H | 1.7594510  | -2.6988990 | -1.4196520 |
| H | 5.1550940  | -0.1616780 | -0.5819170 |
| H | 3.0892300  | -3.8974030 | -3.1701380 |
| H | 6.4853080  | -1.3487390 | -2.3301410 |
| H | 5.4520310  | -3.2245490 | -3.6195230 |
| H | 4.2011600  | -0.5955020 | 1.9567140  |
| H | 3.8094010  | -2.3422960 | 1.5281700  |
| H | 0.4933850  | -1.3394510 | 3.7501160  |
| C | 3.0148700  | 3.7780380  | -0.1129750 |
| H | -0.4538260 | 2.6993980  | -3.7133660 |
| H | -1.9568350 | 2.2062660  | -2.8938370 |
| H | -1.4654380 | 3.9209370  | -2.9186540 |
| H | -4.1362320 | 3.9797870  | 0.0566820  |
| H | -2.3651140 | 3.9128650  | 0.2698360  |
| H | -3.0664750 | 4.0404920  | -1.3601440 |
| C | 3.7369550  | 3.5877230  | 1.0531720  |
| H | 3.3964040  | 4.4079880  | -0.9167990 |
| H | 4.7065550  | 4.0694880  | 1.1787130  |
| C | 3.2189570  | 2.7707200  | 2.0982810  |
| C | 1.9933730  | 2.1325880  | 1.9715250  |
| H | 3.7940710  | 2.6422660  | 3.0154000  |
| H | 1.5952460  | 1.4935260  | 2.7535930  |
| C | -5.8598200 | -2.0569120 | -0.7557920 |
| H | -6.7566910 | -0.0909150 | -0.7005540 |
| H | -6.8118570 | -2.5835670 | -0.8229770 |
| C | -4.6461350 | -2.8015240 | -0.7357510 |
| C | -3.4136170 | -2.1718740 | -0.6445530 |
| H | -4.6838740 | -3.8897630 | -0.7876510 |
| H | -2.4838120 | -2.7328700 | -0.6116200 |

File: P\_BP3\_S\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.5387200  | -0.3291420 | -2.1522790 |
| C  | 5.2193220  | -0.8106990 | -0.8698460 |
| C  | 3.8956920  | -1.1320090 | -0.5476210 |
| C  | 2.8804090  | -0.9608370 | -1.5107890 |
| C  | 3.2017730  | -0.4833210 | -2.7982380 |
| C  | 4.5283680  | -0.1661660 | -3.1164850 |
| C  | 1.4543590  | -1.2279780 | -1.1858250 |
| O  | 1.1659450  | -1.2460730 | 0.1109150  |
| Si | -0.4214900 | -1.5415130 | 0.8914240  |
| O  | -1.2189410 | -0.6362430 | -0.6217280 |
| N  | -2.1598800 | 0.3039210  | -0.4319980 |
| C  | -1.7765250 | 1.5335290  | 0.0037790  |
| C  | -2.7415570 | 2.5387140  | 0.2619800  |
| C  | -4.0774900 | 2.2387350  | 0.0023470  |
| C  | -4.4703280 | 0.9851040  | -0.5178440 |
| C  | -3.4713750 | -0.0229680 | -0.7333730 |
| C  | -0.3166490 | 1.7841180  | 0.1188500  |
| C  | 0.3481350  | 2.7253800  | -0.7108490 |
| C  | 1.7079650  | 2.9313440  | -0.4956550 |
| C  | 2.4082610  | 2.2577680  | 0.5320900  |
| C  | 1.7084930  | 1.3004620  | 1.3413900  |
| N  | 0.3681110  | 1.0896120  | 1.0605020  |
| O  | -0.3020280 | 0.1316170  | 1.7500540  |
| C  | -0.6666060 | -3.2913640 | -0.1746510 |
| C  | 0.1167140  | -3.3650810 | -1.1820550 |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 1.1746810  | -3.0101030 | -1.9874200 |
| Cl | -2.4204510 | -1.7764000 | 1.8645940  |
| Cl | 0.6095240  | -2.5881780 | 2.5608190  |
| C  | -0.3886530 | 3.4479140  | -1.8155800 |
| H  | 2.2519260  | 3.6255670  | -1.1374770 |
| C  | -2.3627980 | 3.8870860  | 0.8347720  |
| H  | -4.8420230 | 2.9896830  | 0.2052480  |
| C  | -5.8262510 | 0.6634380  | -0.8215330 |
| C  | -3.8079510 | -1.3000530 | -1.2413830 |
| H  | 0.7281460  | -0.7182060 | -1.8316770 |
| H  | 3.6321570  | -1.4899440 | 0.4465030  |
| H  | 2.4098980  | -0.3515880 | -3.5390320 |
| H  | 6.0026790  | -0.9292150 | -0.1197270 |
| H  | 4.7739570  | 0.2112120  | -4.1103510 |
| H  | 6.5719850  | -0.0790850 | -2.3989040 |
| H  | 2.1227160  | -3.5320530 | -1.8177460 |
| H  | 0.9838830  | -2.7425810 | -3.0318600 |
| H  | -1.4060970 | -3.9843830 | 0.2166520  |
| C  | 3.7952750  | 2.4653660  | 0.7826770  |
| H  | -0.9342880 | 4.3195060  | -1.4233950 |
| H  | 0.3289000  | 3.8098770  | -2.5641250 |
| H  | -1.1157890 | 2.7910190  | -2.3134050 |
| H  | -1.3079590 | 3.9363420  | 1.1310430  |
| H  | -2.5600840 | 4.6861830  | 0.1038740  |
| H  | -2.9796090 | 4.0921570  | 1.7223010  |
| C  | 4.4335470  | 1.7646980  | 1.7911830  |
| H  | 4.3332630  | 3.1843450  | 0.1647850  |
| H  | 5.4948810  | 1.9253100  | 1.9802050  |
| C  | 3.7125620  | 0.8295410  | 2.5854510  |
| C  | 2.3640090  | 0.5863020  | 2.3695790  |
| H  | 4.2291830  | 0.2874000  | 3.3776230  |
| H  | 1.8117440  | -0.1399080 | 2.9579410  |
| C  | -5.1378490 | -1.5651450 | -1.5306950 |
| H  | -3.0284180 | -2.0419850 | -1.3895680 |
| H  | -5.4122370 | -2.5440280 | -1.9243860 |
| C  | -6.1510040 | -0.5862440 | -1.3191990 |
| H  | -6.5910650 | 1.4222610  | -0.6547890 |
| H  | -7.1880590 | -0.8283660 | -1.5518240 |

File: P\_BP3\_R\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.2938670  | 0.2726430  | -2.4662660 |
| C  | 3.9553440  | 0.6828360  | -2.6077350 |
| C  | 2.9361400  | 0.0014650  | -1.9330360 |
| C  | 3.2555550  | -1.0944020 | -1.1047110 |
| C  | 4.5946470  | -1.5125510 | -0.9733290 |
| C  | 5.6120580  | -0.8258530 | -1.6493550 |
| C  | 2.2062910  | -1.8007460 | -0.3215760 |
| O  | 1.1320240  | -1.0714490 | -0.0538960 |
| Si | -0.3731240 | -1.5243750 | 0.7872810  |
| O  | -1.1842710 | -0.5835220 | -0.6890390 |
| N  | -2.2074860 | 0.2618820  | -0.4594180 |
| C  | -1.9334020 | 1.4835440  | 0.0730700  |
| C  | -2.9815350 | 2.3804370  | 0.3965130  |
| C  | -4.2852950 | 1.9932010  | 0.0926060  |
| C  | -4.5651460 | 0.7594260  | -0.5369900 |
| C  | -3.4833600 | -0.1427010 | -0.8128560 |
| C  | -0.4992940 | 1.8519620  | 0.1912190  |
| C  | 0.0667270  | 2.8935170  | -0.5911500 |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 1.4234620  | 3.1591360  | -0.4304910 |
| C  | 2.2171120  | 2.4423260  | 0.4949680  |
| C  | 1.6097960  | 1.4040900  | 1.2775260  |
| N  | 0.2671950  | 1.1439610  | 1.0549520  |
| O  | -0.3173210 | 0.1120510  | 1.7148440  |
| C  | -0.5677750 | -3.2285890 | -0.3702400 |
| C  | 0.4914390  | -3.4973820 | -1.0322950 |
| C  | 1.7635530  | -3.3037080 | -1.5186180 |
| Cl | -2.3613940 | -1.8866040 | 1.7444130  |
| Cl | 0.6972170  | -2.5855510 | 2.4386880  |
| C  | -0.7665100 | 3.6531640  | -1.5983400 |
| H  | 1.8933590  | 3.9271770  | -1.0459600 |
| C  | -2.7206160 | 3.7019370  | 1.0859710  |
| H  | -5.1135090 | 2.6581150  | 0.3418200  |
| C  | -5.8851860 | 0.3547900  | -0.8944870 |
| H  | 2.5757480  | -2.4256700 | 0.5019830  |
| H  | 1.8963850  | 0.3139040  | -2.0269830 |
| H  | 4.8338010  | -2.3610830 | -0.3287220 |
| H  | 3.7098300  | 1.5366660  | -3.2414760 |
| H  | 6.6497930  | -1.1429870 | -1.5359520 |
| H  | 6.0864230  | 0.8085320  | -2.9912540 |
| H  | 2.5496160  | -4.0126930 | -1.2392250 |
| H  | 1.8564510  | -2.8995770 | -2.5324250 |
| H  | -1.5285230 | -3.7325860 | -0.3193360 |
| C  | 2.3600870  | 0.6475620  | 2.2059580  |
| C  | 3.6134970  | 2.6770730  | 0.6558390  |
| H  | -0.1106910 | 4.1266000  | -2.3412140 |
| H  | -1.4711530 | 2.9903140  | -2.1200240 |
| H  | -1.3505670 | 4.4468130  | -1.1080850 |
| H  | -3.0530530 | 4.5385320  | 0.4527710  |
| H  | -3.2980270 | 3.7446930  | 2.0217780  |
| H  | -1.6614380 | 3.8462430  | 1.3317350  |
| C  | 4.3487850  | 1.9212170  | 1.5518570  |
| H  | 4.0829400  | 3.4555390  | 0.0542730  |
| H  | 5.4184620  | 2.0968190  | 1.6657780  |
| C  | 3.7157700  | 0.9121200  | 2.3309780  |
| H  | 1.8744140  | -0.1318460 | 2.7852500  |
| H  | 4.3069930  | 0.3307170  | 3.0386570  |
| C  | -6.0989880 | -0.8710680 | -1.4998540 |
| H  | -6.7118860 | 1.0332510  | -0.6828550 |
| H  | -7.1090890 | -1.1756850 | -1.7740190 |
| C  | -5.0056460 | -1.7434220 | -1.7698580 |
| C  | -3.7072160 | -1.3960110 | -1.4298850 |
| H  | -5.1919690 | -2.7039180 | -2.2506070 |
| H  | -2.8659350 | -2.0535990 | -1.6271920 |

File:P\_BP4\_S\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -6.8700370 | -2.3072790 | -0.7446610 |
| C  | -5.8210110 | -2.9786980 | -0.0899060 |
| C  | -4.5713470 | -2.3636830 | 0.0540600  |
| C  | -4.3664850 | -1.0697470 | -0.4665520 |
| C  | -5.4186600 | -0.3952620 | -1.1185450 |
| C  | -6.6669510 | -1.0157340 | -1.2607430 |
| C  | -3.0543410 | -0.3753940 | -0.3249380 |
| O  | -2.0006360 | -1.1740900 | -0.1822220 |
| Si | -0.3384180 | -0.9551860 | 0.3765290  |
| O  | 1.3942970  | -0.6374720 | 1.0996500  |
| N  | 2.4574830  | -0.5429770 | 0.2745930  |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 2.6663330  | 0.6435310  | -0.3447940 |
| C  | 3.7452800  | 0.8083010  | -1.2468610 |
| C  | 4.6055630  | -0.2743780 | -1.4262740 |
| C  | 4.4279370  | -1.4903080 | -0.7283880 |
| C  | 3.3009110  | -1.6326450 | 0.1510050  |
| C  | 1.7677520  | 1.7629620  | 0.0342040  |
| C  | 2.2593730  | 2.8851150  | 0.7533390  |
| C  | 1.3816130  | 3.9352550  | 1.0015620  |
| C  | 0.0734950  | 3.9401000  | 0.4608570  |
| C  | -0.3776650 | 2.7995310  | -0.2818540 |
| N  | 0.4702640  | 1.7011390  | -0.3623910 |
| O  | -0.0074100 | 0.5467570  | -0.8686100 |
| C  | -0.9135070 | 0.4022410  | 1.8444150  |
| C  | -2.1284390 | 0.7642560  | 1.7269440  |
| C  | -3.4162760 | 0.7247700  | 1.2405080  |
| Cl | 0.3801270  | -2.2395230 | -1.2558670 |
| Cl | -0.5386390 | -2.6029310 | 1.8817550  |
| C  | 3.6843640  | 2.9107920  | 1.2584670  |
| H  | 1.7140940  | 4.7863370  | 1.5968110  |
| C  | 3.9597930  | 2.0917390  | -2.0194380 |
| H  | 5.4419640  | -0.1829240 | -2.1206950 |
| C  | 5.3135470  | -2.5990330 | -0.8695720 |
| H  | -2.9157900 | 0.4604130  | -1.0175240 |
| H  | -3.7488940 | -2.8735830 | 0.5557820  |
| H  | -5.2526550 | 0.6083260  | -1.5179420 |
| H  | -5.9789580 | -3.9831260 | 0.3062750  |
| H  | -7.4771820 | -0.4960720 | -1.7744850 |
| H  | -7.8421730 | -2.7910060 | -0.8540060 |
| H  | -4.1387460 | 0.1460990  | 1.8257770  |
| H  | -3.8311830 | 1.6270180  | 0.7793140  |
| H  | -0.1462330 | 0.6479740  | 2.5725650  |
| C  | -0.8192930 | 5.0417560  | 0.6079820  |
| H  | 3.7950070  | 3.6954950  | 2.0185710  |
| H  | 3.9723600  | 1.9465450  | 1.7017880  |
| H  | 4.3887740  | 3.1289480  | 0.4413870  |
| H  | 3.1704270  | 2.8309930  | -1.8370030 |
| H  | 4.9292950  | 2.5405910  | -1.7550670 |
| H  | 3.9797220  | 1.8710710  | -3.0972600 |
| C  | -2.0629900 | 5.0228270  | -0.0008430 |
| H  | -0.4895550 | 5.9025530  | 1.1898690  |
| H  | -2.7379710 | 5.8716200  | 0.1077330  |
| C  | -2.4505490 | 3.9146220  | -0.8044450 |
| C  | -1.6237420 | 2.8091450  | -0.9455530 |
| H  | -3.4043550 | 3.9380450  | -1.3320420 |
| H  | -1.8805000 | 1.9853650  | -1.6021790 |
| C  | 5.0822190  | -3.7679510 | -0.1657530 |
| H  | 6.1695470  | -2.4995080 | -1.5374930 |
| H  | 5.7618730  | -4.6133800 | -0.2734070 |
| C  | 3.9580480  | -3.8782810 | 0.7022050  |
| C  | 3.0652010  | -2.8296310 | 0.8658100  |
| H  | 3.7918420  | -4.8072280 | 1.2479820  |
| H  | 2.1968090  | -2.9084540 | 1.5143860  |

