# Giant Spin-Orbit Effects on $^{1}H$ and $^{13}C$ NMR Shifts for Uranium(VI) Complexes Revisited: Role of the Exchange-Correlation Response Kernel, Bonding Analyses, and New Predictions

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## Electronic Supplementary Information

**Table S1.** Comparison of the compositions of the U–C σ-bonding NLMOs in selected U(VI) complexes with different NBO modules at PBE0 level [a]

| | NBO 5.0 (ADF 2012) | | | NBO 6.0 (ADF 2014) | | | NBO 5.9 (G09) | | |
|---|---|---|---|---|---|---|---|---|---|
| Complex | %U | %U(d) | %U(f) | %U | %U(d) | %U(f) | %U | %U(d) | %U(f) |
| **1** | 9.3 | 12.2 | 58.8 | 16.3 | 49.9 | 33.8 | 16.4 | 49.5 | 31.5 |
| **4** | 15.3 | 12.3 | 71.7 | 21.0 | 29.9 | 56.6 | 22.1 | 34.1 | 53.3 |
| **5** | 28.0 | 8.6 | 88.4 | 28.9 | 23.5 | 75.0 | 28.5 | 24.5 | 73.0 |
| **6** | 27.8 | 8.9 | 88.3 | 28.5 | 26.0 | 71.4 | 27.7 | 25.0 | 72.3 |
| **7** | 23.1 | 9.3 | 82.1 | 28.7 | 25.8 | 67.0 | 28.7 | 24.7 | 68.1 |

[a] Scalar-relativistic results with def2-TZVP GTO (Gaussian 09) and TZ2P STO (ADF) basis sets at PBE0-D3-optimized structures.

**Table S2.** Optimized U–C bond lengths (in Ångstroms) with different functionals (with and without dispersion corrections) compared with experimental data [a]

| Complex | PBE | PBE0 | PBE0-D3 | B3LYP | B3LYP-D3 | Expt. |
|---|---|---|---|---|---|---|
| **1** | 2.67 | 2.66 | 2.63 | 2.70 | 2.65 | 2.63 [S1] |
| **2** | 2.66 | 2.66 | 2.61 | 2.70 | 2.62 | – |
| **3** | 2.50 | 2.50 | 2.48 | 2.52 | 2.49 | 2.50 [S2] |
| **3**[c] | – | – | 2.48 | – | – | – |
| **4** | 2.49[b] | 2.48[b] | 2.48[b] | 2.51[b] | 2.49[b] | 2.49[b],[S3] |
| **4**[c] | – | – | 2.56 | – | – | – |
| **5** | 2.36 | 2.30 | 2.30 | 2.34 | 2.34 | 2.35 [S4] |
| **6** | 2.35 | 2.27 | 2.28 | 2.32 | 2.32 | 2.28 [S5] |
| **7** | 2.36 | 2.33 | 2.32 | 2.37 | 2.35 | – |
| **SD**[d] | 0.04 | 0.03 | 0.02 | 0.04 | 0.02 | |
| **8** | – | – | 2.64 | – | 2.65 | 2.65 [S6] |
| **8'** | – | – | 2.72 | – | – | – |
| **9** | – | – | 2.62 | – | 2.62 | 2.62 [S7] |
| **10** | – | – | 2.29 | – | 2.31 | 2.34 [S4] |
| **11** | – | – | 2.36 | – | 2.37 | 2.43 [S6] |
| **12** | – | – | 2.14 | – | 2.17 | 2.18 [S8] |
| **13** | 2.32[e] | 2.26[e] | 2.22[e] | 2.27[e] | 2.24[e] | 2.45 [S9] |
| **14** | – | – | 2.37 | – | 2.38 | 2.40 [S10] |
| **SD**[d] | – | – | 0.10 | – | 0.09 | |

[a] def2-TZVP basis set with small-core ECP for uranium, see Computational Details in main text. [b] Averaged data for two non-equivalent alkyl carbon atoms. [c] Only anionic part of the complex without $Li^+$ counter-ion(s) was considered. [d] Standard deviation. [e] Note that while the structure optimization was done for a U(VI) singlet ground-state, the X-ray structure of **13** feature all U–L bond-lengths characteristic for a U(IV) complex, in accordance with DFT calculations for a triplet structure (see Discussion in main text).

**Table S3.** Optimized U=O and U–N bond lengths (in Ångstroms) with different DFT functionals (with and without dispersion corrections), compared with experimental values [a]

| | PBE0 | | PBE0-D3 | | B3LYP | | B3LYP-D3 | | Expt. [b] | |
|---|---|---|---|---|---|---|---|---|---|---|
| | d(U=O) | d(U–N) | d(U=O) | d(U–N) | d(U=O) | d(U–N) | d(U=O) | d(U–N) | d(U=O) | d(U–N) |
| **1** | 1.78 | 2.31 | 1.79 | 2.30 | 1.81 | 2.34 | 1.81 | 2.32 | 1.80 | 2.28 |
| **3** | 1.77 | 2.49 | 1.78 | 2.46 | 1.79 | 2.52 | 1.78 | 2.48 | 1.78 | 2.46 |
| **4** | 1.86 | – | 1.85 | – | 1.88 | – | 1.88 | – | 1.89 | – |
| **5** | 1.78 | 2.22 | 1.78 | 2.21 | 1.80 | 2.26 | 1.80 | 2.23 | 1.80 | 2.22 |
| **6** | 1.78 | 2.21 | 1.78 | 2.21 | 1.80 | 2.24 | 1.80 | 2.22 | 1.80 | 2.22 |
| **SD** | 0.02 | 0.02 | 0.02 | 0.01 | 0.01 | 0.05 | 0.01 | 0.02 | | |
| **8** | – | – | 1.75 | – | – | – | 1.77 | – | 1.76 | – |
| **9** | – | – | 1.75 | – | – | – | 1.77 | – | 1.74 | – |
| **10** | – | – | 1.78 | 2.19 | – | – | 1.80 | 2.21 | 1.81 | 2.20 |
| **11** | – | – | 1.77 | – | – | – | 1.79 | – | 1.76 | – |
| **12** | – | – | 1.76 | 2.32 | – | – | 1.78 | 2.34 | 1.84 | 2.31 |
| **13** | – | 2.27[c] | – | 2.26[c] | – | 2.30[c] | – | 2.29[c] | – | 2.36 |
| **14** | – | – | 1.79 | 1.89 | – | – | 1.82 | 1.92 | 1.81 | 1.92 |
| **SD** | | | 0.04 | 0.02 | | | 0.03 | 0.02 | | |

[a] def2-TZVP basis with small-core ECP for uranium, see Computational Details in main text. [b] See Table S2 for references to experimental data. [c] Note that while the structure optimization was done for a U(VI) singlet ground-state, the X-ray structure of **13** feature all U–L bond-lengths characteristic for a U(IV) complex, in accordance with DFT calculations for a triplet structure (see Discussion in main text).

**Table S4.** Solvent effects on optimized U–C bond lengths (in Ångstroms) using COSMO [a]

| Complex | gas phase | benzene (ε=2.3) | THF (ε=7.6) |
|---|---|---|---|
| **1** | 2.633 | 2.634 | 2.634 |
| **2** | 2.613 | 2.612 | 2.613 |
| **3** | 2.482 | 2.485 | 2.488 |
| **4**[b] | 2.478 | 2.480 | 2.482 |
| **5** | 2.304 | 2.302 | 2.300 |
| **6** | 2.277 | 2.274 | 2.271 |
| **7** | 2.323 | 2.324 | 2.326 |

[a] PBE0-D3/def2-TZVP/ECP results, see Computational Details in main text. [b] Averaged data for two non-equivalent alkyl carbon atoms.

**Table S5.** Optimized U–H and U–C bond lengths (in Ångstroms) with (SO) and without (SR) consideration of spin-orbit effects [a]

| Complex | d(U–C/H) SR | d(U–C/H) SO | $\Delta d^{SR-SO}$ [Å] |
|---|---|---|---|
| $U(CH_3)_6$ (**7'**) | 2.353 | 2.349 | 0.004 |
| $HUF_5$ (**15**) | 1.906 | 1.901 | 0.004 |
| $H_2UO_2$ ($C_{2v}$, **18**) | 1.957 | 1.962 | –0.006 |
| $H_2UO_2$ ($D_{2h}$, **18**) | 1.999 | 1.987 | 0.012 |

[a] 2c-ZORA/TZ2P/PBE0 results.

**Table S6.** Comparison between calculated $^{13}$C NMR shielding components (in ppm) of U(VI)-bound carbon atoms at PBE level with (XC) and without consideration of the exchange-correlation kernel [a]

| Complex | $\sigma_{2c}^{dia}$ | $\sigma_{2c}^{para}$ | $\sigma_{2c}^{SO}$ | $\sigma_{2c}^{xc,dia}$ | $\sigma_{2c}^{xc,para}$ | $\sigma_{2c}^{xc,SO}$ |
|---|---|---|---|---|---|---|
| **1** | 240.2 | –254.4 | –65.3 | 240.3 | –254.4 | –88.2 |
| **2** | 242.9 | –281.1 | –58.2 | 242.9 | –281.1 | –75.2 |
| **3** | 245.5 | –279.6 | –139.0 | 245.5 | –280.3 | –196.1 |
| **4**-C1[b] | 233.2 | –117.0 | –89.4 | 233.3 | –119.3 | –142.5 |
| **4**-C2[b] | 234.0 | –136.0 | –99.2 | 234.1 | –139.3 | –159.4 |
| **5** | 219.3 | –145.9 | –70.6 | 219.4 | –148.2 | –115.9 |
| **6** | 234.0 | –201.9 | –52.4 | 234.1 | –205.8 | –88.3 |
| **7** | 237.6 | –203.2 | –96.4 | 237.7 | –212.3 | –162.1 |
| **8** | 253.5 | –93.5 | –12.0 | 253.6 | –93.8 | –25.4 |
| **9** | – | – | – | 237.9 | –249.3 | –99.8 |
| **10** | – | – | – | 259.3 | –277.9 | –162.7 |
| **11** | – | – | – | 273.4 | –247.6 | –95.3 |
| **12** | – | – | – | 286.3 | –323.7 | –72.3 |
| **13** | – | – | – | 290.1 | –369.7 | –162.2 |
| **14** | – | – | – | 271.9 | –287.1 | –75.8 |

[a] 2c-ZORA-SO/TZ2P results at PBE0-D3/def2-TZVP/ECP optimized structures, see Computational Details in main text. [b] Data for two non-equivalent alkyl carbon atoms in **4**.

**Table S7.** Comparison between calculated $^{13}$C NMR shielding components (in ppm) of U(VI)-bound carbon atoms at PBE0 level with (XC) and without consideration of exchange-correlation kernel [a]

| Complex | $\sigma_{2c}^{dia}$ | $\sigma_{2c}^{para}$ | $\sigma_{2c}^{SO}$ | $\sigma_{2c}^{xc,dia}$ | $\sigma_{2c}^{xc,para}$ | $\sigma_{2c}^{xc,SO}$ |
|---|---|---|---|---|---|---|
| **1** | 252.0 | –269.6 | –61.6 | 252.1 | –269.6 | –77.7 |
| **2** | 255.6 | –301.5 | –51.3 | 255.7 | –301.5 | –62.2 |
| **3** | 252.0 | –269.6 | –61.6 | 250.8 | –277.5 | –169.0 |
| **4**-C1[b] | 231.8 | –105.1 | –124.7 | 231.9 | –108.1 | –195.0 |
| **4**-C2[b] | 230.9 | –126.1 | –142.8 | 231.0 | –130.8 | –229.0 |
| **5** | 231.7 | –165.3 | –106.7 | 231.7 | –168.2 | –171.9 |
| **6** | 235.0 | –215.5 | –81.8 | 235.1 | –220.8 | –136.5 |
| **7** | 232.0 | –200.8 | –180.3 | 232.1 | –214.6 | –362.7 |
| **8** | 246.2 | –70.6 | –6.4 | 246.3 | –70.7 | –12.6 |
| **9** | – | – | – | 252.9 | –265.9 | –72.1 |
| **10** | – | – | – | 266.7 | –278.8 | –222.3 |
| **11** | – | – | – | 263.7 | –191.4 | –71.4 |
| **12** | – | – | – | 260.5 | –342.4 | –99.1 |
| **13** | – | – | – | 256.6 | –377.5 | –389.7 |
| **14** | – | – | – | 259.2 | –229.9 | –58.2 |

[a] 2c-ZORA-SO/TZ2P results at PBE0-D3/def2-TZVP/ECP optimized structures, see Computational Details in main text. [b] Data for two non-equivalent alkyl carbon atoms in **4**.

**Table S8.** Isotropic $^{13}$C NMR shifts (in ppm vs. TMS) of U(VI)-bound carbon atoms calculated at different levels of theory for B3LYP-D3/def2-TZVP/ECP optimized structures. Spin-orbit-induced shifts are given in parentheses [a]

| Complex | $\delta_{2c}(PBE)$ | $\delta_{2c}^{xc}(PBE)$ | $\delta_{2c}(PBE0)$ | $\delta_{2c}^{xc}(PBE0)$ | $\delta_{exp}$ |
|---|---|---|---|---|---|
| **1** | 270.1 (67.1) | 295.8 (92.6) | 275.7 (64.6) | 294.4 (83.2) | 262.8 [S1] |
| **2** | 285.7 (60.4) | 304.3 (79.0) | 291.1 (53.7) | 303.4 (65.9) | 283.6 [S11] |
| **3** | 365.7 (142.0) | 426.6 (202.0) | 351.0 (131.3) | 392.0 (171.8) | 329.4 [S2] |
| **4**[b] | 178.0 (95.4) | 244.7 (158.7) | 222.8 (143.2) | 324.0 (240.4) | 242.9 [S3] |
| **5** | 186.1 (71.0) | 240.8 (123.2) | 240.2 (112.7) | 323.8 (192.7) | 301.0 [S4] |
| **6** | 207.5 (50.3) | 253.0 (91.4) | 259.7 (83.4) | 333.6 (150.9) | 317.4 [S5] |
| **7** | 255.6 (99.8) | 342.9 (176.1) | 362.1 (196.7) | 690.7 (444.8) | 434.3 [S3] |

[a] 2c-ZORA-SO/TZ2P results, see Computational Details in main text. [b] Averaged data for two non-equivalent alkyl carbon atoms.

**Table S9.** Calculated $^{13}C$ NMR shifts (in ppm vs. TMS) of U(VI)-bound carbon atoms with solvent effects using COSMO both for the structure optimization and NMR shift calculation [a]

| Complex | $\delta_{2c}^{xc}(PBE0)$ gas-phase | $\delta_{2c}^{xc}(PBE0)$ benzene (ε=2.3) | $\delta_{2c}^{xc}(PBE0)$ THF (ε=7.6) | $\delta_{exp}$ |
|---|---|---|---|---|
| **1** | 286.8 | 288.6 | – | 262.8 [S1],[b] |
| **2** | 299.5 | – | 302.3 | 283.6 [S11],[c] |
| **3** | 387.3 | 383.9 | – | 329.4 [S2],[b] |
| **4**[e] | 291.5 | – | 298.3 | 242.9 [S3],[d] |
| **5** | 299.9 | 302.4 | – | 301.0 [S4],[b] |
| **6** | 313.7 | – | 320.2 | 317.4 [S5],[d] |
| **7** | 536.8 | 537.3 | 537.2 | 434.3 [S3],[d] |
| **8** | 28.5 | – | 34.8 | 21.2 [S6],[d] |

[a] 2c-ZORA-SO/TZ2P results; see Computational Details in main text. [b] Experimental value measured in benzene-$d_6$. [c] Experimental value measured in pyridine-$d_5$. [d] Experimental value measured in THF-$d_8$. [e] Averaged data for two non-equivalent alkyl carbon atoms.

**Table S10.** Dependence of $^{13}C$ NMR shifts (in ppm vs. TMS) of U(VI)-bound carbon atoms on EXX admixture. Data for B3LYP-D3/def2-TZVP/ECP optimized structures [a]

| Complex | $\delta_{2c}^{xc}(PBE)$ | $\delta_{2c}^{xc}(PBE-10HF)$ | $\delta_{2c}^{xc}(PBE-15HF)$ | $\delta_{2c}^{xc}(PBE0)$ | $\delta_{2c}(PBE-40HF)$ | $\delta_{exp}$ |
|---|---|---|---|---|---|---|
| **1** | 295.8 | 297.4 | 297.0 | 294.4 | 275.4 | 262.8[S1] |
| **2** | 304.3 | 304.7 | 304.4 | 303.4 | 293.2 | 283.6[S11] |
| **3** | 426.6 | 417.3 | 410.2 | 392.0 | 335.8 | 329.4[S2] |
| **4**[b] | 244.7 | 273.3 | 291.0 | 324.0 | 254.3 | 242.9[S3] |
| **5** | 240.8 | 271.1 | 285.8 | 323.8 | 295.9 | 301.0[S4] |
| **6** | 253.0 | 281.6 | 296.9 | 333.6 | 311.8 | 317.4[S5] |
| **7** | 342.8 | 409.7 | 461.3 | 690.7 | 555.5 | 434.3[S3] |
| **SD** | 54.9 | 38.1 | 36.3 | 93.4 | 41.5 | |

[a] 2c-ZORA-SO/TZ2P results. [b] Averaged data for two non-equivalent alkyl carbon atoms.

