Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Carbodiphosphorane-based nickel pincer complexes and their (de)protonated analogues: dimerisation, ligand tautomers and proton affinities

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1. Syntheses

1.1 Materials and Methods

All experiments were carried out under an atmosphere of purified argon or nitrogen in the MBraun glove boxes LABmaster 130 and UNIlab or using standard Schlenk techniques.

THF and diethyl ether were dried over Na/K alloy, *n*-hexane was dried over $LiAlH_4$, toluene was dried over sodium and dichloromethane was dried over CaH_2. Deuterated solvents were sparged with argon and stored over molecular sieves.

1 was obtained following the reported procedure by REITSAMER *et al.*[1]

^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded using Bruker AVANCE 300 A, DRX 400, DRX 500 and Avance 500 NMR spectrometers at 300 K. ^{1}H and $^{13}C\{^{1}H\}$, ^{13}C-APT (attached proton test) NMR chemical shifts are reported in ppm downfield from tetramethylsilane. The resonance of the residual protons in the deuterated solvent was used as internal standard for ^{1}H NMR. The solvent peak of the deuterated solvent was used as internal standard for ^{13}C NMR. ^{31}P NMR chemical shifts are reported in ppm downfield from H_3PO_4 and referenced to an external 85 % solution of phosphoric acid in D_2O. The following abbreviations are used for the description of NMR data: br (broad), s (singlet), d (doublet), t (triplet), q (quartet), quin (quintet), m (multiplet), v (virtual).

FT-IR spectra were recorded by attenuated total reflection of the solid samples on a Bruker Tensor IF37 spectrometer. The intensity of the absorption band is indicated as w (weak), m (medium), s (strong), vs (very strong) and br (broad).

HR-ESI mass spectra were acquired with a LTQ-FT mass spectrometer (Thermo Fisher Scientific). HR-APCI mass spectra were acquired with a LTQ-FT mass spectrometer (Thermo Fisher Scientific). In both cases the resolution was set to 100.000. Elemental analyses were performed on a Vario Micro Cube Elemental Analyzer.

None of the compounds have been characterised by elemental analysis.

1.2 *Synthesis of Complex* **2**

To a suspension of 100 mg **1** (110 µmol, 1.0 eq.) in 10 ml diethyl ether, 0.15 ml of a solution of $HBF_4 \cdot OEt_2$ in diethyl ether (109 µmol, 1.0 eq.) were added. After stirring for 16 h, the solvent was removed *in vacuo* and the remaining orange solid was dissolved in 10 ml DCM. After filtration, layering of the solution with *n*-hexane yields 72 mg **2** (68.6 µmol, 62 %) as orange crystals.

Due to the low solubility of **2** in CD_2Cl_2 and MeCN-d_3 and its decomposition in DMSO-d_6 and D_3COD, the resonances of the bridging CH and CH_2 carbons could not be observed in 1D spectra and were assigned via 2D crosspeaks.

^{1}H NMR (300 MHz, CD_2Cl_2) δ_H: 4.39 – 4.05 (4H, m, C*H*$_2$), 4.37 (1H, t, $^2J_{H,P}$ = 18.7 Hz, P-C*H*-P), 7.75 – 7.11 (m, 32H, Phenyl-*H*), 7.83 (vq, 4H, *J* = 6.4 Hz, Phenyl-*H*), 7.91 (vq, 4H, *J* = 6.6 Hz, Phenyl-*H*) ppm.

^{13}C APT NMR (75 MHz, CD_2Cl_2) δ_C: 8.8 (P-*C*H-P), 31.5 (P-*C*H$_2$-P), 129.4 (vt, $J_{C,P}$ = 5.6 Hz, Phenyl-*C*), 130.3 (d, $J_{C,P}$ = 4.6 Hz, Phenyl-*C*), 130.4 (d, $J_{C,P}$ = 3.9 Hz, Phenyl-*C*), 133.0 – 132.7 (m, Phenyl-*C*), 133.3 (d, $J_{C,P}$ = 11.5 Hz, Phenyl-*C*), 133.8 (vt, $J_{C,P}$ = 6.4 Hz, Phenyl-*C*), 134.1 (vt, $J_{C,P}$ = 6.1 Hz, Phenyl-*C*), 135.0 (d, $J_{C,P}$ = 1.8 Hz, Phenyl-*C*), 135.8 (s, Phenyl-*C*) ppm.

^{31}P{^{1}H} NMR (121 MHz, CD_2Cl_2) δ_P: 6.1 (t, $^2J_{P,P}$ = 42.5 Hz), 43.6 (t, $^2J_{P,P}$ = 42.5 Hz) ppm.

FT-IR (ATR) $\tilde{}$/cm^{-1}: 3061 (w), 2972 (w), 2914 (w), 2325 (w), 1587 (w), 1485 (w), 1437 (s), 1367 (w), 1339 (w), 1314 (w), 1284 (w), 1191 (w), 1144 (m), 1098 (vs), 1050 (vs), 996 (vs), 884 (m), 838 (w), 783 (m), 732 (vs), 684 (vs), 643 (m), 578 (w), 525 (s), 506 (m), 489 (m), 470 (s).

ESI-MS (+) / : 873 (15%, M - H$^+$), 782 (100, M - NiClHR-ESI-MS (+) / : 873.1430 (calc. for [M] - H$^+$), 873.1436 (found, Δ = 0.7 ppm)

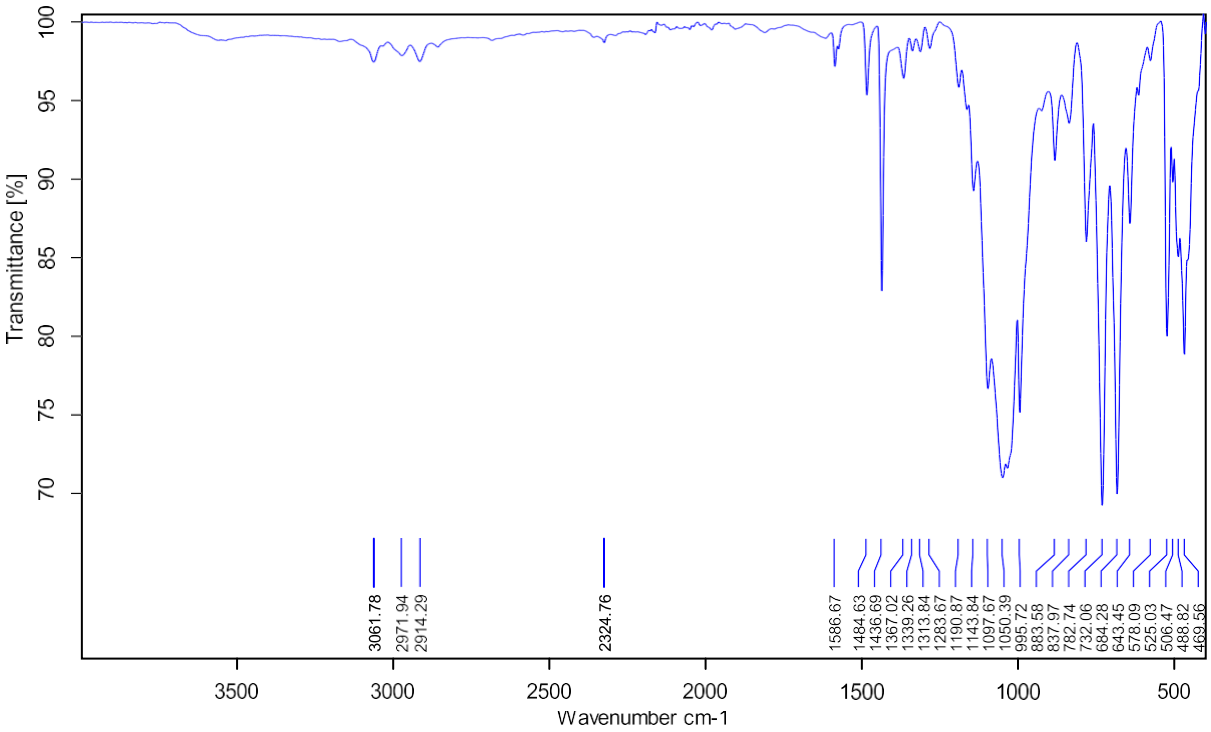


Figure 1- FT-IR spectrum of complex 2.

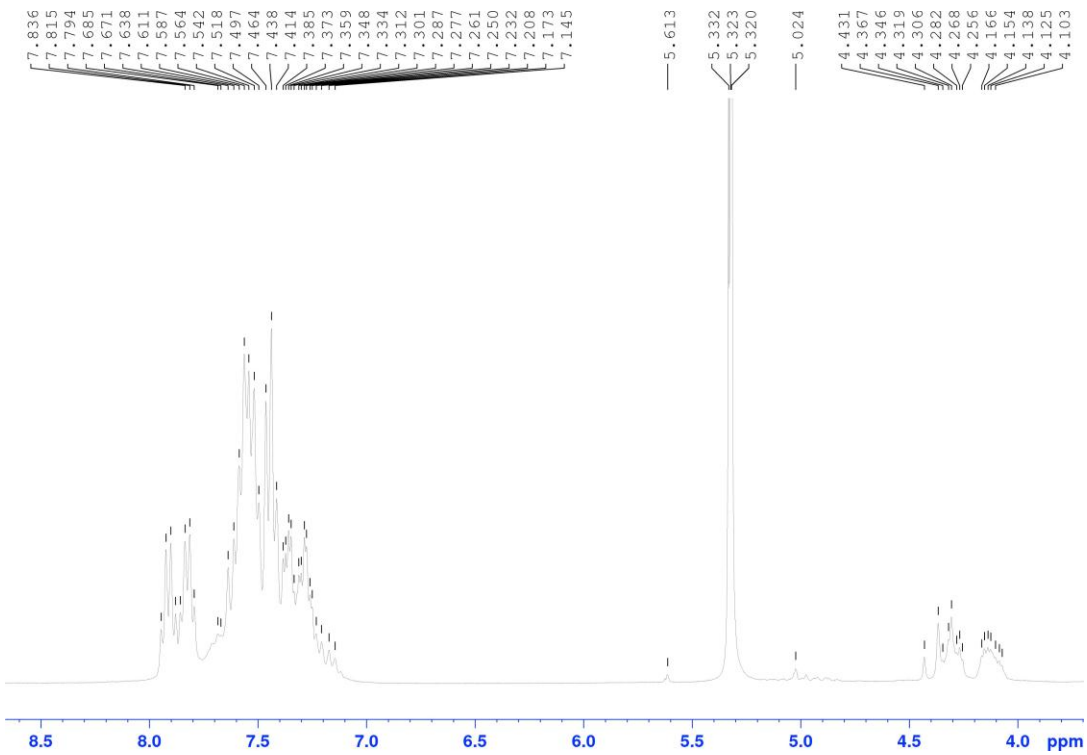


Figure 2 - ^{1}H NMR spectrum of complex 2 in CD_2Cl_2.

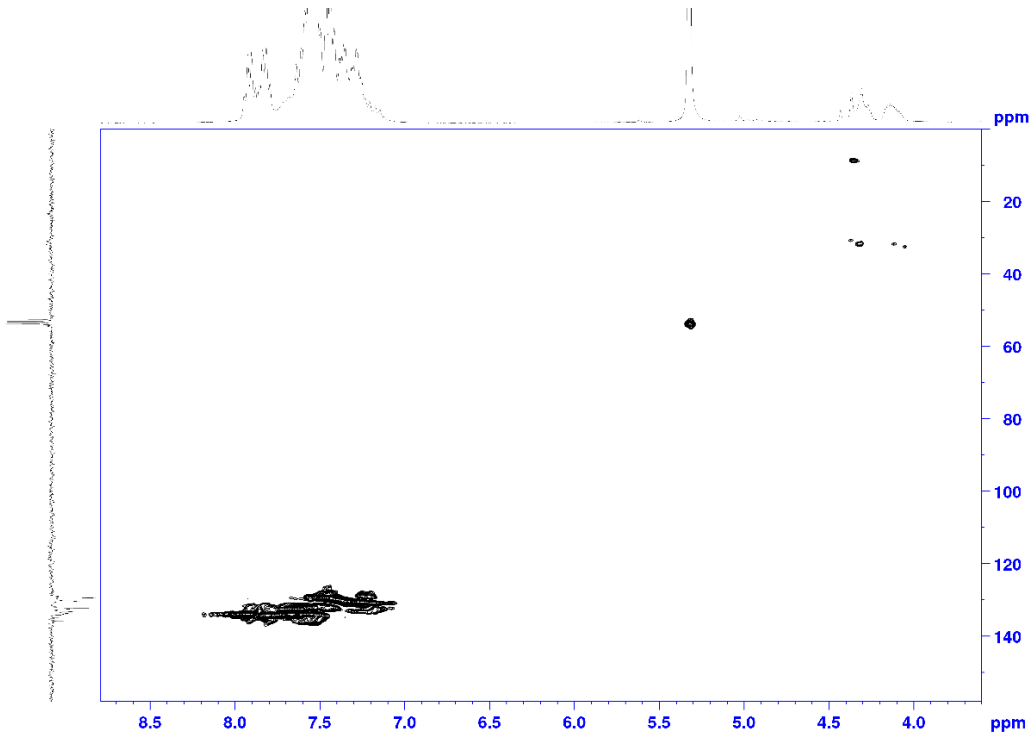


Figure 3 - $^{1}H,^{13}C$ HMQC NMR spectrum of complex 2 in CD_2Cl_2.

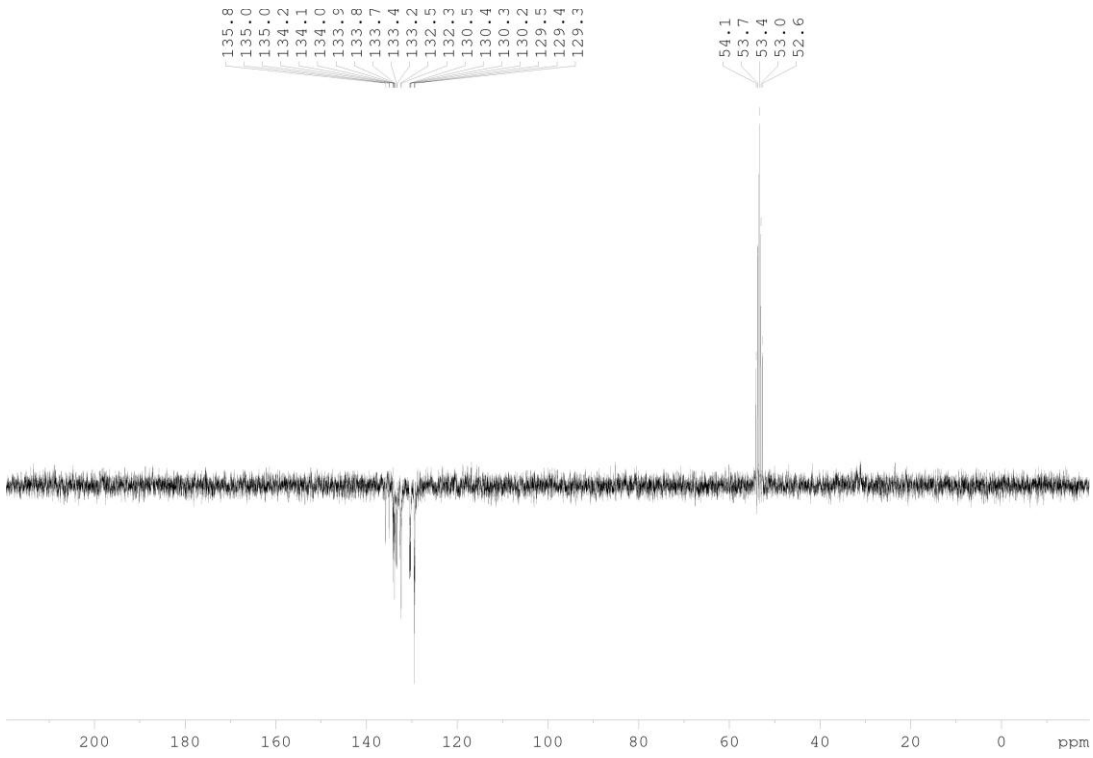


Figure 4 - ^{13}C APT NMR spectrum of complex 2 in CD_2Cl_2.

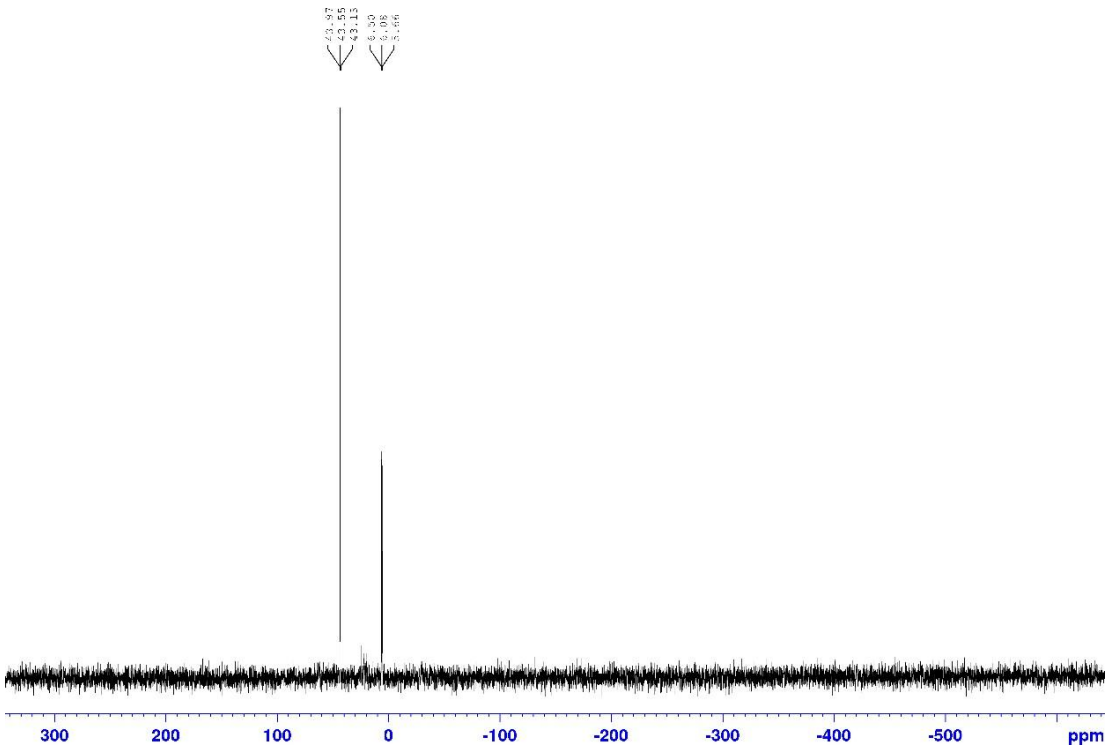


Figure 5 - $^{31}P\{^1H\}$ NMR spectrum of complex 2 in CD_2Cl_2.

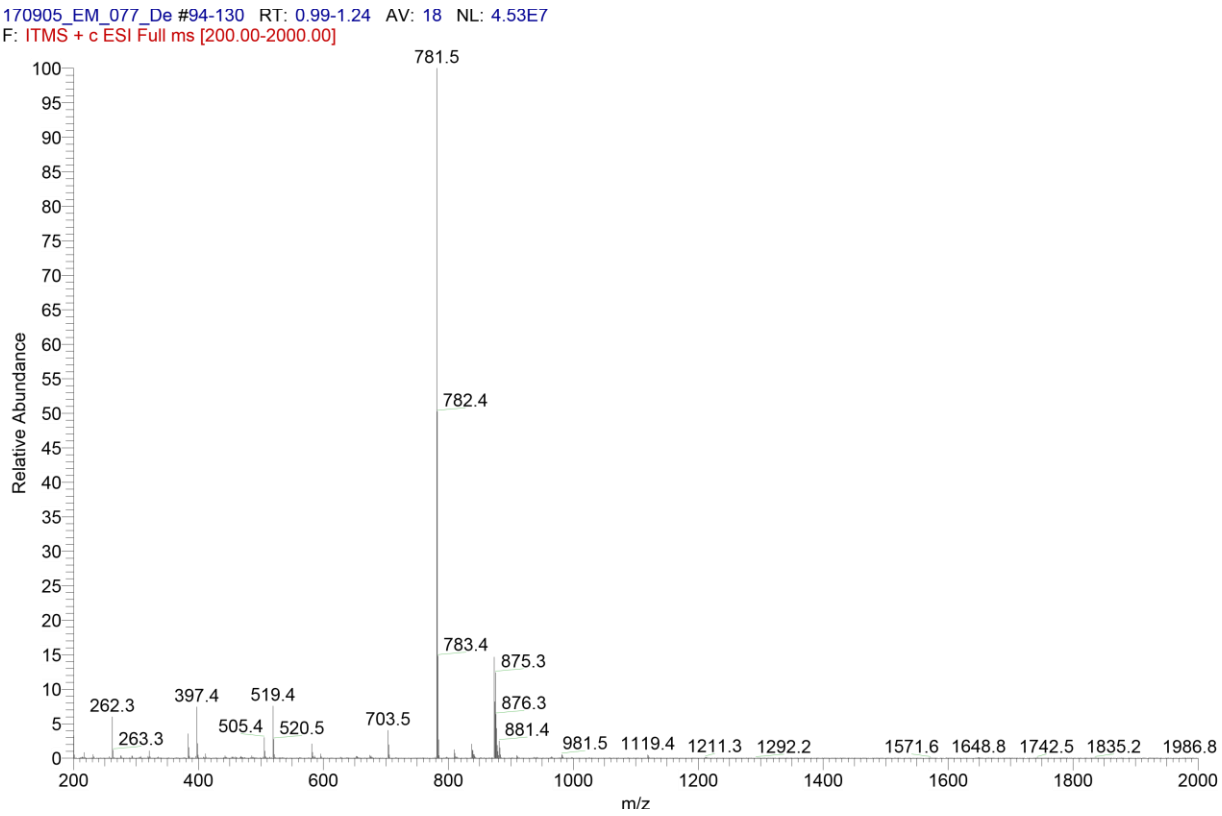


Figure 6 - ESI(+) MS spectrum of complex 2.

1.3 Synthesis of Complex **3**

200 mg **1** (220 µmol, 0.9 eq.) and 41 mg LiHMDS (245 µmol, 1.0 eq.) were dissolved in 20 ml THF and stirred for 16 h. After removal of the solvent in vacuo, the remaining dark brown solid was extracted with 20 ml of toluene. Removal of the solvent in vacuo yielded 120 mg (137 µmol, 56 %) **3** as dark red powder.

Crystals suitable for single-crystal X-ray diffraction measurements were obtained by layering a solution of **3** in THF with *n*-hexane and storing it at 4 °C.

Due to low solubility in most deuterated solvents (e.g. C_6D_6, CD_2Cl_2,...), NMR measurements were carried out in DMSO-d_6. **3** is only stable for a limited amount of time in DMSO-d_6 and shows decomposition to **1** and free ligand.

^{1}H NMR (300 MHz, DMSO-d_6) δ_H: 1.34 (1H, ddvt, $J_{H,P}$ = 16.5 Hz, $J_{H,P}$ = 5.2 Hz, $J_{H,P}$ = 2.4 Hz, P-C*H*-P), 3.46 (vt, 2H, $^2J_{H,P}$ = 9.3 Hz, P-CH_2-P), 6.90 - 7.07 (8H, m, Phenyl-*H*), 7.12 - 7.42 (24H, m, Phenyl-*H*), 7.67 - 7.77 (4H, m, Phenyl-*H*), 7.84 - 7.94 (4H, m, Phenyl-*H*) ppm.

^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ_C: 24.2 (s, P-*C*H-P), 36.8 (d, $^1J_{C,P}$ = 148.7 Hz, P-*C*H_2-P), 127.1 (d, $J_{C,P}$ = 6.7 Hz, Phenyl-*C*), 127.7 (d, $J_{C,P}$ = 13.2 Hz, Phenyl-*C*), 127.7 (s, Phenyl-*C*), 128.3 (d, $J_{C,P}$ = 14.8 Hz, Phenyl-*C*), 128.7 (s, Phenyl-*C*), 129.7 (s, Phenyl-*C*), 129.9 (s, Phenyl-*C*), 130.5 – 130.8 (m Phenyl-*C*), 131.1 (s, Phenyl-*C*), 131.2 (s, Phenyl-*C*), 131.9 (s, Phenyl-*C*), 132.0 (s, Phenyl-*C*), 132.3 (d, $J_{C,P}$ = 10.9 Hz, Phenyl-*C*), 132.6 (d, $J_{C,P}$ = 6.2 Hz, Phenyl-*C*), 133.4 (d, $J_{C,P}$ = 23.5 Hz, Phenyl-*C*), 139.0 (s, Phenyl-*C*), 141.7 (s, Phenyl-*C*) ppm.

^{31}P{^{1}H} NMR (101 MHz, C_6D_6) δ_P: 10.4 (ddd, $J_{P,P}$ = 42.6, 82.5, 348.1 Hz), 17.0 (ddd, $J_{P,P}$ = 28.1, 52.7, 81.8 Hz), 25.0 (ddd, $J_{P,P}$ = 27.1, 143.6, 348.3 Hz), 45.0 (ddd, $J_{P,P}$ = 40.7, 52.5, 144.0 Hz) ppm.

^{31}P{^{1}H} NMR (101 MHz, DMSO-d_6) δ_P: 10.3 (ddd, $J_{P,P}$ = 39.5, 84.1, 338.9 Hz), 20.7 (ddd, $J_{P,P}$ = 25.7, 52.0, 83.6 Hz), 23.8 (ddd, $J_{P,P}$ = 25.2, 147.8, 339.1 Hz), 44.8 (ddd, $J_{P,P}$ = 39.4, 52.0, 147.6 Hz) ppm.