File:P\_BP4\_R\_B97D\_631G.XYZ

|   |           |            |           |
|---|-----------|------------|-----------|
| C | 6.6389710 | -1.5055690 | 1.7117330 |
| C | 5.4928370 | -0.9126620 | 2.2702710 |
| C | 4.2870910 | -0.8998160 | 1.5569760 |
| C | 4.2218900 | -1.4856150 | 0.2761690 |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.3718030  | -2.0842290 | -0.2796470 |
| C  | 6.5747750  | -2.0959240 | 0.4372220  |
| C  | 2.9625080  | -1.4829930 | -0.5239300 |
| O  | 1.8507540  | -1.2152960 | 0.1635060  |
| Si | 0.1843140  | -1.0508640 | -0.4416130 |
| O  | -1.5356430 | -0.5696950 | -1.1322200 |
| N  | -2.5528740 | -0.3330110 | -0.2781950 |
| C  | -2.6195750 | 0.8795480  | 0.3336000  |
| C  | -3.6525470 | 1.1568900  | 1.2666490  |
| C  | -4.6136450 | 0.1724220  | 1.4840950  |
| C  | -4.5845920 | -1.0614380 | 0.7954050  |
| C  | -3.5044550 | -1.3264740 | -0.1123870 |
| C  | -1.5979570 | 1.8970550  | -0.0253800 |
| C  | -1.9300810 | 3.1485590  | -0.6060840 |
| C  | -0.9061210 | 4.0796990  | -0.7758380 |
| C  | 0.4228220  | 3.8079110  | -0.3767990 |
| C  | 0.7321640  | 2.5163510  | 0.1648920  |
| N  | -0.3066480 | 1.6108430  | 0.2914500  |
| O  | -0.0331940 | 0.3909970  | 0.7924560  |
| C  | 0.8194990  | 0.2545520  | -1.9738420 |
| C  | 2.0843740  | 0.2510130  | -2.1151390 |
| C  | 3.3850650  | -0.0888520 | -1.8148890 |
| Cl | -0.5905440 | -2.2992340 | 1.1998970  |
| Cl | 0.2455060  | -2.7352440 | -1.9056540 |
| C  | -3.3341860 | 3.4712990  | -1.0675160 |
| H  | -1.1335530 | 5.0446570  | -1.2310870 |
| C  | -3.7080200 | 2.4655820  | 2.0230470  |
| H  | -5.4092590 | 0.3549000  | 2.2075080  |
| C  | -5.5731120 | -2.0724150 | 0.9777380  |
| H  | 2.8744620  | -2.2947650 | -1.2581660 |
| H  | 3.3888590  | -0.4666560 | 1.9958090  |
| H  | 5.3172670  | -2.5430750 | -1.2693920 |
| H  | 5.5371330  | -0.4671670 | 3.2654190  |
| H  | 7.4591080  | -2.5672470 | 0.0056880  |
| H  | 7.5763770  | -1.5144240 | 2.2703350  |
| H  | 3.9520820  | -0.6708740 | -2.5484840 |
| H  | 3.9811230  | 0.6568590  | -1.2777580 |
| H  | 0.0313800  | 0.7758060  | -2.5081400 |
| C  | 1.4866730  | 4.7483020  | -0.5146760 |
| H  | -4.3531840 | 3.1895120  | 1.5022800  |
| H  | -4.1358600 | 2.2953430  | 3.0205270  |
| H  | -2.7139730 | 2.9171170  | 2.1399070  |
| H  | -3.2968440 | 3.8884530  | -2.0844850 |
| H  | -3.9847010 | 2.5881560  | -1.0794670 |
| H  | -3.7892970 | 4.2320480  | -0.4152610 |
| C  | -5.4836770 | -3.2667880 | 0.2842180  |
| H  | -6.3942590 | -1.8799090 | 1.6684750  |
| H  | -6.2426600 | -4.0367410 | 0.4233780  |
| C  | -4.4025480 | -3.5015070 | -0.6124460 |
| C  | -3.4131090 | -2.5509410 | -0.8150210 |
| H  | -4.3466680 | -4.4490610 | -1.1485090 |
| H  | -2.5768010 | -2.7273730 | -1.4855850 |
| C  | 2.7716830  | 4.4092690  | -0.1274750 |
| H  | 1.2624750  | 5.7321230  | -0.9273380 |
| H  | 3.5810110  | 5.1319070  | -0.2314590 |
| C  | 3.0488710  | 3.1182030  | 0.4081820  |
| C  | 2.0478020  | 2.1703950  | 0.5526390  |
| H  | 4.0667130  | 2.8673320  | 0.7085260  |
| H  | 2.2444180  | 1.1774710  | 0.9444140  |

File:P\_BP5\_S\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -6.9093010 | -0.8246770 | -1.1529660 |
| C  | -5.8550410 | 0.0373810  | -1.5081470 |
| C  | -4.5426280 | -0.2626700 | -1.1254500 |
| C  | -4.2771090 | -1.4263980 | -0.3752270 |
| C  | -5.3315710 | -2.2950270 | -0.0317350 |
| C  | -6.6456510 | -1.9904640 | -0.4150490 |
| C  | -2.8930940 | -1.7817100 | 0.0566640  |
| O  | -2.0897170 | -0.7408840 | 0.2997760  |
| Si | -0.3691090 | -0.7689680 | 0.7658600  |
| O  | -0.0691320 | 0.5282810  | -0.5910520 |
| N  | 0.4702570  | 1.7207780  | -0.2557390 |
| C  | 1.8182050  | 1.7956870  | -0.1086330 |
| C  | 2.4273230  | 3.0085700  | 0.3039920  |
| C  | 1.6067950  | 4.1232810  | 0.4699830  |
| C  | 0.2134500  | 4.0630120  | 0.2429880  |
| C  | -0.3779650 | 2.8034260  | -0.1083820 |
| C  | 2.6114400  | 0.5945980  | -0.4749270 |
| C  | 3.5606670  | 0.6325200  | -1.5325430 |
| C  | 4.3543930  | -0.4920690 | -1.7388950 |
| C  | 4.2395280  | -1.6417200 | -0.9226630 |
| C  | 3.2350940  | -1.6697060 | 0.1023190  |
| N  | 2.4383800  | -0.5396710 | 0.2549520  |
| O  | 1.4958130  | -0.5658800 | 1.2141880  |
| C  | 0.0815410  | -2.0719130 | -0.8086850 |
| C  | -0.9659200 | -2.6035760 | -1.3010210 |
| C  | -2.3175450 | -2.8165850 | -1.4683950 |
| Cl | -0.7496160 | 0.7095420  | 2.3622390  |
| Cl | -0.4829120 | -2.5048060 | 2.1682870  |
| C  | 3.6892720  | 1.8452540  | -2.4269900 |
| H  | 5.0817970  | -0.4929590 | -2.5515450 |
| C  | 3.9071530  | 3.1068680  | 0.6046510  |
| H  | 2.0490020  | 5.0678450  | 0.7903170  |
| C  | -0.6467140 | 5.1915370  | 0.3861910  |
| H  | -2.8375830 | -2.5945230 | 0.7928170  |
| H  | -3.7197650 | 0.3932370  | -1.4082770 |
| H  | -5.1210320 | -3.1971370 | 0.5466430  |
| H  | -6.0586400 | 0.9415470  | -2.0843410 |
| H  | -7.4608380 | -2.6598090 | -0.1359650 |
| H  | -7.9316380 | -0.5880240 | -1.4525240 |
| H  | -2.7875330 | -2.3449420 | -2.3383880 |
| H  | -2.7250960 | -3.8027280 | -1.2211850 |
| H  | 1.1192580  | -2.1984790 | -1.0957220 |
| C  | 5.0560920  | -2.7965840 | -1.0951280 |
| H  | 4.0725780  | 1.5382660  | -3.4094970 |
| H  | 2.7241850  | 2.3507160  | -2.5673830 |
| H  | 4.3965310  | 2.5753170  | -2.0054970 |
| H  | 4.4053470  | 3.7765150  | -0.1127090 |
| H  | 4.0438350  | 3.5379090  | 1.6074790  |
| H  | 4.4082570  | 2.1315300  | 0.5807860  |
| C  | -2.0101540 | 5.0574480  | 0.1896730  |
| H  | -0.2055970 | 6.1513000  | 0.6558700  |
| H  | -2.6647460 | 5.9221160  | 0.2998090  |
| C  | -2.5711810 | 3.7910550  | -0.1442300 |
| C  | -1.7739480 | 2.6665840  | -0.2902300 |
| H  | -3.6492140 | 3.6999300  | -0.2789930 |
| H  | -2.1906630 | 1.6890130  | -0.5097050 |

|   |           |            |            |
|---|-----------|------------|------------|
| C | 4.8730730 | -3.9070170 | -0.2880750 |
| H | 5.8205570 | -2.7810900 | -1.8723250 |
| H | 5.5008130 | -4.7880240 | -0.4218240 |
| C | 3.8654780 | -3.9094370 | 0.7169630  |
| C | 3.0440990 | -2.8087140 | 0.9193290  |
| H | 3.7332840 | -4.7920950 | 1.3428370  |
| H | 2.2665120 | -2.8039970 | 1.6782600  |

File: P\_bp5\_R\_B97D\_631G.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 1.9334140  | 2.6085810  | 0.0982090  |
| C  | 0.5309970  | 2.7698670  | 0.0216230  |
| C  | -0.0541290 | 4.0448470  | -0.2830290 |
| C  | 0.8164350  | 5.1544170  | -0.4896610 |
| C  | 2.1879420  | 4.9934900  | -0.3949730 |
| C  | 2.7432270  | 3.7157720  | -0.1040550 |
| N  | -0.3328280 | 1.7048510  | 0.2285680  |
| C  | -1.6834120 | 1.8217380  | 0.1829160  |
| C  | -2.2923940 | 3.0536500  | -0.1738780 |
| C  | -1.4600660 | 4.1456910  | -0.4007550 |
| O  | 0.1827930  | 0.4947640  | 0.5266740  |
| Si | 0.3310370  | -0.8334090 | -0.8563960 |
| Cl | 0.2933850  | -2.5529710 | -2.2799160 |
| C  | -2.4979740 | 0.6375930  | 0.5568200  |
| C  | -3.3899010 | 0.6560030  | 1.6606470  |
| C  | -4.2442600 | -0.4317130 | 1.8278820  |
| C  | -4.2449880 | -1.5207230 | 0.9270370  |
| C  | -3.2924220 | -1.5346060 | -0.1473680 |
| N  | -2.4273430 | -0.4541200 | -0.2528780 |
| C  | -3.2220170 | -2.6148670 | -1.0594030 |
| C  | -4.1069160 | -3.6721220 | -0.8975720 |
| C  | -5.0623150 | -3.6837780 | 0.1576810  |
| C  | -5.1305220 | -2.6306880 | 1.0537720  |
| C  | -3.7921880 | 3.1674710  | -0.3281720 |
| C  | -3.4012340 | 1.7857670  | 2.6680740  |
| O  | -1.5202010 | -0.4664250 | -1.2491620 |
| O  | 2.0716760  | -1.0255000 | -0.4836620 |
| C  | 2.6521660  | -0.9945880 | 0.7173570  |
| C  | 4.1260250  | -1.2155400 | 0.7224930  |
| C  | 4.7697480  | -1.9127100 | -0.3203400 |
| C  | 6.1572290  | -2.0961050 | -0.2792230 |
| C  | 6.9067200  | -1.5926920 | 0.7999580  |
| C  | 6.2652650  | -0.9002460 | 1.8414320  |
| C  | 4.8768320  | -0.7151200 | 1.8059730  |
| C  | -0.1903490 | -2.1755570 | 0.6338380  |
| C  | 0.7725500  | -2.4453300 | 1.4273570  |
| C  | 2.0800390  | -2.4605750 | 1.8568570  |
| Cl | 0.7921720  | 0.6293150  | -2.4417040 |
| H  | -4.9327850 | -0.4457000 | 2.6740100  |
| H  | -1.8993480 | 5.1031180  | -0.6837490 |
| H  | 2.3044650  | -0.1984620 | 1.3894850  |
| H  | 4.1790330  | -2.2925500 | -1.1537650 |
| H  | 4.3718250  | -0.1766610 | 2.6113830  |
| H  | 6.6568090  | -2.6296100 | -1.0894100 |
| H  | 6.8452450  | -0.5038480 | 2.6762940  |
| H  | 7.9879300  | -1.7381680 | 0.8274370  |
| H  | 2.3234070  | -2.0719850 | 2.8512320  |
| H  | 2.6914880  | -3.3138260 | 1.5427320  |
| H  | -1.1771410 | -2.6256480 | 0.5864990  |

|   |            |            |            |
|---|------------|------------|------------|
| H | -4.3847030 | 2.2790870  | 2.6841680  |
| H | -3.2225000 | 1.3749800  | 3.6733320  |
| H | -2.6323490 | 2.5410580  | 2.4666940  |
| H | -4.0335750 | 4.0442180  | -0.9436980 |
| H | -4.2146490 | 2.2734650  | -0.8082940 |
| H | -4.2858020 | 3.2942620  | 0.6469920  |
| H | -5.8555360 | -2.6274760 | 1.8679560  |
| H | -5.7419770 | -4.5299850 | 0.2576620  |
| H | -4.0677860 | -4.5082550 | -1.5958430 |
| H | -2.4823340 | -2.6000320 | -1.8554850 |
| H | 0.3757930  | 6.1235220  | -0.7240610 |
| H | 2.8503440  | 5.8446200  | -0.5527520 |
| H | 3.8255640  | 3.5992880  | -0.0481960 |
| H | 2.3556070  | 1.6290860  | 0.2868560  |