**Table S11.** Compositions of the U–C bonding NLMOs along with the calculated SO ($\sigma^{SO}$) and paramagnetic ($\sigma^{para}$) contributions to the isotropic $^{13}C$ shielding at the PBE level [a]

| | U–C | %U | %U(s) | %U(d) | %U(f) | %C | %C(s) | %C(p) | $\sigma^{para}$ | $\sigma^{SO}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| **1** | σ | 17.2 | 19 | 47 | 34 | 78.6 | 44 | 56 | –254 | –88 |
| **2** | σ | 15.7 | 19 | 44 | 37 | 79.2 | 40 | 60 | –281 | –75 |
| **3** | σ | 23.8 | 16 | 39 | 45 | 73.1 | 39 | 61 | –280 | –196 |
| **4**-C1[b] | σ | 23.0 | 12 | 31 | 57 | 73.2 | 21 | 79 | –119 | –143 |
| **4**-C2[b] | σ | 23.9 | 11 | 30 | 59 | 72.5 | 22 | 78 | –139 | –159 |
| **5** | σ | 33.0 | 3 | 20 | 78 | 65.2 | 22 | 78 | –148 | –116 |
| **6** | σ | 31.8 | 3 | 20 | 77 | 64.3 | 18 | 82 | –206 | –88 |
| **7** | σ | 29.3 | 7 | 23 | 71 | 68.1 | 20 | 80 | –212 | –162 |
| **8** | σ | 15.9 | 8 | 42 | 50 | 73.7 | 7 | 93 | –94 | –25 |
| **9** | σ | 17.7 | 20 | 43 | 37 | 78.8 | 44 | 56 | –249 | –100 |
| **10** | σ | 29.2 | 6 | 34 | 61 | 67.8 | 50 | 50 | –278 | –163 |
| **11** | σ | 19.8 | 9 | 44 | 47 | 70.1 | 19 | 81 | –248 | –95 |
| | π | 13.9 | 0 | 20 | 80 | 70.1 | 0 | 100 | | |
| **12** | σ | 29.9 | 2 | 20 | 77 | 62.7 | 19 | 81 | –324 | –72 |
| | π | 24.3 | 0 | 35 | 65 | 65.5 | 0 | 100 | | |
| **13** | σ | 26.8 | 2 | 26 | 71 | 68.0 | 32 | 68 | –370 | –162 |
| | π | 25.0 | 0 | 26 | 74 | 64.2 | 0 | 100 | | |
| **14** | σ | 20.7 | 6 | 41 | 53 | 68.4 | 16 | 84 | –287 | –76 |
| | π | 15.0 | 0 | 23 | 76 | 70.0 | 2 | 98 | | |

[a] 2c-ZORA-SO/TZ2P results at PBE0-D3/def2-TZVP/ECP optimized structures; see Computational Details in main text. [b] Data for two non-equivalent alkyl carbon atoms.

**Table S12.** Compositions of the U–C bonding NLMOs along with the calculated SO ($\sigma^{SO}$) and paramagnetic ($\sigma^{para}$) contributions to the isotropic $^{13}C$ shielding at the PBE0 level [a]

| | U–C | %U | %U(s) | %U(d) | %U(f) | %C | %C(s) | %C(p) | $\sigma^{para}$ | $\sigma^{SO}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| **1** | σ | 16.4 | 19 | 49 | 32 | 79.9 | 44 | 56 | –270 | –78 |
| **2** | σ | 14.9 | 19 | 47 | 33 | 80.7 | 40 | 60 | –302 | –62 |
| **3** | σ | 22.2 | 17 | 43 | 40 | 75.0 | 40 | 60 | –278 | –169 |
| **4**-C1[b] | σ | 21.7 | 13 | 35 | 52 | 74.9 | 22 | 78 | –108 | –195 |
| **4**-C2[b] | σ | 22.5 | 12 | 34 | 54 | 74.2 | 23 | 77 | –131 | –229 |
| **5** | σ | 28.5 | 3 | 24 | 73 | 66.0 | 25 | 75 | –168 | –172 |
| **6** | σ | 27.7 | 3 | 25 | 72 | 64.7 | 20 | 80 | –221 | –137 |
| **7** | σ | 28.7 | 7 | 25 | 68 | 69.2 | 22 | 78 | –215 | –363 |
| **8** | σ | 15.3 | 7 | 49 | 43 | 75.4 | 8 | 92 | –71 | –13 |
| **9** | σ | 16.3 | 21 | 47 | 32 | 80.6 | 44 | 56 | –266 | –72 |
| **10** | σ | 28.9 | 5 | 34 | 60 | 68.2 | 49 | 51 | –279 | –222 |
| **11** | σ | 21.5 | 5 | 52 | 42 | 70.2 | 20 | 80 | –191 | –71 |
| | π | 11.2 | 0 | 27 | 73 | 73.4 | 0 | 100 | | |
| **12** | σ | 30.8 | 2 | 21 | 77 | 62.7 | 18 | 82 | –342 | –99 |
| | π | 23.4 | 0 | 37 | 63 | 67.3 | 1 | 99 | | |
| **13** | σ | 28.2 | 5 | 26 | 68 | 67.7 | 31 | 69 | –378 | –390 |
| | π | 24.7 | 0 | 28 | 72 | 65.5 | 0 | 100 | | |
| **14** | σ | 20.9 | 5 | 47 | 49 | 69.7 | 18 | 82 | –230 | –58 |
| | π | 12.9 | 0 | 29 | 70 | 72.8 | 2 | 98 | | |

[a] 2c-ZORA-SO/TZ2P results at PBE0-D3/def2-TZVP/ECP optimized structures; see Computational Details in main text. [b] Data for two non-equivalent alkyl carbon atoms.

**Table S13.** Mulliken atomic spin densities at uranium induced by a finite Fermi contact perturbation (perturbation parameter λ=0.01 a.u.) for a U(VI)-bound carbon atom as function of EXX admixture [a]

| Complex | PBE | PBE0 | PBE-40HF |
|---|---|---|---|
| **3** | 0.1051 | 0.1046 | 0.1031 |
| **4** | 0.0471 | 0.0526 | 0.0542 |

[a] TZVP/def2-TZVP basis sets (G09), PBE0-D3 structures.

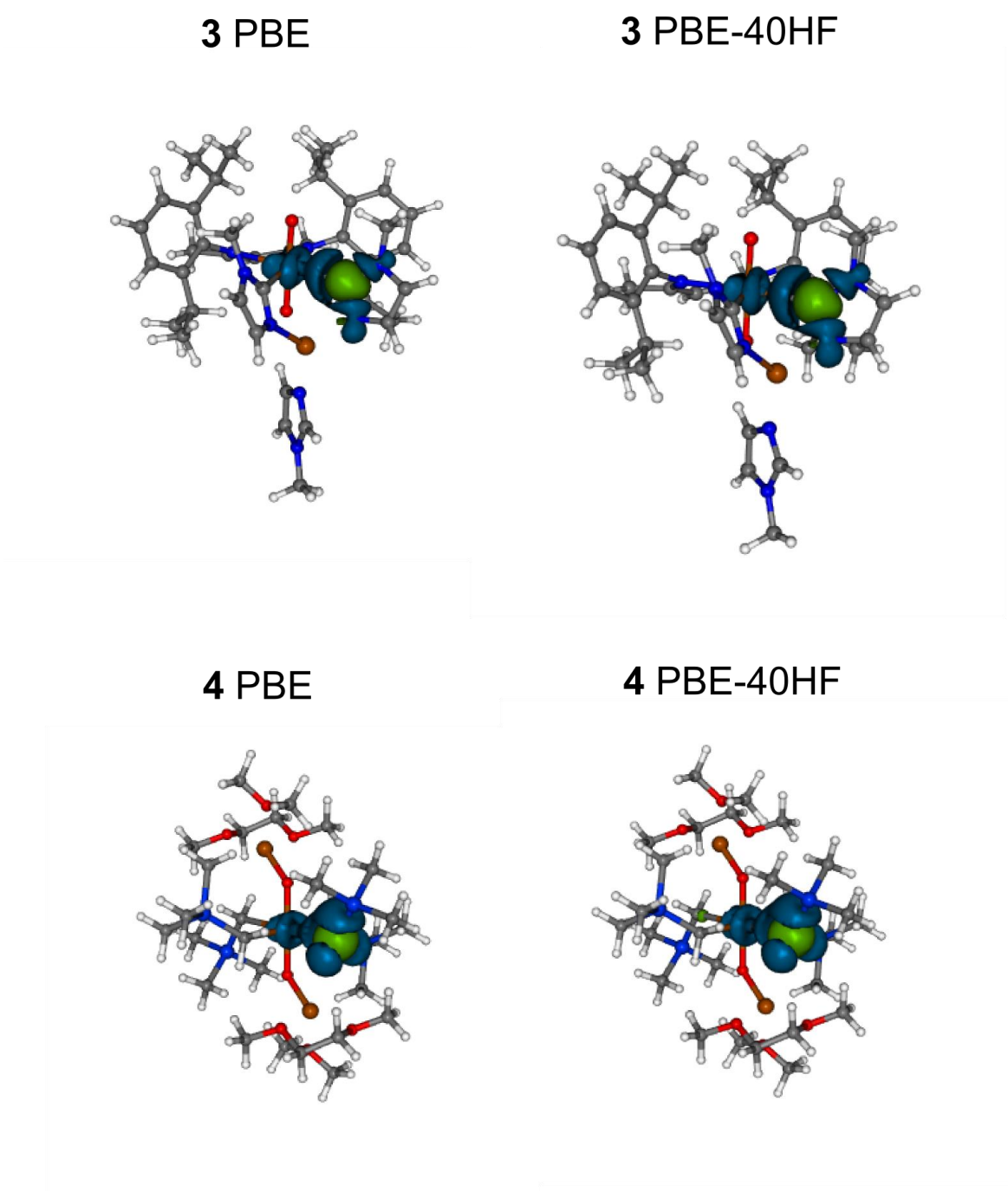


**Figure S1.** Isosurface plots (±0.0005) of spin densities induced by a finite Fermi contact perturbation (λ=0.01) for a uranium-bound carbon atom in **3** and **4** with PBE and PBE-40HF functionals, respectively.

**Table S14.** Comparison of computed hydride $^{1}$H NMR shifts (in ppm vs. TMS) in uranium(VI) hydride complexes with (xc) and without consideration of the exchange-correlation kernel [a]

| Complex | $\delta_{2c}(PBE)$ | $\delta_{2c}^{xc}(PBE)$ | $\delta_{2c}(PBE0)$ | $\delta_{2c}^{xc}(PBE0)$ | $\delta_{4c}(PBE)$ | $\delta_{4c}^{xc}(PBE)$ |
|---|---|---|---|---|---|---|
| **15** | 140.8 | 265.5 | 254.3 | 603.7 | 137.1 | 251.8 |
| **16** | 98.2 | 171.0 | 168.0 | 336.6 | 96.8 | 163.8 |
| **17** | 100.2 | 178.4 | 176.7 | 348.8 | 99.2 | 174.0 |
| **18** | 81.3 | 132.2 | 64.5 | 87.3 | 85.0 | 136.9 |

[a] 2c-ZORA-SO results with TZ2P basis; 4c-mDKS results with Dyall-TZ/IGLO-III basis, see Computational Details in main text**.**

**Table S15.** Comparison of computed hydride $^{1}$H NMR shifts (in ppm vs. TMS) in uranium(VI) hydride complexes for different optimized structures [a]

| Complex | $\delta_{2c}^{xc}(PBE)$ PBE0-D3 | $\delta_{2c}^{xc}(PBE)$ B3LYP-D3 | $\delta_{2c}^{xc}(PBE0)$ PBE0-D3 | $\delta_{2c}^{xc}(PBE0)$ B3LYP-D3 |
|---|---|---|---|---|
| **15** | 265.5 | 295.0 | 603.7 | 759.5 |
| **16** | 171.0 | 190.5 | 336.6 | 411.7 |
| **17** | 178.4 | 195.8 | 348.8 | 413.4 |
| **18** | 132.2 | 153.2 | 87.3 | 101.3 |
| **19** | 212.1 | 240.7 | 163.4 | 205.6 |
| **20** | 93.9 | 90.6 | 83.2 | 74.9 |
| **21** | 124.8 | 100.4 | 84.1 | 64.5 |
| **22** | 55.6 | 59.4 | 49.8 | 53.7 |
| **23** | 117.6 | 125.5 | 170.5 | 188.2 |

[a] 2c-ZORA-SO/TZ2P results, see Computational Details in main text**.**

**Table S16.** Principal $^{13}C$ NMR shift tensor components (δ in ppm vs. TMS), the anisotropy (Δδ)[a] and the asymmetry (η)[b] parameters as computed at the PBE0 level with consideration of the exchange-correlation kernel [c]

| Complex | $\delta_{xx}$ | $\delta_{yy}$ | $\delta_{zz}$ | Δδ | η |
|---|---|---|---|---|---|
| **1** | 236.5 | 236.5 | 467.6 | 231.2 | 0.00 |
| **2** | 162.1 | 247.0 | 490.8 | 286.2 | 0.44 |
| **3** | 228.2 | 262.7 | 672.3 | 426.8 | 0.12 |
| **4** | 36.2 | 239.8 | 600.0 | 462.0 | 0.66 |
| **5** | 414.2 | 412.3 | 74.4 | -338.9 | 0.01 |
| **6** | 528.5 | 353.2 | 60.7 | -380.2 | 0.69 |
| **7** | 764.6 | 708.8 | 138.3 | -598.4 | 0.14 |
| **8** | 52.5 | 31.1 | 3.1 | -38.7 | 0.83 |
| **9** | 129.4 | 214.5 | 487.5 | 315.6 | 0.40 |
| **10** | 622.3 | 615.1 | 41.7 | -577.0 | 0.02 |
| **11** | 20.5 | 182.6 | 370.2 | 268.6 | 0.90 |
| **12** | 29.2 | 352.6 | 737.2 | 546.3 | 0.89 |
| **13** | 1073.6 | 820.2 | 213.9 | -733.0 | 0.52 |
| **14** | 41.7 | 182.6 | 438.3 | 326.2 | 0.65 |

[a] $\Delta\delta = \delta_{zz} - (\delta_{xx} + \delta_{yy})/2$, where $|\delta_{zz} - \delta_{iso}| \geq |\delta_{xx} - \delta_{iso}| \geq |\delta_{yy} - \delta_{iso}|$. [b] $\eta = (\delta_{yy} - \delta_{xx})/(\delta_{zz} - \delta_{iso})$. [c] 2c-ZORA-SO/TZ2P results at PBE0-D3/def2-TZVP/ECP optimized structures, see Computational Details in main text.

**Table S17.** Principal $^{1}$H NMR shift tensor components (δ in ppm vs. TMS), the anisotropy (Δδ)[a] and the asymmetry (η)[b] parameters as computed at the PBE0 level with consideration of the exchange-correlation kernel [c]

| Complex | $\delta_{xx}$ | $\delta_{yy}$ | $\delta_{zz}$ | Δδ | η |
|---|---|---|---|---|---|
| **15** | 860.0 | 859.8 | 91.2 | -768.7 | 0.00 |
| **16** | 424.0 | 416.6 | 169.3 | -251.0 | 0.04 |
| **17** | 489.9 | 479.7 | 76.8 | -408.0 | 0.04 |
| **18** | 23.7 | 71.9 | 166.2 | 118.3 | 0.61 |
| **19** | 73.4 | 116.5 | 316.9 | 221.9 | 0.29 |
| **20** | 27.3 | 62.9 | 159.6 | 114.5 | 0.47 |
| **21** | 56.0 | 79.1 | 114.3 | 46.8 | 0.74 |
| **22** | 69.9 | 51.9 | 27.5 | -33.4 | 0.81 |
| **23** | 220.8 | 219.2 | 71.6 | -148.4 | 0.02 |

[a] $\Delta\delta = \delta_{zz} - (\delta_{xx} + \delta_{yy})/2$, where $|\delta_{zz} - \delta_{iso}| \geq |\delta_{xx} - \delta_{iso}| \geq |\delta_{yy} - \delta_{iso}|$. [b] $\eta = (\delta_{yy} - \delta_{xx})/(\delta_{zz} - \delta_{iso})$. [c] 2c-ZORA-SO/TZ2P results at PBE0-D3/def2-TZVP/ECP optimized structures, see Computational Details in main text.