FT-IR (ATR) $\tilde{}$/cm^{-1}: 3045 (w), 2321 (w), 1585 (w), 1480 (w), 1433 (m), 1377 (w), 1306 (w), 1184 (w), 1131 (m), 1092 (s), 1025 (w), 998 (w), 911 (m), 856 (m), 798 (m), 739 (vs), 689 (vs), 529 (m), 496 (vs), 475 (s), 441 (m), 416 (w).

ESI-MS (+) /: 873 (100%, $[M]H^+$), 782 (17, $[M]H_2^+$ - $NiCl^+$), 704 (28, $[M]H^+$ - PhNiCl).

HR-ESI-MS (+) /: 873.1430 (calc. for $[M]H^+$), 873.1432 (found, Δ = 0.2 ppm).

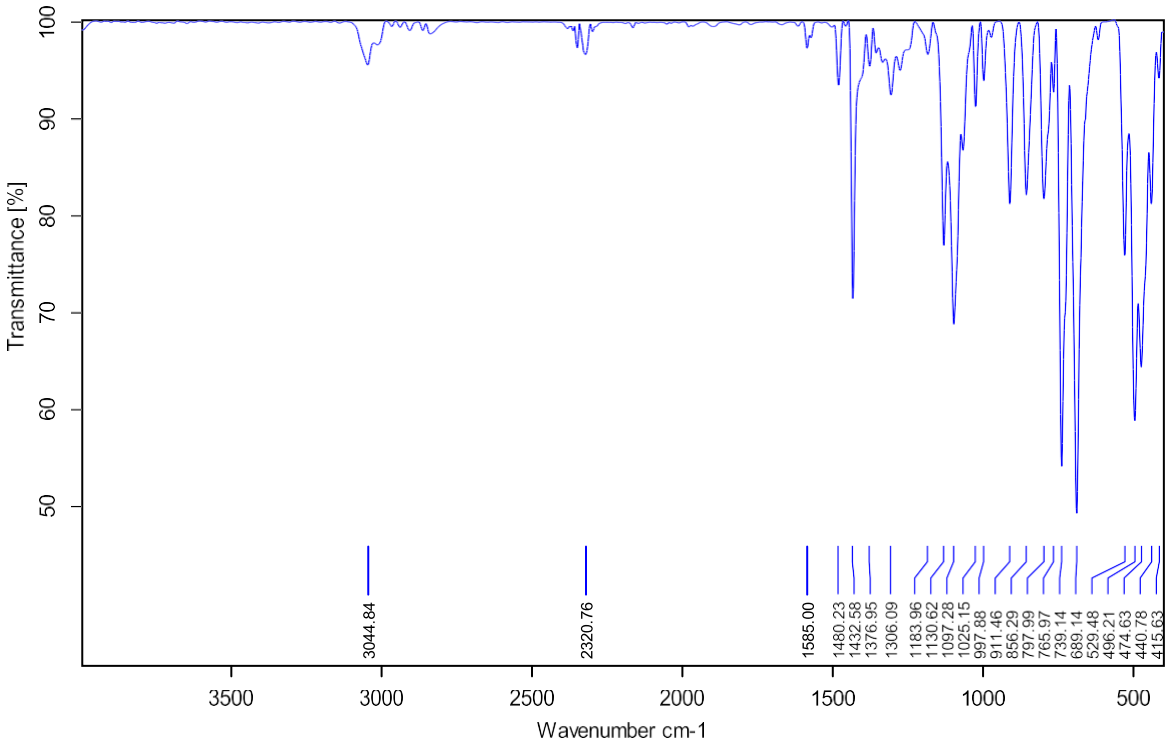


Figure 7 - FT-IR spectrum of complex 3.

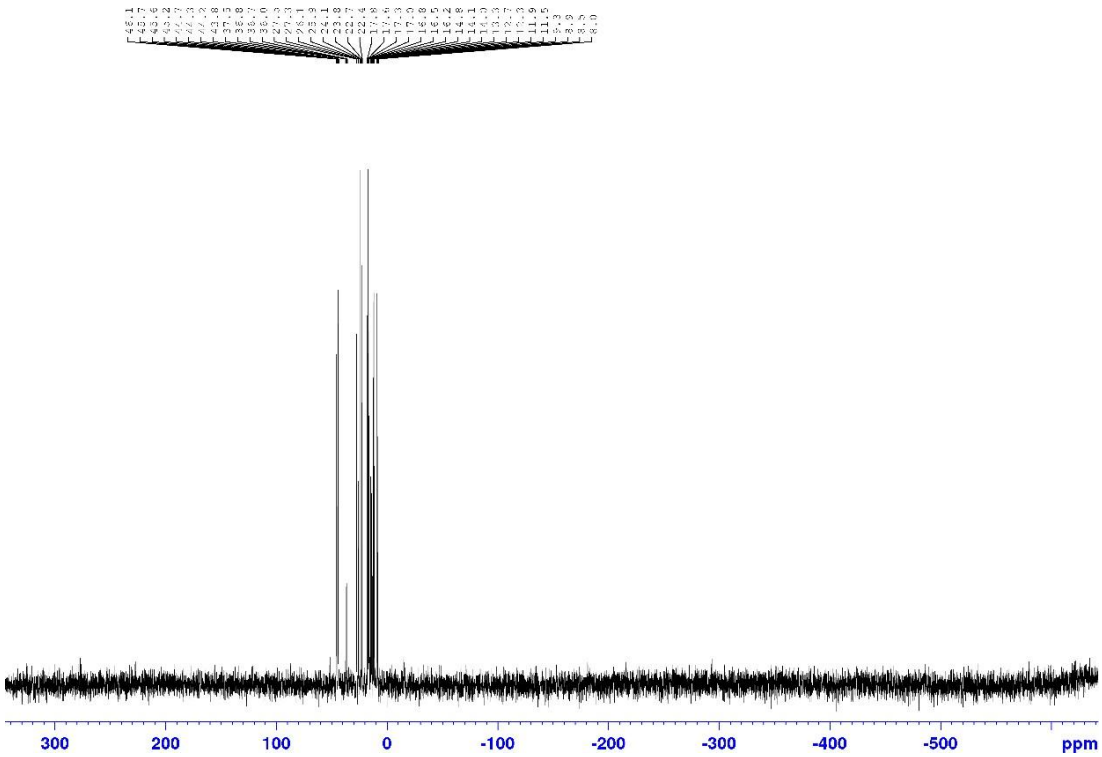


*Figure 8 - $^{31}P\{^{1}H\}$ NMR spectrum of complex **3** in C_6D_6.*

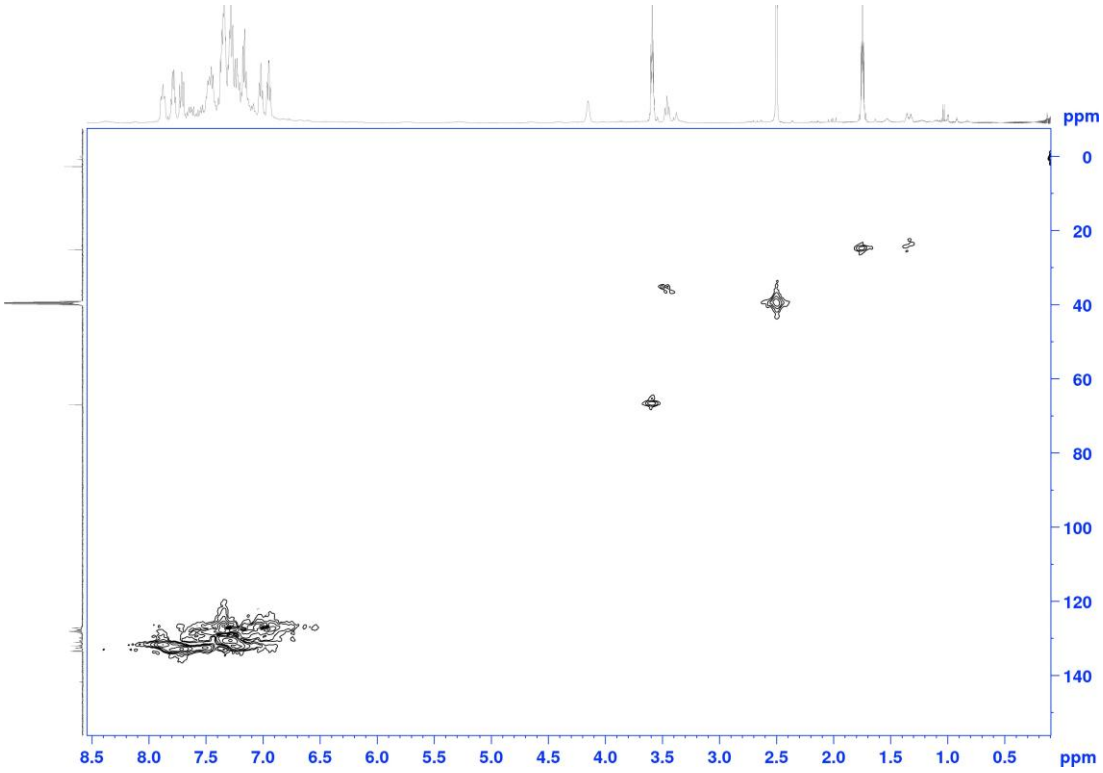


*Figure 9 - $^{1}H,^{13}C$ HMQC NMR spectrum of complex **3** in DMSO-d_6.*

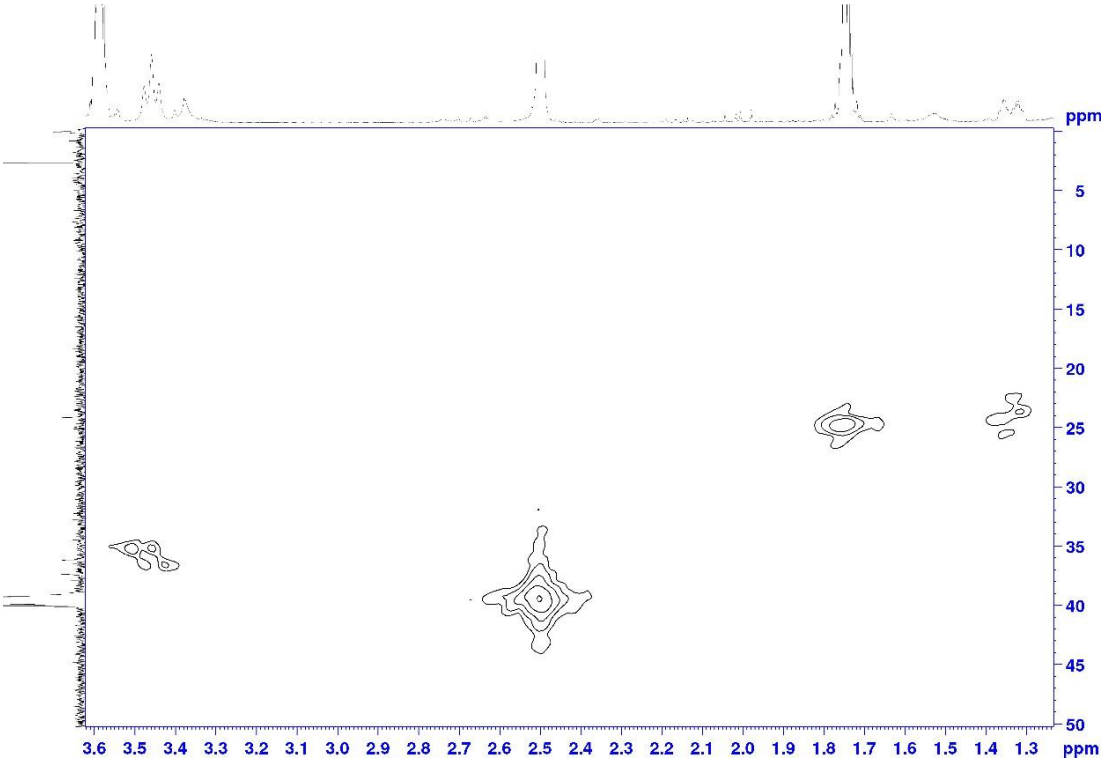


*Figure 10 – Detail of the $^{1}H,^{13}C$ HMQC NMR spectrum of complex **3** in DMSO-d_6, area of PCHP and PCH_2P resonances.*

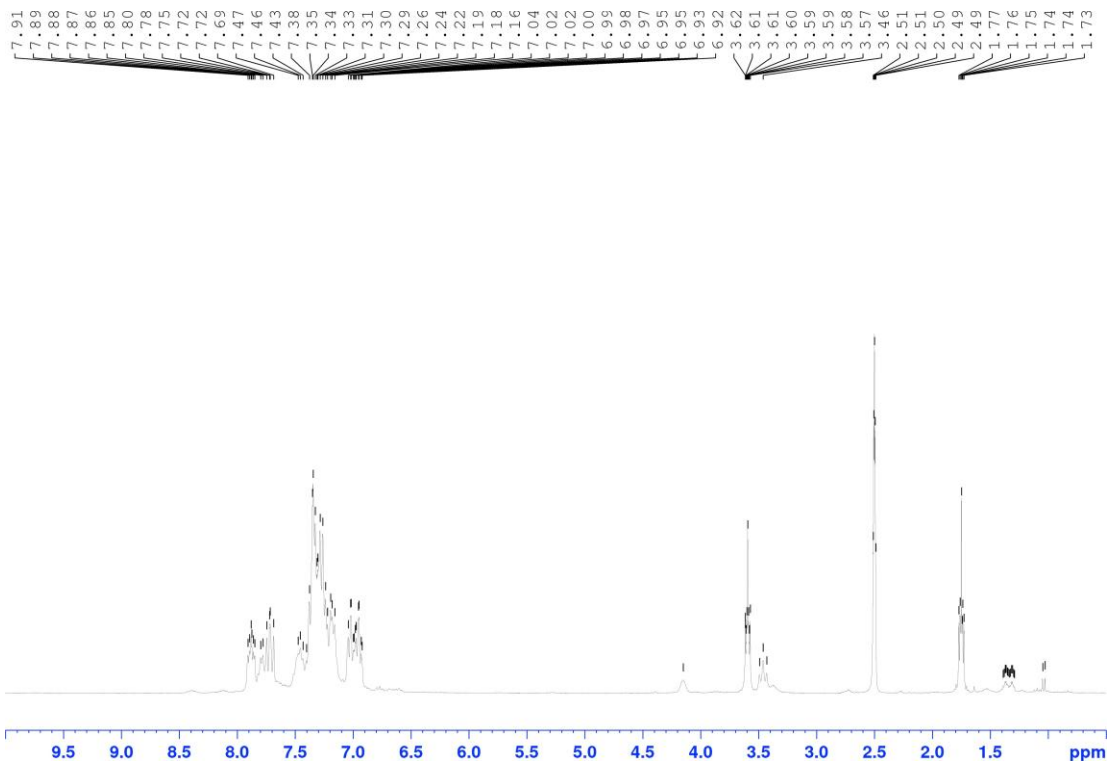


*Figure 11 - ^{1}H NMR spectrum of complex **3** in DMSO-d_6.*

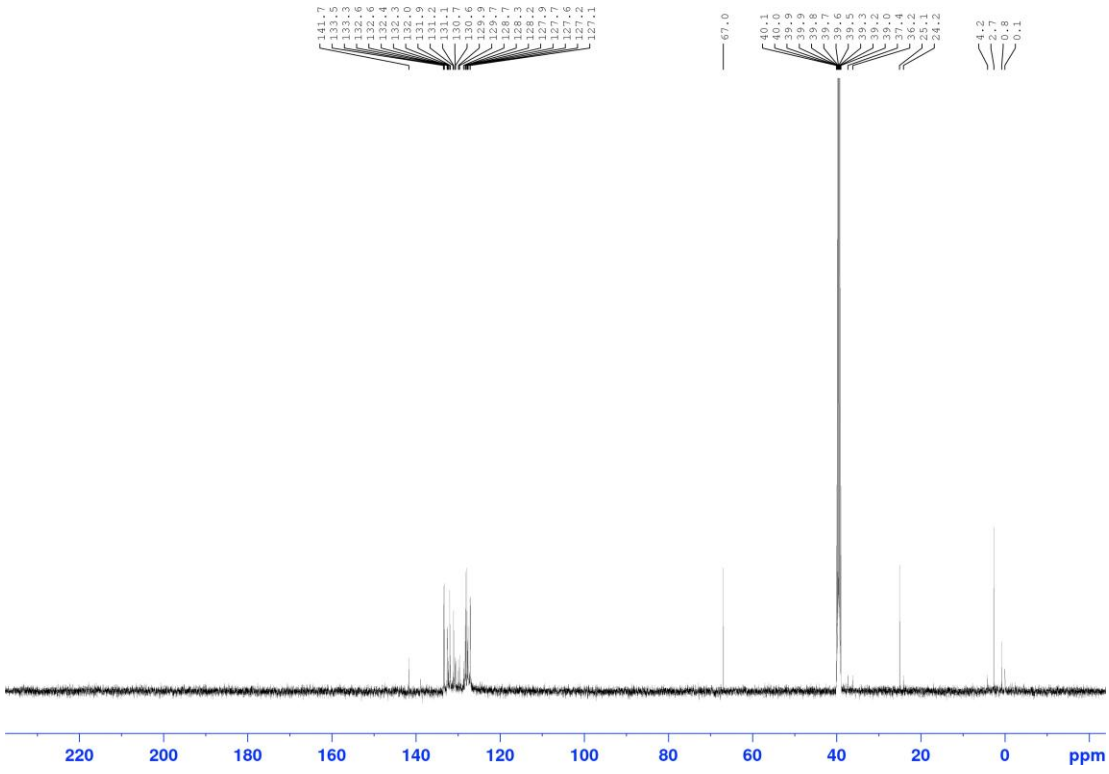


*Figure 12 - $^{13}C\{^{1}H\}$ NMR spectrum of complex **3** in DMSO-d_6.*

1.4 Synthesis of Complex **4**

488 mg **1** (536 µmol, 1.0 eq.) was suspended in 50 ml toluene and 10 ml of a solution of $AlMe_3$ in toluene (163 mmol/L, 1.79 mmol, 3.0 eq.) was added dropwise. After stirring for 15 h, the solvent was evaporated, the solids dissolved in 100 ml THF and filtered. Removal of the solvent *in vacuo* yielded 480 mg **4** (490 µmol, 91 %) as a dark orange solid.

The resonances of the bridging CH and CH_2 carbons could not be observed in 1D spectra and were assigned via 2D crosspeaks.

^{1}H NMR (300 MHz, CD_2Cl_2) δ_H: -0.78 (6H, s, $AlCl_2(CH_3)_2$), -0.74 (3H, t, $^{3}J_{H,P}$ = 9.6 Hz, Ni-CH_3), 3.81 (4H, vq, $^{2}J_{C,P}$ = 4.0 Hz, P-CH_2-P), 7.12 - 7.21 (8H, m, Phenyl-*H*), 7.24 - 7.34 (8H, m, Phenyl-*H*), 7.34 - 7.42 (12H, m, Phenyl-*H)*, 7.43 - 7.53 (12H, m, Phenyl-*H*) ppm.

^{13}C APT NMR (75 MHz, CD_2Cl_2) δ_C: -7.3 (Ni-CH_3), 45.7 (P-CH_2-P), 129.1 (t, $J_{C,P}$ = 5.8 Hz, Phenyl-*C*), 129.3 (t, $J_{C,P}$ = 5.0 Hz, Phenyl-*C*), 131.3 (t, $J_{C,P}$ = 1.1 Hz, Phenyl-*C*), 132.3 (t, $J_{C,P}$ = 1.7 Hz, Phenyl-*C*), 132.5 (t, $J_{C,P}$ = 5.0 Hz, Phenyl-*C*), 133.6 (t, $J_{C,P}$ = 6.4 Hz, Phenyl-*C*) ppm.

^{31}P{^{1}H} NMR (121 MHz, CD_2Cl_2) δ_P: 27.5 (t, $^{2}J_{P,P}$ = 53.5 Hz), 31.8 (t, $^{2}J_{P,P}$ = 53.4 Hz) ppm.

FT-IR (ATR) $\tilde{}$/cm^{-1}: 3057 (w), 2926 (w), 1587 (w), 1574 (w), 1484 (w), 1436 (s), 1362 (w), 1307 (w), 1261 (w), 1173 (m), 1099 (vs), 1025 (m), 999 (m), 816 (m), 774 (s), 760 (m), 735 (vs), 718 (s), 688 (vs), 668 (vs), 572 (m), 528 (m), 495 (s), 481 (s), 471 (s), 443 (m), 422 (w). JHV-8

ESI-MS (+) *m/z*: 874 (100%, $[M]ClH^+$ - Me^-), 798 (23, $[M]OH^+$ - $NiMe^+$), 704 (26, $[M]H^+$ - PhNiMe).

HR-ESI-MS (+) *m/z*: 873.1430 (calc. for $[M]ClH^+$ - Me^-), 873.1432 (found, Δ = 0.2 ppm).