# ALLYLATION- B3LYP/TZV(2d,2p)

File: A\_BP1\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.0521190  | -2.9043710 | -0.9326280 |
| C  | 4.2418540  | -1.7510470 | -0.8003940 |
| C  | 3.1974310  | -1.7673090 | 0.1587050  |
| C  | 2.9788820  | -2.8924180 | 0.9706760  |
| C  | 3.7968210  | -3.9829490 | 0.8213620  |
| C  | 4.8342260  | -3.9955590 | -0.1364850 |
| N  | 2.4196360  | -0.6381000 | 0.2717590  |
| C  | 2.6669020  | 0.4954860  | -0.4006250 |
| C  | 3.6587170  | 0.5298850  | -1.4039420 |
| C  | 4.4169900  | -0.6049860 | -1.5911120 |
| O  | 1.3893040  | -0.6607540 | 1.1430820  |
| Si | -0.3811360 | -0.7735490 | 0.5088120  |
| Cl | -0.8510930 | 0.7279660  | 2.1612000  |
| C  | 1.8936000  | 1.7130520  | -0.0414520 |
| C  | 2.5066530  | 2.8620200  | 0.4945970  |
| C  | 1.7301440  | 3.9952100  | 0.6307220  |
| C  | 0.3857500  | 4.0263690  | 0.2358970  |
| C  | -0.2130000 | 2.8308890  | -0.2384860 |
| N  | 0.5776540  | 1.71117430 | -0.3056660 |
| C  | -1.5614750 | 2.7972760  | -0.6322940 |
| C  | -2.2949080 | 3.9530020  | -0.5578950 |
| C  | -1.7248820 | 5.1550520  | -0.0805100 |
| C  | -0.4152070 | 5.1925940  | 0.3116890  |
| C  | 3.8640860  | 1.7452630  | -2.2668170 |
| C  | 3.9412040  | 2.8737450  | 0.9515000  |
| O  | 0.0145410  | 0.5571420  | -0.7203050 |
| O  | -2.0441730 | -0.7670100 | -0.1047130 |
| C  | -3.1768790 | -0.7943490 | 0.5466050  |
| C  | -4.4006470 | -1.0102610 | -0.2591710 |
| C  | -4.3439690 | -1.5980180 | -1.5255080 |
| C  | -5.5056850 | -1.7600380 | -2.2661150 |
| C  | -6.7300400 | -1.3389520 | -1.7522450 |
| C  | -6.7900610 | -0.7495270 | -0.4932560 |
| C  | -5.6301590 | -0.5869140 | 0.2516780  |
| C  | -0.7361100 | -2.3218600 | 1.7897160  |
| Cl | 0.1923040  | -2.1746040 | -1.1749350 |
| H  | 2.1717570  | 4.8907480  | 1.0475280  |
| H  | 5.1743570  | -0.6157740 | -2.3631420 |
| H  | -3.2866400 | -0.1046350 | -0.1046350 |
| H  | -3.3909710 | -1.9158950 | -1.9231270 |
| H  | -5.6760000 | -0.1254100 | 1.2296180  |
| H  | -5.4580980 | -2.2124020 | -3.2471130 |
| H  | -7.7375150 | -0.4148390 | -0.0941580 |
| H  | -7.6331060 | -1.4669640 | -2.3331430 |
| H  | 3.9891350  | 3.2399620  | 1.9763840  |
| H  | 4.3991160  | 1.8895130  | 0.9292860  |
| H  | 4.5402500  | 3.5465650  | 0.3381260  |
| H  | 4.4176780  | 1.4678780  | -3.1605270 |
| H  | 2.9175030  | 2.1838910  | -2.5769080 |
| H  | 4.4378970  | 2.5146640  | -1.7510760 |
| H  | -1.9894520 | 1.8745710  | -0.9859050 |
| H  | -3.3299750 | 3.9440680  | -0.8684260 |
| H  | 0.0311540  | 6.1055460  | 0.6794540  |
| H  | -2.3325480 | 6.0469050  | -0.0276820 |

|   |            |            |            |
|---|------------|------------|------------|
| H | 2.1879820  | -2.8819700 | 1.6998100  |
| H | 3.6430940  | -4.8491680 | 1.4488960  |
| H | 5.4574290  | -4.8726690 | -0.2349320 |
| H | 5.8441390  | -2.8988750 | -1.6679260 |
| H | 0.0391550  | -2.2174770 | 2.5417100  |
| C | -2.0564170 | -2.2060860 | 2.3279790  |
| H | -0.5923810 | -3.1931220 | 1.1598110  |
| C | -3.1986450 | -2.5257930 | 1.6274670  |
| H | -2.1751010 | -1.6739120 | 3.2641180  |
| H | -4.1574850 | -2.4648820 | 2.1211330  |
| H | -3.1382460 | -3.2007610 | 0.7846800  |

File: A\_BP1\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -1.6360230 | 2.7929080  | -0.5762970 |
| C  | -0.2802550 | 2.8525520  | -0.2116420 |
| C  | 0.3092620  | 4.0627670  | 0.2369260  |
| C  | -0.5073480 | 5.2179620  | 0.3132890  |
| C  | -1.8234750 | 5.1558330  | -0.0532330 |
| C  | -2.3847710 | 3.9388610  | -0.5022050 |
| N  | 0.5273700  | 1.7459070  | -0.2831130 |
| C  | 1.8465370  | 1.7696240  | -0.0407540 |
| C  | 2.4519020  | 2.9335800  | 0.4704600  |
| C  | 1.6610110  | 4.0567230  | 0.6069620  |
| C  | 2.6330350  | 0.5594430  | -0.3964470 |
| N  | 2.4232190  | -0.5666720 | 0.3012010  |
| C  | 3.2337250  | -1.6747050 | 0.1999940  |
| C  | 4.2499950  | -1.6576090 | -0.7888940 |
| C  | 4.3768320  | -0.5266210 | -1.6099570 |
| C  | 3.6014160  | 0.5962010  | -1.4226010 |
| C  | 3.0779290  | -2.7776550 | 1.0549160  |
| C  | 3.9207210  | -3.8501020 | 0.9124900  |
| C  | 4.9228080  | -3.8664490 | -0.0818740 |
| C  | 5.0852820  | -2.7935640 | -0.9153680 |
| O  | 1.4023150  | -0.6003030 | 1.1835490  |
| Si | -0.3801860 | -0.7462200 | 0.5660000  |
| Cl | -0.8427290 | 0.7489310  | 2.2054770  |
| C  | 3.7636080  | 1.8012230  | -2.3086260 |
| C  | 3.8948330  | 2.9719100  | 0.8980160  |
| O  | -0.0240420 | 0.5782890  | -0.6773960 |
| O  | -2.0774350 | -0.6901150 | 0.0526010  |
| C  | -2.8498960 | -1.6507530 | -0.3816060 |
| C  | -4.2879940 | -1.3307760 | -0.5324940 |
| C  | -4.8737940 | -0.2660780 | 0.1570470  |
| C  | -6.2178460 | 0.0233550  | -0.0277180 |
| C  | -6.9874490 | -0.7441650 | -0.8990560 |
| C  | -6.4073360 | -1.8040200 | -1.5889680 |
| C  | -5.0632180 | -2.0982610 | -1.4051360 |
| C  | -0.7388490 | -2.3086240 | 1.8386400  |
| Cl | 0.2188000  | -2.1551710 | -1.1165770 |
| H  | 2.0969530  | 4.9637860  | 1.0045600  |
| H  | 5.1126180  | -0.5380340 | -2.4024230 |
| H  | -2.4389830 | -2.3098200 | -1.1404430 |
| H  | -4.2718070 | 0.3293610  | 0.8282620  |
| H  | -4.6115890 | -2.9216570 | -1.9433450 |
| H  | -6.6676740 | 0.8489290  | 0.5065310  |
| H  | -7.0000440 | -2.3982350 | -2.2705050 |
| H  | -8.0346820 | -0.5149040 | -1.0408070 |
| H  | 2.8023900  | 2.2185770  | -2.6025440 |

|   |            |            |            |
|---|------------|------------|------------|
| H | 4.3357650  | 2.5879660  | -1.8177460 |
| H | 4.3014800  | 1.5201210  | -3.2107440 |
| H | 4.4772670  | 3.6252870  | 0.2484960  |
| H | 3.9601380  | 3.3760130  | 1.9074540  |
| H | 4.3588770  | 1.9902010  | 0.9028880  |
| H | 5.8536720  | -2.7885320 | -1.6754020 |
| H | 5.5660510  | -4.7294670 | -0.1757940 |
| H | 3.8165620  | -4.6966330 | 1.5760460  |
| H | 2.3219390  | -2.7581310 | 1.8196710  |
| H | -0.0679370 | 6.1419800  | 0.6610970  |
| H | -2.4434130 | 6.0392010  | -0.0001350 |
| H | -3.4261370 | 3.9100160  | -0.7895150 |
| H | -2.0593340 | 1.8581530  | -0.9027410 |
| H | 0.2424530  | -2.7245850 | 2.0322010  |
| H | -1.1550480 | -1.8234120 | 2.7139020  |
| C | -1.6310890 | -3.2297320 | 1.2064420  |
| C | -2.9910310 | -3.0248090 | 1.1183380  |
| H | -1.2018750 | -4.0310170 | 0.6174730  |
| H | -3.6143960 | -3.7836400 | 0.6684210  |
| H | -3.4757940 | -2.3700980 | 1.8293490  |

File:a\_BP2\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 2.2257090  | 1.6510590  | 2.0870040  |
| C  | 1.4526090  | 2.0330870  | 0.9788310  |
| C  | 1.8964390  | 3.0494640  | 0.0948740  |
| C  | 3.1517520  | 3.6533060  | 0.3435570  |
| C  | 3.9003750  | 3.2744400  | 1.4258380  |
| C  | 3.4287350  | 2.2754350  | 2.3031470  |
| N  | 0.2246320  | 1.4591280  | 0.7289780  |
| C  | -0.6027970 | 1.9047680  | -0.2248850 |
| C  | -0.1632570 | 2.8525790  | -1.1769330 |
| C  | 1.0863470  | 3.3998670  | -0.9995330 |
| C  | -2.0030110 | 1.4106240  | -0.2227430 |
| N  | -2.2100840 | 0.1249970  | -0.5272800 |
| C  | -3.4540860 | -0.4033910 | -0.7796020 |
| C  | -4.5717460 | 0.4520380  | -0.6009040 |
| C  | -4.3570020 | 1.7622200  | -0.1422010 |
| C  | -3.0897820 | 2.2679700  | 0.0485770  |
| C  | -3.6124280 | -1.7313010 | -1.2069430 |
| C  | -4.8797090 | -2.1895670 | -1.4635170 |
| C  | -6.0094390 | -1.3606910 | -1.2890590 |
| C  | -5.8614350 | -0.0686080 | -0.8622140 |
| O  | -1.1305670 | -0.6769760 | -0.6402090 |
| Si | -0.2998550 | -1.3368760 | 0.8889580  |
| Cl | -0.6491470 | -3.4136360 | 0.0844290  |
| C  | -2.8747370 | 3.6546500  | 0.5920620  |
| C  | -1.0015220 | 3.1974060  | -2.3782640 |
| O  | -0.1924340 | 0.4624180  | 1.5322440  |
| O  | 1.2054600  | -1.0873400 | -0.0496390 |
| C  | 2.1233280  | -1.9798870 | -0.3169490 |
| C  | 3.3274960  | -1.5521880 | -1.0627710 |
| C  | 3.7346410  | -0.2184600 | -1.1262640 |
| C  | 4.8502210  | 0.1350750  | -1.8712330 |
| C  | 5.5713490  | -0.8379090 | -2.5584710 |
| C  | 5.1695530  | -2.1687850 | -2.5010550 |
| C  | 4.0541140  | -2.5248050 | -1.7564380 |
| C  | 0.7765010  | -2.0162620 | 2.4929360  |
| Cl | -2.1943540 | -1.4046600 | 2.0934370  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 1.4573470  | 4.1235940  | -1.7124530 |
| H | -5.2146460 | 2.3882920  | 0.0634590  |
| H | 1.7725110  | -2.9753150 | -0.5653540 |
| H | 3.1732270  | 0.5360670  | -0.5986020 |
| H | 3.7394450  | -3.5595160 | -1.7168150 |
| H | 5.1576560  | 1.1706300  | -1.9188470 |
| H | 5.7217560  | -2.9270110 | -3.0385800 |
| H | 6.4399160  | -0.5589980 | -3.1390340 |
| H | -0.4422490 | 3.8540170  | -3.0395200 |
| H | -1.2659130 | 2.2995730  | -2.9369010 |
| H | -1.9284320 | 3.7031350  | -2.1139760 |
| H | -2.4274170 | 4.3281940  | -0.1375640 |
| H | -3.8274770 | 4.0814200  | 0.8947590  |
| H | -2.2217180 | 3.6322420  | 1.4639150  |
| H | -6.7187830 | 0.5740390  | -0.7207800 |
| H | -6.9947520 | -1.7545200 | -1.4930050 |
| H | -5.0152980 | -3.2068490 | -1.8020740 |
| H | -2.7470210 | -2.3629340 | -1.3183690 |
| H | 3.4996670  | 4.4216610  | -0.3320160 |
| H | 4.8542820  | 3.7444160  | 1.6169040  |
| H | 4.0213720  | 1.9996280  | 3.1635950  |
| H | 1.8540250  | 0.9028730  | 2.7647130  |
| H | 0.0347950  | -2.5300710 | 3.0918240  |
| C | 1.8278570  | -2.8752990 | 2.0389900  |
| H | 1.1203950  | -1.1068760 | 2.9743920  |
| C | 3.0054670  | -2.4320950 | 1.4808160  |
| H | 1.6081820  | -3.9337210 | 1.9667800  |
| H | 3.7618420  | -3.1496680 | 1.1986500  |
| H | 3.3539670  | -1.4291210 | 1.6848020  |