**Table S18.** Optimized Cartesian coordinates of U(VI) complexes **1-23** (PBE0/def2-TZVP/ECP results)

Complex **1**

| | | | |
|---|---|---|---|
| U | 0.0497 | 0.0416 | 1.7879 |
| N | -2.2973 | 0.0373 | -0.0589 |
| N | -1.7190 | 2.8325 | -0.7869 |
| N | -0.5783 | 3.6383 | 0.8232 |
| C | -3.2401 | -0.4152 | 0.9810 |
| C | -2.5684 | -1.4143 | 1.9202 |
| H | -2.1091 | -2.2297 | 1.3533 |
| H | -3.3149 | -1.8482 | 2.5901 |
| H | -1.7969 | -0.9440 | 2.5246 |
| C | -4.4389 | -1.1491 | 0.3605 |
| H | -5.0574 | -0.5045 | -0.2655 |
| H | -5.0789 | -1.5471 | 1.1516 |
| H | -4.0933 | -1.9870 | -0.2505 |
| C | -3.7350 | 0.7654 | 1.8229 |
| H | -2.8850 | 1.2420 | 2.3161 |
| H | -4.4423 | 0.4353 | 2.5893 |
| H | -4.2398 | 1.5191 | 1.2128 |
| C | -2.9821 | 0.7244 | -1.1310 |
| H | -3.9337 | 1.1358 | -0.7707 |
| H | -3.2428 | 0.0547 | -1.9684 |
| C | -2.2334 | 1.8985 | -1.7674 |
| H | -1.3998 | 1.5472 | -2.3690 |
| H | -2.9210 | 2.4428 | -2.4179 |
| C | -0.6873 | 2.5418 | 0.0345 |
| C | -2.2652 | 4.0575 | -0.5082 |
| H | -3.0969 | 4.4652 | -1.0574 |
| C | -1.5438 | 4.5709 | 0.5108 |
| H | -1.6360 | 5.5186 | 1.0081 |
| C | 0.3656 | 3.7799 | 1.9567 |
| C | -0.2088 | 3.0409 | 3.1603 |
| H | -1.1932 | 3.4387 | 3.4193 |
| H | 0.4504 | 3.1692 | 4.0218 |
| H | -0.2989 | 1.9759 | 2.9472 |
| C | 1.7169 | 3.2083 | 1.5605 |
| H | 1.6677 | 2.1455 | 1.3227 |
| H | 2.4131 | 3.3346 | 2.3923 |
| H | 2.1182 | 3.7372 | 0.6932 |
| C | 0.5374 | 5.2570 | 2.2908 |
| H | 0.8441 | 5.8342 | 1.4154 |
| H | 1.3174 | 5.3503 | 3.0474 |
| H | -0.3704 | 5.6973 | 2.7080 |
| O | -0.0495 | -0.0413 | -1.7879 |
| N | 2.2976 | -0.0377 | 0.0591 |
| N | 1.7184 | -2.8327 | 0.7869 |
| N | 0.5777 | -3.6382 | -0.8234 |

| | | | |
|---|---|---|---|
| C | 3.2406 | 0.4148 | -0.9806 |
| C | 2.5691 | 1.4139 | -1.9200 |
| H | 2.1096 | 2.2293 | -1.3533 |
| H | 3.3158 | 1.8477 | -2.5897 |
| H | 1.7977 | 0.9434 | -2.5245 |
| C | 4.4391 | 1.1489 | -0.3597 |
| H | 5.0574 | 0.5043 | 0.2667 |
| H | 5.0795 | 1.5470 | -1.1505 |
| H | 4.0933 | 1.9868 | 0.2513 |
| C | 3.7359 | -0.7656 | -1.8224 |
| H | 2.8861 | -1.2424 | -2.3157 |
| H | 4.4433 | -0.4352 | -2.5887 |
| H | 4.2409 | -1.5192 | -1.2123 |
| C | 2.9822 | -0.7251 | 1.1311 |
| H | 3.9336 | -1.1369 | 0.7708 |
| H | 3.2432 | -0.0556 | 1.9685 |
| C | 2.2330 | -1.8989 | 1.7675 |
| H | 1.3993 | -1.5472 | 2.3690 |
| H | 2.9202 | -2.4435 | 2.4182 |
| C | 0.6869 | -2.5417 | -0.0346 |
| C | 2.2645 | -4.0578 | 0.5081 |
| H | 3.0963 | -4.4654 | 1.0570 |
| C | 1.5429 | -4.5710 | -0.5109 |
| H | 1.6347 | -5.5189 | -1.0079 |
| C | -0.3659 | -3.7794 | -1.9572 |
| C | 0.2086 | -3.0395 | -3.1602 |
| H | 1.1931 | -3.4371 | -3.4193 |
| H | -0.4505 | -3.1676 | -4.0219 |
| H | 0.2985 | -1.9747 | -2.9465 |
| C | -1.7174 | -3.2083 | -1.5609 |
| H | -1.6684 | -2.1458 | -1.3221 |
| H | -2.4134 | -3.3340 | -2.3930 |
| H | -2.1188 | -3.7381 | -0.6941 |
| C | -0.5372 | -5.2563 | -2.2922 |
| H | -0.8441 | -5.8341 | -1.4172 |
| H | -1.3171 | -5.3493 | -3.0490 |
| H | 0.3708 | -5.6962 | -2.7094 |

Complex **2**

| | | | |
|---|---|---|---|
| U | 0.0000 | 0.0000 | 0.0002 |
| O | 0.6210 | -0.3130 | 1.6451 |
| O | -0.6212 | 0.3129 | -1.6447 |
| O | 0.4551 | -2.0457 | -0.5537 |
| O | -0.4546 | 2.0459 | 0.5540 |
| C | -2.0402 | -1.5094 | 0.6237 |
| C | 2.0402 | 1.5093 | -0.6235 |
| N | -1.7957 | -2.7459 | 1.0374 |
| N | -3.3512 | -1.3899 | 0.4110 |
| N | 1.7957 | 2.7458 | -1.0374 |

| | | | |
|---|---|---|---|
| N | 3.3512 | 1.3898 | -0.4106 |
| C | -2.9833 | -3.5986 | 1.0357 |
| H | -3.0903 | -4.1211 | 1.9886 |
| H | -2.9093 | -4.3498 | 0.2424 |
| C | -4.1030 | -2.5913 | 0.7822 |
| H | -4.7777 | -2.8924 | -0.0206 |
| H | -4.7040 | -2.3938 | 1.6761 |
| C | 2.9834 | 3.5985 | -1.0356 |
| H | 3.0904 | 4.1209 | -1.9886 |
| H | 2.9093 | 4.3497 | -0.2424 |
| C | 4.1031 | 2.5912 | -0.7820 |
| H | 4.7778 | 2.8924 | 0.0207 |
| H | 4.7039 | 2.3935 | -1.6760 |
| C | -0.4681 | -3.2667 | 1.2829 |
| H | -0.5748 | -4.2692 | 1.7034 |
| H | 0.0227 | -2.6327 | 2.0237 |
| C | 0.4223 | -3.3064 | 0.0239 |
| C | -0.1390 | -4.2911 | -0.9984 |
| H | -1.1267 | -3.9628 | -1.3304 |
| H | -0.2142 | -5.3040 | -0.5920 |
| H | 0.5114 | -4.3150 | -1.8750 |
| C | 1.8214 | -3.7190 | 0.4619 |
| H | 2.4814 | -3.7501 | -0.4067 |
| H | 1.8254 | -4.7047 | 0.9361 |
| H | 2.2231 | -2.9849 | 1.1638 |
| C | -4.0113 | -0.1712 | 0.0945 |
| C | -4.2515 | 0.7612 | 1.1108 |
| C | -4.9283 | 1.9284 | 0.7764 |
| H | -5.1217 | 2.6679 | 1.5453 |
| C | -5.3512 | 2.1620 | -0.5191 |
| H | -5.8742 | 3.0804 | -0.7607 |
| C | -5.0990 | 1.2295 | -1.5088 |
| H | -5.4242 | 1.4235 | -2.5248 |
| C | -4.4258 | 0.0478 | -1.2236 |
| C | -3.8219 | 0.5288 | 2.5406 |
| H | -3.2410 | -0.3951 | 2.5707 |
| C | -2.9164 | 1.6453 | 3.0511 |
| H | -2.0463 | 1.7812 | 2.4063 |
| H | -2.5656 | 1.4108 | 4.0593 |
| H | -3.4543 | 2.5964 | 3.1042 |
| C | -5.0365 | 0.3510 | 3.4486 |
| H | -5.6454 | 1.2588 | 3.4677 |
| H | -4.7198 | 0.1397 | 4.4732 |
| H | -5.6777 | -0.4680 | 3.1126 |
| C | -4.1695 | -0.9595 | -2.3189 |
| H | -3.5447 | -1.7500 | -1.8962 |
| C | -3.3939 | -0.3491 | -3.4818 |
| H | -3.9650 | 0.4482 | -3.9655 |
| H | -3.1916 | -1.1133 | -4.2368 |

| | | | |
|---|---|---|---|
| H | -2.4418 | 0.0579 | -3.1401 |
| C | -5.4776 | -1.5850 | -2.7988 |
| H | -6.0358 | -2.0419 | -1.9775 |
| H | -5.2805 | -2.3545 | -3.5493 |
| H | -6.1256 | -0.8315 | -3.2553 |
| C | 0.4682 | 3.2666 | -1.2832 |
| H | 0.5749 | 4.2691 | -1.7036 |
| H | -0.0225 | 2.6326 | -2.0241 |
| C | -0.4225 | 3.3063 | -0.0244 |
| C | 0.1378 | 4.2918 | 0.9976 |
| H | 1.1257 | 3.9644 | 1.3300 |
| H | 0.2125 | 5.3046 | 0.5907 |
| H | -0.5128 | 4.3158 | 1.8740 |
| C | -1.8218 | 3.7177 | -0.4629 |
| H | -2.4820 | 3.7490 | 0.4055 |
| H | -1.8264 | 4.7031 | -0.9378 |
| H | -2.2229 | 2.9829 | -1.1644 |
| C | 4.0113 | 0.1712 | -0.0942 |
| C | 4.2519 | -0.7610 | -1.1106 |
| C | 4.9289 | -1.9281 | -0.7762 |
| H | 5.1227 | -2.6673 | -1.5453 |
| C | 5.3519 | -2.1617 | 0.5192 |
| H | 5.8751 | -3.0800 | 0.7607 |
| C | 5.0994 | -1.2293 | 1.5090 |
| H | 5.4245 | -1.4235 | 2.5250 |
| C | 4.4258 | -0.0479 | 1.2239 |
| C | 3.8224 | -0.5284 | -2.5404 |
| H | 3.2417 | 0.3955 | -2.5704 |
| C | 2.9167 | -1.6447 | -3.0510 |
| H | 2.0465 | -1.7805 | -2.4061 |
| H | 2.5659 | -1.4102 | -4.0592 |
| H | 3.4544 | -2.5960 | -3.1040 |
| C | 5.0370 | -0.3508 | -3.4484 |
| H | 5.6458 | -1.2587 | -3.4676 |
| H | 4.7203 | -0.1394 | -4.4729 |
| H | 5.6783 | 0.4681 | -3.1123 |
| C | 4.1691 | 0.9592 | 2.3193 |
| H | 3.5438 | 1.7494 | 1.8968 |
| C | 3.3942 | 0.3483 | 3.4823 |
| H | 3.9658 | -0.4487 | 3.9659 |
| H | 3.1916 | 1.1123 | 4.2375 |
| H | 2.4422 | -0.0592 | 3.1408 |
| C | 5.4769 | 1.5854 | 2.7990 |
| H | 6.0347 | 2.0427 | 1.9777 |
| H | 5.2795 | 2.3547 | 3.5496 |
| H | 6.1255 | 0.8322 | 3.2553 |

Complex **3**

| | | | |
|---|---|---|---|
| U | -0.0531 | -0.6315 | 0.0019 |

| | | | |
|---|---|---|---|
| O | 1.3850 | -1.6727 | 0.0008 |
| O | -1.5518 | 0.3488 | 0.0030 |
| C | -1.2488 | -2.0549 | -1.6431 |
| C | -1.2471 | -2.0555 | 1.6478 |
| N | -0.8690 | -2.9896 | 2.5679 |
| C | -1.9805 | -3.5749 | 3.1050 |
| C | -3.0436 | -2.9864 | 2.4817 |
| N | -2.5902 | -2.0556 | 1.5979 |
| N | -2.5918 | -2.0550 | -1.5913 |
| C | -3.0464 | -2.9855 | -2.4748 |
| C | -1.9842 | -3.5735 | -3.1000 |
| N | -0.8719 | -2.9884 | -2.5643 |
| N | 1.0473 | 0.9714 | -1.5068 |
| C | 1.3309 | 2.2362 | -1.2655 |
| C | 1.8098 | 3.1453 | -2.3700 |
| N | 1.0494 | 0.9710 | 1.5093 |
| C | 1.2814 | 0.4342 | 2.8038 |
| C | 2.5480 | -0.0876 | 3.1185 |
| C | 2.7699 | -0.5768 | 4.4005 |
| C | 1.7668 | -0.5736 | 5.3507 |
| C | 0.5095 | -0.1028 | 5.0159 |
| C | 0.2359 | 0.3989 | 3.7483 |
| C | 0.4861 | -3.2811 | -2.9474 |
| C | 0.4896 | -3.2826 | 2.9489 |
| C | 3.6750 | -0.1223 | 2.1122 |
| C | 4.8189 | 0.8035 | 2.5163 |
| C | -1.1522 | 0.9139 | 3.4303 |
| C | -2.2469 | 0.1458 | 4.1593 |
| C | 1.2780 | 0.4351 | -2.8017 |
| C | 2.5446 | -0.0856 | -3.1184 |
| C | 2.7655 | -0.5729 | -4.4012 |
| C | 1.7612 | -0.5701 | -5.3500 |
| C | 0.5038 | -0.1009 | -5.0132 |
| C | 0.2314 | 0.3999 | -3.7450 |
| C | 3.6724 | -0.1218 | -2.1130 |
| C | 4.8157 | 0.8051 | -2.5161 |
| C | -1.1563 | 0.9146 | -3.4251 |
| C | -1.3025 | 2.4075 | -3.7154 |
| C | 1.3326 | 2.2359 | 1.2681 |
| C | 1.8126 | 3.1448 | 2.3722 |
| C | 1.3149 | 2.8323 | 0.0014 |
| C | 4.1937 | -1.5415 | 1.9058 |
| C | -2.2521 | 0.1468 | -4.1528 |
| C | 4.1918 | -1.5413 | -1.9098 |
| C | -1.2979 | 2.4066 | 3.7220 |
| Li | -3.2511 | -1.0260 | 0.0039 |
| N | -4.7397 | 0.3537 | 0.0008 |
| C | -6.0503 | 0.3046 | -0.0032 |
| N | -6.5935 | 1.5396 | -0.0112 |

| | | | |
|---|---|---|---|
| C | -5.5541 | 2.4336 | -0.0123 |
| C | -4.4147 | 1.6840 | -0.0048 |
| C | -7.9989 | 1.8572 | -0.0174 |
| H | 3.4029 | -2.1991 | -1.5439 |
| H | 4.9997 | -1.5451 | -1.1745 |
| H | 4.5902 | -1.9571 | -2.8387 |
| H | 1.5391 | 3.8917 | 0.0013 |
| H | 3.2750 | 0.2266 | 1.1585 |
| H | 0.6008 | -4.3521 | -3.1215 |
| H | 1.1459 | -2.9831 | -2.1352 |
| H | 0.7688 | -2.7352 | -3.8501 |
| H | 3.7490 | -0.9670 | 4.6564 |
| H | -1.9268 | -4.3394 | -3.8566 |
| H | 3.7448 | -0.9615 | -4.6588 |
| H | 2.8914 | 3.2727 | -2.2860 |
| H | 1.3615 | 4.1331 | -2.2576 |
| H | 1.5923 | 2.7601 | -3.3635 |
| H | 1.5966 | 2.7593 | 3.3658 |
| H | 1.3637 | 4.1325 | 2.2607 |
| H | 2.8941 | 3.2729 | 2.2868 |
| H | -4.0981 | -3.1849 | -2.6190 |
| H | -0.2809 | -0.1296 | 5.7557 |
| H | -1.3220 | 0.7779 | -2.3551 |
| H | 3.2729 | 0.2250 | -1.1583 |
| H | 4.5928 | -1.9594 | 2.8335 |
| H | 5.0011 | -1.5442 | 1.1698 |
| H | 3.4043 | -2.1984 | 1.5392 |
| H | -0.2875 | -0.1279 | -5.7520 |
| H | 1.9514 | -0.9492 | -6.3479 |
| H | 1.9581 | -0.9534 | 6.3480 |
| H | -4.0951 | -3.1857 | 2.6275 |
| H | -6.6526 | -0.5915 | -0.0007 |
| H | -1.9220 | -4.3412 | 3.8610 |
| H | 1.1483 | -2.9845 | 2.1357 |
| H | 0.6044 | -4.3537 | 3.1223 |
| H | 0.7738 | -2.7371 | 3.8514 |
| H | -3.3847 | 2.0037 | -0.0032 |
| H | -1.3193 | 0.7779 | 2.3604 |
| H | -2.2778 | 0.3921 | -5.2186 |
| H | -3.2240 | 0.4154 | -3.7331 |
| H | -2.1342 | -0.9319 | -4.0464 |
| H | 5.2697 | 0.4812 | -3.4568 |
| H | 5.5960 | 0.8020 | -1.7502 |
| H | 4.4776 | 1.8336 | -2.6500 |
| H | 4.4814 | 1.8319 | 2.6520 |
| H | 5.5988 | 0.8012 | 1.7500 |
| H | 5.2732 | 0.4778 | 3.4563 |
| H | -0.6480 | 3.0143 | -3.0913 |
| H | -2.3317 | 2.7219 | -3.5226 |

| | | | |
|---|---|---|---|
| H | -1.0732 | 2.6248 | -4.7631 |
| H | -2.3274 | 2.7211 | 3.5309 |
| H | -0.6443 | 3.0140 | 3.0976 |
| H | -1.0672 | 2.6230 | 4.7696 |
| H | -8.2611 | 2.4274 | -0.9102 |
| H | -8.2670 | 2.4362 | 0.8680 |
| H | -8.5704 | 0.9304 | -0.0147 |
| H | -5.7182 | 3.4983 | -0.0181 |
| H | -2.1289 | -0.9329 | 4.0526 |
| H | -3.2192 | 0.4143 | 3.7408 |
| H | -2.2713 | 0.3910 | 5.2251 |