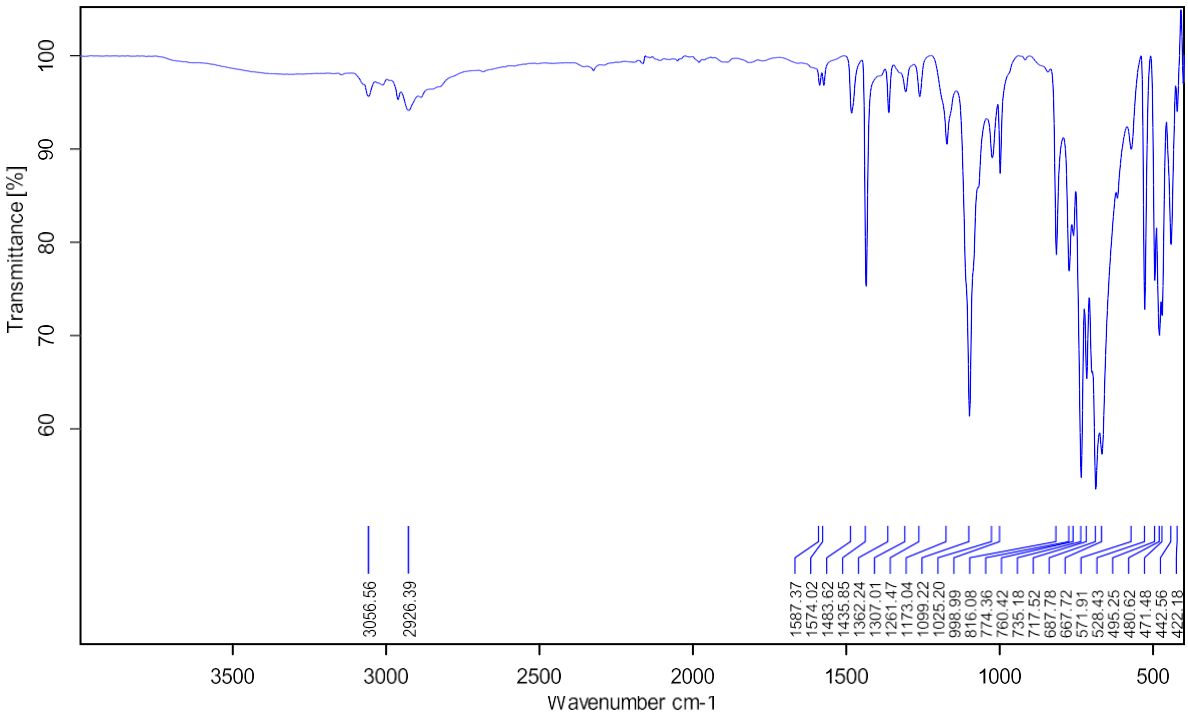


Figure 13 - FT IR spectrum of complex ***4****.*

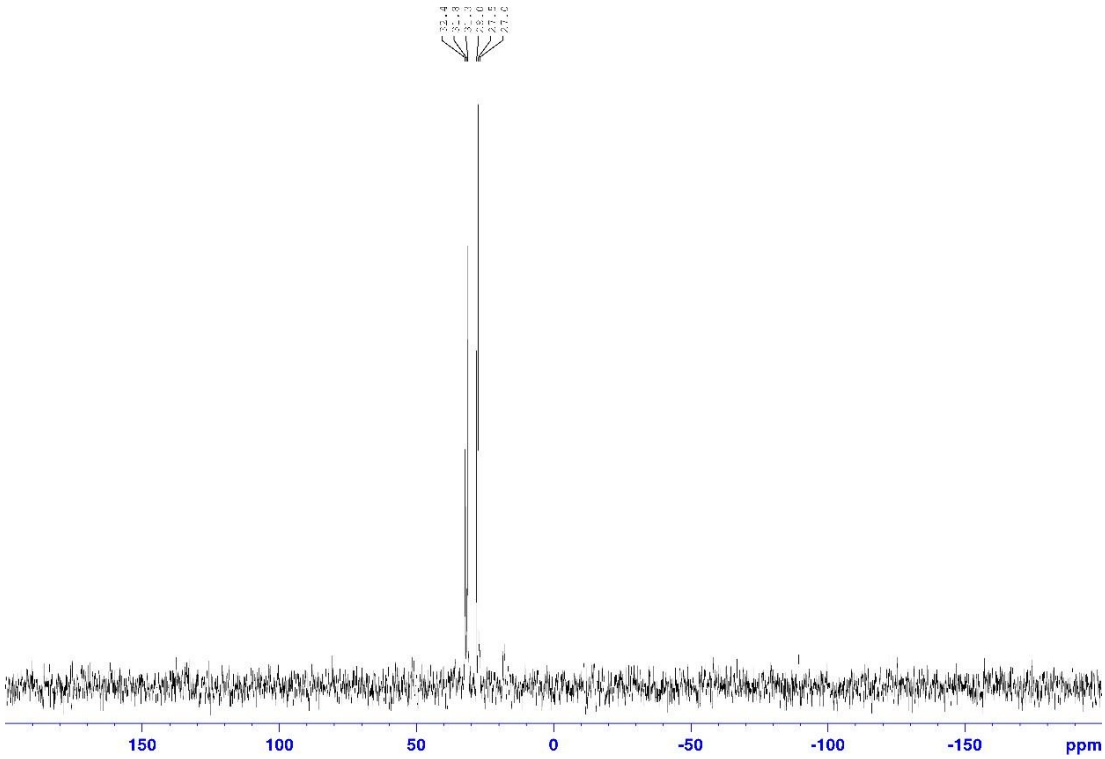


*Figure 14 – $^{31}P\{^{1}H\}$ NMR spectrum of complex **4** in CD_2Cl_2.*

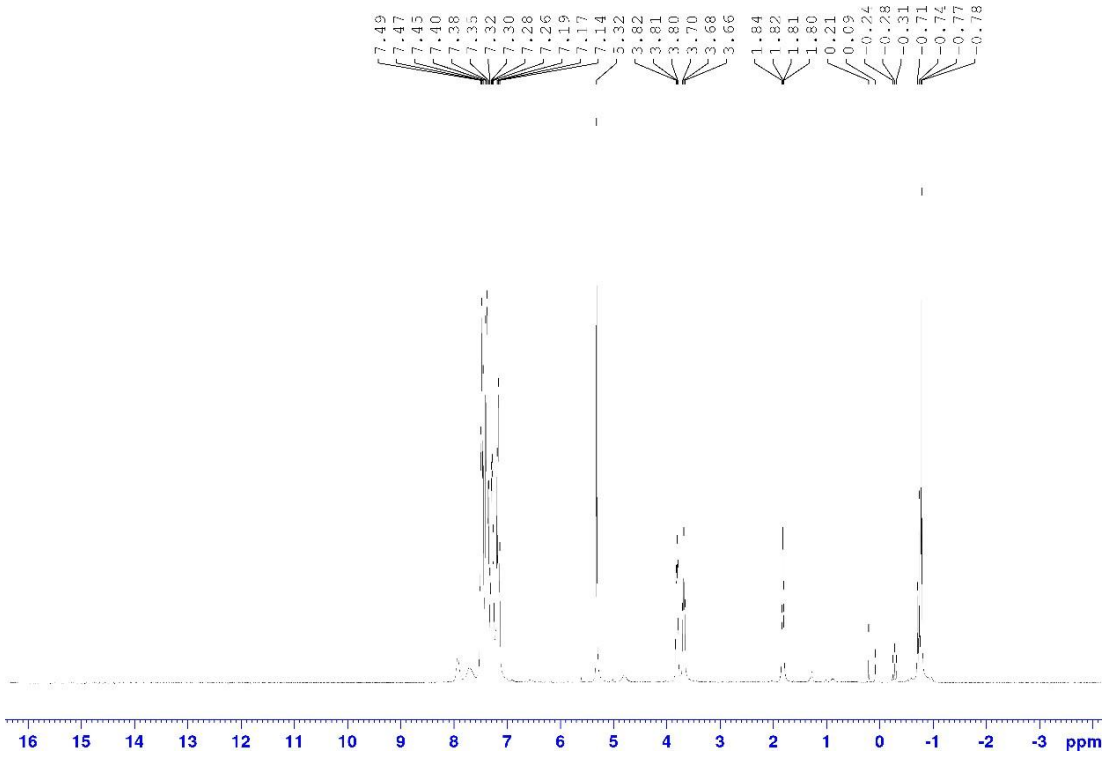


*Figure 15 - ^{1}H NMR spectrum of complex **4** in CD_2Cl_2.*

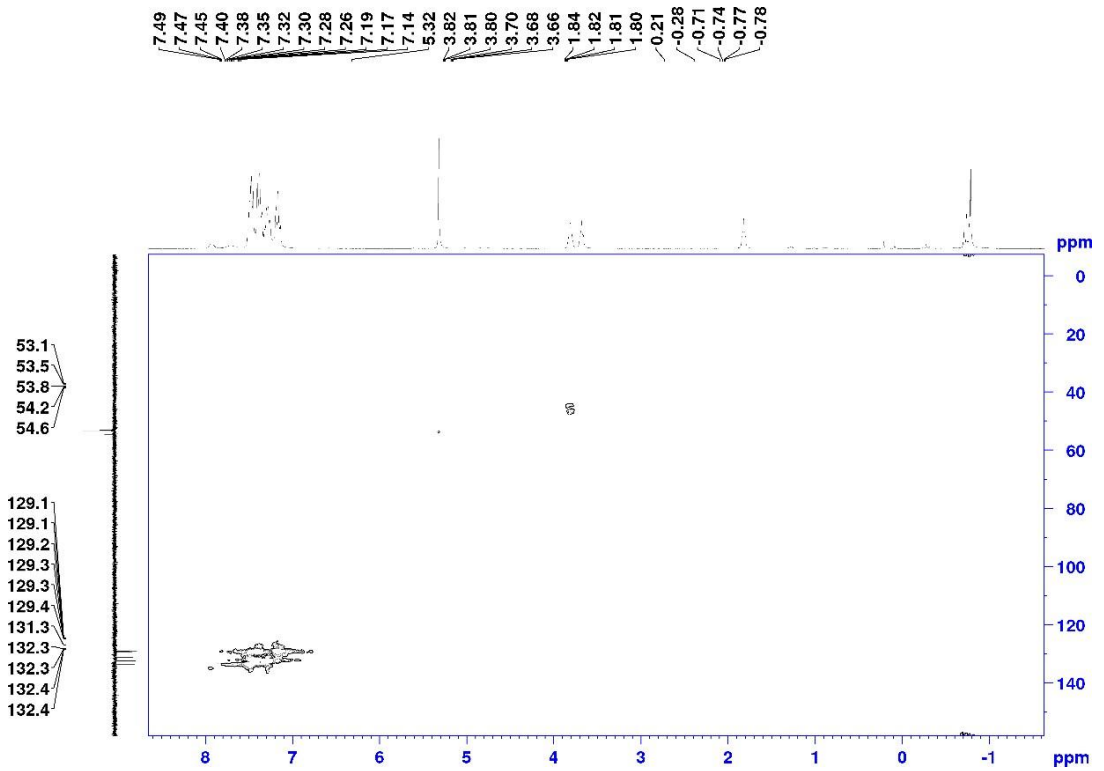


*Figure 16 - $^{1}H,^{13}C$ HMQC NMR spectrum of complex **4** in CD_2Cl_2.*

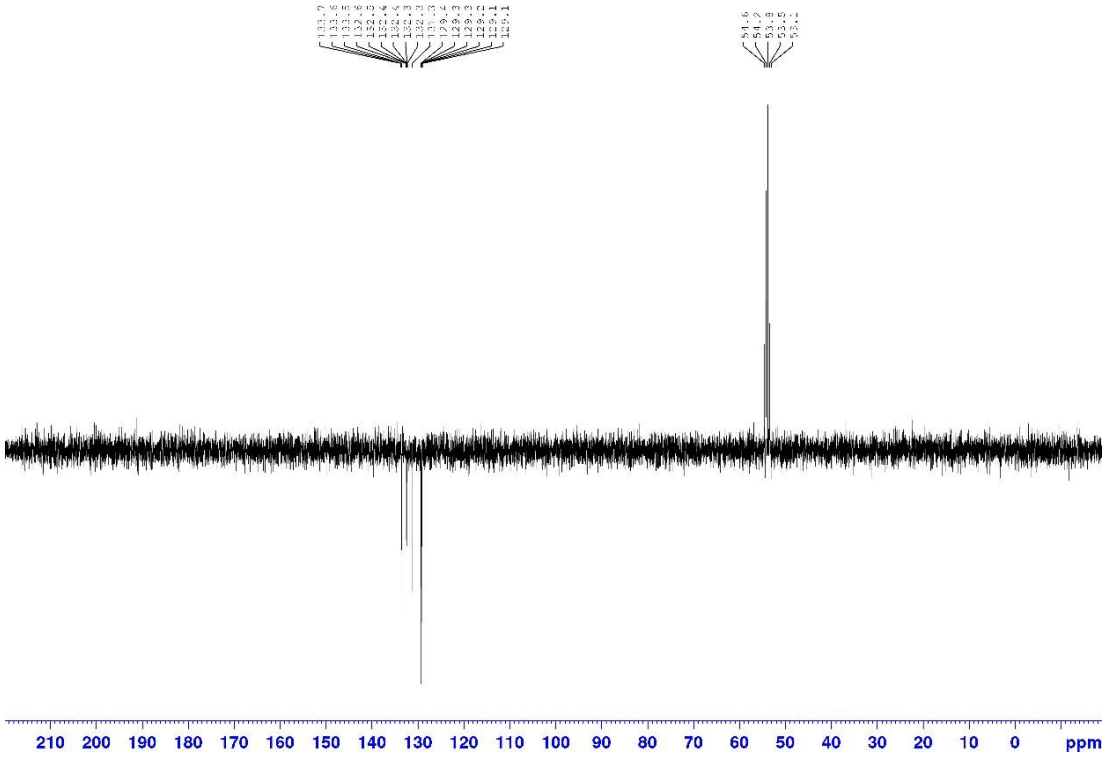


*Figure 17 - $^{13}C\{^{1}H\}$ NMR spectrum of complex **4** in CD_2Cl_2.*

1.5 *Synthesis of Complex* **5**

770 mg **1** (846 µmol, 1.0 eq.) and 460 mg LiHMDS (2.75 mmol, 3.3 eq.) were suspended in 50 ml toluene and stirred for 16 h. The resulting red-brown solution was filtered and layered with 100 ml *n*-hexane. After 7 d at -21 °C, the solvent was decanted from the formed dark brown crystals and they were dried *in vacuo*. 428 mg **5** (60 %, 256 mol) was obtained.

Crystals suitable for single-crystal X-ray diffraction measurements were obtained by layering a solution of **5** in THF with *n*-hexane.

5 decomposes in CD_2Cl_2. For this reason, saturated solution in C_6D_6 (15 mg in 0.6 ml) was used for NMR experiments. Due to the low concentration of the solution, unambiguous assignment of ^{13}C resonances was not possible in all cases. Furthermore, selective ^{31}P decoupling of ^{1}H NMR spectra was used to identify the proton resonances corresponding to the methyl-backbone of the ligand.

^{1}H NMR (300 MHz, C_6D_6) δ_H: 1.01 (2H, ddd, $^{2}J_{H,P}$ = 4.2 Hz, $^{2}J_{H,P}$ = 4.7 Hz, , $^{2}J_{H,P}$ = 10.7 Hz, P-C*H*-P), 1.13-1.23 (2H, br m, P-C*H*-P), 6.60-7.96 (80H, superimposed resonances, Phenyl-*H*) ppm.

$^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) δ_C: 30.2 (m, P-*C*H-P), 125.5-127.8 (m, Phenyl-*C*, *meta*+*para*) 131.0-133.0 (m, Phenyl-*C*, *ortho*) ppm.

$^{31}P\{^{1}H\}$ NMR (122 MHz, C_6D_6) δ_P: 14.8 (dd, $^{2}J_{P,P}$ = 24.7, $^{2}J_{P,P}$ = 48.2 Hz), 23.6 (dd, $^{2}J_{P,P}$ = 21.9, $^{2}J_{P,P}$ = 39.6 Hz), 37.1 (dd, $^{2}J_{P,P}$ = 23.2, $^{2}J_{P,P}$ = 153.4 Hz), 41.5 (dd, $^{2}J_{P,P}$ = 25.8, $^{2}J_{P,P}$ = 153.4 Hz) ppm.

FT-IR (ATR) $\tilde{}$/cm^{-1}: 3374 (br w), 3052 (m), 2953 (m), 2896 (w), 2326 (w), 1980 (w), 1665 (br w), 1586 (w), 1481 (m), 1434 (s), 1307 (w), 1249 (m), 1178 (m), 1132 (m), 1097 (s), 1026 (w), 999 (w), 929 (s), 884 (w), 836 (s), 737 (vs), 690 (vs), 617 (w), 527 (m), 479 (s).

HR-FD-MS (+) /: 1673.32591 (calc. for M^+), 1673.32437 (found, Δ = -0.9 ppm)

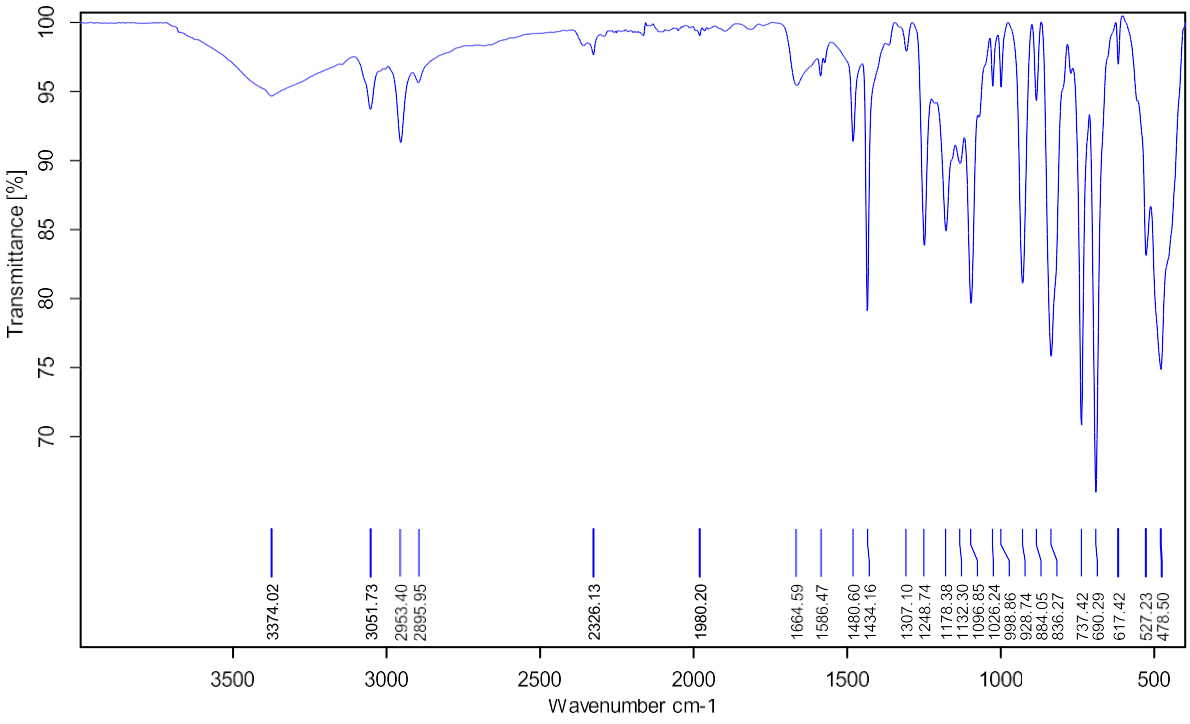


Figure 18 - FT IR spectrum of complex ***5****.*

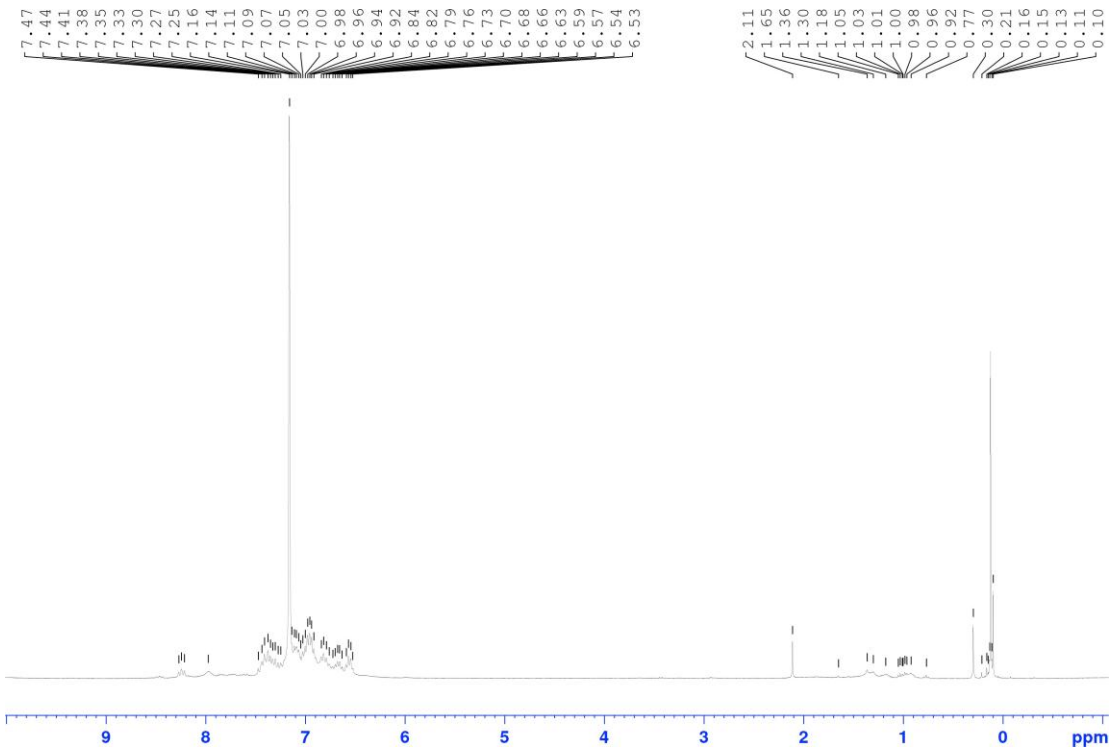


*Figure 19 - ^{1}H NMR spectrum of complex **5** in C_6D_6.*

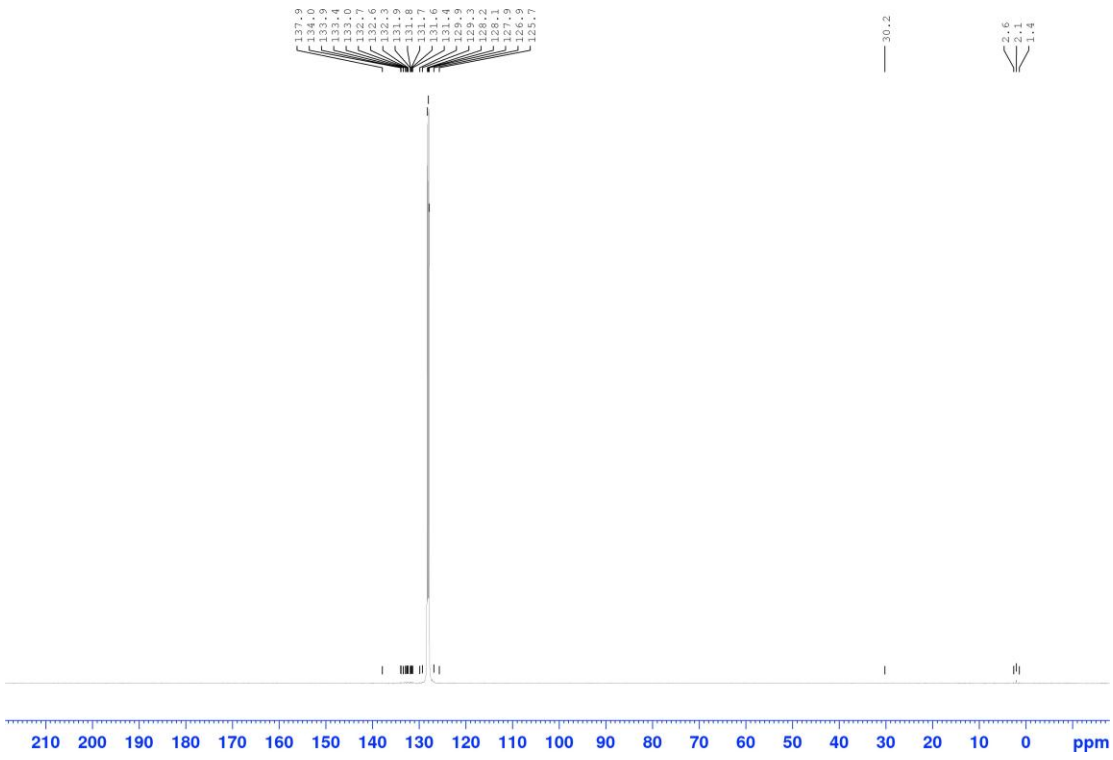


*Figure 20 - $^{13}C\{^{1}H\}$ NMR spectrum of complex **5** in C_6D_6.*

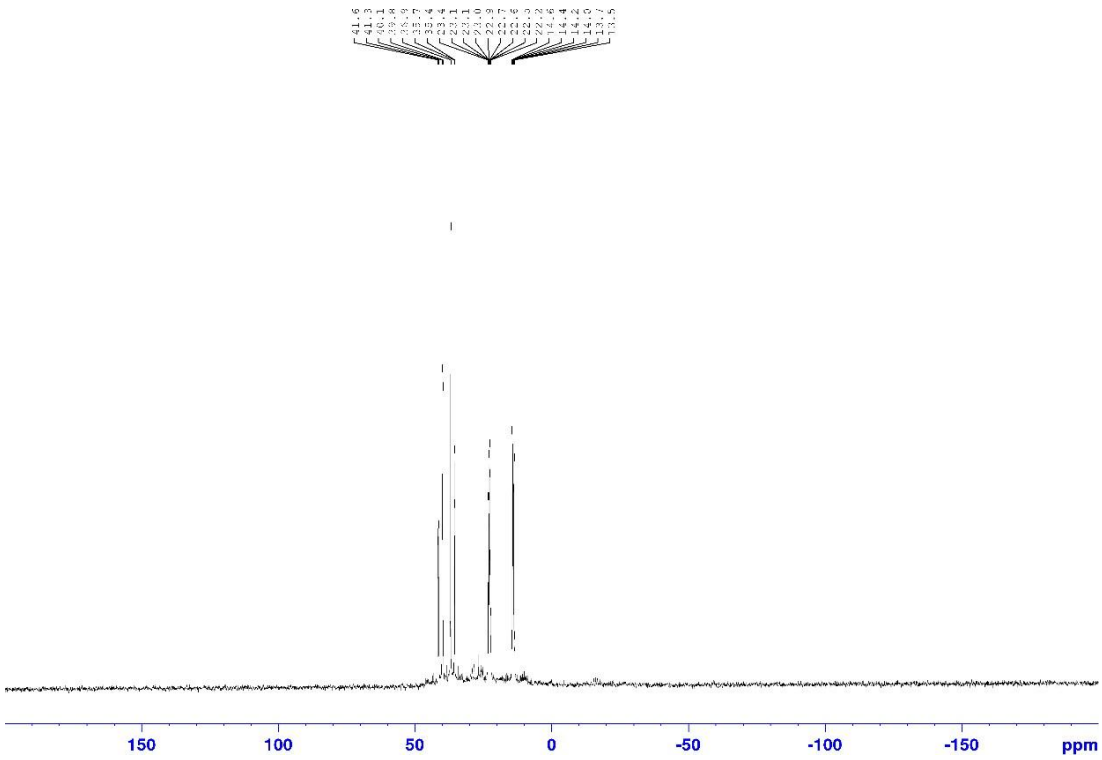


*Figure 21 – $^{31}P\{^{1}H\}$ NMR spectrum of complex **5** in C_6D_6.*

1.6 Synthesis of Complex **6**

To 81.0 mg **5** (48.4 µmol, 1.0 eq.), dissolved in 5 ml toluene, 50 µml HCl in DEE (2 M, 100 µmol, 2.1 eq.) were added. After stirring for 2 h, the solvents were removed in vacuo and 5 ml of DCM were added. After filtration through a syringe filter, the solvent was removed in vacuo and 52 mg **6** (29.8 µmol, 62 %) were obtained in form of a dark red solid.

The $^{31}P\{^{1}H\}$ NMR spectrum shows just three instead of the expected four resonances. This is most likely due to the overlapping of two resonances with similar shifts in the area of 22 to 25 ppm. The presence of two isomers in the crystal structure of **5** suggests a similar equilibrium for **6**, even though only one isomer is present in the isolated single crystals. ^{1}H NMR spectroscopy yields evidence for a second isomer in solution. The phosphorous bridging -CH- and -CH_2- groups of the second isomer display two low intensity resonances shifted +0.2 - 0.3 ppm compared to the main isomer (1.84-1.93 vs. 1.52-1.63 ppm and 3.63-3.81 vs. 3.48 ppm). The absent third resonance is superimposed by the main isomer resonance at 3.48 ppm, as suggested by a slightly bigger integral for the corresponding main isomer resonance and observed via 2D $^{1}H,^{1}H$ COSY and $^{1}H,^{13}C$ HSQC NMR coupling. The shifts of the phosphorous atoms are expected to be nearly identical for the two isomers and thus, no new resonances are expected to be present. ^{13}C NMR spectroscopy proves to be difficult because of low resonance intensities in $^{13}C\{^{1}H\}$ NMR spectra even with a saturated solution (~30 mg in 0.6 ml CD_2Cl_2). ^{13}C NMR shifts had to be extracted from a $^{1}H,^{13}C$ HSQC NMR spectrum. Furthermore, **6** is prone to slow decomposition in CD_2Cl_2 and partially forms complex **1**. In THF-d_8, the solubility is worse and decomposition is observed, whereas in C_6D_6, almost no solubility is observed. The following assignment is for the main isomer only.