File:A\_BP2\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -3.1104680 | -2.4155110 | -0.6333720 |
| C  | -3.2383740 | -1.0221530 | -0.5168270 |
| C  | -4.5124720 | -0.3983020 | -0.4855630 |
| C  | -5.6618560 | -1.2197560 | -0.5713390 |
| C  | -5.5314920 | -2.5766530 | -0.6936220 |
| C  | -4.2512780 | -3.1715820 | -0.7274340 |
| N  | -2.1355720 | -0.2045450 | -0.4404490 |
| C  | -2.2056950 | 1.1314090  | -0.4281920 |
| C  | -3.4504930 | 1.7838350  | -0.3162940 |
| C  | -4.5815610 | 0.9972150  | -0.3433840 |
| O  | -0.9105930 | -0.7725180 | -0.4394120 |
| Si | 0.0550160  | -0.8956870 | 1.1348220  |
| Cl | 0.2002580  | -3.1195680 | 0.7771440  |
| C  | -0.9363100 | 1.8863020  | -0.5846400 |
| C  | -0.6667260 | 2.6508010  | -1.7418640 |
| C  | 0.4663360  | 3.4322000  | -1.7370380 |
| C  | 1.3113090  | 3.4996330  | -0.6155450 |
| C  | 1.0372800  | 2.6684810  | 0.5001940  |
| N  | -0.0590210 | 1.8387790  | 0.4251150  |
| C  | 1.8390370  | 2.7144280  | 1.6522630  |
| C  | 2.9095150  | 3.5734270  | 1.6800700  |
| C  | 3.2191260  | 4.3888840  | 0.5709240  |
| C  | 2.4373680  | 4.3544170  | -0.5527950 |
| C  | -3.5396130 | 3.2698650  | -0.0984130 |
| C  | -1.5490540 | 2.5634060  | -2.9577710 |
| O  | -0.2915210 | 0.9747830  | 1.4330310  |

|    |            |            |            |
|----|------------|------------|------------|
| O  | 1.4280000  | -0.4597460 | 0.0858250  |
| C  | 2.7340120  | -0.4823790 | 0.0458980  |
| C  | 3.4478340  | -1.4365000 | -0.8338390 |
| C  | 2.7953260  | -2.4861630 | -1.4832540 |
| C  | 3.4973010  | -3.3081160 | -2.3556560 |
| C  | 4.8508750  | -3.0915550 | -2.5914950 |
| C  | 5.5048670  | -2.0378360 | -1.9576200 |
| C  | 4.8069790  | -1.2145350 | -1.0883440 |
| C  | 1.2566240  | -1.0409620 | 2.7891130  |
| Cl | -1.7584420 | -1.1583540 | 2.4356820  |
| H  | 0.7131620  | 4.0193050  | -2.6111560 |
| H  | -5.5532490 | 1.4640510  | -0.2554770 |
| H  | 3.1894840  | 0.5058910  | 0.0600000  |
| H  | 1.7450860  | -2.6521260 | -1.3049030 |
| H  | 5.3179590  | -0.3910760 | -0.6055990 |
| H  | 2.9840740  | -4.1180390 | -2.8557550 |
| H  | 6.5541570  | -1.8571470 | -2.1454960 |
| H  | 5.3929620  | -3.7347600 | -3.2710890 |
| H  | -1.1004170 | 3.1186260  | -3.7773510 |
| H  | -1.6728060 | 1.5290910  | -3.2779630 |
| H  | -2.5422870 | 2.9743520  | -2.7833040 |
| H  | -4.5812450 | 3.5796730  | -0.0862050 |
| H  | -3.0947320 | 3.5404690  | 0.8600130  |
| H  | -3.0280280 | 3.8434270  | -0.8682380 |
| H  | 2.6583610  | 4.9834560  | -1.4033000 |
| H  | 4.0727490  | 5.0495700  | 0.6175530  |
| H  | 3.5208090  | 3.6302780  | 2.5693810  |
| H  | 1.5832290  | 2.1056750  | 2.5023120  |
| H  | -6.6363770 | -0.7536580 | -0.5415250 |
| H  | -6.4103720 | -3.2013410 | -0.7632930 |
| H  | -4.1675930 | -4.2446290 | -0.8245660 |
| H  | -2.1306460 | -2.8633300 | -0.6385970 |
| H  | 0.6889080  | -1.7423360 | 3.3875940  |
| C  | 2.5374300  | -1.5269680 | 2.4030480  |
| H  | 1.2533330  | -0.0409800 | 3.2121710  |
| C  | 3.5504520  | -0.7231680 | 1.9347680  |
| H  | 2.6518100  | -2.5994360 | 2.2995100  |
| H  | 4.5085960  | -1.1566850 | 1.6937650  |
| H  | 3.5593780  | 0.3232010  | 2.2058890  |

File:A\_BP3\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -6.0702240 | -1.1418890 | -1.1793830 |
| C  | -5.8278760 | 0.1706110  | -0.8774870 |
| C  | -4.5050310 | 0.6193080  | -0.6481990 |
| C  | -3.4505890 | -0.3262860 | -0.7239600 |
| C  | -3.7093430 | -1.6724930 | -1.0268050 |
| C  | -5.0036780 | -2.0629700 | -1.2576160 |
| N  | -2.1699630 | 0.1294110  | -0.5028570 |
| C  | -1.8783620 | 1.4233450  | -0.3138220 |
| C  | -2.9042220 | 2.3789420  | -0.1520910 |
| C  | -4.2020640 | 1.9505550  | -0.3192510 |
| O  | -1.1622640 | -0.7641700 | -0.5050960 |
| Si | -0.3079770 | -1.2695190 | 1.1396910  |
| Cl | 0.8062700  | -1.7411550 | 3.0309410  |
| C  | -0.4475970 | 1.8189210  | -0.3061550 |
| C  | 0.1053330  | 2.6403860  | -1.3114190 |
| C  | 1.3910010  | 3.0969600  | -1.1193380 |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 2.1320450  | 2.7678740  | 0.0281850  |
| C  | 1.5715010  | 1.8681540  | 0.9719450  |
| N  | 0.3008110  | 1.4049780  | 0.7230090  |
| C  | 2.2789760  | 1.4789720  | 2.1206040  |
| C  | 3.5299250  | 2.0040140  | 2.3264370  |
| C  | 4.1103600  | 2.9019050  | 1.4042960  |
| C  | 3.4305330  | 3.2725880  | 0.2753330  |
| C  | -2.5998220 | 3.7914830  | 0.2685990  |
| C  | -0.6558530 | 2.9562290  | -2.5708310 |
| O  | -0.2551150 | 0.5332490  | 1.5950560  |
| O  | 1.2604450  | -1.1066920 | 0.2827690  |
| C  | 1.6012160  | -1.4231010 | -0.9331640 |
| C  | 3.0388890  | -1.3709340 | -1.2725100 |
| C  | 4.0218990  | -1.3851780 | -0.2794550 |
| C  | 5.3616290  | -1.3135430 | -0.6314080 |
| C  | 5.7312690  | -1.2275630 | -1.9716910 |
| C  | 4.7550110  | -1.2092680 | -2.9634550 |
| C  | 3.4136450  | -1.2825410 | -2.6159950 |
| C  | -0.4585410 | -3.2304960 | 0.5727820  |
| Cl | -2.2629180 | -1.3236010 | 2.2284410  |
| H  | 1.8470230  | 3.7280980  | -1.8699890 |
| H  | -5.0136910 | 2.6542320  | -0.1945780 |
| H  | 0.9244890  | -1.1452220 | -1.7362200 |
| H  | 3.7286430  | -1.4474660 | 0.7583240  |
| H  | 2.6535690  | -1.2727500 | -3.3866860 |
| H  | 6.1202860  | -1.3238380 | 0.1388960  |
| H  | 5.0390230  | -1.1383650 | -4.0041860 |
| H  | 6.7769860  | -1.1733320 | -2.2415360 |
| H  | 0.0025870  | 3.4461240  | -3.2836780 |
| H  | -1.0412140 | 2.0485210  | -3.0342510 |
| H  | -1.5022550 | 3.6184430  | -2.3946400 |
| H  | -3.5278580 | 4.3381840  | 0.4143450  |
| H  | -2.0499890 | 3.8031740  | 1.2098110  |
| H  | -2.0058460 | 4.3336990  | -0.4645280 |
| H  | 3.8669940  | 3.9552490  | -0.4396990 |
| H  | 5.0988070  | 3.2947240  | 1.5945340  |
| H  | 4.0818310  | 1.7230340  | 3.2121000  |
| H  | 1.8335060  | 0.7815330  | 2.8108050  |
| H  | -2.8974200 | -2.3751090 | -1.0799030 |
| H  | -5.2095280 | -3.0956870 | -1.5002240 |
| H  | -6.6358100 | 0.8852930  | -0.8114310 |
| H  | -7.0805420 | -1.4804170 | -1.3582390 |
| H  | -1.5130600 | -3.4477200 | 0.6951670  |
| C  | 0.0174290  | -3.4136620 | -0.7639020 |
| H  | 0.1435400  | -3.7296250 | 1.3247440  |
| C  | 1.3481640  | -3.4833360 | -1.0975690 |
| H  | -0.6943190 | -3.3280450 | -1.5777140 |
| H  | 1.6367330  | -3.6605970 | -2.1229920 |
| H  | 2.0780070  | -3.7397530 | -0.3423530 |

File:A\_BP3\_R\_B3LYP\_TZV2D2P.XYZ

|   |           |            |            |
|---|-----------|------------|------------|
| C | 4.6793980 | -1.5584390 | -0.8403660 |
| C | 3.3390370 | -1.2292330 | -1.0591210 |
| C | 2.9915700 | -0.4551930 | -2.1695790 |
| C | 3.9740700 | -0.0204630 | -3.0467880 |
| C | 5.3089270 | -0.3521680 | -2.8253500 |
| C | 5.6599610 | -1.1196580 | -1.7192660 |
| C | 2.3269160 | -1.6865690 | -0.0830450 |

|    |            |            |            |
|----|------------|------------|------------|
| O  | 1.2050720  | -1.0254240 | -0.0286040 |
| Si | -0.2933010 | -1.4010340 | 0.8792680  |
| Cl | -2.2475670 | -1.6922810 | 1.9325690  |
| O  | -1.1555320 | -0.6731610 | -0.6600890 |
| N  | -2.2107140 | 0.1523300  | -0.5234610 |
| C  | -3.4615050 | -0.3320520 | -0.8260530 |
| C  | -4.5684410 | 0.5315570  | -0.6214370 |
| C  | -4.3393880 | 1.8141720  | -0.1035230 |
| C  | -3.0654770 | 2.2865890  | 0.1312410  |
| C  | -1.9882400 | 1.4212570  | -0.1444830 |
| C  | -5.8643510 | 0.0489020  | -0.9283470 |
| C  | -6.0306900 | -1.2142080 | -1.4258460 |
| C  | -4.9122160 | -2.0515850 | -1.6327170 |
| C  | -3.6427700 | -1.6298720 | -1.3326460 |
| C  | -0.5770210 | 1.8789510  | -0.0725380 |
| C  | -0.0727720 | 2.8828730  | -0.9249630 |
| C  | 1.2116670  | 3.3282350  | -0.6942050 |
| C  | 1.9921610  | 2.8290700  | 0.3593740  |
| C  | 1.4695860  | 1.7814530  | 1.1612650  |
| N  | 0.2067870  | 1.3280790  | 0.8646570  |
| C  | 2.2098490  | 1.2385510  | 2.2246420  |
| C  | 3.4580270  | 1.7470910  | 2.4805720  |
| C  | 4.0048030  | 2.7832490  | 1.6917040  |
| C  | 3.2907080  | 3.3121620  | 0.6512660  |
| C  | -2.8609460 | 3.6664890  | 0.6971940  |
| C  | -0.8811730 | 3.4399390  | -2.0660800 |
| O  | -0.3023610 | 0.3125730  | 1.6000560  |
| Cl | 0.8263070  | -2.1179280 | 2.6997130  |
| C  | -0.3681310 | -3.2467960 | 0.0075880  |
| C  | 0.9381990  | -3.8305910 | -0.0049010 |
| H  | 1.2426520  | -4.4044370 | 0.8618850  |
| H  | 1.6316640  | 4.0897200  | -1.3375220 |
| H  | -5.1885240 | 2.4492890  | 0.1112850  |
| H  | 2.7208860  | -2.0728070 | 0.8512910  |
| H  | 1.9558910  | -0.1967580 | -2.3365750 |
| H  | 4.9531080  | -2.1536860 | 0.0211560  |
| H  | 3.7015500  | 0.5787700  | -3.9047060 |
| H  | 6.6954270  | -1.3742660 | -1.5408880 |
| H  | 6.0718360  | -0.0116640 | -3.5118470 |
| H  | -1.0786410 | -3.7816480 | 0.6271020  |
| H  | -1.4303060 | 4.3318290  | -1.7639340 |
| H  | -0.2159730 | 3.7281830  | -2.8772290 |
| H  | -1.5967110 | 2.7197880  | -2.4552660 |
| H  | -3.6388350 | 3.8744650  | 1.4293740  |
| H  | -1.8991410 | 3.7748170  | 1.1911340  |
| H  | -2.9349180 | 4.4278260  | -0.0796430 |
| H  | 3.6981080  | 4.1061010  | 0.0417610  |
| H  | 4.9929550  | 3.1581170  | 1.9165170  |
| H  | 1.7896770  | 0.4401860  | 2.8135730  |
| H  | 4.0339400  | 1.3459330  | 3.3023260  |
| H  | -6.7111350 | 0.7001710  | -0.7651220 |
| H  | -7.0196870 | -1.5783140 | -1.6640240 |
| H  | -5.0591780 | -3.0449030 | -2.0320770 |
| H  | -2.7907890 | -2.2682990 | -1.4844500 |
| C  | 1.8950880  | -3.5215890 | -0.9424440 |
| H  | -0.7558960 | -3.0440640 | -0.9857320 |
| H  | 2.8542050  | -4.0176320 | -0.9143970 |
| H  | 1.5944600  | -3.1161890 | -1.8986920 |

File: A\_BP4\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -5.8979050 | 0.3454550  | -1.4904660 |
| C  | -4.9812130 | 0.1594840  | -0.4539480 |
| C  | -3.5449280 | -0.0708850 | -0.7914910 |
| H  | -3.4041870 | -0.4535400 | -1.8021880 |
| O  | -2.8667400 | -0.7577150 | 0.1429510  |
| Si | -1.1566460 | -0.8800810 | 0.4195350  |
| Cl | -0.8094270 | -1.8965010 | -1.4064700 |
| C  | -0.8759530 | 1.1044860  | 0.3212870  |
| H  | -0.2188980 | 1.0886630  | -0.5526030 |
| C  | -2.0992100 | 1.7714980  | 0.0753900  |
| H  | -2.5999280 | 2.2592190  | 0.9050580  |
| H  | -0.3696640 | 1.3748510  | 1.2408560  |
| H  | -3.6586340 | 2.2298710  | -1.2960620 |
| C  | -2.8070240 | 1.5902800  | -1.1180050 |
| H  | -2.2130400 | 1.3837080  | -2.0000920 |
| Cl | -1.5676420 | -1.7977500 | 2.2781880  |
| C  | -5.4268660 | 0.1757920  | 0.8679960  |
| C  | -6.7716460 | 0.3798190  | 1.1466110  |
| C  | -7.6821710 | 0.5679810  | 0.1102840  |
| C  | -7.2430080 | 0.5473070  | -1.2093630 |
| O  | 0.6730290  | -1.0059540 | 0.9575110  |
| N  | 1.7286350  | -1.4177540 | 0.2061230  |
| C  | 1.9310930  | -2.7794680 | 0.0612650  |
| C  | 3.0041280  | -3.2003750 | -0.7630550 |
| C  | 3.8366270  | -2.2290770 | -1.3439520 |
| C  | 3.6727990  | -0.8900730 | -1.0812530 |
| C  | 2.5936030  | -0.4992480 | -0.2567040 |
| C  | 3.2140040  | -4.5881340 | -0.9441290 |
| C  | 2.4144260  | -5.4986410 | -0.3074170 |
| C  | 1.3781310  | -5.0577310 | 0.5403920  |
| C  | 1.1269580  | -3.7204000 | 0.7235580  |
| C  | 4.6191020  | 0.1370760  | -1.6340100 |
| C  | 2.4981030  | 0.8993980  | 0.2348640  |
| C  | 2.9377250  | 1.2626200  | 1.5304800  |
| C  | 2.9692860  | 2.5962120  | 1.8520640  |
| C  | 2.5816100  | 3.5771170  | 0.9148170  |
| C  | 2.1399040  | 3.1737470  | -0.3672270 |
| N  | 2.1008870  | 1.8137050  | -0.6692210 |
| C  | 1.7378500  | 4.1118690  | -1.3315230 |
| C  | 1.7844920  | 5.4483580  | -1.0195420 |
| C  | 2.2219240  | 5.8767730  | 0.2508630  |
| C  | 2.6106360  | 4.9635760  | 1.1968750  |
| C  | 3.3723670  | 0.2073070  | 2.5088710  |
| O  | 1.6494230  | 1.4241120  | -1.8190880 |
| H  | 3.3068880  | 2.9064150  | 2.8311580  |
| H  | 4.6509240  | -2.5521770 | -1.9782420 |
| H  | -4.7235030 | 0.0132170  | 1.6718530  |
| H  | -5.5608850 | 0.3251250  | -2.5190750 |
| H  | -7.1114900 | 0.3863320  | 2.1731890  |
| H  | -7.9466960 | 0.6831660  | -2.0189360 |
| H  | -8.7292390 | 0.7242050  | 0.3305840  |
| H  | 3.7335320  | 0.6709340  | 3.4234290  |
| H  | 2.5451040  | -0.4544750 | 2.7667570  |
| H  | 4.1762230  | -0.4080800 | 2.1025410  |
| H  | 5.4087340  | -0.3492050 | -2.2009660 |
| H  | 4.0928960  | 0.8268360  | -2.2937240 |
| H  | 5.0824120  | 0.7206890  | -0.8383130 |

|   |           |            |            |
|---|-----------|------------|------------|
| H | 2.9468880 | 5.2870600  | 2.1722630  |
| H | 2.2497450 | 6.9334810  | 0.4767150  |
| H | 1.4831150 | 6.1801770  | -1.7555750 |
| H | 1.4070680 | 3.7616290  | -2.2954390 |
| H | 4.0246270 | -4.9090590 | -1.5830210 |
| H | 2.5816530 | -6.5576060 | -0.4418110 |
| H | 0.7690830 | -5.7840120 | 1.0595530  |
| H | 0.3390660 | -3.3919500 | 1.3788940  |