Complex **4**

| | | | |
|---|---|---|---|
| U | -0.0004 | -0.0024 | 0.0004 |
| O | 1.6803 | 0.6882 | -0.3623 |
| O | -1.6817 | -0.6918 | 0.3631 |
| C | -1.1621 | 1.8313 | -1.2283 |
| C | 0.0580 | -1.2500 | -2.1204 |
| C | 1.1619 | -1.8375 | 1.2262 |
| C | -0.0591 | 1.2426 | 2.1230 |
| Si | -1.3963 | 2.2742 | 2.8387 |
| C | -3.1055 | 1.5528 | 2.4946 |
| Si | 0.1832 | -3.0823 | 2.1596 |
| C | 1.2521 | -4.3630 | 3.0585 |
| Si | -0.1826 | 3.0706 | -2.1682 |
| C | 0.8753 | 2.2406 | -3.4869 |
| Si | 1.4002 | -2.2729 | -2.8396 |
| C | 1.3751 | -4.0236 | -2.1452 |
| C | 3.1072 | -1.5507 | -2.4863 |
| C | 1.2902 | -2.4188 | -4.7205 |
| C | -1.2512 | 4.3474 | -3.0730 |
| C | 0.9459 | 4.0431 | -1.0158 |
| C | -1.2806 | 2.4336 | 4.7182 |
| C | -1.3694 | 4.0208 | 2.1338 |
| C | -0.9449 | -4.0496 | 1.0024 |
| C | -0.8750 | -2.2590 | 3.4822 |
| Li | -3.3493 | -0.1866 | -0.2707 |
| Li | 3.3486 | 0.1894 | 0.2739 |
| O | 4.5917 | -1.2347 | 1.2151 |
| C | 4.5781 | -2.6391 | 1.0380 |
| C | 4.6778 | -0.8790 | 2.5791 |
| C | 4.7723 | 0.6173 | 2.6690 |
| O | 3.6583 | 1.1492 | 2.0003 |
| C | 3.5950 | 2.5563 | 2.0285 |
| O | -4.5924 | 1.2439 | -1.2049 |
| C | -4.6836 | 0.8908 | -2.5693 |
| C | -4.7819 | -0.6051 | -2.6620 |
| O | -3.6666 | -1.1409 | -1.9984 |
| C | -3.6072 | -2.5482 | -2.0290 |

| | | | |
|---|---|---|---|
| C | -4.5738 | 2.6480 | -1.0259 |
| O | 4.7353 | 1.0421 | -0.8811 |
| C | 4.3005 | 2.0454 | -1.7751 |
| C | 5.9564 | 0.4642 | -1.2748 |
| O | -4.7350 | -1.0409 | 0.8851 |
| C | -4.2995 | -2.0481 | 1.7743 |
| C | -5.9536 | -0.4617 | 1.2844 |
| H | -3.7068 | 3.0892 | -1.5260 |
| H | -4.5073 | 2.8425 | 0.0431 |
| H | -5.4964 | 3.0903 | -1.4184 |
| H | 0.0355 | 0.3243 | 2.7258 |
| H | 0.8980 | 1.7702 | 2.2006 |
| H | 1.7352 | -2.3163 | 0.4209 |
| H | 1.8693 | -1.3209 | 1.8891 |
| H | 3.3341 | -1.6256 | -1.4204 |
| H | 3.1409 | -0.4938 | -2.7587 |
| H | 3.8896 | -2.0787 | -3.0395 |
| H | -1.9276 | 3.8596 | -3.7822 |
| H | -0.6433 | 5.0634 | -3.6351 |
| H | -1.8631 | 4.9176 | -2.3668 |
| H | -1.8725 | 1.3147 | -1.8879 |
| H | -1.7321 | 2.3144 | -0.4233 |
| H | 6.2144 | -0.2903 | -0.5335 |
| H | 6.7481 | 1.2223 | -1.3185 |
| H | -0.8953 | -1.7851 | -2.1931 |
| H | -0.0465 | -0.3331 | -2.7235 |
| H | 0.3690 | 4.6870 | -0.3476 |
| H | 1.6420 | 4.6754 | -1.5742 |
| H | 1.5191 | 3.3492 | -0.3969 |
| H | -1.5177 | -3.3530 | 0.3861 |
| H | -1.6415 | -4.6840 | 1.5579 |
| H | -0.3680 | -4.6910 | 0.3318 |
| H | 1.5378 | 1.5007 | -3.0335 |
| H | 1.4845 | 2.9732 | -4.0250 |
| H | 0.2551 | 1.7218 | -4.2235 |
| H | -1.5372 | -1.5165 | 3.0324 |
| H | -0.2546 | -1.7445 | 4.2216 |
| H | -1.4847 | -2.9941 | 4.0163 |
| H | -1.3364 | 1.4480 | 5.1899 |
| H | -2.0865 | 3.0505 | 5.1286 |
| H | -0.3288 | 2.8848 | 5.0131 |
| H | 2.0993 | -3.0297 | -5.1334 |
| H | 1.3441 | -1.4292 | -5.1840 |
| H | 0.3407 | -2.8708 | -5.0217 |
| H | -0.4048 | 4.5012 | 2.3221 |
| H | -2.1455 | 4.6449 | 2.5863 |
| H | -1.5247 | 4.0147 | 1.0522 |
| H | 1.5261 | -4.0228 | -1.0629 |
| H | 2.1550 | -4.6430 | -2.5975 |

| | | | |
|---|---|---|---|
| H | 0.4127 | -4.5055 | -2.3401 |
| H | -5.7093 | -0.9626 | -2.1916 |
| H | -4.7896 | -0.9081 | -3.7172 |
| H | 3.4917 | 2.9167 | 3.0575 |
| H | 2.7161 | 2.8482 | 1.4567 |
| H | 4.4909 | 2.9969 | 1.5749 |
| H | 3.7879 | -1.2393 | 3.1114 |
| H | 5.5652 | -1.3358 | 3.0363 |
| H | -4.5033 | -2.9870 | -1.5740 |
| H | -2.7277 | -2.8433 | -1.4597 |
| H | -3.5072 | -2.9072 | -3.0589 |
| H | 5.7007 | 0.9759 | 2.2012 |
| H | 4.7755 | 0.9226 | 3.7236 |
| H | -3.7945 | 1.2501 | -3.1037 |
| H | -5.5714 | 1.3505 | -3.0229 |
| H | 5.5008 | -3.0779 | 1.4341 |
| H | 4.5157 | -2.8353 | -0.0309 |
| H | 3.7109 | -3.0824 | 1.5360 |
| H | 0.6441 | -5.0822 | 3.6166 |
| H | 1.9277 | -3.8784 | 3.7708 |
| H | 1.8649 | -4.9293 | 2.3499 |
| H | -3.3358 | 1.6218 | 1.4290 |
| H | -3.8854 | 2.0850 | 3.0471 |
| H | -3.1401 | 0.4974 | 2.7730 |
| H | 3.3128 | 2.3658 | -1.4510 |
| H | 4.9969 | 2.8923 | -1.7680 |
| H | 4.2267 | 1.6526 | -2.7952 |
| H | 5.8614 | -0.0100 | -2.2583 |
| H | -6.7470 | -1.2180 | 1.3275 |
| H | -5.8548 | 0.0086 | 2.2696 |
| H | -6.2118 | 0.2963 | 0.5468 |
| H | -4.2212 | -1.6586 | 2.7954 |
| H | -4.9979 | -2.8934 | 1.7671 |
| H | -3.3136 | -2.3696 | 1.4459 |

Complex **5**

| | | | |
|---|---|---|---|
| U | 0.0086 | -0.0028 | 0.0164 |
| O | -0.6703 | -0.0707 | -1.6260 |
| N | -0.5266 | 2.1375 | 0.1506 |
| N | -1.4351 | -1.5444 | 0.6680 |
| N | 1.9835 | -0.5925 | -0.7815 |
| Si | -1.8355 | -2.8453 | -0.4389 |
| Si | -2.3533 | -1.3851 | 2.1423 |
| Si | 2.4950 | 0.0391 | -2.3357 |
| Si | 2.9436 | -1.8345 | -0.0225 |
| Si | 0.5952 | 3.3299 | 0.7520 |
| Si | -2.0330 | 2.6804 | -0.5651 |
| C | -3.2273 | -2.3595 | -1.5902 |
| H | -3.4786 | -3.1985 | -2.2452 |

| | | | |
|---|---|---|---|
| H | -4.1307 | -2.0748 | -1.0474 |
| H | -2.9266 | -1.5194 | -2.2199 |
| C | -0.3454 | -3.3254 | -1.4701 |
| H | 0.8716 | -2.7067 | 1.1997 |
| H | -0.6734 | -4.0498 | -2.2218 |
| H | 0.1153 | -2.4927 | -2.0024 |
| C | -2.2998 | -4.4243 | 0.4692 |
| H | -3.1795 | -4.3373 | 1.1078 |
| H | -2.5091 | -5.1985 | -0.2753 |
| H | -1.4672 | -4.7767 | 1.0833 |
| C | -3.3578 | 1.3643 | -0.4070 |
| H | -3.0665 | 0.3921 | -0.8056 |
| H | -3.6678 | 1.2367 | 0.6316 |
| H | -4.2347 | 1.6972 | -0.9709 |
| C | -1.8152 | 3.0922 | -2.3765 |
| H | -1.5257 | 2.2002 | -2.9369 |
| H | -2.7571 | 3.4603 | -2.7928 |
| H | -1.0543 | 3.8586 | -2.5360 |
| C | -2.7452 | 4.1683 | 0.3363 |
| H | -3.6941 | 4.4346 | -0.1395 |
| H | -2.9597 | 3.9215 | 1.3793 |
| H | -2.1102 | 5.0545 | 0.3207 |
| C | 0.0795 | 3.9769 | 2.4348 |
| H | -0.8488 | 4.5482 | 2.3864 |
| H | -0.0666 | 3.1675 | 3.1550 |
| H | 0.8582 | 4.6356 | 2.8311 |
| C | 2.3314 | 2.6121 | 0.9451 |
| H | 2.5446 | 2.3650 | 1.9863 |
| H | 2.5437 | 1.7238 | 0.3438 |
| H | 3.0489 | 3.3776 | 0.6356 |
| C | 0.7648 | 4.7826 | -0.4236 |
| H | 1.4640 | 5.5073 | 0.0044 |
| H | 1.1675 | 4.4581 | -1.3858 |
| H | -0.1751 | 5.3026 | -0.6128 |
| C | 4.4595 | -1.1208 | 0.8190 |
| H | 4.1990 | -0.3304 | 1.5279 |
| H | 4.9759 | -1.9080 | 1.3765 |
| H | 5.1651 | -0.7015 | 0.1001 |
| C | 1.9591 | -2.7554 | 1.3005 |
| H | 0.4174 | -3.8131 | -0.8604 |
| H | 2.2305 | -3.8135 | 1.2458 |
| H | 2.2148 | -2.4026 | 2.3008 |
| C | 3.4993 | -3.1371 | -1.2536 |
| H | 4.0997 | -3.8877 | -0.7304 |
| H | 2.6392 | -3.6462 | -1.6942 |
| H | 4.1057 | -2.7386 | -2.0677 |
| C | 4.3647 | 0.1929 | -2.4496 |
| H | 4.7420 | 0.8797 | -1.6878 |
| H | 4.9040 | -0.7498 | -2.3541 |

| | | | |
|---|---|---|---|
| H | 4.6143 | 0.6170 | -3.4271 |
| C | 1.8675 | 1.7876 | -2.5826 |
| H | 2.1065 | 2.0922 | -3.6062 |
| H | 0.7897 | 1.8935 | -2.4561 |
| H | 2.3674 | 2.4861 | -1.9092 |
| C | 1.8671 | -1.0222 | -3.7421 |
| H | 2.2039 | -2.0574 | -3.6597 |
| H | 0.7750 | -1.0178 | -3.7627 |
| H | 2.2238 | -0.6271 | -4.6974 |
| C | -4.1903 | -1.6334 | 1.8491 |
| H | -4.5808 | -0.8726 | 1.1695 |
| H | -4.4381 | -2.6112 | 1.4346 |
| H | -4.7189 | -1.5342 | 2.8019 |
| C | -1.7820 | -2.6053 | 3.4463 |
| H | -1.9882 | -3.6372 | 3.1582 |
| H | -0.7088 | -2.5217 | 3.6378 |
| H | -2.3017 | -2.4100 | 4.3892 |
| C | -2.1739 | 0.3406 | 2.8882 |
| H | -3.1439 | 0.6302 | 3.3020 |
| H | -1.4539 | 0.3442 | 3.7084 |
| H | -1.8842 | 1.1286 | 2.1883 |
| C | 0.8838 | 0.0850 | 2.1460 |
| H | 0.5198 | -0.7779 | 2.7040 |
| H | 1.9710 | 0.0605 | 2.0767 |
| H | 0.5534 | 1.0089 | 2.6199 |

Complex **6**

| | | | |
|---|---|---|---|
| U | 0.0003 | 0.0589 | -0.1538 |
| O | -0.0800 | 0.0092 | -1.9304 |
| C | 0.5568 | 0.0102 | 2.0533 |
| H | 0.2889 | 0.9605 | 2.5200 |
| H | 0.1210 | -0.8241 | 2.5990 |
| Si | 2.3807 | -0.1778 | 1.6082 |
| C | 2.9057 | -1.9419 | 1.9392 |
| C | 3.5166 | 0.9829 | 2.5318 |
| H | 2.1672 | -2.6414 | 1.5397 |
| H | 2.9909 | -2.1188 | 3.0149 |
| H | 3.8716 | -2.1703 | 1.4826 |
| H | 3.4626 | 0.7750 | 3.6038 |
| H | 4.5518 | 0.8272 | 2.2159 |
| H | 3.2648 | 2.0312 | 2.3696 |
| N | 2.1963 | 0.1818 | -0.0877 |
| Si | 3.4749 | 0.5585 | -1.2054 |
| C | 2.8652 | 0.6195 | -2.9702 |
| C | 4.1966 | 2.2479 | -0.8173 |
| C | 4.8478 | -0.7126 | -1.0675 |
| H | 2.5032 | -0.3457 | -3.3268 |
| H | 2.0518 | 1.3381 | -3.0906 |
| H | 3.6899 | 0.9303 | -3.6186 |

| | | | |
|---|---|---|---|
| H | 3.4524 | 3.0380 | -0.9476 |
| H | 5.0241 | 2.4619 | -1.5002 |
| H | 4.5814 | 2.3140 | 0.2025 |
| H | 5.6441 | -0.4881 | -1.7826 |
| H | 5.2959 | -0.7210 | -0.0698 |
| H | 4.4775 | -1.7180 | -1.2819 |
| N | -0.6993 | -2.0246 | 0.0434 |
| Si | -0.2179 | -3.2518 | -1.1061 |
| Si | -1.9237 | -2.3665 | 1.2308 |
| C | 1.5302 | -2.9437 | -1.7013 |
| C | -1.3581 | -3.2543 | -2.5899 |
| C | -0.1987 | -4.9630 | -0.3295 |
| C | -2.5858 | -0.7640 | 1.9904 |
| C | -3.3952 | -3.2539 | 0.4788 |
| C | -1.2648 | -3.4073 | 2.6449 |
| H | 1.6209 | -2.0003 | -2.2403 |
| H | 1.8172 | -3.7470 | -2.3863 |
| H | 2.2448 | -2.9367 | -0.8755 |
| H | -1.0483 | -4.0186 | -3.3081 |
| H | -1.3223 | -2.2855 | -3.0942 |
| H | -2.3942 | -3.4559 | -2.3101 |
| H | 0.1243 | -5.6851 | -1.0853 |
| H | -1.1716 | -5.2890 | 0.0412 |
| H | 0.5137 | -5.0123 | 0.4982 |
| H | -2.4099 | 0.1632 | 1.4350 |
| H | -2.1800 | -0.6140 | 2.9926 |
| H | -3.6719 | -0.8573 | 2.0845 |
| H | -3.8628 | -2.6461 | -0.2990 |
| H | -4.1430 | -3.4411 | 1.2551 |
| H | -3.1285 | -4.2160 | 0.0381 |
| H | -2.0244 | -3.4917 | 3.4279 |
| H | -1.0084 | -4.4163 | 2.3184 |
| H | -0.3713 | -2.9685 | 3.0964 |
| N | -1.2611 | 1.8931 | -0.0825 |
| Si | -2.6413 | 1.8969 | -1.1600 |
| Si | -0.8568 | 3.3540 | 0.7704 |
| C | -3.2910 | 0.1471 | -1.3853 |
| C | -2.1891 | 2.5860 | -2.8382 |
| C | -4.0919 | 2.8510 | -0.4409 |
| C | 0.9453 | 3.3525 | 1.3109 |
| C | -1.9025 | 3.5524 | 2.3125 |
| C | -1.0394 | 4.8708 | -0.3211 |
| H | -2.5431 | -0.5908 | -1.6831 |
| H | -3.7949 | -0.2107 | -0.4859 |
| H | -4.0357 | 0.1741 | -2.1873 |
| H | -1.3669 | 2.0087 | -3.2674 |
| H | -3.0417 | 2.5233 | -3.5202 |
| H | -1.8809 | 3.6315 | -2.7810 |
| H | -4.9323 | 2.7937 | -1.1395 |

| | | | |
|---|---|---|---|
| H | -3.8835 | 3.9071 | -0.2638 |
| H | -4.4166 | 2.4069 | 0.5035 |
| H | 1.6165 | 2.8642 | 0.5999 |
| H | 1.0939 | 2.8901 | 2.2874 |
| H | 1.2727 | 4.3927 | 1.3968 |
| H | -1.7984 | 2.6779 | 2.9610 |
| H | -1.5871 | 4.4314 | 2.8822 |
| H | -2.9622 | 3.6669 | 2.0773 |
| H | -0.7979 | 5.7643 | 0.2624 |
| H | -0.3422 | 4.8238 | -1.1619 |
| H | -2.0432 | 5.0026 | -0.7265 |