^{1}H NMR (300 MHz, CD_2Cl_2) δ_H: 1.52-1.63 (2H, m, P-C*H*-P), 3.22 (2H, ddd, $^{2}J_{H,H}$ = 14.4 Hz, $^{2}J_{H,P}$ = 14.9 Hz, $^{2}J_{H,P}$ = 8.5 Hz), 3.48 (2H, ddd, $^{2}J_{H,H}$ = 14.4 Hz, $^{2}J_{H,P}$ =10.2 Hz, $^{2}J_{H,P}$ = 4.5 Hz), 6.34-6.52 (10H, superimposed resonances, Phenyl-*H*), 6.69 (4H, dt, $J_{H,H}$ = 7.6 Hz, $J_{H,H}$ = 2.6 Hz, Phenyl-*H*), 6.76-6.89 (10H, superimposed resonances, Phenyl-*H*), 6.98-7.47 (44H, superimposed resonances, Phenyl-*H*), 7.54-7.67 (8H, superimposed resonances, Phenyl-*H*), 7.79 (4H, dd, $J_{H,H}$ = 7.9 Hz, $J_{H,H}$ = 11.1 Hz, Phenyl-*H*) ppm.

$^{13}C\{^{1}H\}$ NMR (75 MHz, CD_2Cl_2) δ_C: -9.5-8.3 (m, P-*C*H-P), 42.6 (dd, $^{1}J_{C,P}$ = 24.1 Hz, $^{1}J_{C,P}$ = 64.8 Hz, P-*C*H_2-P), 127.8-130.0 (superimposed resonances, Phenyl-*C*), 130.2-133.4 (superimposed resonances, Phenyl-*C*), 134.6-135.06 (superimposed resonances, Phenyl-*C*) ppm.

$^{31}P\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) δ_P: 22.5-24.8 (m), 28.9 (dd, $^{2}J_{P,P}$ = 81.2 Hz, $^{2}J_{P,P}$ = 28.5 Hz), 38.8 (dd, $^{2}J_{P,P}$ = 81.7 Hz, $^{2}J_{P,P}$ = 16.6 Hz) ppm.

FT-IR (ATR) $\tilde{}$/cm^{-1}: 3049 (w), 2361 (w), 2337 (br w), 1585 (w), 1480 (w), 1434 (m), 1308 (w), 1245 (br w), 1157 (br w), 1096 (m), 1026 (w), 998 (w), 905 (w), 835 (w), 794 (w), 737 (s), 689 (vs), 528 (m), 481 (br s).

HR-ESI-MS (+) /: 1747.2781 (calc. for MH^+), 1747.2812 (found, Δ = 1.8 ppm).

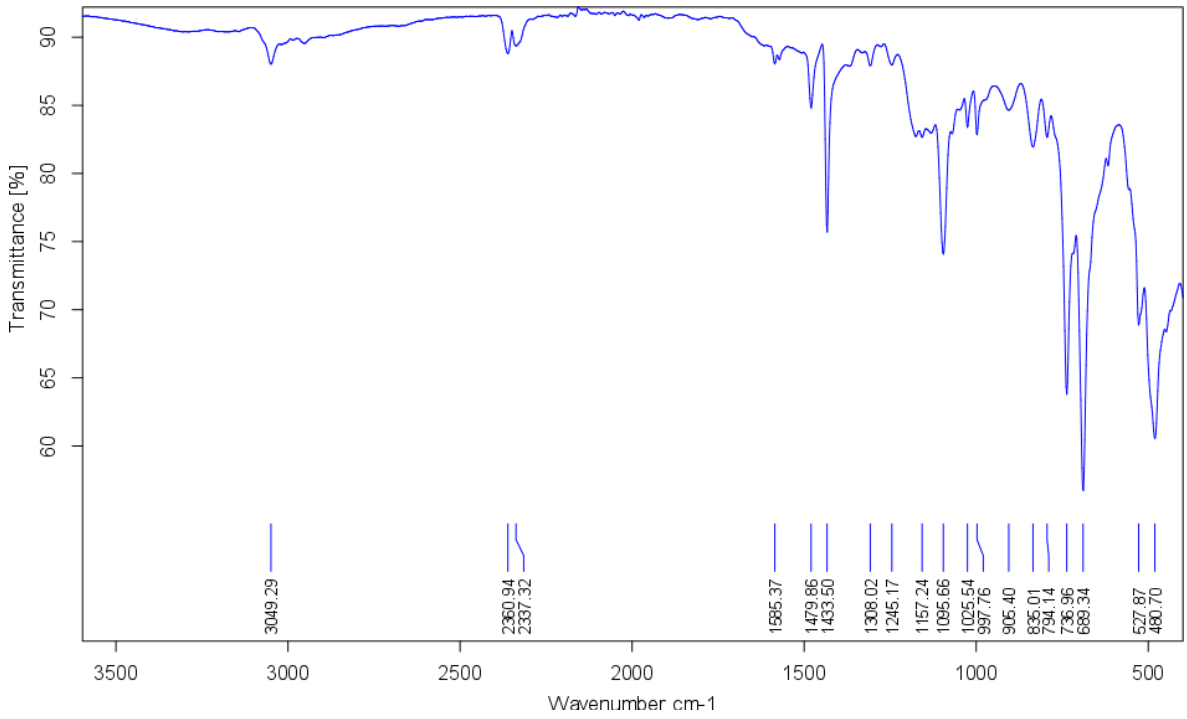


*Figure 22 - FT IR spectrum of complex **6**.*

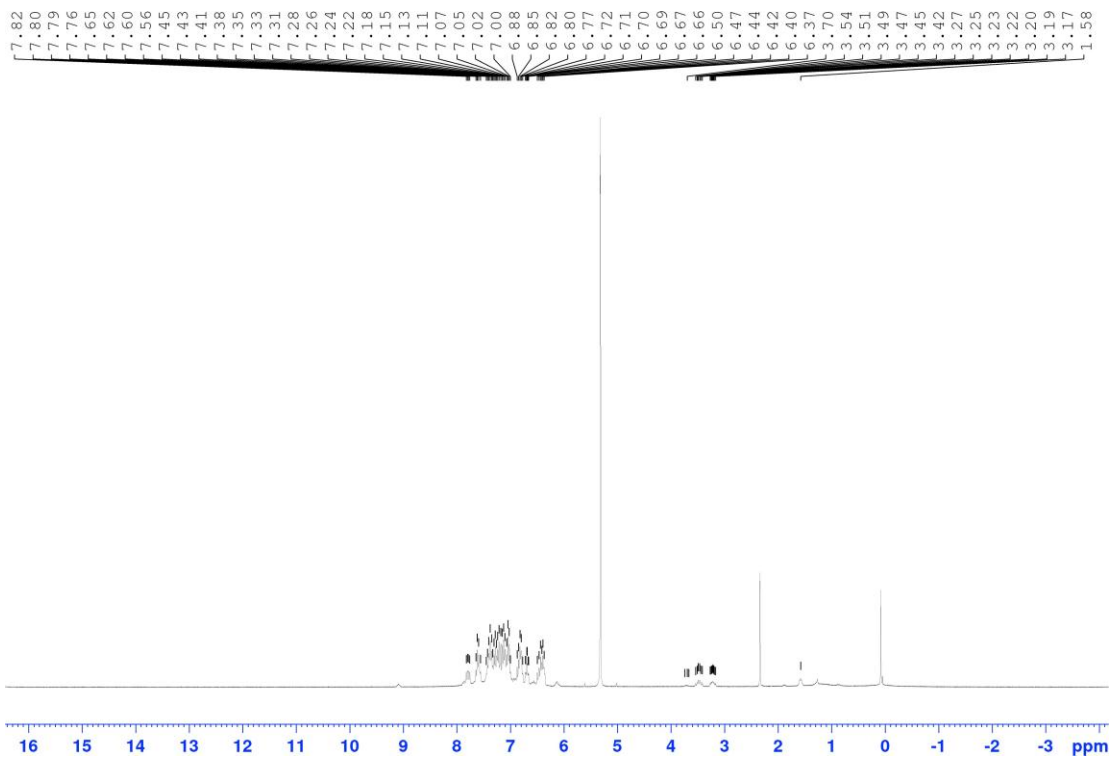


*Figure 23 - ^{1}H NMR spectrum of complex **6** in CD_2Cl_2.*

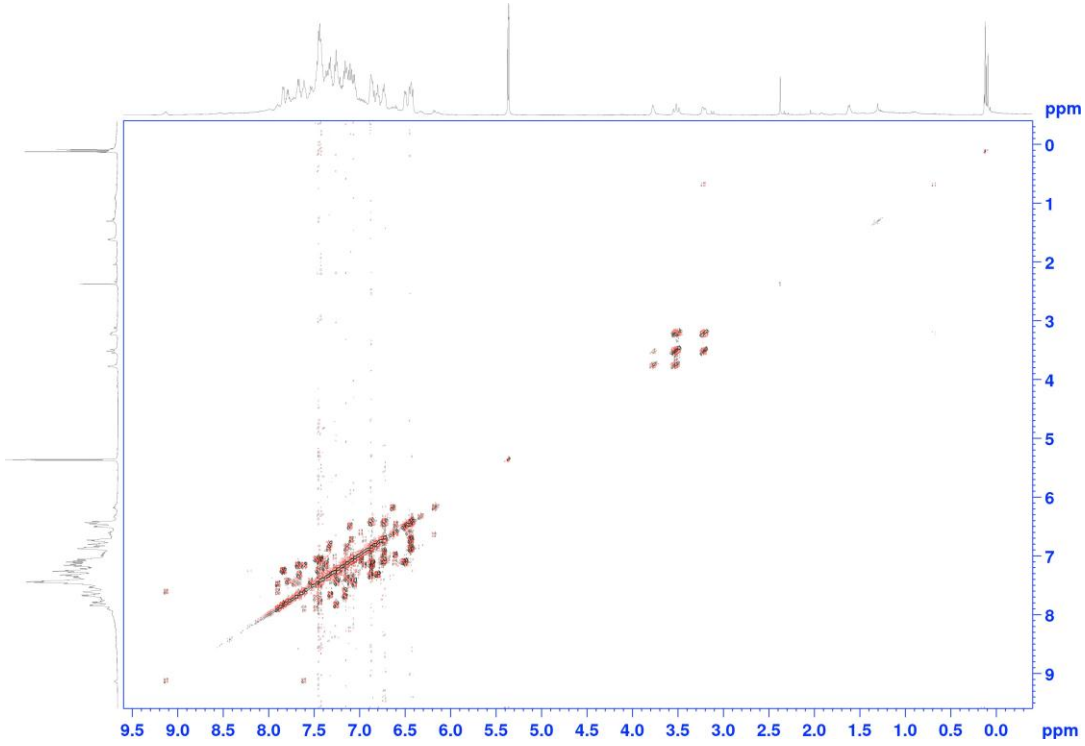


*Figure 24 - $^{1}H,^{1}H$ COSY NMR spectrum of complex **6** in CD_2Cl_2.*

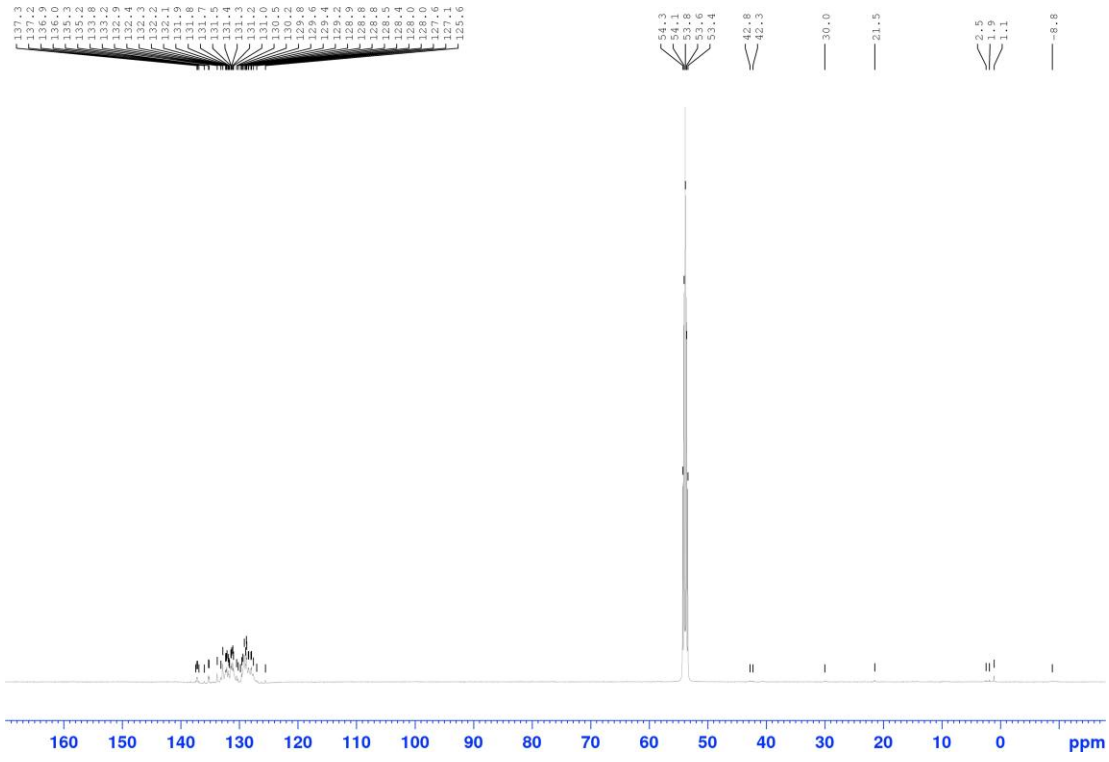


*Figure 25 - $^{13}C\{^{1}H\}$ NMR spectrum of complex **6** in CD_2Cl_2.*

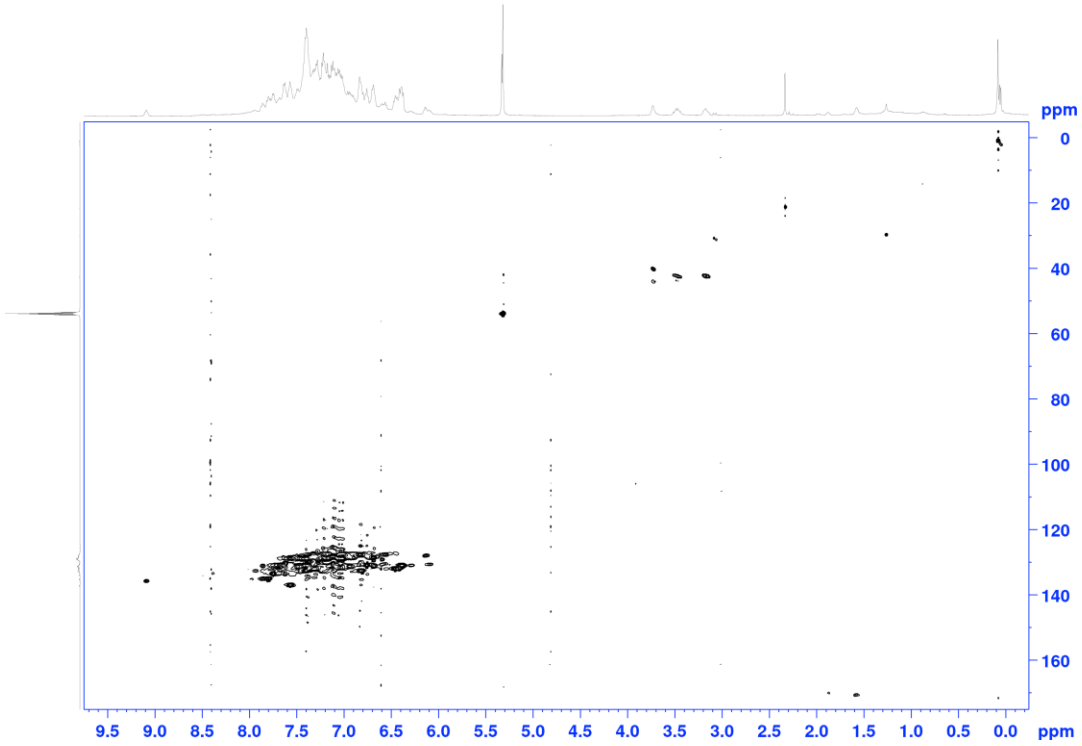


*Figure 26 - $^{1}H,^{1}H$ COSY NMR spectrum of complex **6** in CD_2Cl_2.*

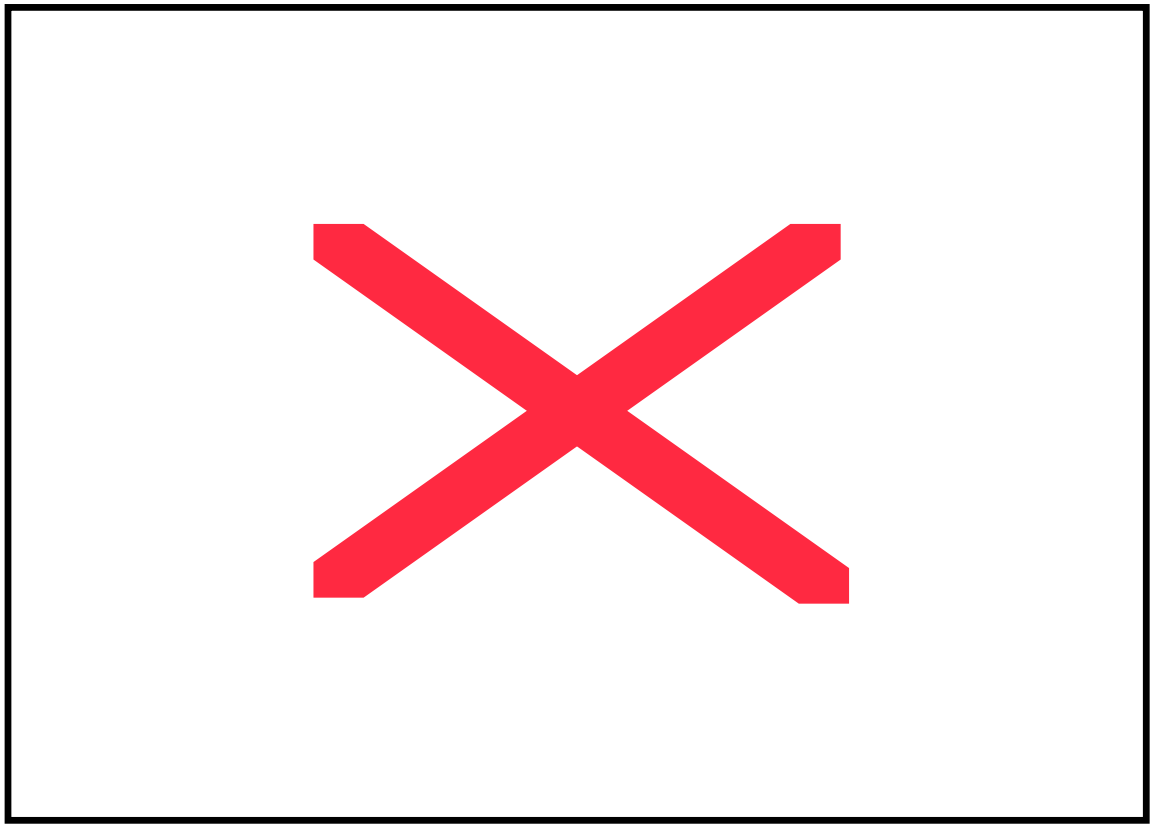


*Figure 27 - $^{13}C\{^{1}H\}$ NMR spectrum of complex **6** in CD_2Cl_2.*

2. X-ray crystallography

The single crystal X-ray diffraction data for the structural analysis were collected using graphite-monochromated Mo-Kα-radiation ($\lambda_{MoK\alpha}$= 0.71073) on the imaging plate detector systems STOE IPDS2 and STOE IPDS2T or on the pixel detector system Bruker Quest D8. The structures were solved with the Olex2 software by direct methods with SHELXT and refined against F^2 by full-matrix-least-square techniques using SHELXL.[2–5]

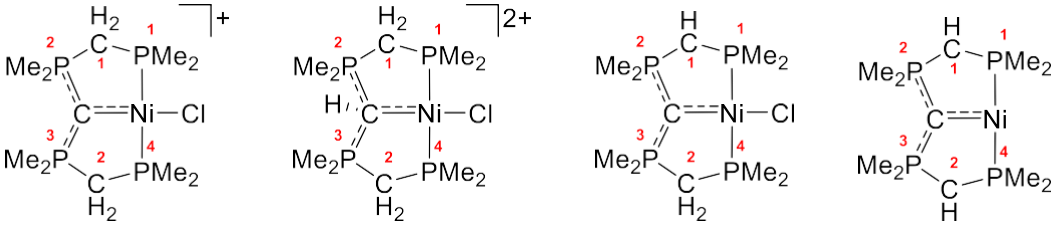
Complex	**2**	**3 · ½ Toluene**	**[4](AlCl$_2$Me$_2$)**	**5 · ¼ THF · $^3/_8$ *n*-hexane**	**6 · 2½ DCM**
Formula	$C_{51}H_{44}B_2ClF_8NiP_4$	$C_{51}H_{43}ClNiP_4$ · ½ C_7H_8	$C_{54}H_{53}AlCl_4NiP_2$	$C_{102}H_{84}Ni_2P_8$ · ¼ C_4H_8O · $^3/_8$ C_6H_{14}	$C_{102}H_{86}Cl_2Ni_2P_8$ · 2½ CH_2Cl_2
$D_{calc.}$/ g cm^{-3}	1.474	1.293	1.326	1.293	1.398
μ/mm^{-1}	0.671	0.639	0.724	0.613	0.791
Formula Weight	1048.52	919.96	991.39	1741.99	1960.10
Colour	orange	red	orange	red	red
Shape	block	block	block	plate	needle
Size/mm^3	0.50×0.41×0.41	0.52×0.36×0.14	0.31×0.26×0.21	0.19×0.18×0.07	0.60×0.22×0.19
T/K	100.0	100.0	100.0	100.0	100.0
Crystal System	monoclinic	monoclinic	monoclinic	triclinic	triclinic
Space Group	$P2_1/c$	$P2_1/c$	$C2/c$	$P\bar{1}$	$P\bar{1}$
a/Å	12.2896(6)	21.4394(11)	13.3928(6)	14.102(3)	13.590(3)
b/Å	18.9342(10)	19.5780(10)	20.9075(10)	14.186(3)	17.439(4)
c/Å	20.4715(11)	23.3621(12)	18.7057(11)	39.126(8)	22.442(5)
α/°	90	90	90	91.13(3)	88.48(3)
β/°	97.295(2)	105.447(2)	108.4890(10)	97.92(3)	72.40(3)
γ/°	90	90	90	119.53(3)	67.39(3)
V/Å^3	4725.0(4)	9451.8(8)	4967.4(4)	6710(3)	4656(2)
Z	4	8	4	3	2
Z'	1	2	0.5	1.5	1
Wavelength/Å	0.710730	0.710730	0.710730	0.710730	0.71073
Radiation type	MoK$_\alpha$	MoK$_\alpha$	MoK$_\alpha$	MoK$_\alpha$	MoK$_\alpha$
Φ_{min}/°	2.128	2.229	2.261	1.585	1.675
Φ_{max}/°	24.971	21.448	24.392	26.772	26.800
Measured Refl.	48535	54585	26730	80180	41177
Independent Refl.	8254	10705	4055	28059	19516
R_{int}	0.0513	0.0687	0.0519	0.0695	0.1289
Parameters	604	1115	284	1584	1111
Restraints	0	0	0	0	0
Largest Peak	1.036	0.397	0.372	1.045	1.431
Deepest Hole	-0.533	-0.349	-0.370	-0.564	-0.933
GooF	1.027	1.013	1.047	0.841	0.949
wR_2 (all data)	0.1118	0.0884	0.0779	0.1379	0.1638
wR_2	0.1035	0.0799	0.0741	0.1099	0.1507
R_1 (all data)	0.0571	0.0570	0.0466	0.1491	0.0931
R_1	0.0445	0.0376	0.0352	0.0536	0.0641
CCDC	1814009	1814006	1814010	1814007	1814008

3. DFT Calculations

DFT calculations were done with Grimme's B97D functional including dispersion[6] and the def2-TZVPP basis set after a preoptimisation with the def2-SVP basis set.[7,8] Crystals structures were used as starting models, where possible, and the phenyl groups were substituted by methyl groups. After optimization, a frequency calculation was run to ascertain that a ground state was found (no imaginary modes). QTAIM charges and critical point data were calculated by the AIMQB module of the AIMStudio software bundle.[9] Laplacian contour line plots were created with the program multiwfn, molecular orbital visualizations with ChemCraft.[10,11]

Table 1 - QTAIM charges for the monomeric complexes

	1^{Me}	**2**^{Me}	**3**^{Me}	**7**^{Me}
Ni	0.39	0.40	0.38	0.29
C^{CDP}	-2.00	-1.38	-1.91	-1.80
P1	1.62	1.60	1.81	1.74
P2	2.60	2.47	2.68	2.68
P3	2.60	2.46	2.54	2.68
P4	1.62	1.60	1.60	1.74
Cl	-0.57	-0.49	-0.62	
C1	-1.02	-1.04	-1.73	-1.73
C2	-1.02	-1.03	-1.02	-1.73

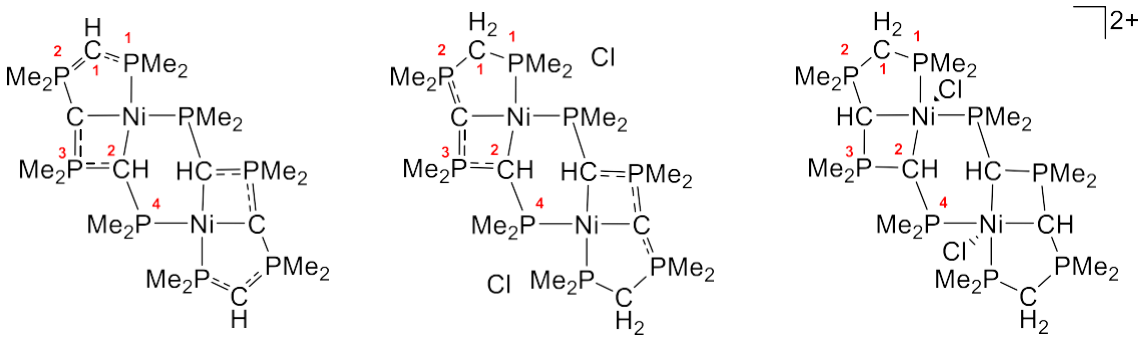


1^{Me} **2**^{Me} **3**^{Me} **7**^{Me}

Figure 28 - Numbering scheme for the monomeric complexes.