File: A\_BP4\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -1.7857230 | 2.6925980  | -0.5022890 |
| C  | -0.4452330 | 2.7990290  | -0.0964470 |
| C  | 0.0608780  | 4.0010080  | 0.4593700  |
| C  | -0.8259620 | 5.0935900  | 0.6100590  |
| C  | -2.1308240 | 4.9849770  | 0.2099320  |
| C  | -2.6075540 | 3.7815310  | -0.3528710 |
| N  | 0.4243650  | 1.7374550  | -0.2315340 |
| C  | 1.7369940  | 1.8340230  | 0.0245340  |
| C  | 2.2653390  | 2.9934470  | 0.6351510  |
| C  | 1.4087060  | 4.0494590  | 0.8526630  |
| C  | 2.6148340  | 0.7100310  | -0.3912050 |
| N  | 2.4626110  | -0.4642070 | 0.2414560  |
| C  | 3.3361010  | -1.5152640 | 0.1103550  |
| C  | 4.4006830  | -1.3676420 | -0.8171760 |
| C  | 4.4861970  | -0.1854450 | -1.5640690 |
| C  | 3.6152910  | 0.8674370  | -1.3689810 |
| C  | 3.1905680  | -2.6878850 | 0.8704170  |
| C  | 4.1082130  | -3.6932950 | 0.7054950  |
| C  | 5.1731710  | -3.5739280 | -0.2155660 |
| C  | 5.3163300  | -2.4385120 | -0.9643140 |
| O  | 1.4191000  | -0.5966110 | 1.0895930  |
| Si | -0.2990760 | -0.9422920 | 0.4137460  |
| Cl | -0.3810480 | -2.8581820 | 1.6146020  |
| C  | 3.7284750  | 2.1030430  | -2.2226170 |
| C  | 3.7054160  | 3.0654660  | 1.0651570  |
| O  | -0.0599370 | 0.5806310  | -0.7176610 |
| O  | -1.9577360 | -1.0279740 | -0.2068790 |
| C  | -3.0230500 | -1.4996060 | 0.3894490  |
| C  | -4.3077890 | -1.3830250 | -0.3422240 |
| C  | -4.4416770 | -0.5521120 | -1.4564500 |
| C  | -5.6493720 | -0.4912960 | -2.1377880 |
| C  | -6.7321290 | -1.2571710 | -1.7149020 |
| C  | -6.6010660 | -2.0937170 | -0.6103010 |
| C  | -5.3948890 | -2.1572000 | 0.0725800  |
| C  | -0.9561210 | 0.1278770  | 2.0493860  |
| Cl | 0.4155560  | -2.0735620 | -1.3561520 |
| H  | 1.7810380  | 4.9457290  | 1.3297740  |
| H  | 5.2632700  | -0.0963430 | -2.3116950 |
| H  | -2.9013350 | -2.4181410 | 0.9549740  |
| H  | -3.5946730 | 0.0234100  | -1.7985480 |
| H  | -5.2931180 | -2.8127840 | 0.9278110  |
| H  | -5.7444460 | 0.1474920  | -3.0051120 |
| H  | -7.4356010 | -2.6993640 | -0.2853120 |
| H  | -7.6711040 | -1.2087930 | -2.2490140 |
| H  | 3.6692990  | 1.8190960  | -3.2730210 |
| H  | 2.9399320  | 2.8241700  | -2.0314360 |
| H  | 4.6896550  | 2.5941080  | -2.0722000 |
| H  | 3.8385690  | 3.8944890  | 1.7557510  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 4.0214090  | 2.1519050  | 1.5661380  |
| H | 4.3732130  | 3.2312330  | 0.2204870  |
| H | 6.1250500  | -2.3358750 | -1.6738760 |
| H | 5.8746320  | -4.3883850 | -0.3257870 |
| H | 4.0118020  | -4.5975970 | 1.2893490  |
| H | 2.3647550  | -2.7804940 | 1.5557110  |
| H | -0.4502100 | 6.0110860  | 1.0400690  |
| H | -2.8030710 | 5.8235590  | 0.3204100  |
| H | -3.6372130 | 3.7165440  | -0.6741930 |
| H | -2.1358960 | 1.7700210  | -0.9326630 |
| H | -0.1314500 | 0.0456540  | 2.7491000  |
| H | -1.0877690 | 1.1445650  | 1.6960010  |
| C | -2.1688300 | -0.4526860 | 2.5321640  |
| C | -3.4010600 | -0.2597040 | 1.9418940  |
| H | -2.0895530 | -1.2286260 | 3.2832650  |
| H | -4.2765780 | -0.6997320 | 2.3965290  |
| H | -3.5759050 | 0.6235460  | 1.3430730  |

File: A\_BP5\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 2.9855340  | -2.8116990 | 0.9614020  |
| C  | 3.1703140  | -1.7177040 | 0.0978360  |
| C  | 4.1681520  | -1.7360640 | -0.9109700 |
| C  | 4.9772490  | -2.8921330 | -1.0323820 |
| C  | 4.7977370  | -3.9509430 | -0.1846010 |
| C  | 3.8007080  | -3.9055150 | 0.8151970  |
| N  | 2.3927700  | -0.5876450 | 0.2054180  |
| C  | 2.6026280  | 0.5242150  | -0.5209770 |
| C  | 3.5357070  | 0.5156380  | -1.5775460 |
| C  | 4.2949380  | -0.6231160 | -1.7537580 |
| C  | 1.8708210  | 1.7559110  | -0.1256580 |
| N  | 0.5377930  | 1.7661710  | -0.2607370 |
| C  | -0.2297440 | 2.8958660  | -0.1047140 |
| C  | 0.4276350  | 4.0840610  | 0.3034230  |
| C  | 1.8073520  | 4.0399110  | 0.5574070  |
| C  | 2.5506620  | 2.8992920  | 0.3450460  |
| C  | -1.6131240 | 2.8756010  | -0.3455210 |
| C  | -2.3240590 | 4.0380370  | -0.1932640 |
| C  | -1.6929490 | 5.2344440  | 0.2136950  |
| C  | -0.3476120 | 5.2579840  | 0.4626130  |
| O  | -0.0756640 | 0.6189990  | -0.6149090 |
| Si | -0.3956320 | -0.7263500 | 0.6690900  |
| Cl | -0.5798610 | -2.4141710 | 2.1489600  |
| C  | 4.0263190  | 2.8752050  | 0.6383670  |
| C  | 3.6907830  | 1.6731640  | -2.5281960 |
| O  | 1.4297150  | -0.5740950 | 1.1488930  |
| O  | -2.1181400 | -0.6456430 | 0.2237830  |
| C  | -2.9806260 | -1.6249130 | 0.1425740  |
| C  | -4.3440840 | -1.2909910 | -0.3332850 |
| C  | -4.5959750 | -0.1785350 | -1.1393820 |
| C  | -5.8924850 | 0.1141700  | -1.5355910 |
| C  | -6.9490770 | -0.7002580 | -1.1342460 |
| C  | -6.7036650 | -1.8096250 | -0.3321510 |
| C  | -5.4063950 | -2.1057220 | 0.0647980  |
| C  | -0.0906150 | -2.0384530 | -0.8970540 |
| Cl | -0.7643140 | 0.7456720  | 2.2913630  |
| H  | 5.0163990  | -0.6588900 | -2.5592660 |
| H  | 2.2984740  | 4.9294890  | 0.9276880  |
| H  | -2.9438910 | -2.3779570 | 0.9236750  |

|   |            |            |            |
|---|------------|------------|------------|
| H | -3.7774280 | 0.4528850  | -1.4527570 |
| H | -5.2164290 | -2.9658770 | 0.6934870  |
| H | -6.0819190 | 0.9783950  | -2.1573200 |
| H | -7.5210000 | -2.4411620 | -0.0127360 |
| H | -7.9587760 | -0.4686810 | -1.4442950 |
| H | 4.7089920  | 2.0600740  | -2.5048180 |
| H | 3.4957070  | 1.3319540  | -3.5448560 |
| H | 3.0066990  | 2.4889210  | -2.3170800 |
| H | 4.2857760  | 3.7258040  | 1.2637150  |
| H | 4.3178200  | 1.9674050  | 1.1636790  |
| H | 4.6224350  | 2.9423180  | -0.2712210 |
| H | 0.1448430  | 6.1660820  | 0.7802450  |
| H | -2.2818750 | 6.1326250  | 0.3316150  |
| H | -3.3882730 | 4.0369730  | -0.3806990 |
| H | -2.0865200 | 1.9528760  | -0.6326970 |
| H | 5.7361090  | -2.9147690 | -1.8015540 |
| H | 5.4203240  | -4.8293770 | -0.2749040 |
| H | 3.6774670  | -4.7484930 | 1.4800620  |
| H | 2.2179820  | -2.7716660 | 1.7169760  |
| H | 0.8853670  | -2.4750830 | -0.7184580 |
| C | -1.1291420 | -3.0191900 | -0.8929140 |
| H | -0.0974360 | -1.3989410 | -1.7739170 |
| C | -2.3867620 | -2.7931790 | -1.4088140 |
| H | -0.9789310 | -3.9119670 | -0.2989150 |
| H | -3.1150390 | -3.5912190 | -1.4035000 |
| H | -2.5196410 | -2.0348680 | -2.1678090 |

File: A\_BP5\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 1.6338260  | 2.8815130  | 0.3501000  |
| C  | 0.2517200  | 2.8683050  | 0.1017420  |
| C  | -0.4200980 | 4.0511520  | -0.3054430 |
| C  | 0.3349110  | 5.2400190  | -0.4578060 |
| C  | 1.6782660  | 5.2425850  | -0.2034710 |
| C  | 2.3255590  | 4.0561220  | 0.2053330  |
| N  | -0.5016410 | 1.7265100  | 0.2470050  |
| C  | -1.8377340 | 1.7087250  | 0.1070070  |
| C  | -2.5261850 | 2.8425540  | -0.3667570 |
| C  | -1.7941630 | 3.9927530  | -0.5710090 |
| O  | 0.1180450  | 0.5706180  | 0.5772410  |
| Si | 0.3996410  | -0.7776790 | -0.7449470 |
| Cl | 0.5406840  | -2.4318340 | -2.2545930 |
| C  | -2.5685110 | 0.4747090  | 0.4946780  |
| C  | -3.4809990 | 0.4581200  | 1.5717920  |
| C  | -4.2479030 | -0.6742870 | 1.7409350  |
| C  | -4.1474740 | -1.7746380 | 0.8731690  |
| C  | -3.1663360 | -1.7496650 | -0.1512480 |
| N  | -2.3841930 | -0.6198340 | -0.2560230 |
| C  | -2.9920410 | -2.8350270 | -1.0254540 |
| C  | -3.8091820 | -3.9281000 | -0.8799220 |
| C  | -4.7945980 | -3.9782520 | 0.1299610  |
| C  | -4.9591520 | -2.9275670 | 0.9923680  |
| C  | -3.9968690 | 2.8157820  | -0.6901710 |
| C  | -3.5869170 | 1.6157610  | 2.5269830  |
| O  | -1.4291410 | -0.5974740 | -1.2046100 |
| O  | 2.1491530  | -0.8508180 | -0.4228090 |
| C  | 2.8334400  | -0.7124280 | 0.6757310  |
| C  | 4.2809540  | -1.0163890 | 0.6086640  |
| C  | 4.8092080  | -1.8084790 | -0.4136260 |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 6.1743490  | -2.0486670 | -0.4668690 |
| C  | 7.0213200  | -1.5028340 | 0.4949160  |
| C  | 6.4990550  | -0.7096730 | 1.5119310  |
| C  | 5.1334840  | -0.4684450 | 1.5701250  |
| C  | 0.0838750  | -2.1306590 | 0.7861110  |
| Cl | 0.7801470  | 0.7316390  | -2.3257980 |
| H  | -4.9503190 | -0.7215050 | 2.5619170  |
| H  | -2.2909070 | 4.8775300  | -0.9457920 |
| H  | 2.5711100  | 0.1071510  | 1.3383590  |
| H  | 4.1500410  | -2.2211570 | -1.1634820 |
| H  | 4.7268320  | 0.1514760  | 2.3589400  |
| H  | 6.5808030  | -2.6587090 | -1.2616920 |
| H  | 7.1543770  | -0.2777540 | 2.2554850  |
| H  | 8.0850180  | -1.6917280 | 0.4485630  |
| H  | -4.1043350 | 1.2980730  | 3.4289230  |
| H  | -2.6048640 | 1.9896630  | 2.8121330  |
| H  | -4.1495880 | 2.4460210  | 2.1024520  |
| H  | -4.3707170 | 1.8090900  | -0.8542550 |
| H  | -4.5873340 | 3.2741500  | 0.1033960  |
| H  | -4.1749890 | 3.3899980  | -1.5975280 |
| H  | -5.7067840 | -2.9575160 | 1.7722490  |
| H  | -5.4194430 | -4.8551780 | 0.2197480  |
| H  | -3.6948130 | -4.7666000 | -1.5519450 |
| H  | -2.2291300 | -2.7907210 | -1.7857530 |
| H  | -0.1747960 | 6.1386470  | -0.7751190 |
| H  | 2.2519310  | 6.1510870  | -0.3162430 |
| H  | 3.3878080  | 4.0713410  | 0.4027420  |
| H  | 2.1330050  | 1.9793340  | 0.6502150  |
| H  | -0.9644360 | -2.0488240 | 1.0444350  |
| H  | 0.3051400  | -3.0773750 | 0.3071790  |
| C  | 0.9321460  | -1.8371910 | 1.8975130  |
| C  | 2.2550230  | -2.2101790 | 1.9553790  |
| H  | 0.5679240  | -1.1434160 | 2.6471220  |
| H  | 2.8367280  | -1.9914140 | 2.8388010  |
| H  | 2.6051810  | -3.0298920 | 1.3436280  |