Complex **7**

| | | | |
|---|---|---|---|
| U | 0.0000 | 0.0001 | 0.0000 |
| C | 0.9350 | 1.6784 | -1.3106 |
| H | 1.6073 | 1.0372 | -1.9020 |
| H | 1.5453 | 2.1015 | -0.4959 |
| C | -0.9817 | 1.6524 | 1.3047 |
| H | -0.0866 | 1.9273 | 1.8839 |
| H | -1.0576 | 2.3816 | 0.4815 |
| C | -1.9155 | -0.0213 | -1.3116 |
| H | -1.6879 | 0.8828 | -1.8975 |
| H | -2.5859 | 0.2971 | -0.4968 |
| C | 0.9816 | -1.6523 | -1.3046 |
| H | 1.0575 | -2.3815 | -0.4815 |
| H | 0.0865 | -1.9272 | -1.8839 |
| C | 1.9155 | 0.0214 | 1.3116 |
| H | 2.5858 | -0.2970 | 0.4967 |
| H | 1.6879 | -0.8828 | 1.8974 |
| C | -0.9350 | -1.6783 | 1.3107 |
| H | -1.5454 | -2.1012 | 0.4960 |
| H | -1.6072 | -1.0370 | 1.9022 |
| Si | 0.2947 | 3.0605 | -2.3849 |
| C | 1.6841 | 4.2776 | -2.7302 |
| C | -1.1050 | 4.0031 | -1.5608 |
| C | -0.3230 | 2.3840 | -4.0222 |
| H | 2.5111 | 3.7911 | -3.2544 |
| H | 2.0799 | 4.6931 | -1.7994 |
| H | 1.3374 | 5.1099 | -3.3494 |
| H | 0.4581 | 1.8259 | -4.5442 |
| H | -1.1788 | 1.7171 | -3.8952 |
| H | -0.6383 | 3.2036 | -4.6735 |
| H | -1.9836 | 3.3737 | -1.3956 |
| H | -1.4129 | 4.8371 | -2.1977 |
| H | -0.8022 | 4.4208 | -0.5968 |
| Si | -2.4921 | 1.7872 | 2.3881 |
| C | -2.8498 | 3.5990 | 2.7334 |
| C | -4.0107 | 1.0471 | 1.5674 |
| C | -2.2082 | 0.9148 | 4.0243 |

| | | | |
|---|---|---|---|
| H | -2.0123 | 4.0731 | 3.2522 |
| H | -3.0167 | 4.1475 | 1.8023 |
| H | -3.7406 | 3.7168 | 3.3569 |
| H | -4.2332 | 1.5300 | 0.6119 |
| H | -4.8820 | 1.1837 | 2.2140 |
| H | -3.8992 | -0.0255 | 1.3872 |
| H | -3.0751 | 1.0491 | 4.6768 |
| H | -2.0539 | -0.1589 | 3.8972 |
| H | -1.3347 | 1.3158 | 4.5443 |
| Si | -2.8058 | -1.2544 | -2.3886 |
| C | -1.8868 | -1.5110 | -4.0039 |
| C | -4.5241 | -0.6032 | -2.7817 |
| C | -2.9977 | -2.9140 | -1.5324 |
| H | -0.9067 | -1.9694 | -3.8548 |
| H | -1.7341 | -0.5654 | -4.5300 |
| H | -2.4613 | -2.1691 | -4.6615 |
| H | -4.4698 | 0.3481 | -3.3179 |
| H | -5.0955 | -0.4354 | -1.8646 |
| H | -5.0851 | -1.3073 | -3.4029 |
| H | -2.0321 | -3.3914 | -1.3435 |
| H | -3.5217 | -2.8204 | -0.5772 |
| H | -3.5818 | -3.5913 | -2.1616 |
| Si | 2.4920 | -1.7872 | -2.3880 |
| C | 2.8496 | -3.5991 | -2.7333 |
| C | 4.0106 | -1.0472 | -1.5674 |
| C | 2.2082 | -0.9149 | -4.0242 |
| H | 2.0121 | -4.0731 | -3.2521 |
| H | 3.0165 | -4.1475 | -1.8021 |
| H | 3.7405 | -3.7169 | -3.3568 |
| H | 3.0751 | -1.0491 | -4.6767 |
| H | 2.0537 | 0.1588 | -3.8972 |
| H | 1.3347 | -1.3160 | -4.5444 |
| H | 4.8819 | -1.1838 | -2.2139 |
| H | 4.2331 | -1.5300 | -0.6118 |
| H | 3.8992 | 0.0255 | -1.3872 |
| Si | 2.8058 | 1.2544 | 2.3887 |
| C | 2.9977 | 2.9141 | 1.5325 |
| C | 4.5241 | 0.6031 | 2.7817 |
| C | 1.8868 | 1.5109 | 4.0040 |
| H | 2.0322 | 3.3915 | 1.3437 |
| H | 3.5819 | 3.5913 | 2.1618 |
| H | 3.5218 | 2.8204 | 0.5773 |
| H | 5.0851 | 1.3071 | 3.4030 |
| H | 5.0955 | 0.4354 | 1.8646 |
| H | 4.4697 | -0.3483 | 3.3178 |
| H | 1.7341 | 0.5652 | 4.5299 |
| H | 0.9067 | 1.9692 | 3.8549 |
| H | 2.4613 | 2.1688 | 4.6616 |
| Si | -0.2946 | -3.0604 | 2.3848 |

| | | | |
|---|---|---|---|
| C | 0.3233 | -2.3840 | 4.0221 |
| C | 1.1050 | -4.0031 | 1.5604 |
| C | -1.6841 | -4.2775 | 2.7302 |
| H | -0.4577 | -1.8258 | 4.5441 |
| H | 1.1792 | -1.7172 | 3.8950 |
| H | 0.6386 | -3.2037 | 4.6733 |
| H | 1.9836 | -3.3737 | 1.3952 |
| H | 1.4129 | -4.8371 | 2.1973 |
| H | 0.8021 | -4.4207 | 0.5965 |
| H | -1.3373 | -5.1098 | 3.3493 |
| H | -2.0799 | -4.6929 | 1.7994 |
| H | -2.5110 | -3.7910 | 3.2545 |

Complex **8**

| | | | |
|---|---|---|---|
| U | -0.8793 | -0.1255 | -0.3866 |
| S | -0.7878 | -3.0099 | -0.2390 |
| S | -3.1642 | 1.6560 | -0.5094 |
| S | 2.1733 | -0.5422 | 1.2272 |
| P | -2.6856 | -2.8092 | 0.3278 |
| P | -4.2254 | 0.0064 | -0.1095 |
| O | -1.0622 | -0.0268 | 1.3535 |
| O | -0.7415 | -0.2148 | -2.1279 |
| O | 1.3679 | -0.5575 | -0.0389 |
| O | 2.4097 | 0.7931 | 1.6940 |
| O | 1.7593 | -1.5395 | 2.1636 |
| O | 0.1330 | 2.1725 | -0.2863 |
| F | 4.6843 | -1.1715 | 1.5435 |
| F | 3.6773 | -2.3223 | 0.0222 |
| F | 4.2378 | -0.2759 | -0.3679 |
| C | -3.2106 | -1.3500 | -0.4721 |
| H | -3.1328 | -1.4995 | -1.5518 |
| C | 3.7920 | -1.1165 | 0.5628 |
| C | -0.0871 | 2.9329 | 0.9169 |
| H | 0.8706 | 3.0217 | 1.4366 |
| H | -0.7428 | 2.3270 | 1.5389 |
| C | 1.3353 | 2.5918 | -0.9579 |
| H | 1.3216 | 3.6836 | -1.0031 |
| C | 1.4234 | 2.0200 | -2.3446 |
| C | -0.7220 | 4.2717 | 0.6326 |
| H | 2.1798 | 2.2775 | -0.3379 |
| C | -2.8287 | -2.7782 | 2.1293 |
| C | -3.6976 | -4.2192 | -0.1846 |
| C | -4.8300 | -0.0223 | 1.5889 |
| C | -5.7160 | 0.0047 | -1.1338 |
| C | -5.0682 | -4.0596 | -0.3649 |
| C | -5.8536 | -5.1427 | -0.7249 |
| C | -5.2702 | -6.3878 | -0.9099 |
| C | -3.9029 | -6.5477 | -0.7362 |
| C | -3.1152 | -5.4668 | -0.3743 |

| | | | |
|---|---|---|---|
| H | -5.5208 | -3.0834 | -0.2311 |
| H | -6.9200 | -5.0123 | -0.8687 |
| H | -5.8818 | -7.2349 | -1.1982 |
| H | -3.4459 | -7.5183 | -0.8885 |
| H | -2.0440 | -5.5810 | -0.2508 |
| C | -4.0409 | -3.0606 | 2.7549 |
| C | -4.1178 | -3.0819 | 4.1356 |
| C | -2.9859 | -2.8326 | 4.8988 |
| C | -1.7747 | -2.5688 | 4.2787 |
| C | -1.6904 | -2.5454 | 2.8958 |
| H | -4.9237 | -3.2779 | 2.1678 |
| H | -5.0645 | -3.2979 | 4.6159 |
| H | -3.0479 | -2.8554 | 5.9809 |
| H | -0.8826 | -2.3865 | 4.8657 |
| H | -0.7387 | -2.3567 | 2.4150 |
| C | -5.9644 | -1.0065 | -2.0525 |
| C | -7.1119 | -0.9700 | -2.8326 |
| C | -8.0090 | 0.0766 | -2.6963 |
| C | -7.7574 | 1.0956 | -1.7853 |
| C | -6.6132 | 1.0641 | -1.0095 |
| H | -5.2641 | -1.8256 | -2.1604 |
| H | -7.3000 | -1.7607 | -3.5493 |
| H | -8.9052 | 0.1052 | -3.3049 |
| H | -8.4547 | 1.9190 | -1.6848 |
| H | -6.4088 | 1.8625 | -0.3047 |
| C | -6.0939 | -0.5322 | 1.8751 |
| C | -6.5606 | -0.5332 | 3.1790 |
| C | -5.7633 | -0.0397 | 4.2002 |
| C | -4.4987 | 0.4557 | 3.9187 |
| C | -4.0338 | 0.4762 | 2.6153 |
| H | -6.7219 | -0.9113 | 1.0777 |
| H | -7.5503 | -0.9180 | 3.3961 |
| H | -6.1278 | -0.0430 | 5.2209 |
| H | -3.8708 | 0.8325 | 4.7170 |
| H | -3.0539 | 0.8745 | 2.3870 |
| H | -0.9008 | 4.7886 | 1.5785 |
| H | -0.0872 | 4.9155 | 0.0214 |
| H | -1.6813 | 4.1438 | 0.1286 |
| H | 2.2906 | 2.4588 | -2.8427 |
| H | 1.5573 | 0.9391 | -2.3339 |
| H | 0.5335 | 2.2575 | -2.9299 |

Complex **9**

| | | | |
|---|---|---|---|
| U | 0.0090 | -0.0110 | 0.0014 |
| Cl | 3.3932 | 2.7255 | 4.5630 |
| Cl | 0.6797 | 1.1802 | 6.1598 |
| Cl | -1.6024 | 2.0724 | -0.0950 |
| N | 1.9861 | 1.5762 | 2.5608 |
| N | 0.3254 | 0.6404 | 3.5333 |

| | | | |
|---|---|---|---|
| O | 1.2624 | 0.8976 | -0.8144 |
| C | 0.8788 | 0.8392 | 2.3147 |
| C | 2.8832 | 2.0586 | 1.5541 |
| C | 3.9853 | 1.2807 | 1.2134 |
| C | 4.8097 | 1.7505 | 0.2030 |
| H | 5.6697 | 1.1548 | -0.0865 |
| C | 4.5586 | 2.9532 | -0.4466 |
| C | 3.4592 | 3.7035 | -0.0571 |
| H | 3.2531 | 4.6470 | -0.5522 |
| C | 2.5996 | 3.2745 | 0.9454 |
| C | 4.2498 | -0.0283 | 1.8837 |
| H | 4.1947 | 0.0543 | 2.9718 |
| H | 5.2416 | -0.3965 | 1.6219 |
| H | 3.5173 | -0.7771 | 1.5677 |
| C | 5.4575 | 3.4186 | -1.5496 |
| H | 5.1826 | 4.4167 | -1.8924 |
| H | 5.4009 | 2.7415 | -2.4066 |
| H | 6.5010 | 3.4451 | -1.2266 |
| C | 1.3925 | 4.0702 | 1.3231 |
| H | 1.4209 | 5.0531 | 0.8533 |
| H | 1.3216 | 4.2123 | 2.4046 |
| H | 0.4776 | 3.5676 | 0.9937 |
| C | 2.1249 | 1.8335 | 3.9077 |
| C | 1.0737 | 1.2391 | 4.5241 |
| C | -0.9052 | -0.0535 | 3.7698 |
| C | -2.0797 | 0.6906 | 3.8127 |
| C | -3.2676 | -0.0009 | 4.0044 |
| H | -4.1978 | 0.5573 | 4.0287 |
| C | -3.2933 | -1.3811 | 4.1558 |
| C | -2.0937 | -2.0793 | 4.1141 |
| H | -2.0996 | -3.1593 | 4.2220 |
| C | -0.8797 | -1.4357 | 3.9203 |
| C | -2.0675 | 2.1738 | 3.6268 |
| H | -3.0664 | 2.5842 | 3.7730 |
| H | -1.7424 | 2.4335 | 2.6158 |
| H | -1.3938 | 2.6642 | 4.3346 |
| C | -4.5864 | -2.0987 | 4.3897 |
| H | -5.4313 | -1.5383 | 3.9861 |
| H | -4.7652 | -2.2388 | 5.4601 |
| H | -4.5786 | -3.0885 | 3.9307 |
| C | 0.3965 | -2.2077 | 3.8276 |
| H | 1.2021 | -1.7335 | 4.3929 |
| H | 0.7273 | -2.2860 | 2.7870 |
| H | 0.2594 | -3.2182 | 4.2127 |
| Cl | -2.9343 | -3.2544 | -4.5402 |
| Cl | -1.0503 | -0.7851 | -6.1672 |
| Cl | 1.6229 | -2.0926 | 0.1114 |
| N | -1.7067 | -1.9049 | -2.5429 |
| N | -0.5674 | -0.3902 | -3.5355 |

| | | | |
|---|---|---|---|
| O | -1.2430 | -0.9217 | 0.8181 |
| C | -0.8676 | -0.8706 | -2.3074 |
| C | -2.2558 | -2.7564 | -1.5311 |
| C | -3.4042 | -2.3501 | -0.8615 |
| C | -3.8938 | -3.1861 | 0.1318 |
| H | -4.7831 | -2.8842 | 0.6760 |
| C | -3.2657 | -4.3805 | 0.4568 |
| C | -2.1209 | -4.7438 | -0.2397 |
| H | -1.6141 | -5.6705 | 0.0094 |
| C | -1.5965 | -3.9479 | -1.2474 |
| C | -4.0594 | -1.0409 | -1.1591 |
| H | -4.1341 | -0.8555 | -2.2330 |
| H | -5.0641 | -1.0121 | -0.7373 |
| H | -3.4882 | -0.2159 | -0.7223 |
| C | -3.8283 | -5.2767 | 1.5157 |
| H | -3.0485 | -5.8829 | 1.9798 |
| H | -4.3301 | -4.7031 | 2.2965 |
| H | -4.5680 | -5.9624 | 1.0909 |
| C | -0.3587 | -4.3450 | -1.9845 |
| H | -0.0092 | -5.3187 | -1.6427 |
| H | -0.5340 | -4.4077 | -3.0620 |
| H | 0.4422 | -3.6216 | -1.8117 |
| C | -1.9296 | -2.0683 | -3.8935 |
| C | -1.2059 | -1.1099 | -4.5226 |
| C | 0.2979 | 0.7232 | -3.7847 |
| C | 1.6654 | 0.4942 | -3.8735 |
| C | 2.4854 | 1.5953 | -4.0829 |
| H | 3.5575 | 1.4410 | -4.1511 |
| C | 1.9711 | 2.8794 | -4.1894 |
| C | 0.5949 | 3.0564 | -4.1043 |
| H | 0.1772 | 4.0544 | -4.1908 |
| C | -0.2678 | 1.9892 | -3.9065 |
| C | 2.2377 | -0.8752 | -3.7009 |
| H | 3.2940 | -0.8845 | -3.9695 |
| H | 2.1540 | -1.2018 | -2.6598 |
| H | 1.7220 | -1.6132 | -4.3202 |
| C | 2.8737 | 4.0591 | -4.3783 |
| H | 3.9001 | 3.7484 | -4.5772 |
| H | 2.5402 | 4.6857 | -5.2087 |
| H | 2.8810 | 4.6856 | -3.4817 |
| C | -1.7449 | 2.1935 | -3.8003 |
| H | -2.2962 | 1.5151 | -4.4560 |
| H | -2.0824 | 2.0210 | -2.7745 |
| H | -2.0086 | 3.2152 | -4.0728 |

Complex **10**

| | | | |
|---|---|---|---|
| U | -0.3223 | 0.0158 | -0.7821 |
| O | -1.0049 | -0.0856 | -2.4264 |
| N | -0.7685 | 2.1507 | -0.6477 |

| | | | |
|---|---|---|---|
| N | -1.7314 | -1.4676 | -0.0280 |
| N | 1.6463 | -0.6801 | -1.4514 |
| Si | -2.1574 | -2.8449 | -1.0300 |
| Si | -2.5088 | -1.2665 | 1.5316 |
| Si | 2.2848 | -0.0573 | -2.9627 |
| Si | 2.5702 | -1.8785 | -0.5685 |
| Si | 0.3945 | 3.2787 | 0.0176 |
| Si | -2.2806 | 2.7458 | -1.3107 |
| C | -3.7754 | -2.5604 | -1.9251 |
| H | -3.9998 | -3.4234 | -2.5589 |
| H | -4.6187 | -2.4065 | -1.2515 |
| H | -3.6917 | -1.6862 | -2.5752 |
| C | -0.8778 | -3.1626 | -2.3668 |
| H | 0.7753 | -2.3850 | 1.1545 |
| H | -1.0163 | -4.1869 | -2.7266 |
| H | -1.0168 | -2.4870 | -3.2106 |
| C | -2.2587 | -4.4148 | -0.0047 |
| H | -3.0092 | -4.3736 | 0.7862 |
| H | -2.5170 | -5.2491 | -0.6634 |
| H | -1.2955 | -4.6419 | 0.4586 |
| C | -3.6104 | 1.4253 | -1.2379 |
| H | -3.3502 | 0.5131 | -1.7752 |
| H | -3.8726 | 1.1624 | -0.2117 |
| H | -4.5092 | 1.8348 | -1.7091 |
| C | -2.0584 | 3.2558 | -3.0958 |
| H | -1.7781 | 2.3908 | -3.7016 |
| H | -2.9952 | 3.6548 | -3.4947 |
| H | -1.2874 | 4.0192 | -3.2137 |
| C | -2.9669 | 4.1763 | -0.3064 |
| H | -3.9182 | 4.4843 | -0.7508 |
| H | -3.1703 | 3.8615 | 0.7203 |
| H | -2.3194 | 5.0527 | -0.2719 |
| C | -0.1079 | 3.7931 | 1.7459 |
| H | -1.0269 | 4.3806 | 1.7570 |
| H | -0.2635 | 2.9022 | 2.3584 |
| H | 0.6840 | 4.3908 | 2.2068 |
| C | 2.1282 | 2.5416 | 0.1098 |
| H | 2.4180 | 2.4002 | 1.1521 |
| H | 2.2594 | 1.5751 | -0.3805 |
| H | 2.8341 | 3.2372 | -0.3537 |
| C | 0.5467 | 4.8019 | -1.0701 |
| H | 1.2703 | 5.4878 | -0.6189 |
| H | 0.9204 | 4.5319 | -2.0612 |
| H | -0.3889 | 5.3470 | -1.2012 |
| C | 3.8915 | -1.0631 | 0.4766 |
| H | 3.4469 | -0.3510 | 1.1749 |
| H | 4.4337 | -1.8166 | 1.0557 |
| H | 4.6185 | -0.5276 | -0.1365 |
| C | 1.4807 | -2.9382 | 0.5359 |