Table 2 - QTAIM charges for the dimeric complexes

	***cis*-5**^{Me}	***trans*-5**^{Me}	***cis*-6**^{Me}	**8**^{Me}
Ni	0.30 / 0.30	0.31 / 0.31	0.34 / 0.37	0.38 / 0.38
C^{CDP}	-2.01 / -2.02	-2.02 / -2.02	-2.08 / -2.03	-1.55 / -1.55
P1	1.76 / 1.75	1.76 / 1.76	1.61 / 1.62	1.52 / 1.52
P2	2.73 / 2.73	2.74 / 2.74	2.63 / 2.62	2.56 / 2.56
P3	2.65 / 2.65	2.64 / 2.64	2.68 / 2.66	2.60 / 2.60
P4	1.63 / 1.63	1.62 / 1.62	1.68 / 1.66	1.74 / 1.74
C1	-1.71 / -1.71	-1.71 / -1.71	-1.05 / -1.04	-1.02 / -1.02
C2	-1.41 / -1.41	-1.40 / -1.40	-1.39 / -1.41	-1.43 / -1.43



5^{Me} **6**^{Me} **8**^{Me}

Figure 29 - Numbering scheme for the dimeric complexes.

Table 3 - Bond critical point data in atomic units for ***1***^{Me}.

Bond	ρ	∇ ρ	ε	K	V	H
Ni—Cl	7.7819929557E-02	2.2181081510E-01	8.7875160579E-02	2.2576453210E-02	-1.2885065495E-01	-1.0627420174E-01
Ni—C^{CDP}	1.0312936845E-01	1.9335851481E-01	4.4694435662E-02	4.0255513124E-02	-1.2885065495E-01	-8.8595141826E-02
Ni—P^1	1.0000341562E-01	1.2488957623E-01	2.4765883313E-02	4.2316537577E-02	-1.1585546921E-01	-7.3538931633E-02
Ni—P^4	9.9879996194E-02	1.2527452645E-01	2.5191501105E-02	4.2211315226E-02	-1.1574126206E-01	-7.3529946834E-02
C^{CDP}—P^2	1.9259576604E-01	-3.1807034153E-02	2.0883773828E-01	1.9295253512E-01	-3.7795331169E-01	-1.8500077657E-01
C^{CDP}—P^3	1.9256151834E-01	-3.2988339036E-02	2.0752867024E-01	1.9294284997E-01	-3.7763861517E-01	-1.8469576520E-01
C^1—P^1	1.5336636795E-01	-2.3611257883E-01	9.4722245481E-02	1.4071579481E-01	-2.2240344491E-01	-8.1687650100E-02
C^2—P^4	1.5347020994E-01	-2.3478459830E-01	9.4566512067E-02	1.4087743051E-01	-2.2305871145E-01	-8.2181280940E-02
C^1—P^2	1.6749618925E-01	-2.7423720639E-01	3.0325424187E-02	1.6253976852E-01	-2.5652023544E-01	-9.3980466920E-02
C^2—P^3	1.6752565952E-01	-2.7340462009E-01	3.1204734505E-02	1.6257553389E-01	-2.5679991277E-01	-9.4224378880E-02
C^1—H	2.7644941915E-01	-9.6288428438E-01	1.2525170948E-02	2.8841433328E-01	-3.3610759546E-01	-4.7693262180E-02
C^1—H‘	2.7710488995E-01	-9.6903880263E-01	9.5183203650E-03	2.8908765694E-01	-3.3591561323E-01	-4.6827956290E-02
C^2—H	2.7645999359E-01	-9.6288827059E-01	1.3123924426E-02	2.8844223335E-01	-3.3616239905E-01	-4.7720165700E-02
C^2—H‘	2.7706567731E-01	-9.6902509095E-01	9.6888542281E-03	2.8903192127E-01	-3.3580756981E-01	-4.6775648540E-02

Table 4 - Bond critical point data in atomic units for ***2***^{Me}.

Bond	ρ	∇ ρ	ε	K	V	H
Ni—Cl	8.7034415332E-02	2.2244556475E-01	7.8279026363E-02	2.8173140155E-02	-1.1195767150E-01	-8.3784531345E-02
Ni—C^{CDP}	8.6566512754E-02	2.0243840378E-01	9.9767303730E-02	2.7349319763E-02	-1.0530824047E-01	-7.7958920707E-02
Ni—P^1	9.6311499621E-02	1.1524253304E-01	2.1220749829E-02	3.9045614423E-02	-1.0690186211E-01	-6.7856247687E-02
Ni—P^4	9.8530697766E-02	1.1591583586E-01	6.2038183095E-03	4.0992075266E-02	-1.1096310950E-01	-6.9971034234E-02
C^{CDP}—P^2	1.7326632469E-01	-2.5374400290E-01	5.0579948604E-02	1.7000059839E-01	-2.7656519606E-01	-1.0656459767E-01
C^{CDP}—P^3	1.7138607006E-01	-2.8405612669E-01	3.8944957540E-02	1.6721978949E-01	-2.6342554730E-01	-9.6205757810E-02
C^{CDP}—H	2.7008562022E-01	-9.0740558063E-01	2.2585187362E-02	2.7824977002E-01	-3.2964814489E-01	-5.1398374870E-02
C^1—P^1	1.4872424108E-01	-2.2039020691E-01	1.0552449368E-01	1.3409791946E-01	-2.1309828720E-01	-7.9000367740E-02
C^2—P^4	1.4864986771E-01	-2.1668539376E-01	9.5106480354E-02	1.3401975496E-01	-2.1386816148E-01	-7.9848406520E-02
C^1—P^2	1.7322329479E-01	-3.1504197714E-01	1.5787527233E-02	1.7048212126E-01	-2.6220374824E-01	-9.1721626980E-02
C^2—P^3	1.7450367485E-01	-2.9777355229E-01	2.4996015707E-02	1.7243005716E-01	-2.7041672626E-01	-9.7986669100E-02
C^1—H	2.7775108663E-01	-9.7964363966E-01	5.9774417084E-03	2.8966344047E-01	-3.3441597103E-01	-4.4752530560E-02
C^1—H‘	2.7630789130E-01	-9.6615658374E-01	3.8870417403E-03	2.8747792031E-01	-3.3341669469E-01	-4.5938774380E-02

C^{2}—H	2.7713558623E-01	-9.7615652234E-01	7.3436619885E-03	2.8856811604E-01	-3.3309710148E-01	-4.4528985440E-02
C^{2}—H‘	2.7564654360E-01	-9.5963565249E-01	6.1422704426E-03	2.8684058856E-01	-3.3377226399E-01	-8.3784531345E-02

Table 5 - Bond critical point data in atomic units for ***3^{Me}***.

Bond	ρ	∇ ρ	ε	K	V	H
Ni—Cl	7.0724447948E-02	2.1466043483E-01	9.5536525902E-02	1.8541979834E-02	-9.0749068376E-02	-7.2207088542E-02
Ni—C^{CDP}	1.0540748784E-01	1.8908602834E-01	3.5047022575E-02	4.2223070587E-02	-1.3171764826E-01	-8.9494577673E-02
Ni—P^{1}	9.7925285290E-02	9.2706245507E-02	1.3635439603E-02	4.0555921790E-02	-1.0428840496E-01	-6.3732483170E-02
Ni—P^{4}	1.0151514258E-01	1.5028055473E-01	1.5875378264E-02	4.3859647289E-02	-1.2528943326E-01	-8.1429785971E-02
C^{CDP}—P^{2}	1.8170578921E-01	-1.3252718596E-01	1.4260667846E-01	1.8018283374E-01	-3.2723387098E-01	-1.4705103724E-01
C^{CDP}—P^{3}	1.9639325357E-01	-4.4289122888E-02	2.7487731681E-01	1.9949076703E-01	-3.8790925335E-01	-1.8841848632E-01
C^{1}—P^{1}	1.8004703534E-01	-3.9372684078E-02	1.3221125750E-01	1.7403244441E-01	-3.3822171781E-01	-1.6418927340E-01
C^{2}—P^{4}	1.5309446555E-01	-2.2165598033E-01	9.5968649468E-02	1.4043062518E-01	-2.2544725527E-01	-8.5016630090E-02
C^{1}—P^{2}	1.9490650037E-01	-3.4307894427E-02	2.9560013071E-01	1.9612306314E-01	-3.8366915267E-01	-1.8754608953E-01
C^{2}—P^{3}	1.6657314657E-01	-2.5230849427E-01	3.9434657512E-02	1.6108718684E-01	-2.5909725011E-01	-9.8010063270E-02
C^{1}—H	2.7255738213E-01	-9.2574581707E-01	6.4785031932E-02	2.8764858597E-01	-3.4386071767E-01	-5.6212131700E-02
C^{2}—H	2.7616437553E-01	-9.5862973123E-01	1.6310172028E-02	2.8844473810E-01	-3.3723204338E-01	-4.8787305280E-02
C^{2}—H‘	2.7571515070E-01	-9.5668541192E-01	1.1704353023E-02	2.8758556447E-01	-3.3599977596E-01	-4.8414211490E-02

Table 6 - Bond critical point data in atomic units for ***7^{Me}***.

Bond	ρ	∇ ρ	ε	K	V	H
Ni—C^{CDP}	1.2364308535E-01	1.1355553875E-01	2.2545212155E-02	5.9718955321E-02	-1.4782679533E-01	-8.8107840009E-02
Ni—P^{1}	9.6107139736E-02	1.1039272239E-01	9.8909277442E-03	3.9082655774E-02	-1.0576349215E-01	-6.6680836376E-02
Ni—P^{4}	9.6731827180E-02	1.0962775526E-01	8.7108590924E-03	3.9589183184E-02	-1.0658530518E-01	-6.6996121996E-02
C^{CDP}—P^{2}	1.8380349677E-01	-1.0373922121E-01	2.1544752992E-01	1.8240540970E-01	-3.3887601409E-01	-1.5647060439E-01
C^{CDP}—P^{3}	1.8376345353E-01	-1.0501970413E-01	2.1561292998E-01	1.8238246566E-01	-3.3851000529E-01	-1.5612753963E-01
C^{1}—P^{1}	1.8372841055E-01	-1.9271540208E-02	1.5392144088E-01	1.7874028279E-01	-3.5266268053E-01	-1.7392239774E-01
C^{2}—P^{4}	1.8379554269E-01	-1.9371897802E-02	1.5519609638E-01	1.7883791576E-01	-3.5283285706E-01	-1.7399494130E-01
C^{1}—P^{2}	1.9155286698E-01	-5.9287230913E-02	2.6466101829E-01	1.9199765930E-01	-3.6917351088E-01	-1.7717585158E-01
C^{2}—P^{3}	1.9154359180E-01	-5.8201321863E-02	2.6402180281E-01	1.9193890150E-01	-3.6932747253E-01	-1.7738857103E-01
C^{1}—H	2.7265352958E-01	-9.2569876437E-01	6.6977287165E-02	2.8788732036E-01	-3.4434994963E-01	-5.6462629270E-02
C^{2}—H	2.7272055563E-01	-9.2627350189E-01	6.7063805306E-02	2.8799343080E-01	-3.4441848613E-01	-5.6425055330E-02

Table 7 - Bond critical point data in atomic units for ***trans-5^{Me}***.

Bond	ρ	∇ ρ	ε	K	V	H
Ni—P^{1}	9.7701999899E-02	1.0885138534E-01	1.2730821185E-02	4.0347555111E-02	-1.0790795656E-01	-6.7560401449E-02
Ni—C^{CDP}	1.0824975677E-01	1.8280046870E-01	4.7105307880E-02	4.5113124736E-02	-1.3592636665E-01	-9.0813241914E-02
Ni—C^{2}	8.0544861682E-02	1.6892490216E-01	1.6952808795E-01	2.3620649345E-02	-8.9472524231E-02	-6.5851874886E-02

Ni—P$^{4'}$	9.7972124906E-02	1.4618299518E-01	1.9447294673E-02	4.0927927226E-02	-1.1840160325E-01	-7.7473676024E-02
C$^{CDP'}$—P$^{2'}$	1.8874486804E-01	-3.3260300298E-02	1.2722331843E-01	1.8689308703E-01	-3.6547109899E-01	-1.7857801196E-01
C$^{CDP'}$—P$^{3'}$	1.9791384453E-01	6.6666902757E-02	1.8187828883E-01	1.9720419320E-01	-4.1107511208E-01	-2.1387091888E-01
C$^{1'}$—P$^{1'}$	1.8041031068E-01	-6.1624578174E-02	1.6845040122E-01	1.7551874984E-01	-3.3563135514E-01	-1.6011260530E-01
C$^{2'}$—P$^{4'}$	1.6415131755E-01	-1.8754884371E-01	4.5368931650E-02	1.5554209818E-01	-2.6419698543E-01	-1.0865488725E-01
C$^{1'}$—P$^{2'}$	1.9250419262E-01	-4.1546368779E-02	2.7096654376E-01	1.9271660128E-01	-3.7504661036E-01	-1.8233000908E-01
C$^{2'}$—P$^{3'}$	1.7560483183E-01	-1.8107802411E-01	1.1114491716E-01	1.7249643829E-01	-2.9972337055E-01	-1.2722693226E-01
Ni'—P$^{1'}$	9.7702417071E-02	1.0885067081E-01	1.2731947821E-02	4.0347904507E-02	-1.0790847672E-01	-6.7560572213E-02
Ni'—C$^{CDP'}$	1.0824960687E-01	1.8280011740E-01	4.7102633011E-02	4.5112997463E-02	-1.3592602428E-01	-9.0813026817E-02
Ni'—C$^{2'}$	8.0543945818E-02	1.6892363665E-01	1.6952474985E-01	2.3620057435E-02	-8.9471024033E-02	-6.5850966598E-02
Ni'—P$^{4'}$	9.7971465370E-02	1.4618341174E-01	1.9440979810E-02	4.0927328351E-02	-1.1840050964E-01	-7.7473181289E-02
C$^{CDP'}$—P$^{2'}$	1.8874479587E-01	-3.3262432293E-02	1.2722460903E-01	1.8689306200E-01	-3.6547051592E-01	-1.7857745392E-01
C$^{CDP'}$—P$^{3'}$	1.9791428898E-01	6.6669803206E-02	1.8187918233E-01	1.9720474078E-01	-4.1107693236E-01	-2.1387219158E-01
C$^{1'}$—P$^{1'}$	1.8041032249E-01	-6.1625440544E-02	1.6845217772E-01	1.7551880021E-01	-3.3563124028E-01	-1.6011244007E-01
C$^{2'}$—P$^{4'}$	1.6415134549E-01	-1.8754858363E-01	4.5365904329E-02	1.5554210769E-01	-2.6419706947E-01	-1.0865496178E-01
C$^{1'}$—P$^{2'}$	1.9250416828E-01	-4.1546145335E-02	2.7096682458E-01	1.9271655660E-01	-3.7504657686E-01	-1.8233002026E-01
C$^{2'}$—P$^{3'}$	1.7560557846E-01	-1.8107384387E-01	1.1114093174E-01	1.7249742926E-01	-2.9972639754E-01	-1.2722896828E-01
C^{1}—H	2.7247445158E-01	-9.2453624341E-01	6.8204003872E-02	2.8764975195E-01	-3.4416544305E-01	-5.6515691100E-02
C$^{1'}$—H	2.7247536593E-01	-9.2454196294E-01	6.8204122232E-02	2.8765148684E-01	-3.4416748293E-01	-5.6515996090E-02
C^{2}—H	2.7604156316E-01	-9.4441666922E-01	3.0771980182E-02	2.8987896012E-01	-3.4365375293E-01	-5.3774792810E-02
C$^{2'}$—H	2.7604192366E-01	-9.4441886419E-01	3.0772245873E-02	2.8987955659E-01	-3.4365439713E-01	-5.3774840540E-02

Table 8 - Bond critical point data in atomic units for ***cis-5^{Me}****.*

Bond	ρ	∇ ρ	ε	K	V	H
Ni—P$^{4'}$	9.8282487699E-02	1.1005573198E-01	2.5580517277E-02	4.0954968359E-02	-1.0942386971E-01	-6.8468901351E-02
Ni—C^{CDP}	1.0471137949E-01	1.8261612561E-01	5.5469007052E-02	4.2026397249E-02	-1.2970682590E-01	-8.7680428651E-02
Ni—C$^{2'}$	8.6691769438E-02	1.7488788976E-01	1.3102872043E-01	2.7788957653E-02	-9.9299887747E-02	-7.1510930094E-02
Ni—P$^{4'}$	9.8403314142E-02	1.4636023743E-01	1.4590951488E-02	4.1169092445E-02	-1.1892824425E-01	-7.7759151805E-02
C$^{CDP'}$—P$^{2'}$	1.8823582371E-01	-4.0941951500E-02	1.2465196184E-01	1.8646979774E-01	-3.6270410761E-01	-1.7623430987E-01
C$^{CDP'}$—P$^{3'}$	1.9736196477E-01	4.9892114007E-02	1.6777269636E-01	1.9710013084E-01	-4.0667329017E-01	-2.0957315933E-01
C$^{1'}$—P$^{1'}$	1.8039663792E-01	-6.3457887084E-02	1.7012507842E-01	1.7554549062E-01	-3.3522650948E-01	-1.5968101886E-01
C$^{2'}$—P$^{4'}$	1.6605898418E-01	-1.7380343874E-01	7.9330590060E-02	1.5816798110E-01	-2.7288510252E-01	-1.1471712142E-01
C$^{1'}$—P$^{2'}$	1.9173343518E-01	-5.4449699696E-02	2.6595890408E-01	1.9205873275E-01	-3.7050504057E-01	-1.7844630782E-01
C$^{2'}$—P$^{3'}$	1.7701914237E-01	-1.7066323779E-01	1.0702002400E-01	1.7428579137E-01	-3.0590577329E-01	-1.3161998192E-01
Ni'—P$^{1'}$	9.8031850885E-02	1.1096068160E-01	2.3658705985E-02	4.0720747090E-02	-1.0918166458E-01	-6.8460917490E-02
Ni'—C$^{CDP'}$	1.0509501611E-01	1.8309977998E-01	5.3638568497E-02	4.2359628452E-02	-1.3049420190E-01	-8.8134573448E-02
Ni'—C$^{2'}$	8.6094334957E-02	1.7337297559E-01	1.3253884596E-01	2.7375057619E-02	-9.8093359136E-02	-7.0718301517E-02
Ni'—P^{4}	9.8950364806E-02	1.4581211706E-01	1.2916551367E-02	4.1640615901E-02	-1.1973426107E-01	-7.8093645169E-02
C$^{CDP'}$—P$^{2'}$	1.8852644352E-01	-3.4979281441E-02	1.2586011511E-01	1.8666164749E-01	-3.6457847461E-01	-1.7791682712E-01
C$^{CDP'}$—P$^{3'}$	1.9764115546E-01	5.5855160569E-02	1.6986673335E-01	1.9727849273E-01	-4.0852077561E-01	-2.1124228288E-01
C$^{1'}$—P$^{1'}$	1.8033196311E-01	-6.3413024685E-02	1.6930479336E-01	1.7545252197E-01	-3.3505178777E-01	-1.5959926580E-01
C$^{2'}$—P$^{4'}$	1.6594927288E-01	-1.7340700743E-01	7.8243943476E-02	1.5800892806E-01	-2.7266610426E-01	-1.1465717620E-01
C$^{1'}$—P$^{2'}$	1.9179321359E-01	-5.3441711020E-02	2.6686942886E-01	1.9210789736E-01	-3.7085536697E-01	-1.7874746961E-01
C$^{2'}$—P$^{3'}$	1.7702311367E-01	-1.6985658941E-01	1.0602814983E-01	1.7426870859E-01	-3.0607326982E-01	-1.3180456123E-01

C^{1}—H	2.7219647256E-01	-9.2288417872E-01	6.7495772305E-02	2.8712792142E-01	-3.4353479816E-01	-5.6406876740E-02
$C^{1'}$—H	2.7217430288E-01	-9.2260953450E-01	6.7527093062E-02	2.8709835010E-01	-3.4354431657E-01	-5.6445966470E-02
C^{2}—H	2.7496185438E-01	-9.3650366714E-01	2.9966227323E-02	2.8878750320E-01	-3.4344908962E-01	-5.4661586420E-02
$C^{2'}$—H	2.7508124835E-01	-9.3718863371E-01	2.9825679088E-02	2.8895042918E-01	-3.4360369994E-01	-5.4653270760E-02

Table 9 - Bond critical point data in atomic units for ***cis-6^{Me}***.

Bond	ρ	∇ ρ	ε	K	V	H
Ni—P^{1}	1.0142507744E-01	1.3514828329E-01	3.1925753366E-02	4.4027800501E-02	-1.2184267182E-01	-7.7814871319E-02
Ni—C^{CDP}	9.8811836487E-02	1.9429705357E-01	9.1469508730E-02	3.7287569161E-02	-1.2314940171E-01	-8.5861832549E-02
Ni—C^{2}	8.9926361103E-02	1.6785851968E-01	1.2546803080E-01	3.0077850099E-02	-1.0212033012E-01	-7.2042480021E-02
Ni—$P^{4'}$	1.0138806086E-01	1.2328956102E-01	1.3442869211E-02	4.3684763767E-02	-1.1819191779E-01	-7.4507154023E-02
C^{CDP}—P^{2}	1.9597661606E-01	5.0126402180E-02	1.6067691129E-01	1.9480644466E-01	-4.0214448986E-01	-2.0733804520E-01
C^{CDP}—P^{3}	1.9409230361E-01	4.9934220197E-02	1.1875131556E-01	1.9183419488E-01	-3.9615194481E-01	-2.0431774993E-01
C^{1}—P^{1}	1.5711863437E-01	-2.5654278943E-01	6.2051419698E-02	1.4618410550E-01	-2.2823251364E-01	-8.2048408140E-02
C^{2}—P^{4}	1.6253575939E-01	-1.7073557365E-01	8.2609828103E-02	1.5329226072E-01	-2.6390062802E-01	-1.1060836730E-01
C^{1}—P^{2}	1.6792917106E-01	-2.7910574641E-01	2.8140695052E-02	1.6323157274E-01	-2.5668670887E-01	-9.3455136130E-02
C^{2}—P^{3}	1.7826066051E-01	-1.9112662278E-01	8.8099259835E-02	1.7656151111E-01	-3.0534136652E-01	-1.2877985541E-01
Ni'—$P^{1'}$	1.0247707601E-01	1.3290748226E-01	4.6944905712E-02	4.4924326825E-02	-1.2307552422E-01	-7.8151197395E-02
Ni'—$C^{CDP'}$	9.4470637280E-02	1.8502748030E-01	9.4915454857E-02	3.3894477319E-02	-1.1404582471E-01	-8.0151347391E-02
Ni'—$C^{2'}$	9.0360637427E-02	1.7701477809E-01	1.1934324830E-01	3.0460131684E-02	-1.0517395789E-01	-7.4713826206E-02
Ni'—P^{4}	1.0121686636E-01	1.2933066342E-01	2.8888703379E-02	4.3689902534E-02	-1.1971247092E-01	-7.6022568386E-02
$C^{CDP'}$—$P^{2'}$	1.9602432218E-01	-9.1207953626E-03	1.3513266932E-01	1.9722010168E-01	-3.9216000453E-01	-1.9493990285E-01
$C^{CDP'}$—$P^{3'}$	1.9299600553E-01	1.5300933361E-02	1.0676603017E-01	1.9173234734E-01	-3.8728992802E-01	-1.9555758068E-01
$C^{1'}$—$P^{1'}$	1.5587582094E-01	-2.4540898350E-01	6.1008946040E-02	1.4454324121E-01	-2.2773423654E-01	-8.3190995330E-02
$C^{2'}$—$P^{4'}$	1.6710381678E-01	1.7513617421E-01	7.8890945620E-02	1.5962100208E-01	-2.7545796061E-01	-1.1583695853E-01
$C^{1'}$—$P^{2'}$	1.6890345503E-01	-2.6748839033E-01	2.1375993559E-02	1.6455998665E-01	-2.6224787571E-01	-9.7687889060E-02
$C^{2'}$—$P^{3'}$	1.7674922323E-01	-1.6840905386E-01	1.0885672069E-01	1.7385704357E-01	-3.0561182368E-01	-1.3175478011E-01
C^{1}—H	2.7454904618E-01	-9.4776806501E-01	2.5169490210E-03	2.8600905349E-01	-3.3507609072E-01	-4.9067037230E-02
C^{1}—H'	2.7862904150E-01	-9.9039226886E-01	1.4311750984E-02	2.9034669484E-01	-3.3309532248E-01	-4.2748627640E-02
$C^{1'}$—H	2.7474020630E-01	-9.4979732420E-01	3.5521464630E-03	2.8615121077E-01	-3.3485309050E-01	-4.8701879730E-02
$C^{1'}$—H'	2.7888570564E-01	-9.8572601405E-01	1.7157644084E-02	2.9100262945E-01	-3.3557375539E-01	-4.4571125940E-02
C^{2}—H	2.7532326390E-01	-9.4143902082E-01	2.3541475379E-02	2.8862708146E-01	-3.4189440772E-01	-5.3267326260E-02
$C^{2'}$—H	2.7548411437E-01	-9.4247968575E-01	2.9063286755E-02	2.8909846435E-01	-3.4257700726E-01	-5.3478542910E-02

*Table 10 - Bond critical point data in atomic units for t****rans-8^{Me}***.