# **PROPARGYLATION - B3LYP/TZV(2d,2p)**

File:P\_BP1\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 6.7098080  | -1.3476090 | 1.7053230  |
| C  | 5.4839350  | -1.7091730 | 2.2591460  |
| C  | 4.3196690  | -1.5978980 | 1.5126970  |
| C  | 4.3756070  | -1.1224590 | 0.2005100  |
| C  | 5.6063300  | -0.7601210 | -0.3513000 |
| C  | 6.7688060  | -0.8700070 | 0.4000380  |
| C  | 3.1459060  | -0.9756370 | -0.6190650 |
| O  | 2.0250980  | -0.8326920 | 0.0598600  |
| Si | 0.3631780  | -0.7912100 | -0.5242220 |
| O  | -1.4103730 | -0.6352790 | -1.1635840 |
| N  | -2.4350140 | -0.5824440 | -0.2831330 |
| C  | -2.6202280 | 0.5480550  | 0.4116450  |
| C  | -3.5695210 | 0.6046970  | 1.4543760  |
| C  | -4.3700010 | -0.4995050 | 1.6451770  |
| C  | -4.2754380 | -1.6325150 | 0.8211280  |
| C  | -3.2643660 | -1.6752150 | -0.1728130 |
| C  | -1.8188730 | 1.7427660  | 0.0392490  |
| C  | -2.4098000 | 2.9003440  | -0.5085300 |
| C  | -1.6091860 | 4.0134820  | -0.6505150 |
| C  | -0.2587080 | 4.0129380  | -0.2640620 |
| C  | 0.3162680  | 2.8057760  | 0.2086170  |
| N  | -0.5058240 | 1.7088810  | 0.2930590  |
| O  | 0.0244940  | 0.5378140  | 0.7072030  |
| C  | 0.6492470  | -2.3572200 | -1.7707960 |
| C  | 1.8631980  | -2.6765910 | -1.8735630 |
| C  | 3.2010610  | -2.6613320 | -1.6353570 |
| Cl | -0.2499990 | -2.2197570 | 1.0945910  |
| Cl | 0.8510240  | 0.6391680  | -2.1989430 |
| C  | -3.8325070 | 2.9006310  | -0.9976420 |
| H  | -2.0306260 | 4.9177070  | -1.0685540 |
| C  | -3.6572930 | 1.7981550  | 2.3668820  |
| H  | -5.0965460 | -0.4976370 | 2.4460990  |
| C  | -3.1320750 | -2.7861690 | -1.0203170 |
| H  | 3.2508170  | -0.3400950 | -1.4949460 |
| H  | 3.3656930  | -1.8702490 | 1.9403420  |
| H  | 5.6524750  | -0.3847340 | -1.3653140 |
| H  | 5.4368930  | -2.0752770 | 3.2755290  |
| H  | 7.7172980  | -0.5807110 | -0.0308370 |
| H  | 7.6147500  | -1.4348040 | 2.2908620  |
| H  | 3.5974170  | -3.4038940 | -0.9528160 |
| H  | 3.8699680  | -2.3751750 | -2.4385150 |
| H  | -0.2227100 | -2.8004540 | -2.2178440 |
| C  | 1.6673790  | 2.7367320  | 0.5849590  |
| C  | 0.5694060  | 5.1576110  | -0.3509140 |
| H  | -4.1381110 | 3.9126060  | -1.2500230 |
| H  | -3.9190210 | 2.2874840  | -1.8959300 |
| H  | -4.5358320 | 2.5066490  | -0.2680510 |
| H  | -4.3330740 | 1.5807570  | 3.1900680  |
| H  | -2.6812900 | 2.0418990  | 2.7854410  |
| H  | -4.0295210 | 2.6866780  | 1.8588450  |
| C  | 2.4294200  | 3.8738000  | 0.4979890  |
| H  | 2.0763630  | 1.8037330  | 0.9345740  |
| H  | 3.4680010  | 3.8391200  | 0.7944580  |
| C  | 1.8832640  | 5.0878950  | 0.0261480  |
| H  | 0.1428060  | 6.0807410  | -0.7165210 |

|   |            |            |            |
|---|------------|------------|------------|
| H | 2.5118590  | 5.9645040  | -0.0362150 |
| C | -3.9954610 | -3.8410000 | -0.8693940 |
| H | -2.3777420 | -2.7863510 | -1.7863620 |
| H | -3.9091210 | -4.6939310 | -1.5272210 |
| C | -4.9946520 | -3.8310380 | 0.1276450  |
| C | -5.1327470 | -2.7505850 | 0.9560270  |
| H | -5.6542480 | -4.6807220 | 0.2291050  |
| H | -5.8969810 | -2.7275430 | 1.7198720  |

File: P\_BP1\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -6.9599290 | -0.7798390 | -1.0274160 |
| C  | -6.2001380 | 0.0614140  | -0.2179590 |
| C  | -4.8700590 | -0.2343370 | 0.0434880  |
| C  | -4.2889090 | -1.3793580 | -0.5064540 |
| C  | -5.0536340 | -2.2203630 | -1.3177700 |
| C  | -6.3838000 | -1.9197600 | -1.5788790 |
| C  | -2.8647690 | -1.7172360 | -0.2605540 |
| O  | -2.0818760 | -0.7042690 | 0.0527960  |
| Si | -0.3931690 | -0.7283120 | 0.5561700  |
| O  | 1.3824250  | -0.6073020 | 1.1698920  |
| N  | 2.4015730  | -0.6031810 | 0.2834300  |
| C  | 2.6284870  | 0.5174460  | -0.4220230 |
| C  | 3.6013780  | 0.5335040  | -1.4407660 |
| C  | 4.3739740  | -0.5978770 | -1.6034370 |
| C  | 4.2242220  | -1.7217230 | -0.7800950 |
| C  | 3.1874740  | -1.7261180 | 0.1891060  |
| C  | 1.8559130  | 1.7361070  | -0.0639800 |
| C  | 2.4810870  | 2.8867050  | 0.4593600  |
| C  | 1.7084060  | 4.0189860  | 0.6070830  |
| C  | 0.3540140  | 4.0482020  | 0.2399640  |
| C  | -0.2554540 | 2.8512200  | -0.2151500 |
| N  | 0.5371950  | 1.7328150  | -0.2990380 |
| O  | -0.0371990 | 0.5741360  | -0.6914030 |
| C  | -0.7095080 | -2.2030310 | 1.9038770  |
| C  | -1.8211410 | -2.7703100 | 1.7376230  |
| C  | -3.0644800 | -2.9931440 | 1.2360180  |
| Cl | 0.1759230  | -2.2008730 | -1.0531620 |
| Cl | -0.8405680 | 0.7399380  | 2.2066520  |
| C  | 3.9258180  | 2.8774710  | 0.8797600  |
| H  | 2.1571020  | 4.9155570  | 1.0129350  |
| C  | 3.7861870  | 1.7114040  | -2.3602770 |
| H  | 5.1214770  | -0.6205360 | -2.3852300 |
| C  | 5.0471220  | -2.8693810 | -0.8914700 |
| H  | -2.4402190 | -2.4465860 | -0.9451090 |
| H  | -4.2761100 | 0.4169050  | 0.6682470  |
| H  | -4.6046550 | -3.1045250 | -1.7514080 |
| H  | -6.6465830 | 0.9493840  | 0.2081790  |
| H  | -6.9679730 | -2.5713310 | -2.2137930 |
| H  | -7.9961350 | -0.5456190 | -1.2293750 |
| H  | -3.2557790 | -3.9143380 | 0.6985650  |
| H  | -3.9042700 | -2.6118000 | 1.8045540  |
| H  | 0.0430110  | -2.3352600 | 2.6621270  |
| C  | -0.4447610 | 5.2135770  | 0.3303390  |
| H  | 4.6814540  | 2.2778750  | -2.1028780 |
| H  | 3.9127180  | 1.3540370  | -3.3807370 |
| H  | 2.9379370  | 2.3896810  | -2.3475200 |
| H  | 4.1132890  | 3.7103640  | 1.5531490  |
| H  | 4.1887790  | 1.9578630  | 1.3992670  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 4.5976280  | 2.9863940  | 0.0291240  |
| C | 4.8471770  | -3.9435360 | -0.0690660 |
| H | 5.8329380  | -2.8721900 | -1.6334000 |
| H | 5.4794250  | -4.8158080 | -0.1511930 |
| C | 3.8140960  | -3.9211800 | 0.8943240  |
| C | 2.9853810  | -2.8370610 | 1.0247010  |
| H | 3.6724670  | -4.7756760 | 1.5404670  |
| H | 2.1962530  | -2.8206840 | 1.7549340  |
| C | -1.7643600 | 5.1733900  | -0.0292900 |
| H | 0.0094470  | 6.1282780  | 0.6838500  |
| H | -2.3709600 | 6.0652200  | 0.0349410  |
| C | -2.3456110 | 3.9690790  | -0.4846570 |
| C | -1.6134160 | 2.8128600  | -0.5723170 |
| H | -3.3888450 | 3.9573930  | -0.7662840 |
| H | -2.0518450 | 1.8870480  | -0.9046590 |

File: P\_BP2\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.5012400  | -0.8790670 | -2.6698260 |
| C  | 4.7057750  | 0.1177930  | -2.1119800 |
| C  | 3.6306670  | -0.2175890 | -1.3009330 |
| C  | 3.3405410  | -1.5573740 | -1.0403950 |
| C  | 4.1389930  | -2.5549170 | -1.6080000 |
| C  | 5.2132620  | -2.2171840 | -2.4186070 |
| C  | 2.1863940  | -1.9700570 | -0.2051080 |
| O  | 1.2156510  | -1.0943800 | -0.0369600 |
| Si | -0.2812970 | -1.3356280 | 0.8964560  |
| O  | -1.1218260 | -0.7067980 | -0.6221020 |
| N  | -2.2087570 | 0.0875210  | -0.5131150 |
| C  | -2.0179400 | 1.3868540  | -0.2319300 |
| C  | -3.1213220 | 2.2339140  | -0.0130790 |
| C  | -4.3810600 | 1.7025290  | -0.2021210 |
| C  | -4.5746090 | 0.3781380  | -0.6149880 |
| C  | -3.4411890 | -0.4637850 | -0.7621580 |
| C  | -0.6207970 | 1.8929720  | -0.2117660 |
| C  | -0.1745610 | 2.8698060  | -1.1285410 |
| C  | 1.0802140  | 3.4033490  | -0.9328520 |
| C  | 1.8918810  | 3.0124030  | 0.1438460  |
| C  | 1.4396220  | 1.9744440  | 0.9986110  |
| N  | 0.2034040  | 1.4293240  | 0.7394640  |
| O  | -0.2345600 | 0.4351220  | 1.5386040  |
| C  | 0.8008630  | -1.8988350 | 2.5338070  |
| C  | 1.9887060  | -2.2107060 | 2.2527250  |
| C  | 3.1125260  | -2.3707340 | 1.5080240  |
| Cl | -2.1517680 | -1.4819300 | 2.1222080  |
| Cl | -0.5554660 | -3.4336000 | 0.1718170  |
| C  | -1.0175840 | 3.3035570  | -2.2972510 |
| H  | 1.4519820  | 4.1500230  | -1.6213200 |
| C  | -2.9713910 | 3.6585670  | 0.4503870  |
| H  | -5.2475280 | 2.3279270  | -0.0329710 |
| C  | -5.8559330 | -0.1696510 | -0.8693840 |
| H  | 1.8642310  | -2.9937510 | -0.3656550 |
| H  | 3.0084340  | 0.5547620  | -0.8777300 |
| H  | 3.9122000  | -3.5966930 | -1.4214750 |
| H  | 4.9220480  | 1.1579950  | -2.3131450 |
| H  | 5.8210360  | -2.9958790 | -2.8579180 |
| H  | 6.3375440  | -0.6144250 | -3.3020960 |
| H  | 3.8862700  | -1.6170500 | 1.5932070  |
| H  | 3.4692430  | -3.3742580 | 1.3101340  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 0.2799140  | -1.8849600 | 3.4755290  |
| C | 3.1568680  | 3.5921670  | 0.4038400  |
| H | -0.3727670 | 3.6664810  | -3.0944460 |
| H | -1.6175030 | 2.4872720  | -2.6929980 |
| H | -1.6904820 | 4.1171770  | -2.0267730 |
| H | -3.6366540 | 3.8328230  | 1.2948840  |
| H | -1.9605520 | 3.8937170  | 0.7692880  |
| H | -3.2557630 | 4.3574800  | -0.3359590 |
| C | -5.9809240 | -1.4739160 | -1.2612440 |
| H | -6.7234330 | 0.4639240  | -0.7510090 |
| H | -6.9583310 | -1.8893450 | -1.4601520 |
| C | -4.8358870 | -2.2891190 | -1.4076690 |
| C | -3.5777160 | -1.8054050 | -1.1569350 |
| H | -4.9537330 | -3.3169510 | -1.7200040 |
| H | -2.7030440 | -2.4272160 | -1.2486890 |
| C | 3.9071730  | 3.1644070  | 1.4656490  |
| H | 3.5096830  | 4.3793730  | -0.2470790 |
| H | 4.8686930  | 3.6144500  | 1.6664080  |
| C | 3.4308640  | 2.1363340  | 2.3080410  |
| C | 2.2175750  | 1.5361700  | 2.0832270  |
| H | 4.0318220  | 1.8171500  | 3.1475950  |
| H | 1.8476870  | 0.7529250  | 2.7224190  |