| | | | |
|---|---|---|---|
| H | 0.1579 | -3.0724 | -2.0369 |
| H | 0.9251 | -3.6747 | -0.0470 |
| H | 2.1430 | -3.4931 | 1.2087 |
| C | 3.3713 | -3.1229 | -1.7269 |
| H | 3.9167 | -3.8561 | -1.1245 |
| H | 2.6120 | -3.6661 | -2.2957 |
| H | 4.0767 | -2.6897 | -2.4367 |
| C | 4.1368 | 0.2359 | -2.8588 |
| H | 4.3636 | 0.9705 | -2.0820 |
| H | 4.7247 | -0.6603 | -2.6589 |
| H | 4.4776 | 0.6489 | -3.8130 |
| C | 1.5613 | 1.6277 | -3.3571 |
| H | 1.9512 | 1.9259 | -4.3354 |
| H | 0.4738 | 1.6400 | -3.4248 |
| H | 1.8755 | 2.3861 | -2.6386 |
| C | 1.8792 | -1.2069 | -4.3794 |
| H | 2.3154 | -2.1983 | -4.2465 |
| H | 0.7965 | -1.3209 | -4.4681 |
| H | 2.2545 | -0.7947 | -5.3201 |
| C | -4.3237 | -1.7455 | 1.4516 |
| H | -4.8651 | -1.1048 | 0.7514 |
| H | -4.5002 | -2.7836 | 1.1669 |
| H | -4.7609 | -1.5967 | 2.4442 |
| C | -1.6868 | -2.3083 | 2.8512 |
| H | -1.6910 | -3.3699 | 2.5990 |
| H | -0.6532 | -1.9974 | 3.0125 |
| H | -2.2227 | -2.1850 | 3.7974 |
| C | -2.4978 | 0.5343 | 2.0961 |
| H | -3.5276 | 0.8746 | 2.2364 |
| H | -1.9784 | 0.6111 | 3.0535 |
| H | -2.0111 | 1.2410 | 1.4215 |
| C | 0.5312 | 0.1557 | 1.3346 |
| C | 0.9752 | 0.1580 | 2.4721 |
| C | 1.4991 | 0.1109 | 3.7872 |
| C | 1.2375 | 1.1344 | 4.7039 |
| C | 1.7513 | 1.0645 | 5.9858 |
| C | 2.5279 | -0.0200 | 6.3701 |
| C | 2.7914 | -1.0399 | 5.4658 |
| C | 2.2825 | -0.9795 | 4.1819 |
| H | 0.6313 | 1.9781 | 4.3977 |
| H | 1.5442 | 1.8609 | 6.6908 |
| H | 2.9277 | -0.0710 | 7.3761 |
| H | 3.3968 | -1.8876 | 5.7645 |
| H | 2.4805 | -1.7700 | 3.4684 |

Complex **11**

| | | | |
|---|---|---|---|
| U | -0.4755 | -0.0008 | 0.0006 |
| S | -1.5774 | 2.6643 | 0.0152 |
| S | -1.5789 | -2.6652 | -0.0116 |

| | | | |
|---|---|---|---|
| P | -3.2884 | 1.5939 | 0.1069 |
| P | -3.2895 | -1.5940 | -0.1007 |
| O | -0.2821 | 0.0044 | -1.7619 |
| O | -0.2813 | -0.0061 | 1.7630 |
| N | 1.5646 | 1.6331 | 0.0249 |
| N | 1.5639 | -1.6356 | -0.0247 |
| C | -2.8387 | 0.0000 | 0.0012 |
| C | 1.9023 | 2.2540 | 1.1559 |
| H | 1.3203 | 1.9895 | 2.0314 |
| C | 2.9213 | 3.1875 | 1.2137 |
| H | 3.1570 | 3.6696 | 2.1536 |
| C | 3.6140 | 3.4896 | 0.0530 |
| H | 4.4158 | 4.2189 | 0.0635 |
| C | 3.2596 | 2.8495 | -1.1233 |
| H | 3.7670 | 3.0607 | -2.0557 |
| C | 2.2267 | 1.9303 | -1.0933 |
| H | 1.8985 | 1.4137 | -1.9882 |
| C | 2.2253 | -1.9342 | 1.0935 |
| H | 1.8965 | -1.4188 | 1.9888 |
| C | 3.2582 | -2.8535 | 1.1231 |
| H | 3.7649 | -3.0660 | 2.0556 |
| C | 3.6134 | -3.4921 | -0.0537 |
| H | 4.4153 | -4.2214 | -0.0646 |
| C | 2.9215 | -3.1884 | -1.2146 |
| H | 3.1580 | -3.6693 | -2.1549 |
| C | 1.9025 | -2.2550 | -1.1563 |
| H | 1.3212 | -1.9894 | -2.0318 |
| C | -4.1953 | -1.9971 | -1.6190 |
| C | -4.4284 | -2.1055 | 1.2199 |
| C | -4.4299 | 2.1075 | -1.2108 |
| C | -4.1904 | 1.9958 | 1.6278 |
| C | -5.7639 | -1.7161 | 1.1466 |
| C | -6.6213 | -1.9646 | 2.2042 |
| C | -6.1497 | -2.6031 | 3.3435 |
| C | -4.8214 | -2.9948 | 3.4189 |
| C | -3.9609 | -2.7481 | 2.3588 |
| H | -6.1296 | -1.2178 | 0.2551 |
| H | -7.6592 | -1.6578 | 2.1424 |
| H | -6.8209 | -2.7968 | 4.1726 |
| H | -4.4530 | -3.4976 | 4.3061 |
| H | -2.9188 | -3.0461 | 2.4010 |
| C | -4.1325 | -1.1098 | -2.6860 |
| C | -4.8047 | -1.3936 | -3.8644 |
| C | -5.5355 | -2.5663 | -3.9805 |
| C | -5.5911 | -3.4601 | -2.9187 |
| C | -4.9224 | -3.1775 | -1.7398 |
| H | -3.5558 | -0.1984 | -2.5776 |
| H | -4.7618 | -0.6917 | -4.6895 |
| H | -6.0655 | -2.7869 | -4.9002 |

| | | | |
|---|---|---|---|
| H | -6.1606 | -4.3781 | -3.0109 |
| H | -4.9680 | -3.8711 | -0.9071 |
| C | -4.1217 | 1.1092 | 2.6951 |
| C | -4.7903 | 1.3923 | 3.8758 |
| C | -5.5231 | 2.5636 | 3.9939 |
| C | -5.5846 | 3.4565 | 2.9318 |
| C | -4.9197 | 3.1746 | 1.7505 |
| H | -3.5435 | 0.1991 | 2.5852 |
| H | -4.7428 | 0.6910 | 4.7011 |
| H | -6.0503 | 2.7836 | 4.9154 |
| H | -6.1558 | 4.3733 | 3.0255 |
| H | -4.9698 | 3.8676 | 0.9177 |
| C | -5.7650 | 1.7169 | -1.1360 |
| C | -6.6243 | 1.9668 | -2.1917 |
| C | -6.1551 | 2.6077 | -3.3307 |
| C | -4.8271 | 3.0004 | -3.4075 |
| C | -3.9647 | 2.7524 | -2.3493 |
| H | -6.1288 | 1.2166 | -0.2449 |
| H | -7.6619 | 1.6591 | -2.1288 |
| H | -6.8278 | 2.8024 | -4.1583 |
| H | -4.4606 | 3.5050 | -4.2945 |
| H | -2.9229 | 3.0510 | -2.3928 |

Complex **12**

| | | | |
|---|---|---|---|
| U | -0.0900 | 2.2500 | 0.4870 |
| O | -0.1043 | 3.9490 | 0.9616 |
| Cl | 0.0414 | 1.5928 | 2.9938 |
| Cl | -0.2730 | 3.0129 | -1.9984 |
| C | -0.0109 | 0.2201 | -0.1944 |
| P | -1.6405 | -0.1900 | 0.0053 |
| C | -2.4216 | -0.7517 | -1.5156 |
| C | -3.5482 | -1.5704 | -1.5005 |
| H | -3.9239 | -1.9608 | -0.5621 |
| C | -4.1859 | -1.8910 | -2.6881 |
| H | -5.0618 | -2.5290 | -2.6742 |
| C | -3.7035 | -1.3951 | -3.8908 |
| H | -4.2042 | -1.6472 | -4.8186 |
| C | -2.5845 | -0.5744 | -3.9075 |
| H | -2.2116 | -0.1788 | -4.8448 |
| C | -1.9444 | -0.2503 | -2.7236 |
| H | -1.0883 | 0.4136 | -2.7217 |
| C | -1.8737 | -1.4972 | 1.2153 |
| C | -2.0769 | -1.1589 | 2.5492 |
| H | -2.1548 | -0.1158 | 2.8278 |
| C | -2.1384 | -2.1552 | 3.5098 |
| H | -2.2901 | -1.8888 | 4.5489 |
| C | -1.9951 | -3.4853 | 3.1442 |
| H | -2.0450 | -4.2622 | 3.8986 |
| C | -1.7831 | -3.8243 | 1.8150 |

| | | | |
|---|---|---|---|
| H | -1.6643 | -4.8629 | 1.5297 |
| C | -1.7184 | -2.8332 | 0.8510 |
| H | -1.5489 | -3.0959 | -0.1874 |
| N | -2.1892 | 1.2506 | 0.4862 |
| Si | -3.7885 | 1.9378 | 0.5969 |
| C | -4.9780 | 0.7120 | 1.3630 |
| H | -5.0851 | -0.1835 | 0.7456 |
| H | -5.9688 | 1.1654 | 1.4581 |
| H | -4.6532 | 0.4000 | 2.3578 |
| C | -4.3760 | 2.4080 | -1.1111 |
| H | -3.6477 | 3.0635 | -1.5959 |
| H | -5.3336 | 2.9337 | -1.0641 |
| H | -4.5043 | 1.5256 | -1.7432 |
| C | -3.6296 | 3.4450 | 1.6825 |
| H | -3.2181 | 3.1788 | 2.6598 |
| H | -4.6049 | 3.9137 | 1.8384 |
| H | -2.9677 | 4.1935 | 1.2382 |
| P | 1.6645 | -0.0133 | -0.1114 |
| C | 2.1011 | -1.2521 | 1.1134 |
| C | 2.5079 | -0.8434 | 2.3783 |
| H | 2.6153 | 0.2134 | 2.5869 |
| C | 2.7316 | -1.7866 | 3.3684 |
| H | 3.0432 | -1.4647 | 4.3548 |
| C | 2.5411 | -3.1337 | 3.1014 |
| H | 2.7136 | -3.8694 | 3.8786 |
| C | 2.1184 | -3.5429 | 1.8440 |
| H | 1.9550 | -4.5944 | 1.6393 |
| C | 1.8947 | -2.6051 | 0.8517 |
| H | 1.5523 | -2.9230 | -0.1271 |
| C | 2.3832 | -0.5230 | -1.6824 |
| C | 3.4210 | -1.4451 | -1.7760 |
| H | 3.7995 | -1.9313 | -0.8849 |
| C | 3.9747 | -1.7394 | -3.0130 |
| H | 4.7809 | -2.4602 | -3.0833 |
| C | 3.5004 | -1.1110 | -4.1543 |
| H | 3.9353 | -1.3430 | -5.1198 |
| C | 2.4755 | -0.1786 | -4.0609 |
| H | 2.1118 | 0.3248 | -4.9489 |
| C | 1.9174 | 0.1174 | -2.8302 |
| H | 1.1366 | 0.8665 | -2.7459 |
| N | 2.0932 | 1.4873 | 0.3006 |
| Si | 3.6218 | 2.3313 | 0.3075 |
| C | 5.0374 | 1.1237 | 0.5133 |
| H | 4.9460 | 0.5371 | 1.4305 |
| H | 5.9849 | 1.6682 | 0.5572 |
| H | 5.0947 | 0.4313 | -0.3306 |
| C | 3.8062 | 3.2475 | -1.3076 |
| H | 3.8703 | 2.5489 | -2.1462 |
| H | 4.7086 | 3.8647 | -1.3098 |

| | | | |
|---|---|---|---|
| H | 2.9455 | 3.8979 | -1.4847 |
| C | 3.5630 | 3.5212 | 1.7414 |
| H | 2.7407 | 4.2328 | 1.6269 |
| H | 4.4932 | 4.0908 | 1.8160 |
| H | 3.4080 | 2.9918 | 2.6850 |

Complex **13**

| | | | |
|---|---|---|---|
| C | 0.8927 | -0.6268 | -5.3163 |
| C | 0.1287 | 1.7183 | -4.9397 |
| C | 2.5743 | 1.2073 | -5.1561 |
| C | -2.6174 | -1.9829 | -4.8220 |
| C | 1.2260 | 0.7041 | -4.6691 |
| C | -2.9965 | -0.6590 | -4.6739 |
| C | -1.9423 | -2.6236 | -3.7925 |
| C | -2.7067 | 0.0218 | -3.4993 |
| C | 5.2901 | -1.3803 | -3.2174 |
| C | 1.6186 | 4.0887 | -2.5133 |
| C | 5.9280 | 0.9467 | -2.5748 |
| C | -1.6637 | -1.9466 | -2.6200 |
| C | -5.0002 | -2.6016 | -2.0690 |
| C | -2.0386 | -0.6151 | -2.4567 |
| C | 3.9212 | 3.8295 | -1.6825 |
| C | 5.3043 | -0.3534 | -2.1012 |
| C | 2.4582 | 3.5792 | -1.3522 |
| C | -4.0676 | 3.4462 | -1.3792 |
| C | -3.6326 | 2.1376 | -1.2478 |
| C | -3.1584 | 4.4939 | -1.3215 |
| C | -4.3883 | -2.5802 | -0.6746 |
| C | 6.0378 | -0.9029 | -0.8895 |
| C | -1.8102 | 4.2280 | -1.1381 |
| C | -2.2736 | 1.8635 | -1.0781 |
| C | -1.3723 | 2.9170 | -1.0244 |
| C | 2.0685 | 4.2864 | -0.0627 |
| C | -4.7038 | -3.8785 | 0.0633 |
| C | -0.0346 | 0.0681 | -0.4945 |
| C | -4.8346 | -1.3894 | 0.1372 |
| C | -6.1863 | -1.2526 | 0.4270 |
| C | 3.9048 | -4.1493 | 0.5327 |
| C | -3.9101 | -0.4553 | 0.6564 |
| C | -0.3294 | -3.0462 | 0.6678 |
| C | -6.6579 | -0.2451 | 1.2476 |
| C | -1.0327 | -4.1987 | 0.9566 |
| C | 4.9399 | 2.0773 | 1.2817 |
| C | 2.8407 | -3.4128 | 1.3400 |
| C | -4.3861 | 0.5230 | 1.5629 |
| C | -5.7447 | 0.6147 | 1.8299 |
| C | -0.2867 | -1.9944 | 1.5783 |
| C | 3.1294 | -0.8796 | 1.7260 |
| C | 3.4309 | -2.2195 | 2.0490 |

| | | | |
|---|---|---|---|
| C | 3.6869 | 1.6232 | 2.0239 |
| C | -1.7118 | -4.3157 | 2.1603 |
| C | 2.1587 | -4.3732 | 2.3071 |
| C | 3.8185 | 0.1618 | 2.3842 |
| C | -3.4248 | 1.3925 | 2.3314 |
| C | -0.0840 | 1.9798 | 2.2258 |
| C | -3.7963 | 2.8671 | 2.3581 |
| C | 0.3550 | 0.6808 | 2.4466 |
| C | 4.3593 | -2.4793 | 3.0505 |
| C | -0.9873 | -2.1080 | 2.7741 |
| C | -1.6925 | -3.2649 | 3.0628 |
| C | 3.4767 | 2.5231 | 3.2347 |
| C | 4.7357 | -0.1585 | 3.3785 |
| C | 5.0026 | -1.4657 | 3.7292 |
| C | -0.1937 | 2.8708 | 3.2810 |
| C | -3.2777 | 0.8501 | 3.7513 |
| C | 0.7150 | 0.2896 | 3.7376 |
| C | 0.1141 | 2.4625 | 4.5692 |
| C | 0.5745 | 1.1730 | 4.7953 |
| H | 0.7784 | -0.4900 | -6.3943 |
| H | 0.0403 | 1.8887 | -6.0149 |
| H | 2.5439 | 1.3751 | -6.2345 |
| H | -2.8428 | -2.5149 | -5.7393 |
| H | -3.5186 | -0.1474 | -5.4744 |
| H | -0.8237 | 1.3428 | -4.5689 |
| H | 1.6816 | -1.3567 | -5.1331 |
| H | -0.0377 | -1.0245 | -4.9127 |
| H | 0.3426 | 2.6700 | -4.4551 |
| H | 2.8458 | 2.1466 | -4.6712 |
| H | 3.3498 | 0.4694 | -4.9457 |
| H | -1.6244 | -3.6536 | -3.9036 |
| H | 4.7233 | -1.0187 | -4.0766 |
| H | 1.9710 | 3.6577 | -3.4492 |
| H | 5.3786 | 1.3436 | -3.4305 |
| H | 6.3148 | -1.5794 | -3.5388 |
| H | -3.0029 | 1.0582 | -3.4004 |
| H | 1.7153 | 5.1743 | -2.5871 |
| H | 4.1939 | 3.3104 | -2.6022 |
| H | 6.9612 | 0.7698 | -2.8805 |
| H | -4.6369 | -3.4623 | -2.6362 |
| H | -4.7501 | -1.7005 | -2.6309 |
| H | 4.8355 | -2.3120 | -2.8824 |
| H | 4.0894 | 4.8983 | -1.8310 |
| H | 0.5655 | 3.8439 | -2.3970 |
| H | -6.0901 | -2.6747 | -2.0171 |
| H | 5.9262 | 1.6935 | -1.7807 |
| H | -1.1440 | -2.4551 | -1.8196 |
| H | 4.5735 | 3.4853 | -0.8839 |
| H | -5.1243 | 3.6478 | -1.5116 |