Bond	ρ	∇ ρ	ε	K	V	H
Ni—P^{1}	9.0803576173E-02	1.4894693266E-01	1.5596554590E-02	3.4544545104E-02	-1.0632582337E-01	-7.1781278266E-02
Ni—C^{CDP}	7.9901080481E-02	1.8187583251E-01	1.2550093290E-01	2.3521234519E-02	-9.2511427164E-02	-6.8990192645E-02
Ni—C^{2}	8.1565337017E-02	1.7964687689E-01	1.2340836724E-01	2.3728019094E-02	-9.2367757409E-02	-6.8639738315E-02
Ni—$P^{4'}$	1.0379056046E-01	1.0379056046E-01	1.8214762908E-02	4.5897664366E-02	-1.1443841475E-01	-6.8540750384E-02
Ni—Cl	4.3249341463E-02	1.2995552405E-01	3.7112708384E-02	5.6557866059E-03	-4.3800454225E-02	-3.8144667619E-02
C^{CDP}—P^{2}	1.8125691977E-01	-1.7892913454E-01	8.6434423569E-02	1.8030517120E-01	-3.1587805878E-01	-1.3557288758E-01
C^{CDP}—P^{3}	1.7785815018E-01	-1.1985066695E-01	1.0415527247E-01	1.7376799276E-01	-3.1757331878E-01	-1.4380532602E-01

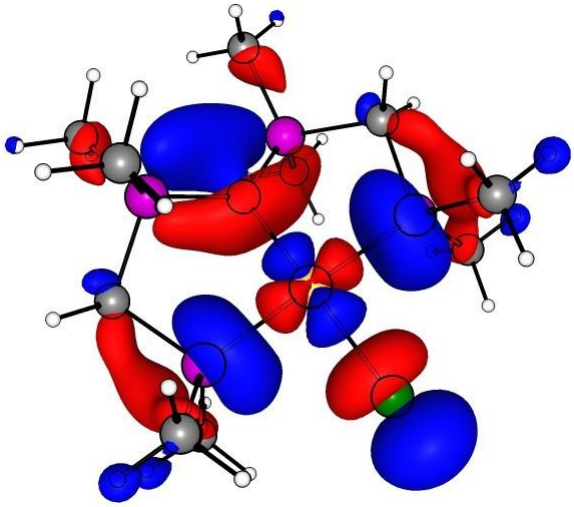
C^{1}—P^{1}	1.4820687686E-01	-2.1980167739E-01	8.7263969666E-02	1.3327541403E-01	-2.1160040872E-01	-7.8324994690E-02
C^{2}—P^{4}	1.6479647940E-01	-1.9377827763E-01	6.6309155831E-02	1.5680381012E-01	-2.6516305083E-01	-1.0835924071E-01
C^{1}—P^{2}	1.7240226980E-01	-2.7954704518E-01	2.3291608931E-02	1.6944902219E-01	-2.6901128309E-01	-9.9562260900E-02
C^{2}—P^{3}	1.8192743366E-01	-1.9960374846E-01	9.2980759458E-02	1.8191591983E-01	-3.1393090255E-01	-1.3201498272E-01
Ni^{1}—$P^{1'}$	9.0804035933E-02	1.4894721348E-01	1.5595730899E-02	3.4544919084E-02	-1.0632664154E-01	-7.1781722456E-02
Ni^{1}—$C^{CDP'}$	7.9900676279E-02	1.8187428190E-01	1.2549953128E-01	2.3520984932E-02	-9.2510540340E-02	-6.8989555408E-02
Ni^{1}—$C^{2'}$	8.1564155626E-02	1.7964479073E-01	1.2340760098E-01	2.3727239546E-02	-9.2365676775E-02	-6.8638437229E-02
Ni^{1}—P^{4}	1.0379094407E-01	9.0572915975E-02	1.8214765905E-02	4.5898016058E-02	-1.1443926111E-01	-6.8541245052E-02
Ni^{1}—Cl^{1}	4.3250136333E-02	1.2995838154E-01	3.7110808067E-02	5.6560249956E-03	-4.3801645376E-02	-3.8145620380E-02
$C^{CDP'}$—$P^{2'}$	1.8125700014E-01	-1.7892830272E-01	8.6435221315E-02	1.8030526503E-01	-3.1587845438E-01	-1.3557318935E-01
$C^{CDP'}$—$P^{3'}$	1.7785807316E-01	-1.1985169699E-01	1.0415470652E-01	1.7376790820E-01	-3.1757289216E-01	-1.4380498396E-01
$C^{1'}$—$P^{1'}$	1.4820704301E-01	-2.1980131289E-01	8.7262830856E-02	1.3327565744E-01	-2.1160098665E-01	-7.8325329210E-02
$C^{2'}$—$P^{4'}$	1.6479658510E-01	-1.9377758572E-01	6.6308662967E-02	1.5680393883E-01	-2.6516348123E-01	-1.0835954240E-01
$C^{1'}$—$P^{2'}$	1.7240218103E-01	-2.7954644954E-01	2.3291597430E-02	1.6944888496E-01	-2.6901115754E-01	-9.9562272580E-02
$C^{2'}$—$P^{3'}$	1.8192790654E-01	-1.9959931852E-01	9.2980415266E-02	1.8191652481E-01	-3.1393321999E-01	-1.3201669518E-01
C^{1}—H	2.7699641488E-01	-9.7104170635E-01	7.6514856820E-03	2.8864425514E-01	-3.3452808370E-01	-4.5883828560E-02
C^{1}—H’	2.7622511210E-01	-9.5933876869E-01	8.3977826276E-03	2.8807007367E-01	-3.3630545516E-01	-4.8235381490E-02
$C^{1'}$—H	2.7699595231E-01	-9.7103877534E-01	7.6516503992E-03	2.8864338878E-01	-3.3452708373E-01	-4.5883694950E-02
$C^{1'}$—H’	2.7622477350E-01	-9.5933692318E-01	8.3980225158E-03	2.8806943179E-01	-3.3630463279E-01	-4.8235201000E-02
C^{2}—H	2.7790846899E-01	-9.6687295250E-01	1.8608761733E-02	2.9053128175E-01	-3.3934432539E-01	-4.8813043640E-02
$C^{2'}$—H	2.7790834766E-01	-9.6687201294E-01	1.8609129218E-02	2.9053107318E-01	-3.3934414312E-01	-4.8813069940E-02
C^{CDP}—H	2.7540372870E-01	-9.4868918562E-01	2.3611531652E-02	2.8742294267E-01	-3.3767358893E-01	-5.0250646260E-02
$C^{CDP'}$—H	2.7540360991E-01	-9.4868875709E-01	2.3611131645E-02	2.8742270824E-01	-3.3767322721E-01	-5.0250518970E-02

3.1 Molecular orbitals

All Molecular Orbitals are shown with a contour value of 0.03 and the atoms are color-coded as follows: Ni: orange; P: violet; Cl: green; C: grey.

1^{Me}

LUMO



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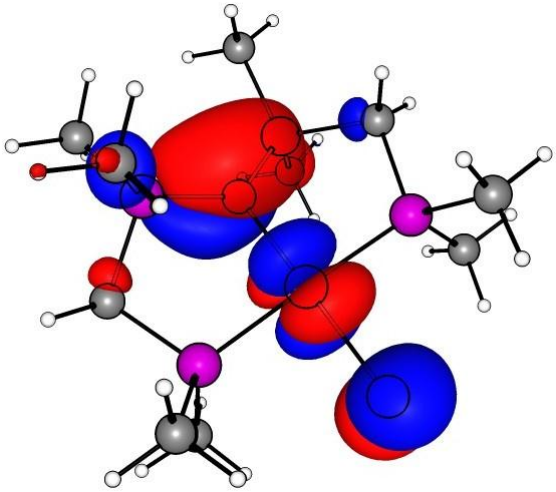

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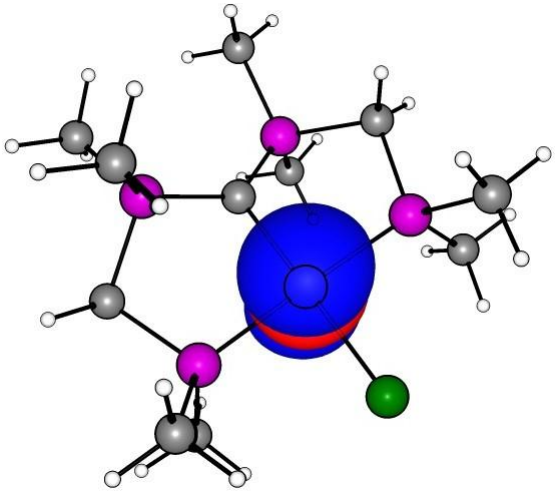

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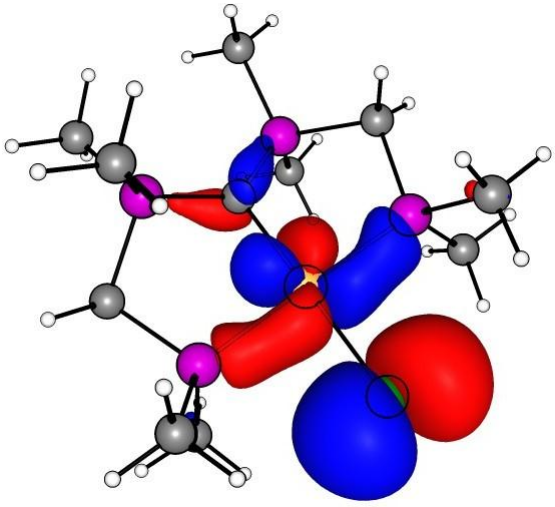

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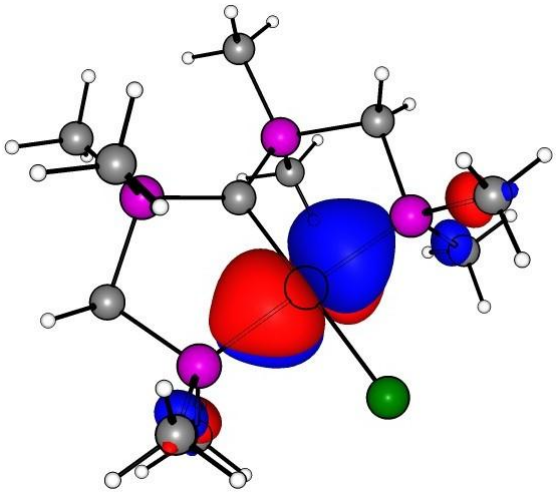

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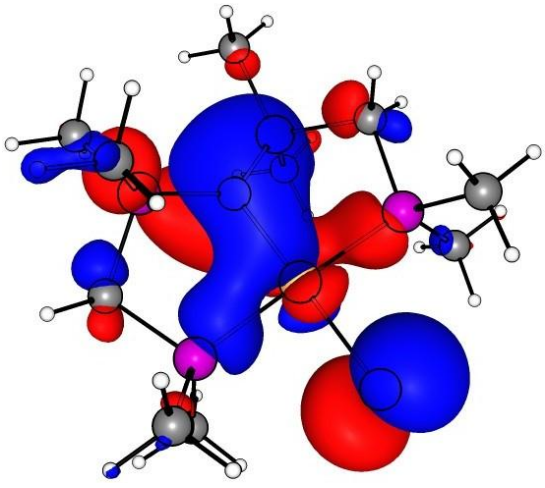

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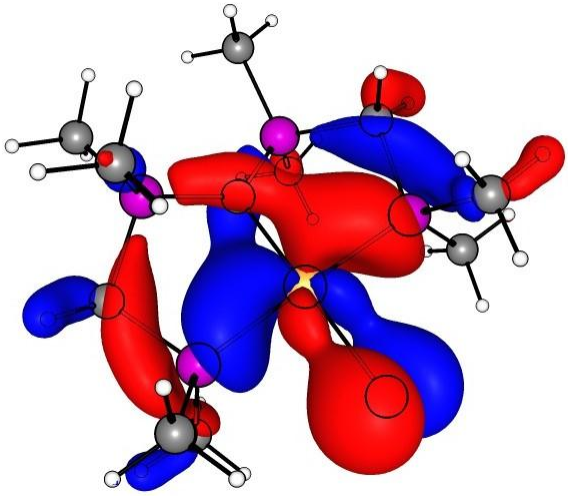

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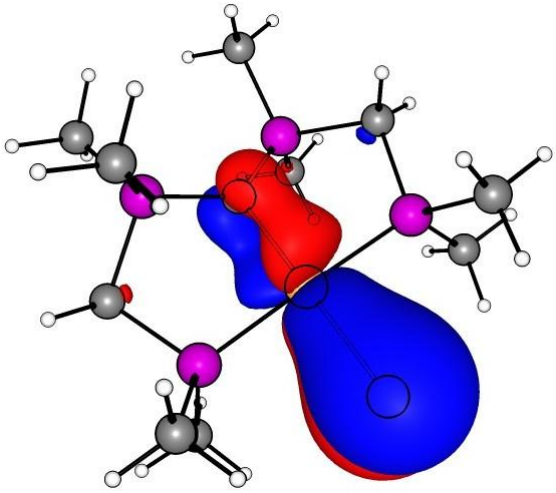

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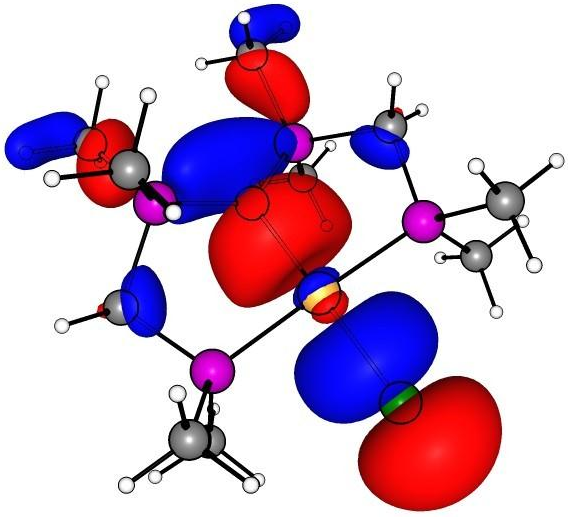

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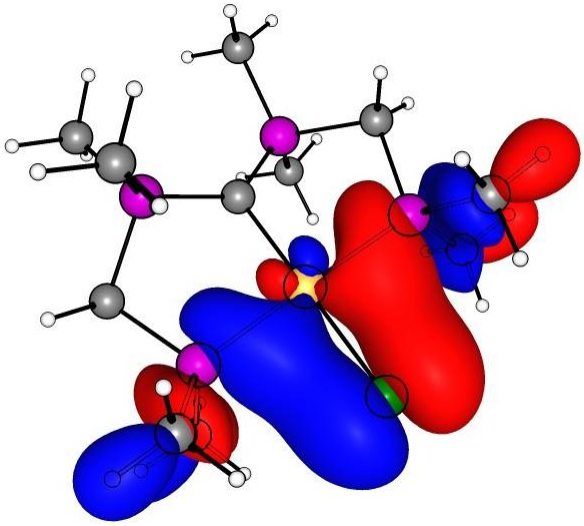

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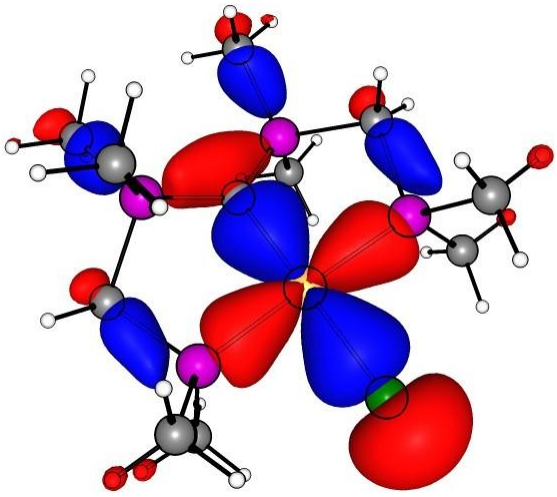

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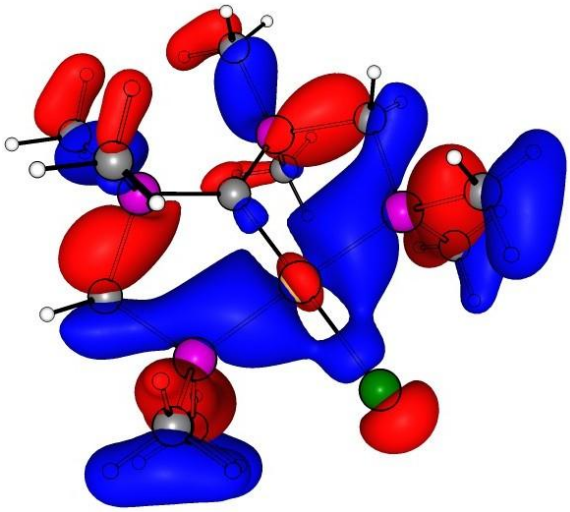

2^{Me}

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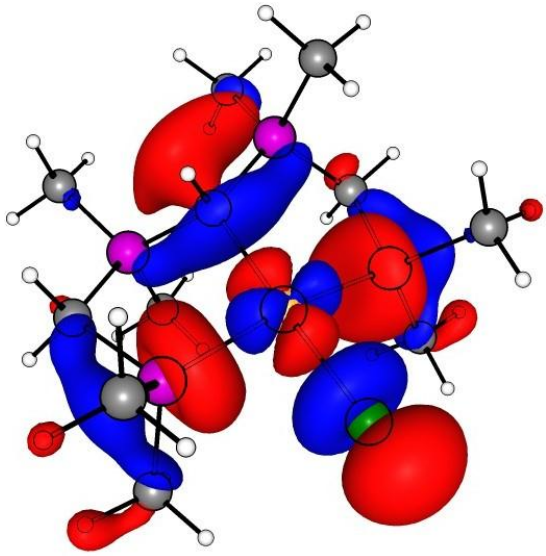

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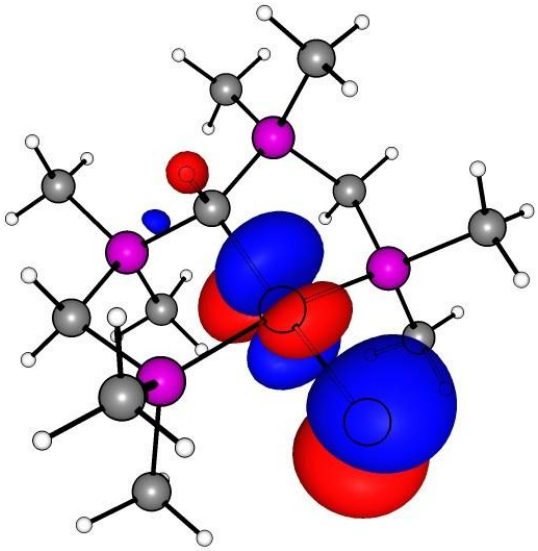

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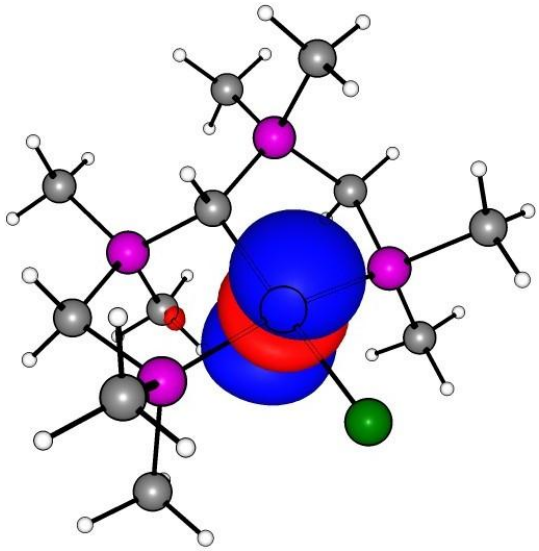

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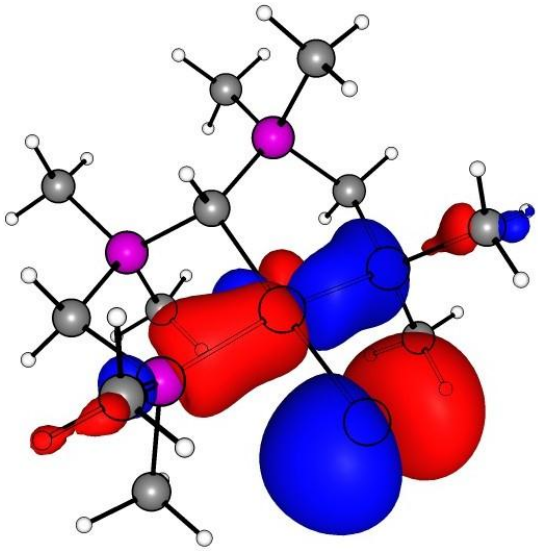

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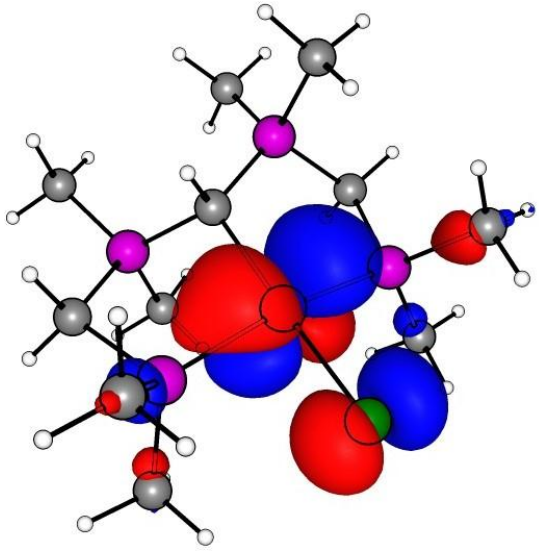

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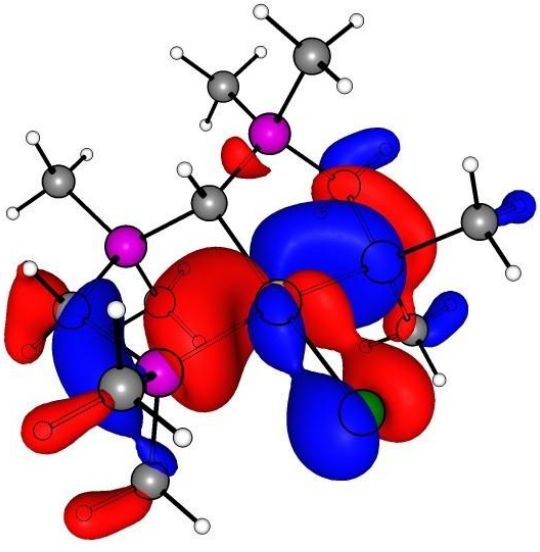

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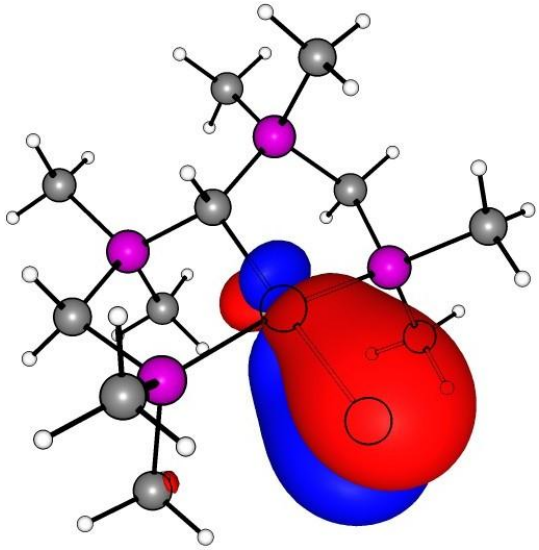

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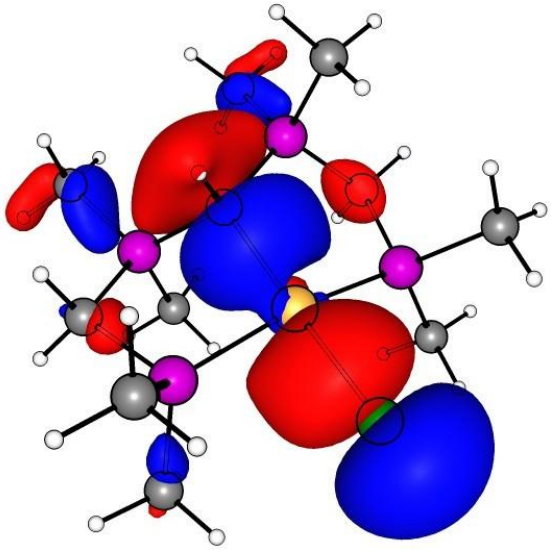

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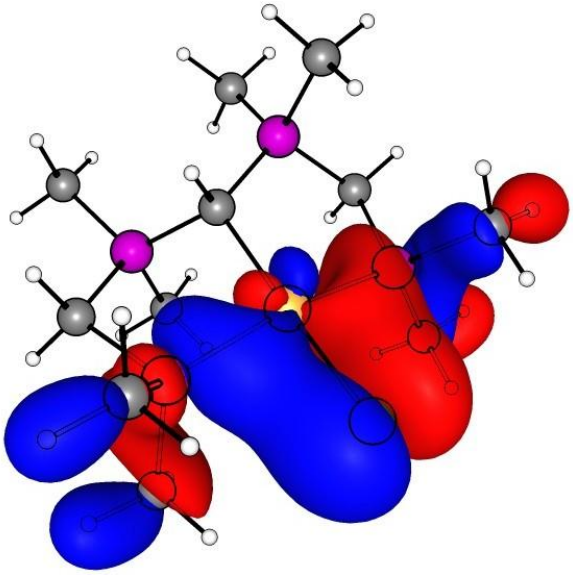