File: P\_BP2\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 4.9006220  | -2.8540450 | -2.7400530 |
| C  | 3.5955920  | -3.2330840 | -2.4371870 |
| C  | 2.8671040  | -2.5363520 | -1.4833190 |
| C  | 3.4461900  | -1.4508170 | -0.8219140 |
| C  | 4.7563580  | -1.0717260 | -1.1306460 |
| C  | 5.4794790  | -1.7695720 | -2.0869860 |
| C  | 2.6899360  | -0.6589840 | 0.1765130  |
| O  | 1.3803120  | -0.6937970 | 0.1206900  |
| Si | -0.0365490 | -0.9709730 | 1.1474130  |
| O  | -0.9575850 | -0.7856180 | -0.4386610 |
| N  | -2.1434610 | -0.1409670 | -0.4591070 |
| C  | -2.1359500 | 1.1989380  | -0.4450440 |
| C  | -3.3466430 | 1.9183580  | -0.3772290 |
| C  | -4.5196570 | 1.1960920  | -0.4287930 |
| C  | -4.5265080 | -0.2007760 | -0.5634110 |
| C  | -3.2886910 | -0.8940340 | -0.5646340 |
| C  | -0.8226140 | 1.8875920  | -0.5455530 |
| C  | -0.4842180 | 2.7013370  | -1.6458230 |
| C  | 0.6899760  | 3.4211890  | -1.5714240 |
| C  | 1.5153430  | 3.3769960  | -0.4389710 |
| C  | 1.1721200  | 2.4997210  | 0.6223060  |
| N  | 0.0302320  | 1.7490000  | 0.4829170  |
| O  | -0.2869530 | 0.8769920  | 1.4635760  |
| C  | 1.0951690  | -1.1361920 | 2.8137050  |
| C  | 2.3280680  | -1.2579530 | 2.5827160  |
| C  | 3.4864760  | -1.3801780 | 1.8956760  |
| Cl | -1.8766490 | -1.1858110 | 2.4144410  |
| Cl | 0.0354470  | -3.1901200 | 0.8089940  |
| C  | -1.3262090 | 2.7717930  | -2.8922380 |
| H  | 0.9795310  | 4.0476060  | -2.4045850 |
| C  | -3.3668130 | 3.4150250  | -0.2250950 |
| H  | -5.4651770 | 1.7181870  | -0.3701910 |
| C  | -5.7182190 | -0.9569890 | -0.6745190 |
| H  | 3.1099130  | 0.3245510  | 0.3752650  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 1.8542120  | -2.8243910 | -1.2448100 |
| H | 5.2065410  | -0.2262210 | -0.6265300 |
| H | 3.1443970  | -4.0723400 | -2.9484210 |
| H | 6.4899590  | -1.4677400 | -2.3250710 |
| H | 5.4635870  | -3.3992830 | -3.4851680 |
| H | 4.2615030  | -0.6361120 | 2.0281340  |
| H | 3.8376350  | -2.3804210 | 1.6718530  |
| H | 0.5517250  | -1.2063790 | 3.7404750  |
| C | 2.6880100  | 4.1605040  | -0.3085950 |
| H | -0.7082480 | 2.5312180  | -3.7568660 |
| H | -2.1618010 | 2.0792440  | -2.8794430 |
| H | -1.7143340 | 3.7791700  | -3.0412870 |
| H | -3.1999680 | 3.9196130  | -1.1763950 |
| H | -4.3387850 | 3.7298130  | 0.1468540  |
| H | -2.6086400 | 3.7594740  | 0.4757870  |
| C | 3.4486560  | 4.0815230  | 0.8260290  |
| H | 2.9603490  | 4.8237770  | -1.1171820 |
| H | 4.3372690  | 4.6877990  | 0.9264810  |
| C | 3.0761580  | 3.2142280  | 1.8768880  |
| C | 1.9596990  | 2.4219480  | 1.7845930  |
| H | 3.6797320  | 3.1761620  | 2.7724760  |
| H | 1.6674970  | 1.7601400  | 2.5822860  |
| C | -5.6609520 | -2.3188920 | -0.7937070 |
| H | -6.6655090 | -0.4369250 | -0.6670930 |
| H | -6.5713290 | -2.8939020 | -0.8836420 |
| C | -4.4150640 | -2.9841510 | -0.7979760 |
| C | -3.2365380 | -2.2930350 | -0.6777850 |
| H | -4.3888270 | -4.0603490 | -0.8924090 |
| H | -2.2839830 | -2.7958740 | -0.6593280 |

File: P\_BP3\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.6738660  | -1.2548710 | -2.0585920 |
| C  | 5.3323470  | -1.3141330 | -0.7096970 |
| C  | 4.0011190  | -1.4040520 | -0.3290980 |
| C  | 2.9988200  | -1.4362880 | -1.3013370 |
| C  | 3.3448820  | -1.3750830 | -2.6536570 |
| C  | 4.6777300  | -1.2823230 | -3.0299370 |
| C  | 1.5666530  | -1.5244950 | -0.9270930 |
| O  | 1.2618460  | -1.1404570 | 0.2931520  |
| Si | -0.2893130 | -1.2454400 | 1.1583920  |
| O  | -1.1016330 | -0.7420410 | -0.4815740 |
| N  | -2.1393990 | 0.1150960  | -0.4882660 |
| C  | -1.8958090 | 1.4214130  | -0.2827430 |
| C  | -2.9632470 | 2.3312960  | -0.1579940 |
| C  | -4.2409240 | 1.8491380  | -0.3587530 |
| C  | -4.4849760 | 0.5106430  | -0.6928100 |
| C  | -3.3900610 | -0.3903140 | -0.7446190 |
| C  | -0.4749870 | 1.8577590  | -0.2588770 |
| C  | 0.0487080  | 2.7301370  | -1.2366960 |
| C  | 1.3416640  | 3.1766540  | -1.0663720 |
| C  | 2.1183820  | 2.7999680  | 0.0399670  |
| C  | 1.5798760  | 1.8728230  | 0.9693190  |
| N  | 0.3026900  | 1.4185810  | 0.7409170  |
| O  | -0.2270660 | 0.5363280  | 1.6198410  |
| C  | -0.4928540 | -3.1968890 | 0.6559870  |
| C  | 0.2651150  | -3.5499830 | -0.2863070 |
| C  | 1.2754980  | -3.4848200 | -1.1891320 |
| Cl | -2.2624620 | -1.3101670 | 2.2141850  |

|    |            |            |            |
|----|------------|------------|------------|
| Cl | 0.7816850  | -1.7887900 | 3.0327870  |
| C  | -0.7564200 | 3.1451810  | -2.4382590 |
| H  | 1.7731150  | 3.8414010  | -1.8023820 |
| C  | -2.7599000 | 3.7717580  | 0.2312110  |
| H  | -5.0805440 | 2.5243370  | -0.2608200 |
| C  | -5.7828440 | 0.0060760  | -0.9549730 |
| C  | -3.5802390 | -1.7474360 | -1.0566750 |
| H  | 0.8665190  | -1.2401830 | -1.7084840 |
| H  | 3.7299400  | -1.4456080 | 0.7155910  |
| H  | 2.5710960  | -1.3983550 | -3.4103930 |
| H  | 6.1058820  | -1.2891600 | 0.0454100  |
| H  | 4.9389710  | -1.2309360 | -4.0778040 |
| H  | 6.7125630  | -1.1854680 | -2.3511860 |
| H  | 2.2220170  | -3.9318650 | -0.9104410 |
| H  | 1.0440340  | -3.5193970 | -2.2467150 |
| H  | -1.2031300 | -3.7556090 | 1.2405500  |
| C  | 3.4265130  | 3.2915000  | 0.2643700  |
| H  | -1.3528720 | 2.3239780  | -2.8306450 |
| H  | -1.4314260 | 3.9680270  | -2.2043680 |
| H  | -0.0880360 | 3.4851620  | -3.2257110 |
| H  | -1.7253090 | 4.0072470  | 0.4603500  |
| H  | -3.1010000 | 4.4407220  | -0.5585500 |
| H  | -3.3525920 | 3.9893730  | 1.1192970  |
| C  | -4.1359620 | 2.8841760  | 1.3613600  |
| H  | 3.8445080  | 3.9946290  | -0.4417760 |
| H  | 5.1314570  | 3.2664770  | 1.5354140  |
| C  | 3.5757400  | 1.9624870  | 2.2730820  |
| C  | 2.3171260  | 1.4491490  | 2.0873100  |
| H  | 4.1504140  | 1.6532920  | 3.1345240  |
| H  | 1.8885000  | 0.7354350  | 2.7713070  |
| C  | -4.8510770 | -2.1898050 | -1.3182550 |
| H  | -2.7335700 | -2.4116620 | -1.0884350 |
| H  | -5.0086910 | -3.2293720 | -1.5679090 |
| C  | -5.9591760 | -1.3144420 | -1.2635550 |
| H  | -6.6223790 | 0.6849780  | -0.9086270 |
| H  | -6.9489990 | -1.6967500 | -1.4671630 |

File: P\_BP3\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | 5.2728840  | -0.4557880 | -2.7786700 |
| C  | 3.9572810  | -0.0294680 | -2.9446330 |
| C  | 2.9637040  | -0.4784570 | -2.0867170 |
| C  | 3.2805870  | -1.3626420 | -1.0525740 |
| C  | 4.6012870  | -1.7865160 | -0.8885890 |
| C  | 5.5935530  | -1.3319960 | -1.7468640 |
| C  | 2.2455640  | -1.8524390 | -0.1089250 |
| O  | 1.1879270  | -1.0845950 | 0.0351770  |
| Si | -0.3048230 | -1.3814550 | 0.9472410  |
| O  | -1.1466480 | -0.7110590 | -0.6124670 |
| N  | -2.1860040 | 0.1407750  | -0.5092070 |
| C  | -1.9405000 | 1.4151900  | -0.1685560 |
| C  | -3.0040490 | 2.3094700  | 0.0714240  |
| C  | -4.2846820 | 1.8521640  | -0.1543370 |
| C  | -4.5345450 | 0.5575870  | -0.6347980 |
| C  | -3.4423170 | -0.3299300 | -0.8090220 |
| C  | -0.5213050 | 1.8518970  | -0.1001850 |
| C  | 0.0085170  | 2.8200190  | -0.9756330 |
| C  | 1.2959400  | 3.2577980  | -0.7390390 |
| C  | 2.0593150  | 2.7768890  | 0.3334620  |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 1.5151730  | 1.7548040  | 1.1545670  |
| N  | 0.2477090  | 1.3179670  | 0.8607400  |
| O  | -0.2848740 | 0.3329660  | 1.6227750  |
| C  | -0.4906570 | -3.2392820 | 0.1470110  |
| C  | 0.5483990  | -3.6291360 | -0.4486200 |
| C  | 1.8018390  | -3.5915380 | -0.9670990 |
| Cl | -2.2565110 | -1.6277690 | 2.0072610  |
| Cl | 0.7991590  | -2.1306690 | 2.7425170  |
| C  | -0.7610130 | 3.3499340  | -2.1562080 |
| H  | 1.7308980  | 3.9979380  | -1.3975560 |
| C  | -2.7649610 | 3.7036810  | 0.5849570  |
| H  | -5.1233710 | 2.5085720  | 0.0346490  |
| C  | -5.8357240 | 0.0871150  | -0.9359450 |
| H  | 2.6252200  | -2.3075200 | 0.8018170  |
| H  | 1.9434030  | -0.1452140 | -2.2094480 |
| H  | 4.8541380  | -2.4646440 | -0.0840060 |
| H  | 3.7079580  | 0.6548060  | -3.7440430 |
| H  | 6.6147670  | -1.6591570 | -1.6092160 |
| H  | 6.0445990  | -0.1037460 | -3.4493400 |
| H  | 2.5662960  | -4.2191300 | -0.5248870 |
| H  | 1.9035450  | -3.4255930 | -2.0328350 |
| H  | -1.4357930 | -3.7292270 | 0.3052810  |
| C  | 2.2417100  | 1.2210120  | 2.2323690  |
| C  | 3.3628100  | 3.2480890  | 0.6250330  |
| H  | -0.1215690 | 3.3402250  | -3.0376160 |
| H  | -1.6458780 | 2.7612810  | -2.3797970 |
| H  | -1.0681670 | 4.3825840  | -1.9909250 |
| H  | -2.5706760 | 4.4027500  | -0.2284680 |
| H  | -3.6504350 | 4.0539760  | 1.1104100  |
| H  | -1.9249190 | 3.7459590  | 1.2748440  |
| C  | 4.0620570  | 2.7296820  | 1.6801670  |
| H  | 3.7858050  | 4.0230400  | 0.0019090  |
| H  | 5.0542470  | 3.0941070  | 1.9042910  |
| C  | 3.4956060  | 1.7159160  | 2.4850500  |
| H  | 1.8077060  | 0.4398840  | 2.8341530  |
| H  | 4.0617990  | 1.3210340  | 3.3165340  |
| C  | -6.0183300 | -1.1863600 | -1.4016180 |
| H  | -6.6736080 | 0.7549030  | -0.7954120 |
| H  | -7.0116490 | -1.5409910 | -1.6361010 |
| C  | -4.9123090 | -2.0459450 | -1.5826510 |
| C  | -3.6377670 | -1.6367940 | -1.2856560 |
| H  | -5.0731460 | -3.0453480 | -1.9609610 |
| H  | -2.7902510 | -2.2861000 | -1.4217000 |

File: P\_BP4\_S\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -6.8441350 | -2.2175620 | -0.8784390 |
| C  | -5.7719030 | -2.9248610 | -0.3400210 |
| C  | -4.5590460 | -2.2903680 | -0.1136820 |
| C  | -4.4131540 | -0.9369830 | -0.4255540 |
| C  | -5.4897640 | -0.2300610 | -0.9656080 |
| C  | -6.7004930 | -0.8699960 | -1.1936990 |
| C  | -3.1191440 | -0.2391320 | -0.2126890 |
| O  | -2.0556640 | -1.0084810 | -0.1920180 |
| Si | -0.4041260 | -0.8644430 | 0.3794280  |
| O  | 1.3175780  | -0.6505680 | 1.0920540  |
| N  | 2.3854530  | -0.6293750 | 0.2677810  |
| C  | 2.6378120  | 0.5098830  | -0.3827990 |
| C  | 3.6620610  | 0.5748920  | -1.3490240 |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 4.4589250  | -0.5400790 | -1.4978490 |
| C  | 4.2707240  | -1.6973680 | -0.7238310 |
| C  | 3.1765710  | -1.7491040 | 0.1781400  |
| C  | 1.8491380  | 1.7040020  | 0.0126190  |
| C  | 2.4629380  | 2.7798270  | 0.6917120  |
| C  | 1.7107870  | 3.9122170  | 0.9060240  |
| C  | 0.4015430  | 4.0283030  | 0.4112020  |
| C  | -0.1902690 | 2.9114500  | -0.2315140 |
| N  | 0.5480640  | 1.7481490  | -0.3098710 |
| O  | -0.0492440 | 0.6348780  | -0.7877620 |
| C  | -0.9558300 | 0.3481460  | 1.9163950  |
| C  | -2.1742030 | 0.6633260  | 1.8962720  |
| C  | -3.4780650 | 0.6510200  | 1.5180000  |
| Cl | 0.2509480  | -2.1215120 | -1.2957490 |
| Cl | -0.6562620 | -2.6157080 | 1.7690220  |
| C  | 3.8671050  | 2.6679080  | 1.2222560  |
| H  | 2.1406890  | 4.7424720  | 1.4491460  |
| C  | 3.8335630  | 1.7819270  | -2.2302590 |
| H  | 5.2562490  | -0.5275040 | -2.2285790 |
| C  | 5.1091400  | -2.8331850 | -0.8224910 |
| H  | -3.0216400 | 0.6928250  | -0.7602890 |
| H  | -3.7202860 | -2.8355090 | 0.2942980  |
| H  | -5.3785020 | 0.8172920  | -1.2162580 |
| H  | -5.8813830 | -3.9737220 | -0.1011600 |
| H  | -7.5280410 | -0.3203740 | -1.6202890 |
| H  | -7.7867780 | -2.7167470 | -1.0562020 |
| H  | -4.1400210 | -0.0228800 | 2.0487800  |
| H  | -3.9382950 | 1.5712820  | 1.1798030  |
| H  | -0.1931430 | 0.5491070  | 2.6504750  |
| C  | -0.3571220 | 5.2179040  | 0.5239180  |
| H  | 4.0764520  | 3.5077990  | 1.8798330  |
| H  | 4.0021560  | 1.7491030  | 1.7916280  |
| H  | 4.6129890  | 2.6769210  | 0.4283970  |
| H  | 4.7103560  | 1.6583130  | -2.8603680 |
| H  | 2.9657650  | 1.9040920  | -2.8797410 |
| H  | 3.9510740  | 2.7053580  | -1.6668160 |
| C  | -1.6132760 | 5.2923920  | -0.0150700 |
| H  | 0.0832190  | 6.0661700  | 1.0285190  |
| H  | -2.1850130 | 6.2056200  | 0.0641570  |
| C  | -2.1592240 | 4.1860760  | -0.6997080 |
| C  | -1.4671330 | 3.0058210  | -0.8050560 |
| H  | -3.1330490 | 4.2724220  | -1.1600530 |
| H  | -1.8589900 | 2.1718840  | -1.3594460 |
| C  | 4.8622540  | -3.9399090 | -0.0556950 |
| H  | 5.9423830  | -2.8046980 | -1.5101160 |
| H  | 5.5060000  | -4.8045860 | -0.1296290 |
| C  | 3.7657340  | -3.9643680 | 0.8339900  |
| C  | 2.9202430  | -2.8908430 | 0.9537920  |
| H  | 3.5859100  | -4.8478790 | 1.4297610  |
| H  | 2.0693530  | -2.9075230 | 1.6149660  |