| | | | |
|---|---|---|---|
| H | -4.3514 | 1.3267 | -1.2717 |
| H | -3.5026 | 5.5174 | -1.4143 |
| H | 7.0642 | -1.1533 | -1.1656 |
| H | -3.3047 | -2.5089 | -0.7685 |
| H | 2.2282 | 5.3625 | -0.1579 |
| H | -4.2877 | -4.7356 | -0.4748 |
| H | -1.0964 | 5.0434 | -1.0936 |
| H | -6.8864 | -1.9669 | 0.0053 |
| H | 5.5489 | -1.8053 | -0.5240 |
| H | -0.3202 | 2.6887 | -0.8998 |
| H | 4.3453 | -3.5014 | -0.2256 |
| H | 6.0672 | -0.1774 | -0.0770 |
| H | 1.0168 | 4.1157 | 0.1714 |
| H | -5.7831 | -4.0315 | 0.1515 |
| H | 0.1936 | -2.9599 | -0.2768 |
| H | 3.4546 | -4.9974 | 0.0119 |
| H | -1.0556 | -5.0051 | 0.2327 |
| H | 5.0198 | 1.5996 | 0.3060 |
| H | 2.6655 | 3.9212 | 0.7722 |
| H | -4.2829 | -3.8685 | 1.0700 |
| H | 2.1017 | -3.0502 | 0.6294 |
| H | 4.9306 | 3.1602 | 1.1391 |
| H | -7.7176 | -0.1507 | 1.4549 |
| H | 4.7051 | -4.5251 | 1.1760 |
| H | 2.8295 | 1.7391 | 1.3598 |
| H | 5.8354 | 1.8315 | 1.8582 |
| H | -0.3550 | 2.2865 | 1.2241 |
| H | -3.8683 | 3.2788 | 1.3503 |
| H | 1.6921 | -5.1908 | 1.7542 |
| H | -2.4579 | 1.2959 | 1.8405 |
| H | -2.2704 | -5.2168 | 2.3855 |
| H | -6.0940 | 1.3758 | 2.5199 |
| H | 2.8749 | -4.8140 | 3.0056 |
| H | 3.2568 | 3.5430 | 2.9093 |
| H | 1.3803 | -3.8754 | 2.8881 |
| H | 4.5850 | -3.5111 | 3.2932 |
| H | -3.0397 | 3.4349 | 2.9066 |
| H | -4.7516 | 3.0365 | 2.8618 |
| H | -0.5379 | 3.8811 | 3.0952 |
| H | 5.2599 | 0.6447 | 3.8829 |
| H | 4.3744 | 2.5734 | 3.8559 |
| H | -1.0243 | -1.2828 | 3.4687 |
| H | -3.0137 | -0.2091 | 3.7347 |
| H | 2.6517 | 2.1817 | 3.8544 |
| H | -2.2441 | -3.3326 | 3.9931 |
| H | 5.7174 | -1.6920 | 4.5118 |
| H | 1.1045 | -0.7048 | 3.9180 |
| H | -4.2193 | 0.9452 | 4.2997 |
| H | -2.5043 | 1.3932 | 4.3004 |

| | | | |
|---|---|---|---|
| H | 0.0097 | 3.1533 | 5.3981 |
| H | 0.8412 | 0.8560 | 5.7964 |
| I | 1.8988 | -2.7188 | -2.3527 |
| N | -2.5543 | -0.5296 | 0.3536 |
| N | 2.1571 | -0.5772 | 0.7260 |
| O | 1.3033 | 0.5077 | -3.2531 |
| O | 3.9490 | -0.0797 | -1.7039 |
| O | 2.2452 | 2.1843 | -1.1717 |
| P | -1.7609 | 0.1421 | -0.8202 |
| P | 0.5178 | -0.4618 | 1.0548 |
| U | 1.9902 | 0.1621 | -1.4029 |

Complex **14**

| | | | |
|---|---|---|---|
| U | -0.3674 | 0.0407 | 0.4976 |
| P | 2.2615 | 1.6066 | 0.1852 |
| P | 2.1990 | -1.5799 | 0.0440 |
| Si | 0.4313 | 3.8130 | 1.1778 |
| Si | 0.5013 | -3.6554 | 1.4004 |
| O | -0.3267 | 0.0693 | 2.2902 |
| N | 0.8352 | 2.2700 | 0.5417 |
| N | 0.7917 | -2.2123 | 0.5108 |
| N | -0.8328 | 0.0012 | -1.3332 |
| N | -2.5161 | 1.5012 | 0.7323 |
| N | -2.5018 | -1.4264 | 0.8405 |
| N | -5.9390 | 3.8635 | 1.0818 |
| N | -5.8297 | -3.8891 | 1.3642 |
| C | 1.9062 | 0.0322 | -0.1641 |
| C | -0.5446 | -0.0376 | -2.6885 |
| C | -0.4455 | -1.2700 | -3.3636 |
| C | -0.0913 | -1.2800 | -4.7040 |
| H | 0.0108 | -2.2405 | -5.2023 |
| C | 0.1460 | -0.1131 | -5.4199 |
| C | -0.0052 | 1.0920 | -4.7495 |
| H | 0.1618 | 2.0234 | -5.2839 |
| C | -0.3468 | 1.1567 | -3.4050 |
| C | -0.7350 | -2.5571 | -2.6615 |
| H | -0.3392 | -2.5616 | -1.6459 |
| H | -0.3018 | -3.3955 | -3.2085 |
| H | -1.8136 | -2.7341 | -2.5942 |
| C | 0.5730 | -0.1595 | -6.8555 |
| H | 1.6097 | -0.4995 | -6.9483 |
| H | 0.5059 | 0.8262 | -7.3198 |
| H | -0.0445 | -0.8495 | -7.4364 |
| C | -0.4894 | 2.4820 | -2.7320 |
| H | -1.5371 | 2.7031 | -2.5041 |
| H | -0.1133 | 3.2831 | -3.3705 |
| H | 0.0479 | 2.5101 | -1.7831 |
| C | 3.0845 | 2.4044 | -1.2308 |
| C | 2.8431 | 1.8602 | -2.4893 |

| | | | |
|---|---|---|---|
| H | 2.2074 | 0.9851 | -2.5661 |
| C | 3.4049 | 2.4274 | -3.6211 |
| H | 3.1983 | 1.9942 | -4.5935 |
| C | 4.2280 | 3.5386 | -3.5045 |
| H | 4.6761 | 3.9803 | -4.3878 |
| C | 4.4834 | 4.0802 | -2.2521 |
| H | 5.1320 | 4.9438 | -2.1550 |
| C | 3.9125 | 3.5178 | -1.1208 |
| H | 4.1224 | 3.9416 | -0.1465 |
| C | 3.4458 | 1.7755 | 1.5510 |
| C | 4.8126 | 1.6016 | 1.3498 |
| H | 5.1929 | 1.4507 | 0.3456 |
| C | 5.6862 | 1.6173 | 2.4248 |
| H | 6.7480 | 1.4767 | 2.2578 |
| C | 5.2030 | 1.8045 | 3.7120 |
| H | 5.8883 | 1.8177 | 4.5519 |
| C | 3.8404 | 1.9586 | 3.9220 |
| H | 3.4541 | 2.0891 | 4.9268 |
| C | 2.9661 | 1.9330 | 2.8474 |
| H | 1.8980 | 2.0162 | 3.0058 |
| C | 2.8038 | -2.3262 | -1.4998 |
| C | 2.3790 | -3.5729 | -1.9394 |
| H | 1.6679 | -4.1322 | -1.3446 |
| C | 2.8306 | -4.0836 | -3.1474 |
| H | 2.4837 | -5.0531 | -3.4871 |
| C | 3.7152 | -3.3507 | -3.9237 |
| H | 4.0649 | -3.7474 | -4.8704 |
| C | 4.1426 | -2.1020 | -3.4925 |
| H | 4.8214 | -1.5172 | -4.1030 |
| C | 3.6859 | -1.5926 | -2.2888 |
| H | 3.9901 | -0.6051 | -1.9608 |
| C | 3.5143 | -1.8992 | 1.2520 |
| C | 4.7465 | -2.4516 | 0.9255 |
| H | 4.9418 | -2.7646 | -0.0934 |
| C | 5.7203 | -2.6115 | 1.9014 |
| H | 6.6781 | -3.0476 | 1.6398 |
| C | 5.4689 | -2.2174 | 3.2058 |
| H | 6.2316 | -2.3390 | 3.9669 |
| C | 4.2404 | -1.6582 | 3.5354 |
| H | 4.0436 | -1.3336 | 4.5505 |
| C | 3.2691 | -1.4979 | 2.5644 |
| H | 2.3111 | -1.0533 | 2.8117 |
| C | -0.9532 | 4.6134 | 0.1963 |
| H | -0.6636 | 4.7341 | -0.8501 |
| H | -1.1609 | 5.6070 | 0.6058 |
| H | -1.8806 | 4.0397 | 0.2238 |
| C | 1.8475 | 5.0484 | 1.1505 |
| H | 2.7213 | 4.6837 | 1.6963 |
| H | 1.5142 | 5.9707 | 1.6370 |

| | | | |
|---|---|---|---|
| H | 2.1540 | 5.2994 | 0.1330 |
| C | -0.1185 | 3.6763 | 2.9796 |
| H | -0.4428 | 2.6616 | 3.2187 |
| H | -0.9400 | 4.3643 | 3.1981 |
| H | 0.7073 | 3.9244 | 3.6512 |
| C | 1.9440 | -4.8638 | 1.4581 |
| H | 2.2989 | -5.1872 | 0.4776 |
| H | 1.6095 | -5.7565 | 1.9971 |
| H | 2.7952 | -4.4481 | 2.0003 |
| C | -0.9311 | -4.6002 | 0.6343 |
| H | -1.8485 | -4.0119 | 0.5821 |
| H | -1.1400 | -5.5009 | 1.2194 |
| H | -0.6823 | -4.9134 | -0.3838 |
| C | 0.1215 | -3.2665 | 3.1999 |
| H | 1.0581 | -3.2077 | 3.7607 |
| H | -0.4969 | -4.0415 | 3.6618 |
| H | -0.3777 | -2.3033 | 3.3087 |
| C | -3.2578 | -1.8128 | -0.1916 |
| H | -2.9330 | -1.4597 | -1.1619 |
| C | -4.3706 | -2.6106 | -0.0727 |
| H | -4.9108 | -2.8845 | -0.9672 |
| C | -4.7662 | -3.0682 | 1.1970 |
| C | -3.9910 | -2.6226 | 2.2826 |
| H | -4.2247 | -2.9049 | 3.2987 |
| C | -2.8967 | -1.8232 | 2.0532 |
| H | -2.2897 | -1.4801 | 2.8814 |
| C | -6.5715 | -4.3488 | 0.2174 |
| H | -7.0267 | -3.5162 | -0.3293 |
| H | -7.3695 | -5.0083 | 0.5506 |
| H | -5.9362 | -4.9077 | -0.4786 |
| C | -6.1673 | -4.3710 | 2.6797 |
| H | -5.3355 | -4.9206 | 3.1340 |
| H | -7.0169 | -5.0457 | 2.6044 |
| H | -6.4435 | -3.5524 | 3.3529 |
| C | -3.2682 | 1.8081 | -0.3295 |
| H | -2.9170 | 1.4144 | -1.2751 |
| C | -4.4082 | 2.5731 | -0.2670 |
| H | -4.9430 | 2.7832 | -1.1817 |
| C | -4.8392 | 3.0806 | 0.9718 |
| C | -4.0602 | 2.7277 | 2.0881 |
| H | -4.3127 | 3.0631 | 3.0834 |
| C | -2.9388 | 1.9513 | 1.9163 |
| H | -2.3322 | 1.6745 | 2.7696 |
| C | -6.6474 | 4.2770 | -0.1036 |
| H | -6.0116 | 4.8633 | -0.7772 |
| H | -7.4954 | 4.8935 | 0.1859 |
| H | -7.0322 | 3.4167 | -0.6598 |
| C | -6.2876 | 4.4372 | 2.3573 |
| H | -6.4708 | 3.6616 | 3.1070 |

| | | | |
|---|---|---|---|
| H | -7.2009 | 5.0177 | 2.2486 |
| H | -5.5020 | 5.1013 | 2.7367 |

Complex **15**

| | | | |
|---|---|---|---|
| U | 0.0000 | 0.0000 | -0.0880 |
| H | 0.0000 | 0.0000 | 1.8228 |
| F | 1.9851 | 0.0001 | 0.0842 |
| F | -1.9852 | 0.0001 | 0.0842 |
| F | 0.0001 | 1.9851 | 0.0842 |
| F | 0.0001 | -1.9852 | 0.0842 |
| F | 0.0000 | 0.0000 | -2.0715 |

Complex **16**

| | | | |
|---|---|---|---|
| U | 0.0000 | 0.0005 | 0.0970 |
| H | 0.0000 | 0.0629 | 2.0923 |
| C | -0.0001 | -0.0998 | -2.2318 |
| C | 1.6615 | -1.6051 | 0.2093 |
| C | -1.6615 | -1.6051 | 0.2093 |
| C | -1.6241 | 1.6459 | 0.1358 |
| C | 1.6241 | 1.6458 | 0.1358 |
| H | -0.8944 | 0.3931 | -2.6291 |
| H | 0.8941 | 0.3935 | -2.6292 |
| H | 0.0002 | -1.1527 | -2.5370 |
| H | 2.5169 | -1.3726 | -0.4308 |
| H | 1.9573 | -1.5278 | 1.2668 |
| H | 1.2983 | -2.6154 | 0.0044 |
| H | -2.5169 | -1.3726 | -0.4309 |
| H | -1.2982 | -2.6154 | 0.0044 |
| H | -1.9573 | -1.5277 | 1.2668 |
| H | -1.6616 | 1.8564 | 1.2161 |
| H | -2.6016 | 1.2936 | -0.2030 |
| H | -1.3358 | 2.5508 | -0.4054 |
| H | 1.3359 | 2.5508 | -0.4054 |
| H | 1.6616 | 1.8564 | 1.2161 |
| H | 2.6017 | 1.2935 | -0.2029 |

Complex **17**

| | | | |
|---|---|---|---|
| U | 0.0786 | -0.0070 | 0.1642 |
| H | -0.0212 | 0.0693 | 2.1160 |
| O | 0.1580 | -0.0904 | -1.8736 |
| O | -1.9155 | 0.4226 | 0.2302 |
| O | 2.0499 | -0.4107 | 0.4950 |
| O | 0.4741 | 1.9856 | 0.3573 |
| O | -0.3616 | -1.9798 | 0.4379 |
| C | -0.3797 | -0.0255 | -3.1580 |
| H | 0.0151 | -0.8421 | -3.7715 |
| H | -1.4718 | -0.1082 | -3.1308 |
| H | -0.1146 | 0.9249 | -3.6335 |
| C | -1.3211 | -2.9921 | 0.3934 |

| | | | |
|---|---|---|---|
| H | -1.2090 | -3.6447 | 1.2649 |
| H | -2.3308 | -2.5676 | 0.4003 |
| H | -1.1960 | -3.5948 | -0.5124 |
| C | -2.8852 | 1.4268 | 0.2918 |
| H | -3.4903 | 1.4227 | -0.6209 |
| H | -3.5439 | 1.2530 | 1.1480 |
| H | -2.4157 | 2.4099 | 0.4020 |
| C | 1.4440 | 2.9833 | 0.4741 |
| H | 1.4766 | 3.5874 | -0.4387 |
| H | 1.2015 | 3.6368 | 1.3179 |
| H | 2.4322 | 2.5429 | 0.6433 |
| C | 3.0506 | -1.3844 | 0.4892 |
| H | 3.7534 | -1.1927 | 1.3060 |
| H | 2.6194 | -2.3821 | 0.6237 |
| H | 3.5995 | -1.3601 | -0.4581 |

Complex **18**

| | | | |
|---|---|---|---|
| U | 0.0000 | 0.0000 | 0.4695 |
| H | 0.0000 | 1.5251 | -0.7674 |
| H | 0.0000 | -1.5251 | -0.7674 |
| O | 1.7428 | 0.0000 | 0.5327 |
| O | -1.7428 | 0.0000 | 0.5327 |

Complex **19**

| | | | |
|---|---|---|---|
| U | -0.4043 | -0.2318 | 0.0356 |
| O | -0.3251 | -0.3680 | -1.7308 |
| O | -0.5004 | -0.0859 | 1.8019 |
| H | -0.6053 | -2.2750 | 0.2451 |
| H | -1.0396 | 1.7295 | -0.1952 |
| O | 1.8637 | -1.4233 | -0.0134 |
| O | -2.8373 | -0.3682 | -0.0679 |
| O | 1.5474 | 1.4070 | 0.2015 |
| C | 2.1027 | -2.3974 | -1.0486 |
| H | 1.1355 | -2.8089 | -1.3427 |
| H | 2.5496 | -1.8821 | -1.9005 |
| C | 3.0021 | -3.4466 | -0.4225 |
| H | 4.0562 | -3.1810 | -0.5438 |
| H | 2.8468 | -4.4310 | -0.8651 |
| C | 2.6002 | -3.3751 | 1.0453 |
| H | 3.3495 | -3.7865 | 1.7226 |
| H | 1.6526 | -3.8941 | 1.2053 |
| C | 2.4014 | -1.8881 | 1.2339 |
| H | 1.6949 | -1.6327 | 2.0234 |
| H | 3.3504 | -1.3704 | 1.4172 |
| C | -3.5686 | 0.0002 | -1.2571 |
| H | -3.3886 | -0.7648 | -2.0126 |
| H | -3.1628 | 0.9525 | -1.6046 |
| C | -5.0170 | 0.1119 | -0.8190 |
| H | -5.5632 | 0.8497 | -1.4070 |

| | | | |
|---|---|---|---|
| H | -5.5270 | -0.8497 | -0.9196 |
| C | -4.8853 | 0.4894 | 0.6518 |
| H | -5.7805 | 0.2742 | 1.2359 |
| H | -4.6481 | 1.5511 | 0.7552 |
| C | -3.7032 | -0.3497 | 1.0801 |
| H | -3.1348 | 0.0551 | 1.9160 |
| H | -3.9928 | -1.3806 | 1.3069 |
| C | 2.1978 | 1.8092 | -1.0177 |
| H | 1.4788 | 1.6993 | -1.8326 |
| H | 3.0391 | 1.1355 | -1.1926 |
| C | 2.6081 | 3.2579 | -0.8130 |
| H | 3.6219 | 3.3209 | -0.4085 |
| H | 2.5792 | 3.8236 | -1.7446 |
| C | 1.5947 | 3.7383 | 0.2186 |
| H | 1.9200 | 4.6236 | 0.7662 |
| H | 0.6314 | 3.9437 | -0.2545 |
| C | 1.4629 | 2.5209 | 1.1029 |
| H | 0.5106 | 2.4493 | 1.6246 |
| H | 2.2864 | 2.4482 | 1.8237 |