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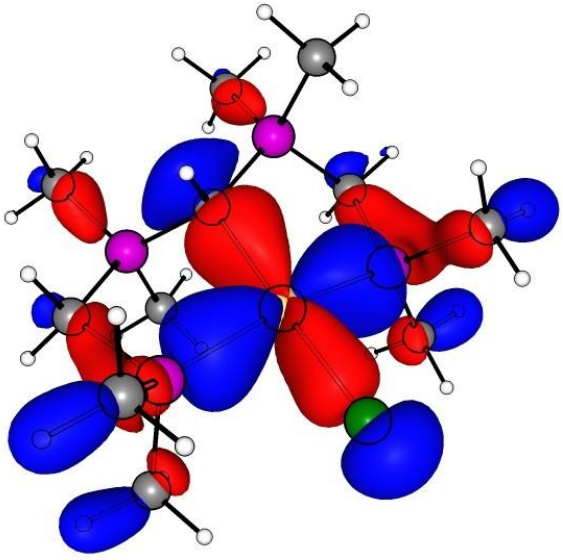

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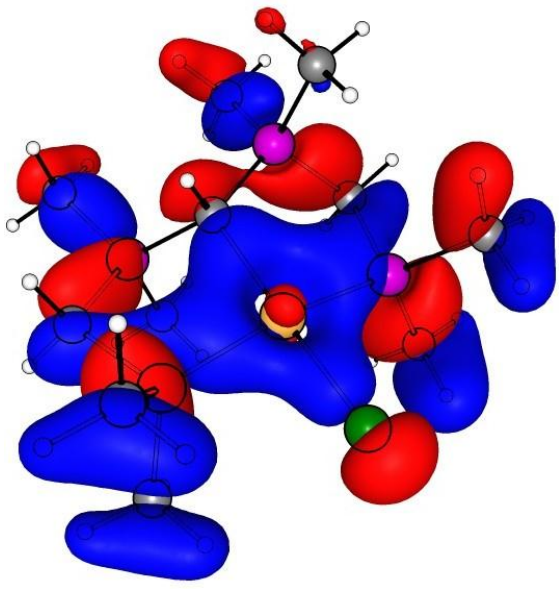

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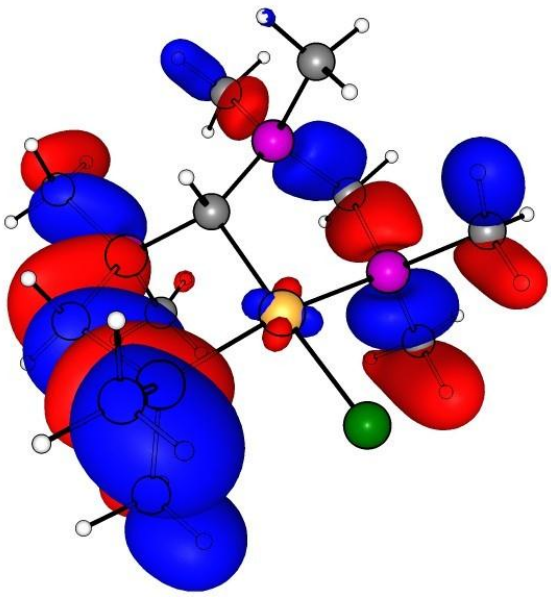

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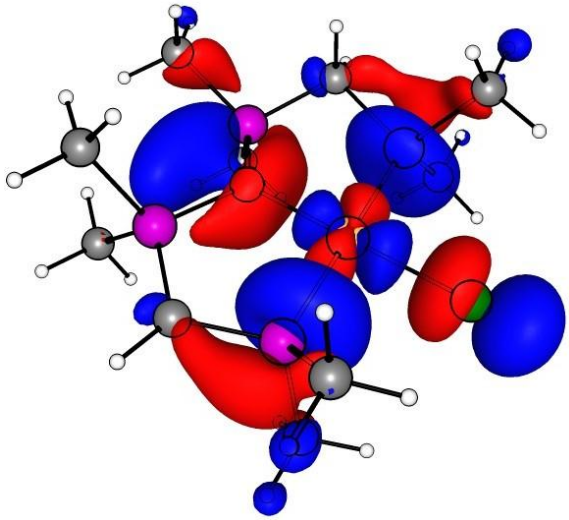

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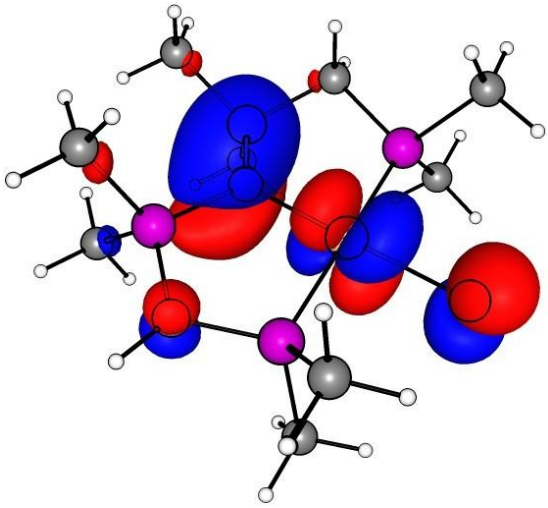

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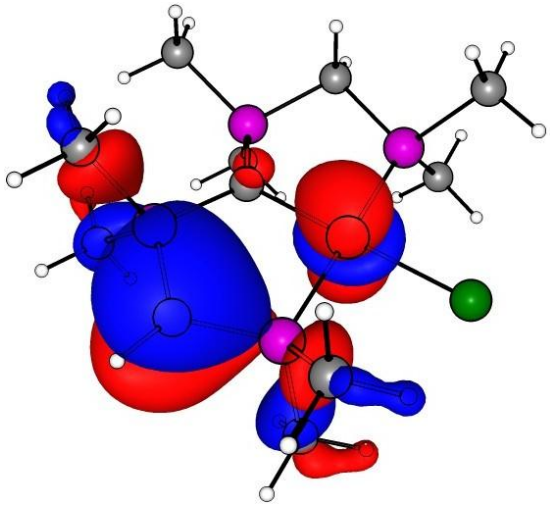

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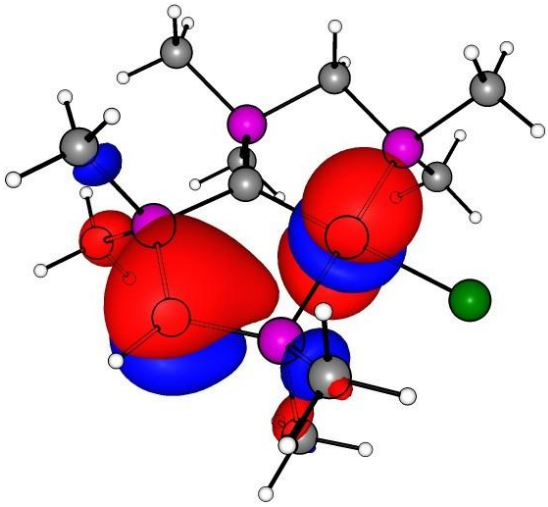

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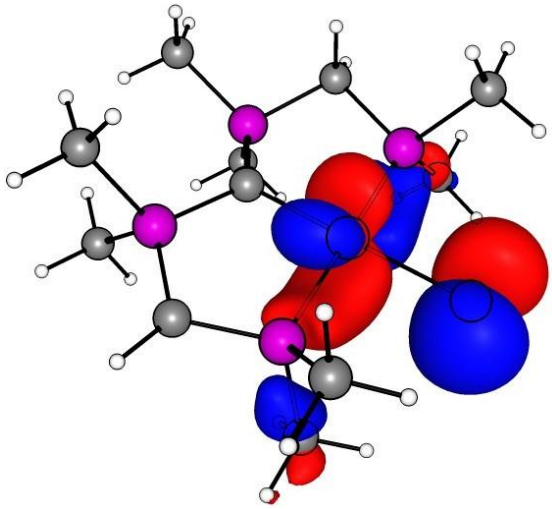

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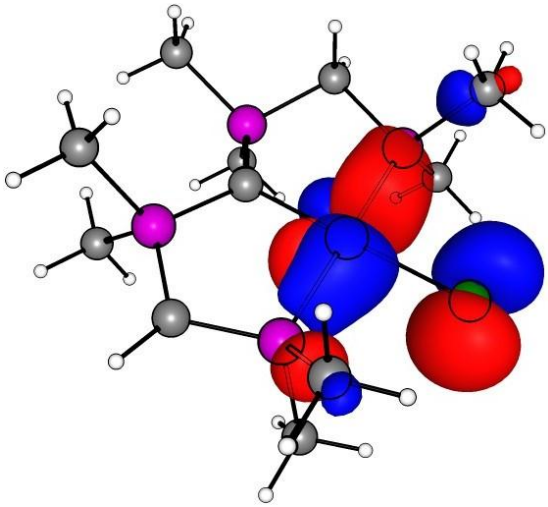

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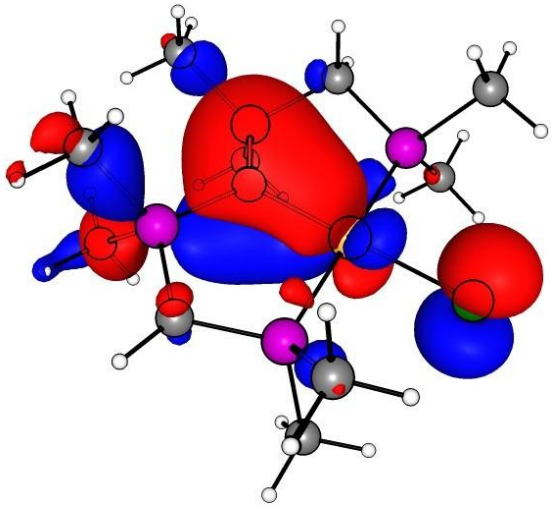

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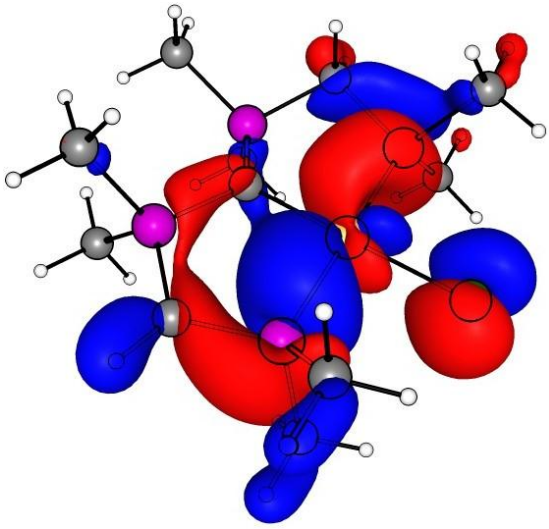

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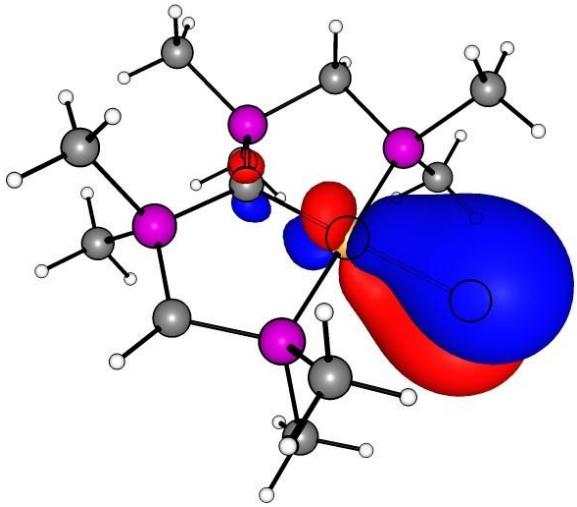

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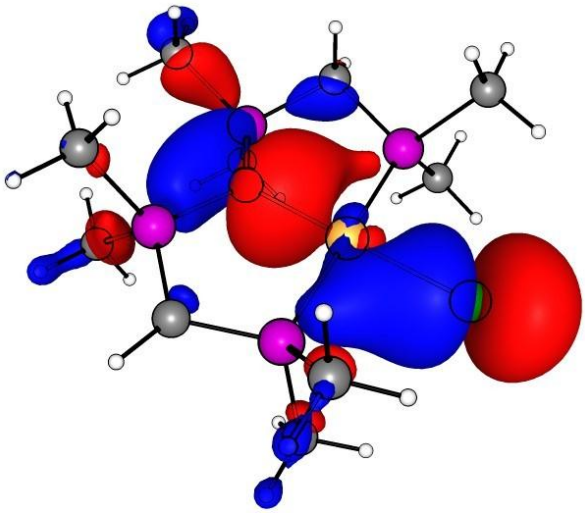

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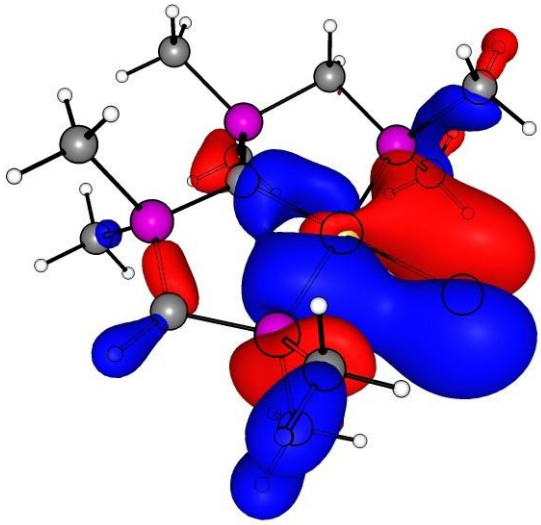

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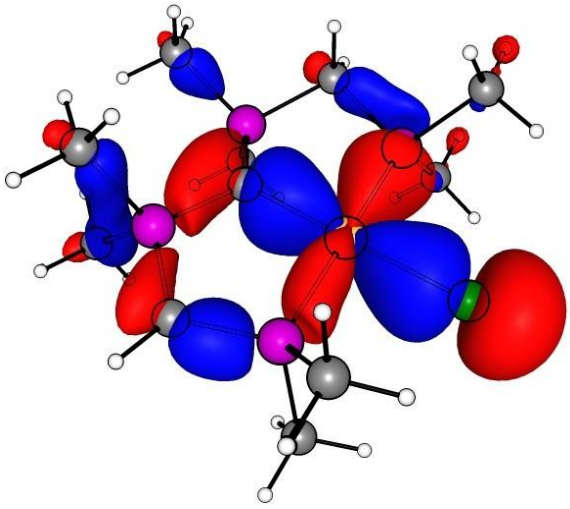

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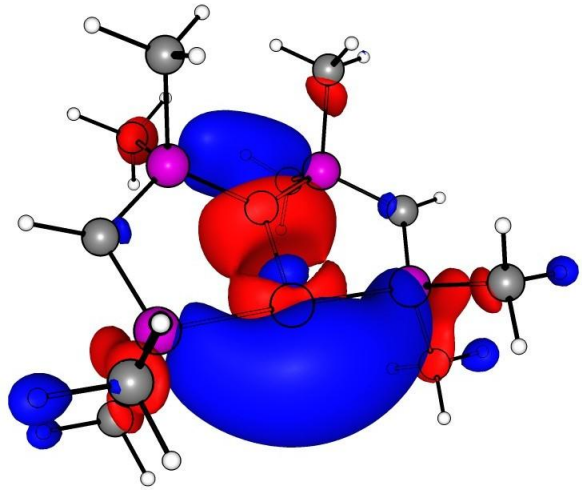

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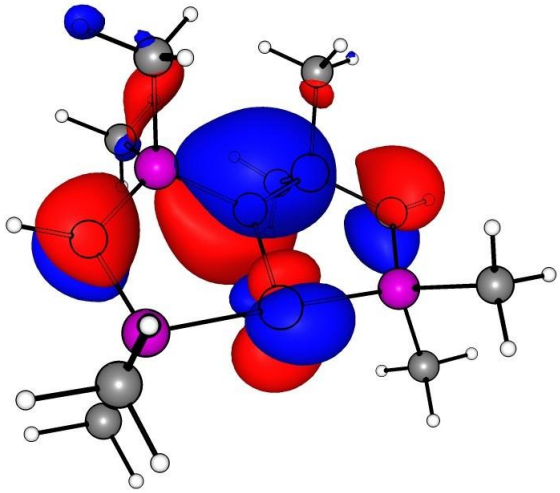

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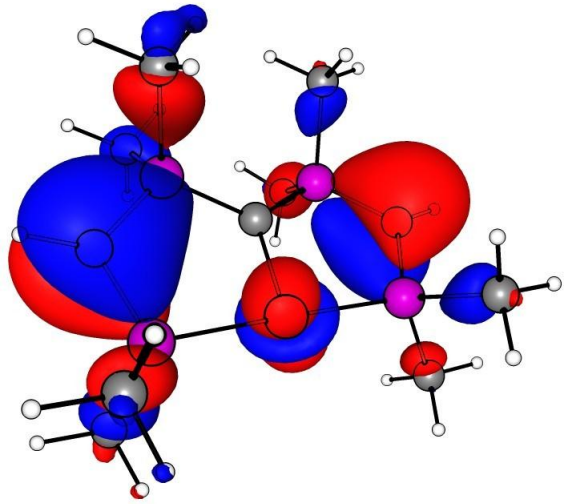

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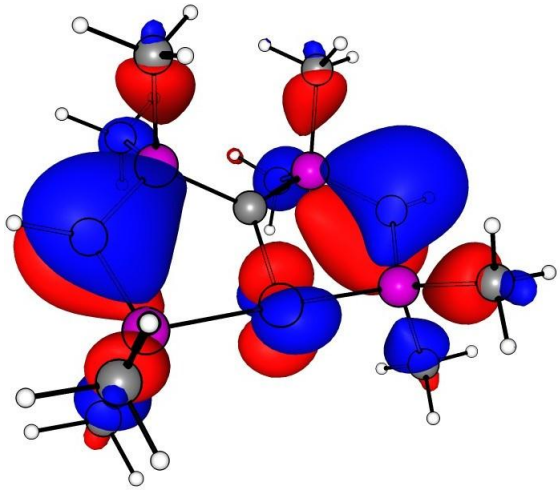

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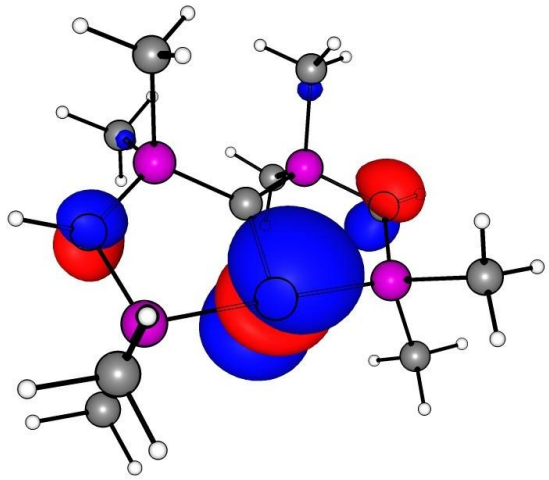

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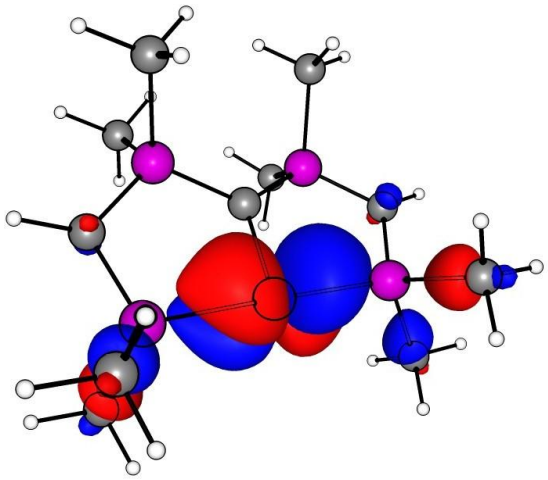

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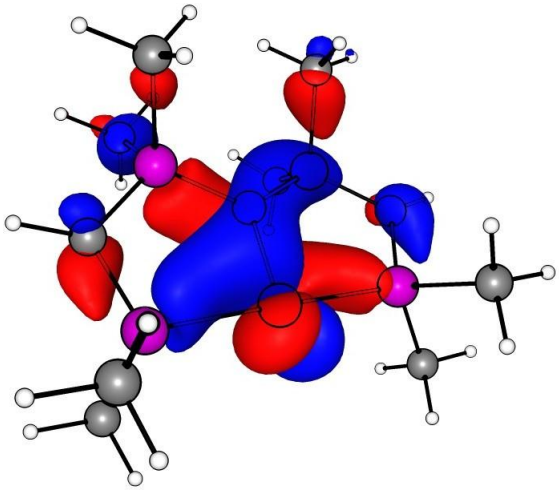

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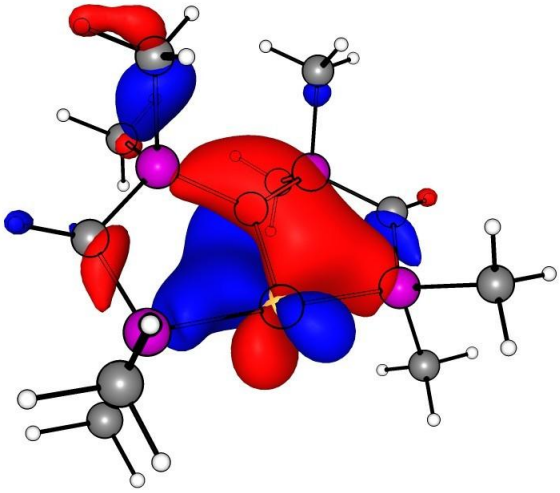

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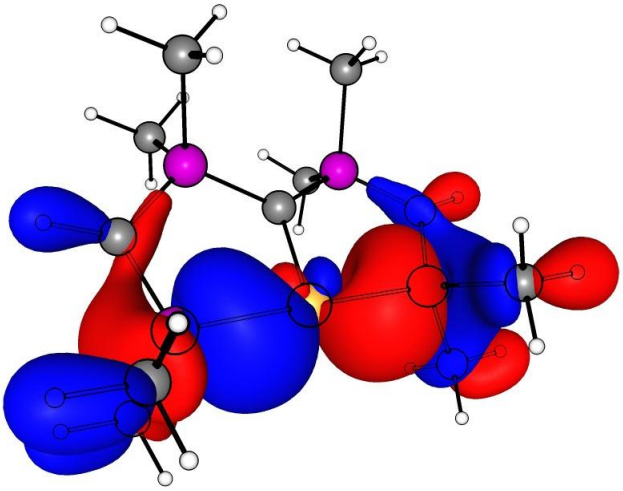

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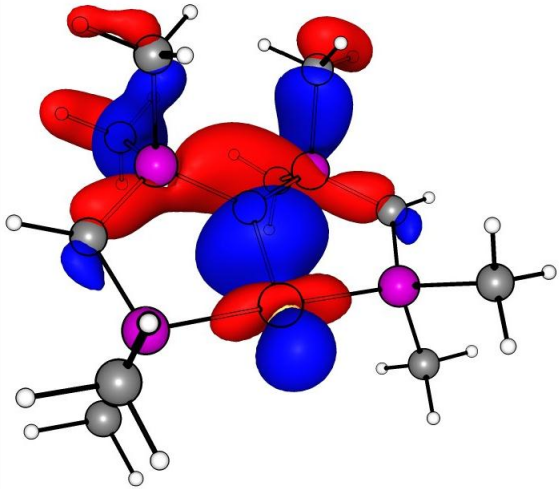

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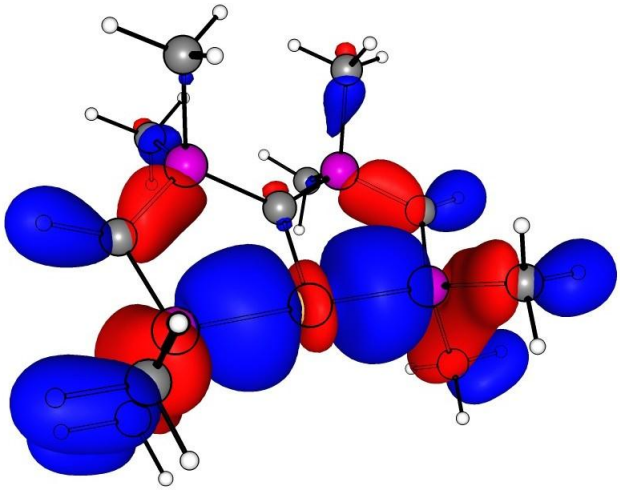

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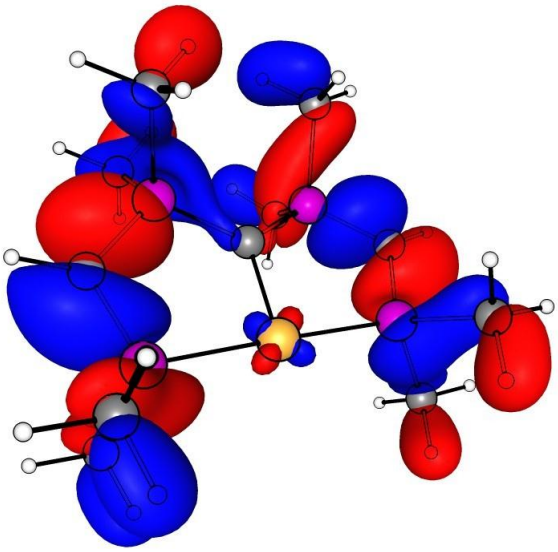