File: P\_BP4\_R\_B3LYP\_TZV2D2P.XYZ

|   |           |            |            |
|---|-----------|------------|------------|
| C | 6.7000470 | -1.4645420 | 1.6658840  |
| C | 5.6022930 | -0.7853590 | 2.1863580  |
| C | 4.4035730 | -0.7537420 | 1.4866990  |
| C | 4.2942770 | -1.4039990 | 0.2562640  |
| C | 5.3969140 | -2.0911790 | -0.2585160 |
| C | 6.5934100 | -2.1212760 | 0.4433670  |

|    |            |            |            |
|----|------------|------------|------------|
| C  | 3.0201260  | -1.4128730 | -0.5087440 |
| O  | 1.9391480  | -1.0735750 | 0.1660130  |
| Si | 0.2788350  | -0.9608990 | -0.4160370 |
| O  | -1.4332970 | -0.5980850 | -1.0986050 |
| N  | -2.4757450 | -0.4442570 | -0.2537600 |
| C  | -2.6133380 | 0.7333100  | 0.3783160  |
| C  | -3.6259220 | 0.9085030  | 1.3404610  |
| C  | -4.5182890 | -0.1288280 | 1.5232510  |
| C  | -4.4425060 | -1.3139010 | 0.7800930  |
| C  | -3.3681290 | -1.4805540 | -0.1324970 |
| C  | -1.6976700 | 1.8351580  | -0.0152850 |
| C  | -2.1728990 | 3.0195290  | -0.6185100 |
| C  | -1.2707440 | 4.0428620  | -0.8155090 |
| C  | 0.0710030  | 3.9356620  | -0.4162510 |
| C  | 0.5249240  | 2.7069200  | 0.1266330  |
| N  | -0.3909980 | 1.6878570  | 0.2524530  |
| O  | 0.0338850  | 0.5068410  | 0.7445710  |
| C  | 0.8862800  | 0.2348880  | -1.9885500 |
| C  | 2.1319800  | 0.2089260  | -2.1570630 |
| C  | 3.4329310  | -0.1135920 | -1.9250170 |
| Cl | -0.4282870 | -2.1755230 | 1.2784690  |
| Cl | 0.3816810  | -2.7401730 | -1.7692450 |
| C  | -3.6053530 | 3.1619040  | -1.0568840 |
| H  | -1.6033080 | 4.9593490  | -1.2834220 |
| C  | -3.7337970 | 2.1475270  | 2.1895560  |
| H  | -5.3043720 | -0.0242830 | 2.2592810  |
| C  | -5.3781800 | -2.3690820 | 0.9151590  |
| H  | 2.9026830  | -2.2541110 | -1.1866310 |
| H  | 3.5452000  | -0.2460530 | 1.9006650  |
| H  | 5.3159110  | -2.6092590 | -1.2054130 |
| H  | 5.6781320  | -0.2864790 | 3.1427240  |
| H  | 7.4394240  | -2.6608510 | 0.0408370  |
| H  | 7.6316860  | -1.4893790 | 2.2142450  |
| H  | 3.9346870  | -0.7592550 | -2.6358560 |
| H  | 4.0657770  | 0.6404480  | -1.4716110 |
| H  | 0.1096060  | 0.7283390  | -2.5477550 |
| C  | 1.0021640  | 4.9943430  | -0.5457950 |
| H  | -4.6510080 | 2.6933480  | 1.9685140  |
| H  | -3.7725870 | 1.8598570  | 3.2395610  |
| H  | -2.8927180 | 2.8222550  | 2.0625230  |
| H  | -3.6815490 | 3.9493970  | -1.8028660 |
| H  | -3.9894600 | 2.2425300  | -1.4943540 |
| H  | -4.2542600 | 3.4347140  | -0.2250390 |
| C  | -5.2437820 | -3.5071380 | 0.1688600  |
| H  | -6.1949930 | -2.2523240 | 1.6131550  |
| H  | -5.9606790 | -4.3093240 | 0.2692090  |
| C  | -4.1678880 | -3.6457640 | -0.7369060 |
| C  | -3.2309240 | -2.6564470 | -0.8896090 |
| H  | -4.0787400 | -4.5522410 | -1.3185150 |
| H  | -2.3980470 | -2.7624630 | -1.5646720 |
| C  | 2.2978450  | 4.8269420  | -0.1378300 |
| H  | 0.6665860  | 5.9329470  | -0.9633570 |
| H  | 3.0039940  | 5.6395470  | -0.2298110 |
| C  | 2.7225020  | 3.5957320  | 0.4087450  |
| C  | 1.8575920  | 2.5389540  | 0.5362560  |
| H  | 3.7472080  | 3.4845300  | 0.7334270  |
| H  | 2.1681150  | 1.5942610  | 0.9485750  |

|    |            |            |            |
|----|------------|------------|------------|
| C  | -6.9645010 | -0.7525580 | -1.0267120 |
| C  | -5.9351250 | 0.1040270  | -1.4103730 |
| C  | -4.6213410 | -0.1901750 | -1.0763830 |
| C  | -4.3249190 | -1.3464330 | -0.3523540 |
| C  | -5.3590120 | -2.2041320 | 0.0270380  |
| C  | -6.6742640 | -1.9056840 | -0.3058950 |
| C  | -2.9333980 | -1.6930280 | 0.0412470  |
| O  | -2.1131770 | -0.6749400 | 0.2324120  |
| Si | -0.4077600 | -0.7236430 | 0.6906160  |
| O  | -0.0705160 | 0.5824170  | -0.6101910 |
| N  | 0.5392440  | 1.7375890  | -0.2620260 |
| C  | 1.8723050  | 1.7334220  | -0.1090260 |
| C  | 2.5391720  | 2.8830780  | 0.3601390  |
| C  | 1.7865860  | 4.0233280  | 0.5501150  |
| C  | 0.4123210  | 4.0598930  | 0.2759940  |
| C  | -0.2347300 | 2.8640920  | -0.1288930 |
| C  | 2.6100730  | 0.5021180  | -0.4921420 |
| C  | 3.5530830  | 0.4951340  | -1.5411340 |
| C  | 4.3033290  | -0.6484030 | -1.7213080 |
| C  | 4.1586390  | -1.7689650 | -0.8906100 |
| C  | 3.1517470  | -1.7521670 | 0.1096870  |
| N  | 2.3867390  | -0.6123970 | 0.2253030  |
| O  | 1.4185120  | -0.6003370 | 1.1625880  |
| C  | -0.0269810 | -2.0241800 | -0.8634350 |
| C  | -1.0749670 | -2.5490390 | -1.3195350 |
| C  | -2.4044110 | -2.7861330 | -1.4832730 |
| Cl | -0.7729590 | 0.7391810  | 2.2989970  |
| Cl | -0.5897820 | -2.4377820 | 2.1105370  |
| C  | 3.7319750  | 1.6675760  | -2.4680900 |
| H  | 5.0283660  | -0.6847770 | -2.5234490 |
| C  | 4.0103020  | 2.8825410  | 0.6798760  |
| H  | 2.2685110  | 4.9186900  | 0.9188600  |
| C  | -0.3699600 | 5.2325490  | 0.4140440  |
| H  | -2.8637700 | -2.4908760 | 0.7756440  |
| H  | -3.8234760 | 0.4728940  | -1.3766600 |
| H  | -5.1355060 | -3.0983550 | 0.5943120  |
| H  | -6.1590840 | 1.0020580  | -1.9695770 |
| H  | -7.4701640 | -2.5700830 | 0.0007770  |
| H  | -7.9878330 | -0.5196190 | -1.2870820 |
| H  | -2.8871580 | -2.3372670 | -2.3433190 |
| H  | -2.7980340 | -3.7538320 | -1.1954300 |
| H  | 0.9856670  | -2.1716890 | -1.1955230 |
| C  | 4.9542950  | -2.9328200 | -1.0208290 |
| H  | 3.8630950  | 1.3053070  | -3.4860630 |
| H  | 2.8793060  | 2.3405690  | -2.4590840 |
| H  | 4.6230790  | 2.2403600  | -2.2111820 |
| H  | 4.5991160  | 3.2510110  | -0.1601830 |
| H  | 4.1964870  | 3.5460030  | 1.5219880  |
| H  | 4.3769980  | 1.8939970  | 0.9442310  |
| C  | -1.7113840 | 5.2007340  | 0.1484820  |
| H  | 0.1149820  | 6.1454110  | 0.7295170  |
| H  | -2.3058740 | 6.0971800  | 0.2502940  |
| C  | -2.3320760 | 3.9972410  | -0.2552760 |
| C  | -1.6151300 | 2.8363880  | -0.3873240 |
| H  | -3.3936680 | 3.9901330  | -0.4569380 |
| H  | -2.0811800 | 1.9096390  | -0.6730830 |
| C  | 4.7520200  | -4.0019510 | -0.1909100 |
| H  | 5.7206830  | -2.9537300 | -1.7824750 |

File: P\_BP5\_S\_B3LYP\_TZV2D2P.XYZ

|   |           |            |            |
|---|-----------|------------|------------|
| H | 5.3642500 | -4.8868930 | -0.2880670 |
| C | 3.7438290 | -3.9594770 | 0.7972410  |
| C | 2.9417050 | -2.8570160 | 0.9524180  |
| H | 3.6003900 | -4.8119050 | 1.4457320  |
| H | 2.1645400 | -2.8202310 | 1.6979440  |

File: P\_BP5\_R\_B3LYP\_TZV2D2P.XYZ

|    |            |            |            |
|----|------------|------------|------------|
| C  | -2.3737970 | 2.9446480  | -0.2907140 |
| C  | -1.7264820 | 1.7717790  | 0.1513840  |
| N  | -0.3912100 | 1.7186140  | 0.2419630  |
| C  | 0.4191540  | 2.8187680  | 0.0745510  |
| C  | -0.2041370 | 4.0399070  | -0.2914930 |
| C  | -1.5914250 | 4.0574820  | -0.5050260 |
| C  | 0.6088680  | 5.1862670  | -0.4608990 |
| C  | 1.9607640  | 5.1097550  | -0.2645420 |
| C  | 2.5586790  | 3.8841260  | 0.0996170  |
| C  | 1.8085990  | 2.7475210  | 0.2613170  |
| C  | -2.5021140 | 0.5689920  | 0.5473550  |
| C  | -3.3731560 | 0.5741270  | 1.6588190  |
| C  | -4.1992230 | -0.5159310 | 1.8239110  |
| C  | -4.1895350 | -1.5973990 | 0.9263040  |
| C  | -3.2412460 | -1.6023830 | -0.1288500 |
| N  | -2.3977280 | -0.5173760 | -0.2297690 |
| C  | -3.1630450 | -2.6694580 | -1.0393520 |
| C  | -4.0385250 | -3.7171330 | -0.8944090 |
| C  | -4.9900820 | -3.7382320 | 0.1478090  |
| C  | -5.0641310 | -2.7035680 | 1.0418630  |
| C  | -3.3450100 | 1.6881580  | 2.6698540  |
| O  | -1.4689730 | -0.5227170 | -1.2079920 |
| Si | 0.3553760  | -0.8015710 | -0.7908670 |
| Cl | 0.3877380  | -2.5026700 | -2.2311770 |
| O  | 0.1735980  | 0.5301440  | 0.5487450  |
| C  | -3.8509210 | 2.9681330  | -0.5792000 |
| O  | 2.0777370  | -0.9561520 | -0.4261300 |
| C  | 2.6973240  | -0.9428170 | 0.7362020  |
| C  | 4.1648020  | -1.1719480 | 0.6830520  |
| C  | 4.7520290  | -1.8473530 | -0.3889580 |
| C  | 6.1268210  | -2.0309760 | -0.4215110 |
| C  | 6.9247680  | -1.5429780 | 0.6105060  |
| C  | 6.3434200  | -0.8651710 | 1.6772320  |
| C  | 4.9675650  | -0.6819420 | 1.7153440  |
| C  | -0.0950580 | -2.1515260 | 0.6744020  |
| C  | 0.8706020  | -2.4060960 | 1.4424990  |
| C  | 2.1514550  | -2.4288820 | 1.8941700  |
| Cl | 0.7937930  | 0.6528600  | -2.3811440 |
| H  | -1.0585080 | -2.6324000 | 0.6508290  |
| H  | 2.3848640  | -0.1715520 | 1.4372510  |
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| H  | 2.7699720  | -3.2633180 | 1.5846090  |
| H  | 4.1303630  | -2.2150420 | -1.1922100 |
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| H  | -4.8782360 | -0.5443380 | 2.6651110  |
| H  | -5.7874160 | -2.7123640 | 1.8448600  |
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| H  | -3.9977480 | -4.5403280 | -1.5932910 |

|   |            |            |            |
|---|------------|------------|------------|
| H | -2.4262300 | -2.6469200 | -1.8259170 |
| H | -2.4032190 | 1.6731270  | 3.2204900  |
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| H | 2.2666400  | 1.8115100  | 0.5230040  |
| H | 3.6280600  | 3.8373920  | 0.2473140  |
| H | 2.5785470  | 5.9869880  | -0.3914380 |
| H | 0.1387940  | 6.1164680  | -0.7466280 |
| H | -2.0541160 | 4.9719930  | -0.8501100 |
| H | -4.1066150 | 3.8941470  | -1.0876790 |
| H | -4.4547750 | 2.9104010  | 0.3254230  |
| H | -4.1391630 | 2.1382610  | -1.2234160 |