Complex **20**

| | | | |
|---|---|---|---|
| U | 0.0283 | 0.3618 | 0.0015 |
| O | 0.4706 | 0.3100 | -1.7201 |
| O | -0.3560 | 0.7819 | 1.6835 |
| H | 0.2113 | 2.4006 | -0.2292 |
| C | -0.6879 | -2.2214 | -0.8415 |
| C | -1.4509 | -1.9851 | 0.3337 |
| C | -0.5720 | -2.0011 | 1.4395 |
| C | 0.7400 | -2.1649 | 0.9439 |
| C | 0.6630 | -2.3288 | -0.4658 |
| C | -1.2084 | -2.3438 | -2.2319 |
| H | -1.2365 | -3.3890 | -2.5589 |
| H | -0.5836 | -1.7934 | -2.9397 |
| H | -2.2265 | -1.9576 | -2.3158 |
| C | -2.9368 | -1.8633 | 0.4108 |
| H | -3.3586 | -1.4518 | -0.5081 |
| H | -3.2439 | -1.2123 | 1.2329 |
| H | -3.4102 | -2.8371 | 0.5788 |
| C | -0.9604 | -1.8685 | 2.8695 |
| H | -1.8630 | -1.2660 | 2.9850 |
| H | -0.1782 | -1.3818 | 3.4548 |
| H | -1.1551 | -2.8464 | 3.3241 |
| C | 1.9766 | -2.2629 | 1.7740 |
| H | 1.8937 | -1.6682 | 2.6866 |
| H | 2.8585 | -1.9148 | 1.2324 |
| H | 2.1716 | -3.2963 | 2.0818 |
| C | 1.8011 | -2.5796 | -1.3940 |
| H | 1.8887 | -3.6429 | -1.6436 |
| H | 2.7540 | -2.2759 | -0.9549 |

| | | | |
|---|---|---|---|
| H | 1.6772 | -2.0305 | -2.3304 |
| O | -2.2061 | 1.1352 | -0.6964 |
| C | -2.9968 | 1.9696 | 0.1721 |
| H | -3.8740 | 1.3968 | 0.4922 |
| H | -2.3851 | 2.2160 | 1.0381 |
| C | -3.3791 | 3.1537 | -0.6834 |
| H | -2.5492 | 3.8633 | -0.7200 |
| H | -4.2667 | 3.6667 | -0.3121 |
| C | -3.5834 | 2.4977 | -2.0433 |
| H | -3.5140 | 3.1980 | -2.8759 |
| H | -4.5609 | 2.0105 | -2.0876 |
| C | -2.4670 | 1.4714 | -2.0781 |
| H | -2.7277 | 0.5527 | -2.6058 |
| H | -1.5438 | 1.8737 | -2.4965 |
| O | 2.4061 | 0.7700 | 0.5040 |
| C | 3.3972 | 0.9691 | -0.5207 |
| H | 4.0741 | 0.1073 | -0.5179 |
| H | 2.8771 | 1.0183 | -1.4753 |
| C | 4.1093 | 2.2387 | -0.1182 |
| H | 3.5192 | 3.1062 | -0.4231 |
| H | 5.1034 | 2.3169 | -0.5593 |
| C | 4.1293 | 2.1103 | 1.4002 |
| H | 4.2696 | 3.0623 | 1.9124 |
| H | 4.9289 | 1.4338 | 1.7136 |
| C | 2.7680 | 1.5085 | 1.6948 |
| H | 2.7640 | 0.8143 | 2.5358 |
| H | 2.0011 | 2.2680 | 1.8514 |

Complex **21**

| | | | |
|---|---|---|---|
| U | -0.0501 | 0.0085 | -0.0391 |
| N | -0.0659 | -0.0929 | -1.8845 |
| N | -0.0145 | 0.1319 | 1.8077 |
| H | -0.5161 | -2.0315 | 0.1049 |
| H | -0.7932 | 1.9641 | -0.1590 |
| O | 2.1910 | -1.2984 | -0.1048 |
| O | -2.5576 | -0.1811 | 0.0045 |
| O | 1.9576 | 1.5645 | -0.0728 |
| C | 2.1838 | -2.5548 | -0.7921 |
| H | 1.3084 | -2.5575 | -1.4366 |
| H | 3.0958 | -2.6189 | -1.3974 |
| C | 2.1419 | -3.6345 | 0.2921 |
| H | 2.9221 | -4.3800 | 0.1282 |
| H | 1.1753 | -4.1365 | 0.2958 |
| C | 2.3573 | -2.8586 | 1.5995 |
| H | 3.0402 | -3.3554 | 2.2902 |
| H | 1.3989 | -2.7032 | 2.0972 |
| C | 2.8838 | -1.5213 | 1.1201 |
| H | 2.6648 | -0.6841 | 1.7796 |
| H | 3.9633 | -1.5587 | 0.9181 |

| | | | |
|---|---|---|---|
| C | -3.4573 | 0.9093 | -0.2539 |
| H | -3.0647 | 1.4824 | -1.0925 |
| H | -3.4636 | 1.5609 | 0.6244 |
| C | -4.8066 | 0.2636 | -0.5011 |
| H | -5.6330 | 0.9260 | -0.2414 |
| H | -4.9100 | -0.0156 | -1.5534 |
| C | -4.7258 | -0.9837 | 0.3689 |
| H | -5.4307 | -1.7640 | 0.0801 |
| H | -4.9061 | -0.7304 | 1.4178 |
| C | -3.2861 | -1.4087 | 0.1673 |
| H | -2.8457 | -1.9514 | 1.0013 |
| H | -3.1555 | -2.0104 | -0.7364 |
| C | 2.7523 | 1.7827 | -1.2438 |
| H | 2.0806 | 1.9403 | -2.0923 |
| H | 3.3394 | 0.8806 | -1.4210 |
| C | 3.5749 | 3.0187 | -0.9427 |
| H | 4.4791 | 2.7548 | -0.3870 |
| H | 3.8731 | 3.5462 | -1.8496 |
| C | 2.6194 | 3.8146 | -0.0624 |
| H | 3.1156 | 4.5684 | 0.5495 |
| H | 1.8626 | 4.3101 | -0.6759 |
| C | 1.9746 | 2.7266 | 0.7713 |
| H | 0.9442 | 2.9401 | 1.0543 |
| H | 2.5639 | 2.4895 | 1.6646 |
| C | -0.3717 | -0.1592 | -3.2986 |
| C | -1.6618 | -0.9532 | -3.4920 |
| C | 0.7763 | -0.8529 | -4.0281 |
| H | 1.7136 | -0.3190 | -3.8569 |
| H | 0.8949 | -1.8776 | -3.6709 |
| H | 0.5873 | -0.8839 | -5.1048 |
| H | -1.5539 | -1.9528 | -3.0667 |
| H | -1.9094 | -1.0430 | -4.5535 |
| H | -2.4905 | -0.4538 | -2.9849 |
| C | -0.3650 | 0.2507 | 3.2095 |
| C | 0.8638 | -0.0635 | 4.0588 |
| C | -1.4827 | -0.7383 | 3.5310 |
| H | -2.3718 | -0.5006 | 2.9428 |
| H | -1.1711 | -1.7544 | 3.2819 |
| H | -1.7472 | -0.6963 | 4.5914 |
| H | 1.2101 | -1.0820 | 3.8714 |
| H | 0.6332 | 0.0299 | 5.1237 |
| H | 1.6760 | 0.6285 | 3.8225 |
| C | -0.5479 | 1.2571 | -3.8409 |
| H | 0.3754 | 1.8286 | -3.7262 |
| H | -0.8117 | 1.2360 | -4.9024 |
| H | -1.3310 | 1.7777 | -3.2875 |
| C | -0.8370 | 1.6740 | 3.4954 |
| H | -1.6885 | 1.9240 | 2.8603 |
| H | -1.1300 | 1.7814 | 4.5440 |

| | | | |
|---|---|---|---|
| H | -0.0409 | 2.3901 | 3.2829 |

Complex **22**

| | | | |
|---|---|---|---|
| U | -0.0067 | 1.8443 | 0.0110 |
| O | -0.0060 | 1.6544 | -1.7351 |
| O | -0.0098 | 1.6657 | 1.7575 |
| U | -0.0005 | -1.8443 | 0.0110 |
| O | -0.0019 | -1.6543 | -1.7351 |
| O | 0.0011 | -1.6657 | 1.7575 |
| H | 1.1804 | 0.0021 | 0.0165 |
| H | -1.1879 | -0.0022 | 0.0161 |
| C | 0.7037 | 4.3355 | -0.9819 |
| C | 1.1373 | 4.3045 | 0.3753 |
| C | -0.0028 | 4.3603 | 1.2074 |
| C | -1.1396 | 4.3108 | 0.3705 |
| C | -0.7003 | 4.3395 | -0.9848 |
| C | 1.5823 | 4.3449 | -2.1842 |
| H | 1.8047 | 5.3684 | -2.5042 |
| H | 1.1145 | 3.8277 | -3.0231 |
| H | 2.5413 | 3.8570 | -1.9933 |
| C | 2.5555 | 4.2994 | 0.8413 |
| H | 3.2222 | 3.8237 | 0.1181 |
| H | 2.6655 | 3.7760 | 1.7937 |
| H | 2.9293 | 5.3182 | 0.9903 |
| C | -0.0056 | 4.4458 | 2.6919 |
| H | 0.8691 | 3.9589 | 3.1254 |
| H | -0.8857 | 3.9653 | 3.1217 |
| H | -0.0025 | 5.4896 | 3.0238 |
| C | -2.5598 | 4.3135 | 0.8307 |
| H | -2.6765 | 3.7904 | 1.7825 |
| H | -3.2261 | 3.8415 | 0.1047 |
| H | -2.9286 | 5.3342 | 0.9784 |
| C | -1.5738 | 4.3540 | -2.1908 |
| H | -1.7855 | 5.3788 | -2.5142 |
| H | -2.5380 | 3.8754 | -2.0026 |
| H | -1.1074 | 3.8305 | -3.0266 |
| C | -1.1362 | -4.3085 | 0.3753 |
| C | 0.0040 | -4.3603 | 1.2074 |
| C | 1.1407 | -4.3067 | 0.3705 |
| C | 0.7015 | -4.3370 | -0.9848 |
| C | -0.7025 | -4.3379 | -0.9819 |
| C | -2.5545 | -4.3084 | 0.8414 |
| H | -2.9246 | -5.3284 | 0.9907 |
| H | -3.2228 | -3.8352 | 0.1179 |
| H | -2.6663 | -3.7850 | 1.7935 |
| C | 0.0071 | -4.4459 | 2.6919 |
| H | -0.8699 | -3.9631 | 3.1254 |
| H | 0.8849 | -3.9612 | 3.1219 |
| H | 0.0090 | -5.4896 | 3.0238 |

| | | | |
|---|---|---|---|
| C | 2.5609 | -4.3045 | 0.8308 |
| H | 2.6758 | -3.7813 | 1.7827 |
| H | 3.2255 | -3.8301 | 0.1049 |
| H | 2.9333 | -5.3240 | 0.9783 |
| C | 1.5751 | -4.3485 | -2.1907 |
| H | 2.5374 | -3.8660 | -2.0027 |
| H | 1.1066 | -3.8271 | -3.0267 |
| H | 1.7908 | -5.3725 | -2.5138 |
| C | -1.5811 | -4.3504 | -2.1842 |
| H | -1.7988 | -5.3746 | -2.5050 |
| H | -1.1156 | -3.8304 | -3.0228 |
| H | -2.5422 | -3.8669 | -1.9930 |

Complex **23**

| | | | |
|---|---|---|---|
| U | -0.0709 | -0.0038 | -0.1867 |
| H | 0.6388 | 0.0603 | 1.5741 |
| O | -0.7502 | -0.0655 | -1.8360 |
| N | -0.5361 | 2.1142 | 0.1261 |
| N | -1.4313 | -1.5129 | 0.6308 |
| N | 1.9502 | -0.5934 | -0.7997 |
| Si | -1.8747 | -2.8668 | -0.3917 |
| Si | -2.1693 | -1.3275 | 2.2053 |
| Si | 2.5589 | -0.0031 | -2.3345 |
| Si | 2.8865 | -1.7396 | 0.1307 |
| Si | 0.6046 | 3.1903 | 0.8989 |
| Si | -2.0239 | 2.7505 | -0.5504 |
| C | -3.3483 | -2.4365 | -1.4588 |
| H | -3.6440 | -3.2988 | -2.0631 |
| H | -4.2096 | -2.1345 | -0.8590 |
| H | -3.1011 | -1.6181 | -2.1385 |
| C | -0.4325 | -3.3259 | -1.4994 |
| H | 0.8671 | -2.8436 | 1.1972 |
| H | -0.7595 | -4.1236 | -2.1733 |
| H | -0.0726 | -2.5068 | -2.1236 |
| C | -2.2527 | -4.4197 | 0.5932 |
| H | -3.0859 | -4.3099 | 1.2887 |
| H | -2.5126 | -5.2169 | -0.1100 |
| H | -1.3787 | -4.7519 | 1.1587 |
| C | -3.3648 | 1.4405 | -0.4895 |
| H | -3.1066 | 0.5195 | -1.0146 |
| H | -3.6337 | 1.1882 | 0.5385 |
| H | -4.2608 | 1.8449 | -0.9700 |
| C | -1.7713 | 3.2758 | -2.3272 |
| H | -1.4979 | 2.4157 | -2.9430 |
| H | -2.6941 | 3.7001 | -2.7326 |
| H | -0.9849 | 4.0277 | -2.4216 |
| C | -2.7013 | 4.1967 | 0.4371 |
| H | -3.6304 | 4.5292 | -0.0358 |
| H | -2.9417 | 3.8979 | 1.4602 |

| | | | |
|---|---|---|---|
| H | -2.0292 | 5.0545 | 0.4823 |
| C | 0.0198 | 3.7381 | 2.5906 |
| H | -0.8845 | 4.3464 | 2.5486 |
| H | -0.1829 | 2.8753 | 3.2290 |
| H | 0.8022 | 4.3340 | 3.0703 |
| C | 2.2641 | 2.3506 | 1.1663 |
| H | 2.2370 | 1.6709 | 2.0201 |
| H | 2.6365 | 1.7901 | 0.3067 |
| H | 2.9977 | 3.1327 | 1.3865 |
| C | 0.9197 | 4.7030 | -0.1673 |
| H | 1.6366 | 5.3610 | 0.3323 |
| H | 1.3410 | 4.4215 | -1.1354 |
| H | 0.0152 | 5.2841 | -0.3560 |
| C | 4.3505 | -0.9297 | 0.9700 |
| H | 4.0261 | -0.0979 | 1.5997 |
| H | 4.8515 | -1.6603 | 1.6121 |
| H | 5.0860 | -0.5490 | 0.2603 |
| C | 1.8597 | -2.5085 | 1.5027 |
| H | 0.4073 | -3.7150 | -0.9203 |
| H | 2.4020 | -3.3858 | 1.8697 |
| H | 1.7346 | -1.8210 | 2.3411 |
| C | 3.4948 | -3.1443 | -0.9562 |
| H | 4.0725 | -3.8501 | -0.3523 |
| H | 2.6590 | -3.6898 | -1.4001 |
| H | 4.1378 | -2.8036 | -1.7697 |
| C | 4.4295 | 0.1565 | -2.3545 |
| H | 4.7733 | 0.8769 | -1.6086 |
| H | 4.9548 | -0.7845 | -2.1858 |
| H | 4.7310 | 0.5299 | -3.3379 |
| C | 1.9094 | 1.7280 | -2.6483 |
| H | 2.2425 | 2.0475 | -3.6403 |
| H | 0.8205 | 1.7998 | -2.6376 |
| H | 2.3102 | 2.4420 | -1.9253 |
| C | 2.0207 | -1.1170 | -3.7368 |
| H | 2.3562 | -2.1460 | -3.5908 |
| H | 0.9320 | -1.1215 | -3.8248 |
| H | 2.4334 | -0.7589 | -4.6842 |
| C | -4.0316 | -1.5421 | 2.0991 |
| H | -4.4779 | -0.7893 | 1.4450 |
| H | -4.3255 | -2.5238 | 1.7236 |
| H | -4.4708 | -1.4242 | 3.0941 |
| C | -1.4766 | -2.5443 | 3.4476 |
| H | -1.6955 | -3.5814 | 3.1904 |
| H | -0.3925 | -2.4381 | 3.5311 |
| H | -1.9094 | -2.3458 | 4.4328 |
| C | -1.8539 | 0.3812 | 2.9180 |
| H | -2.5317 | 0.5127 | 3.7678 |
| H | -0.8322 | 0.4784 | 3.2891 |
| H | -2.0357 | 1.2040 | 2.2249 |

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