***cis*-5^{Me}**

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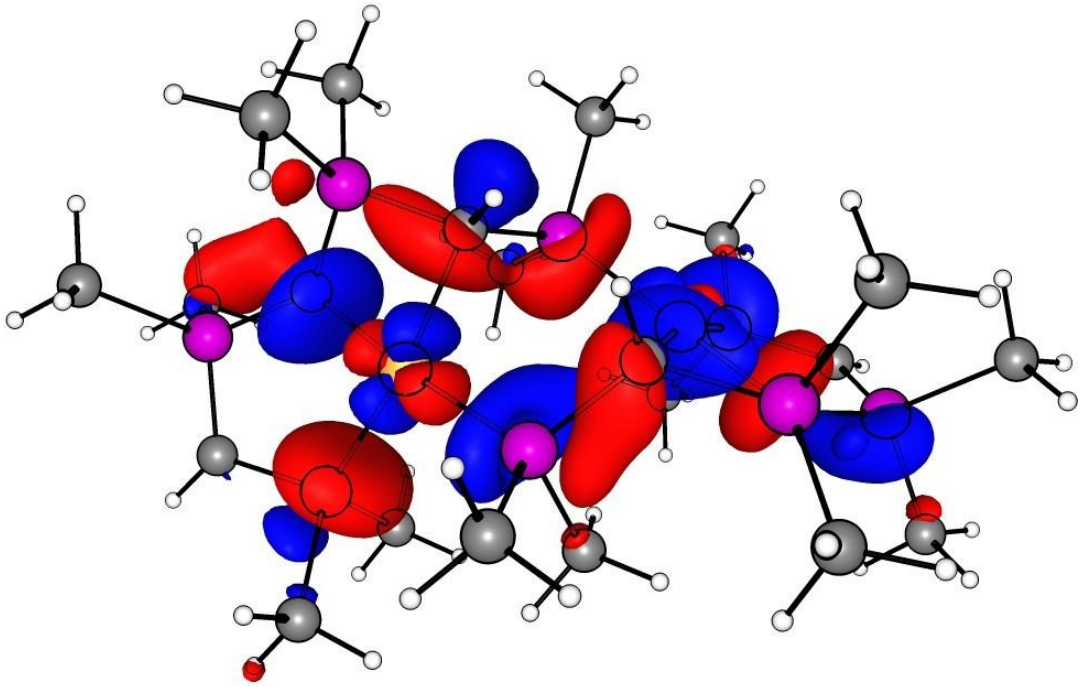

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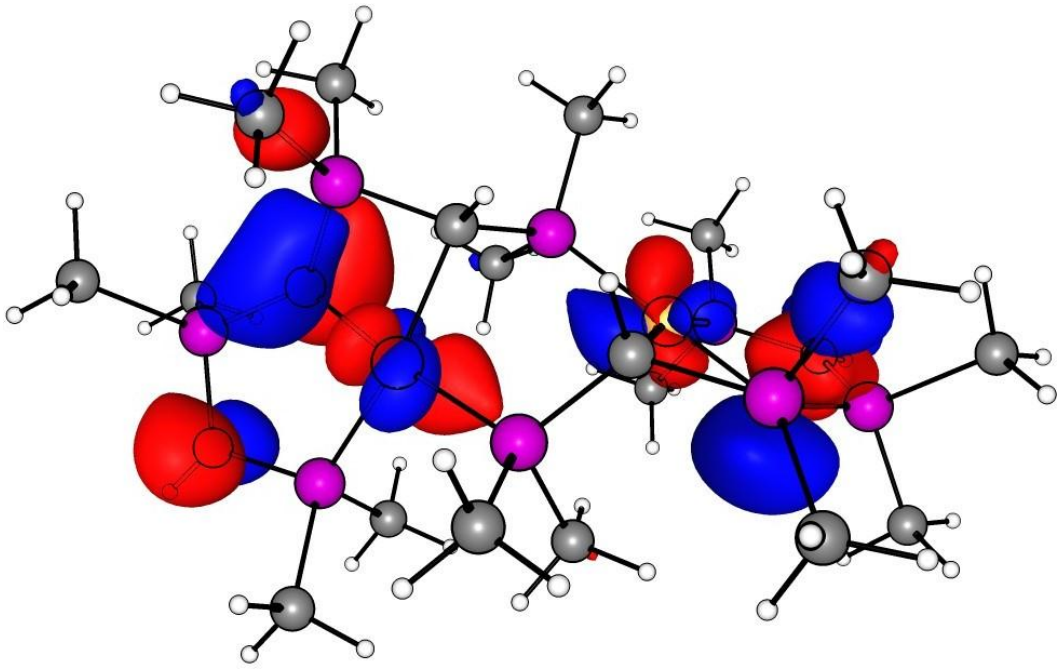

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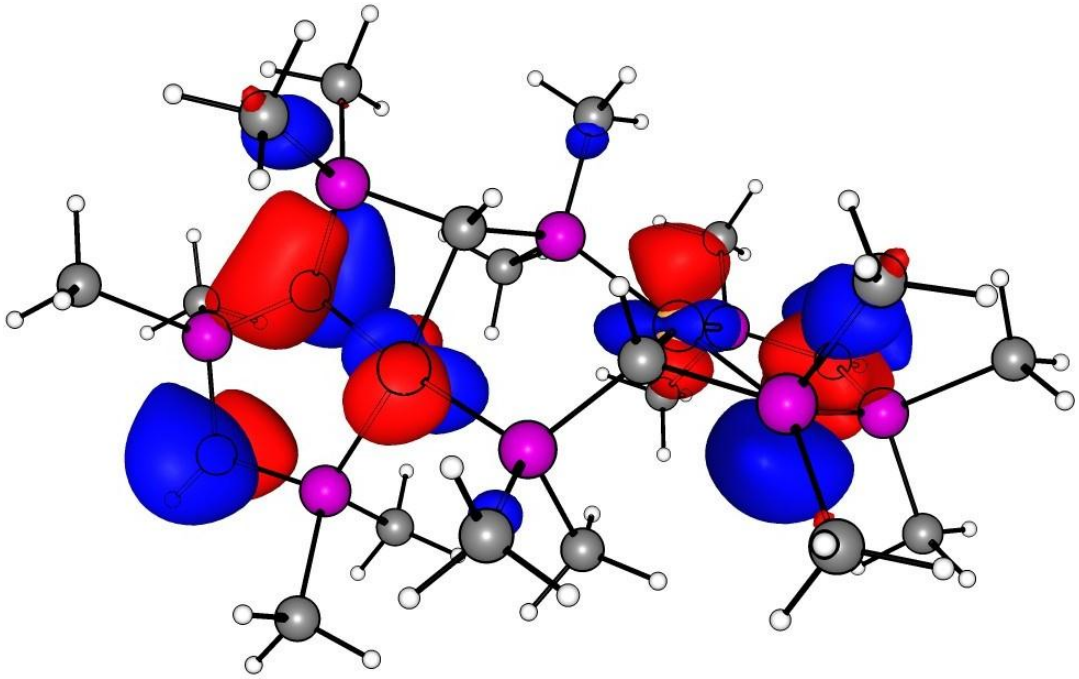

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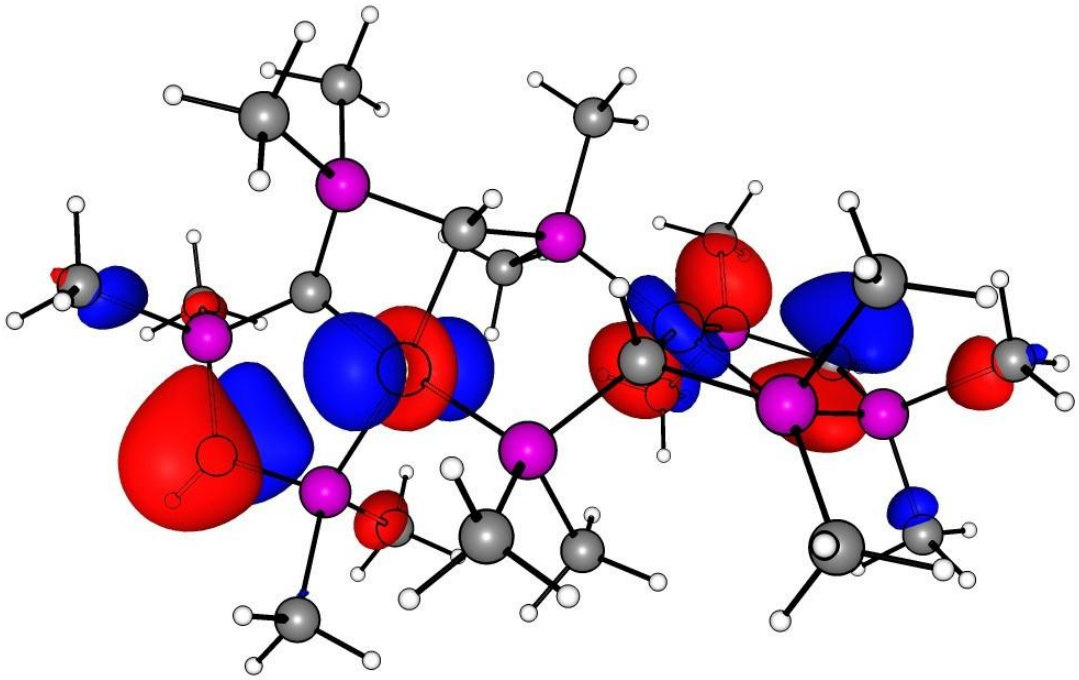

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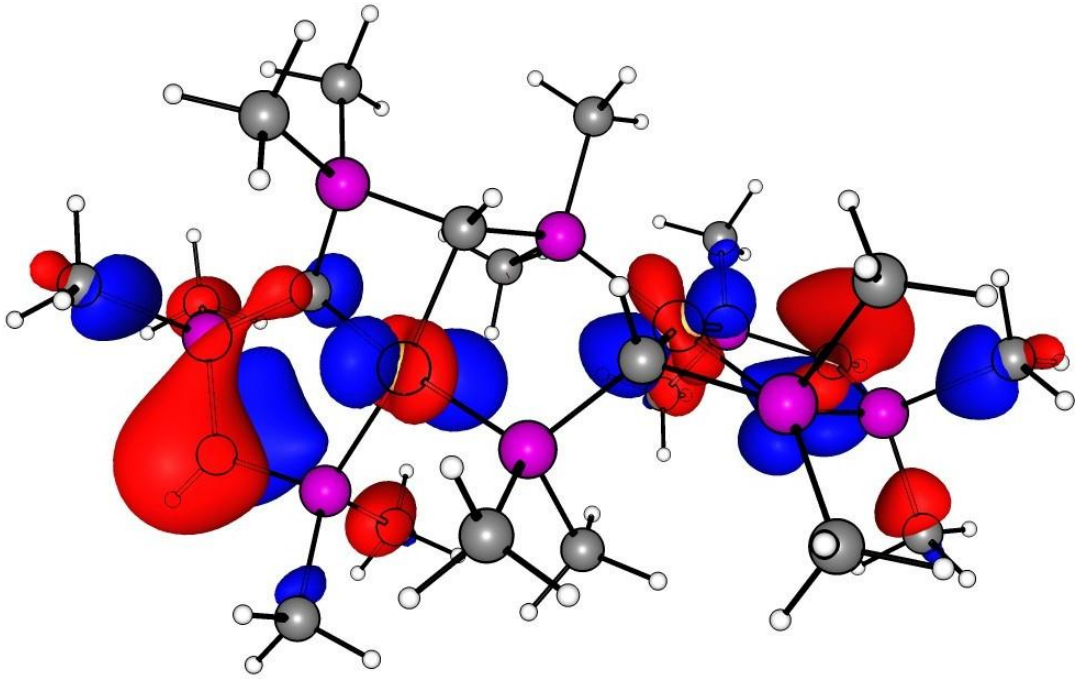

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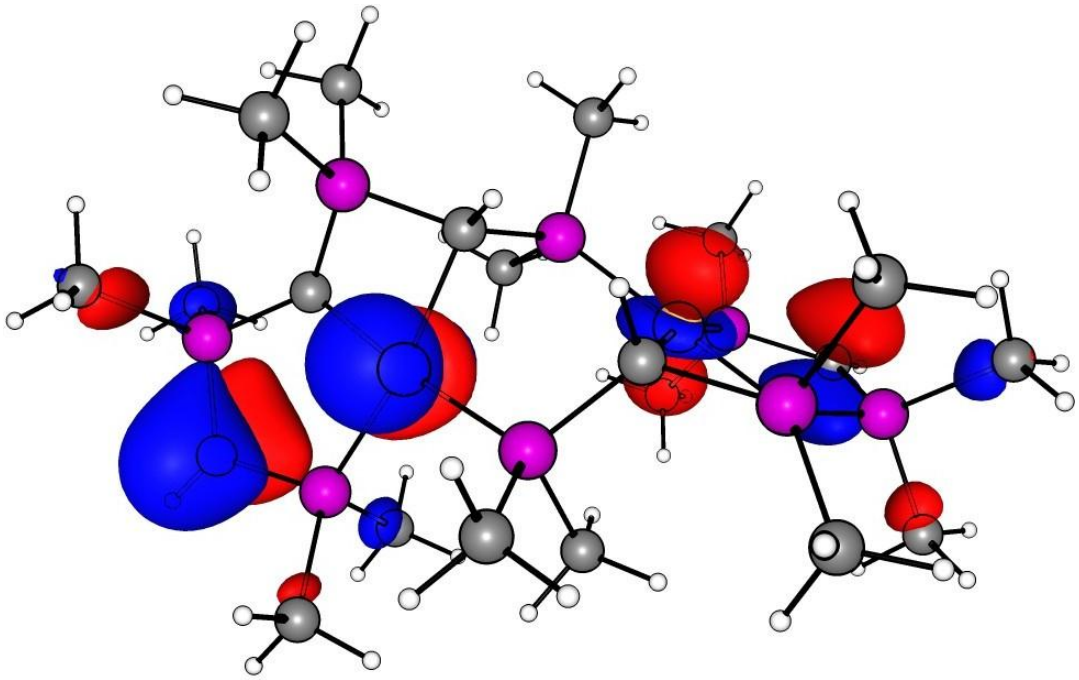

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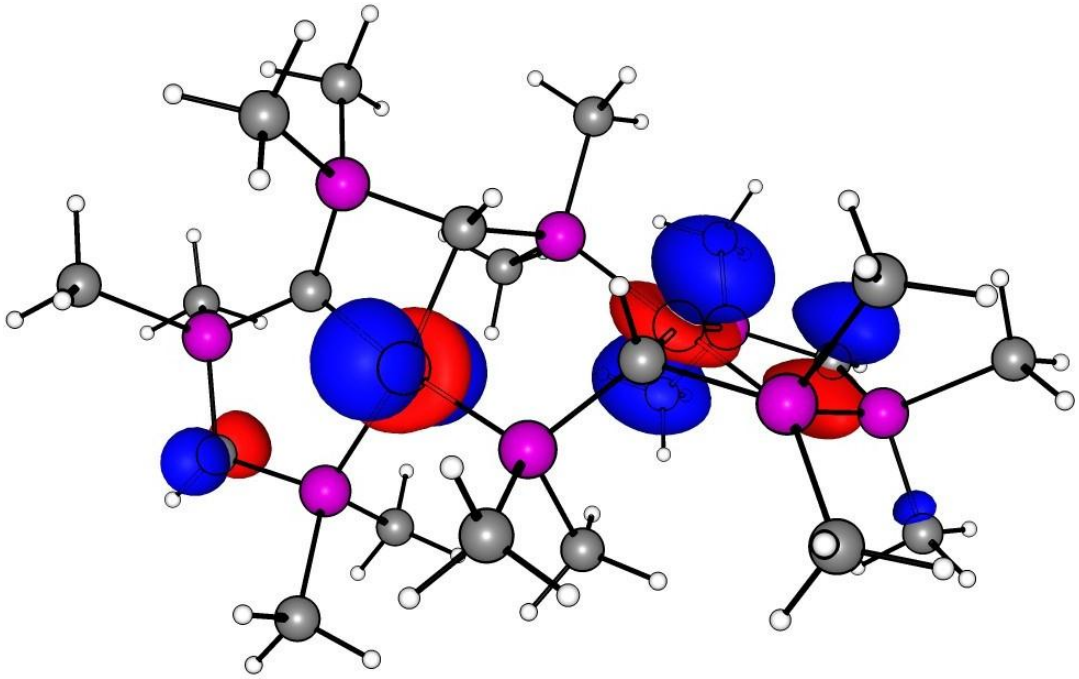
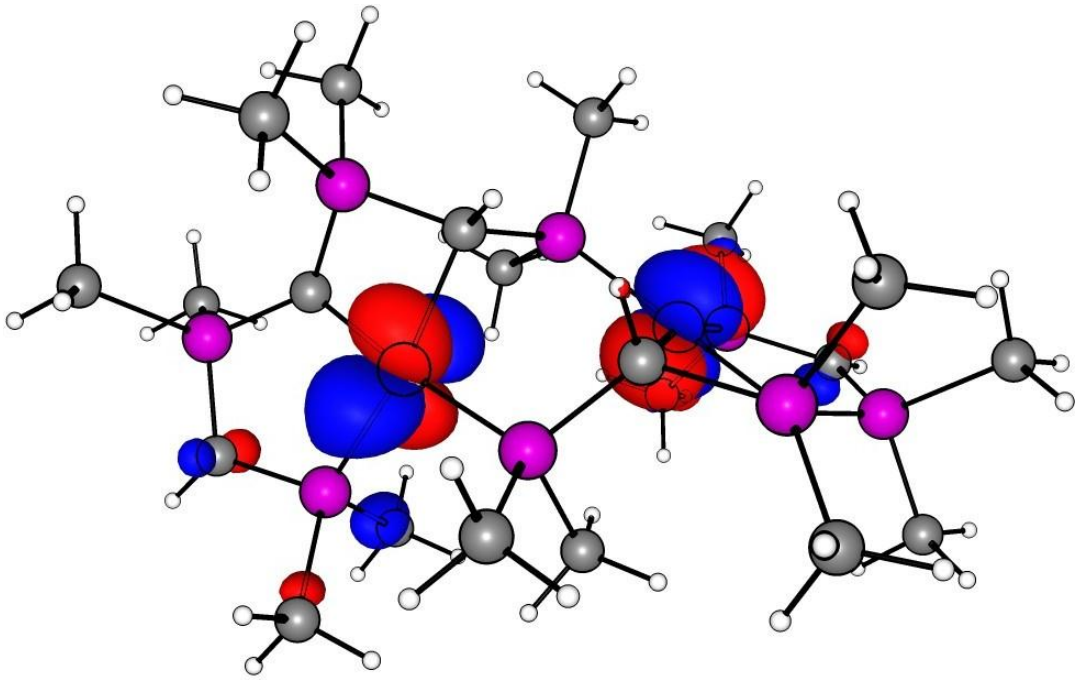
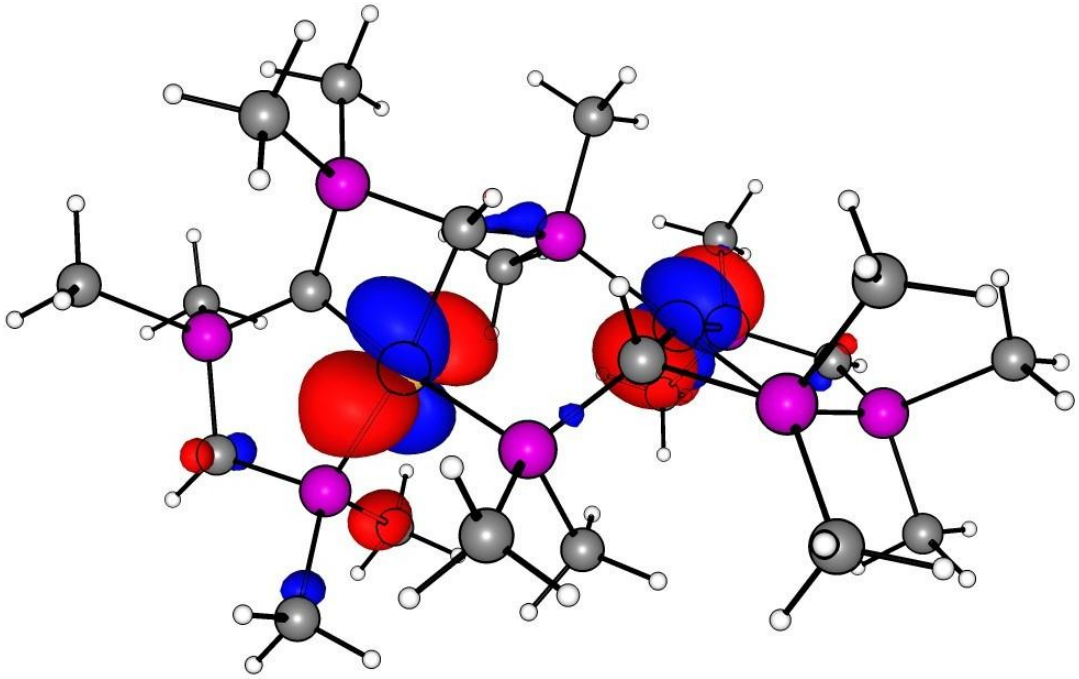


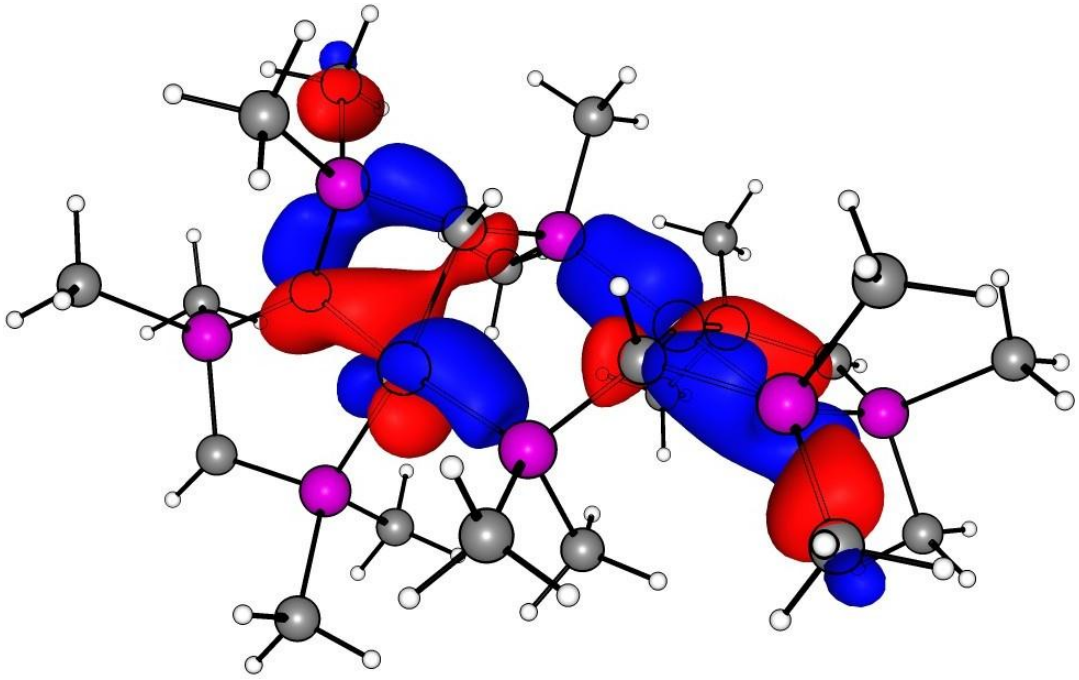
HOMO-6



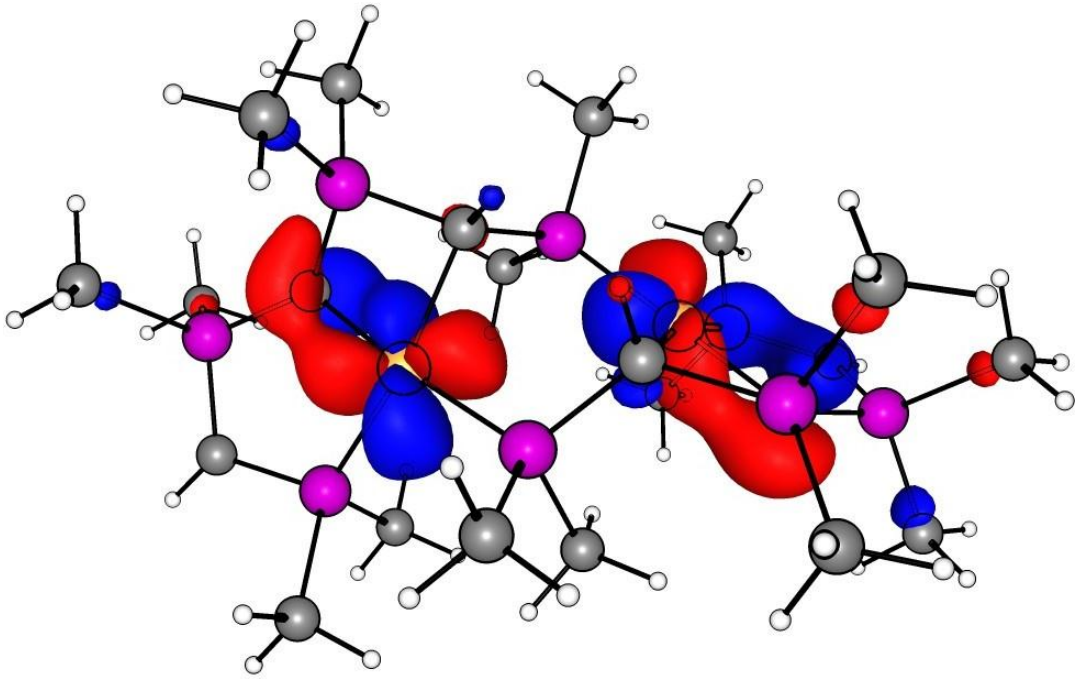
HOMO-7



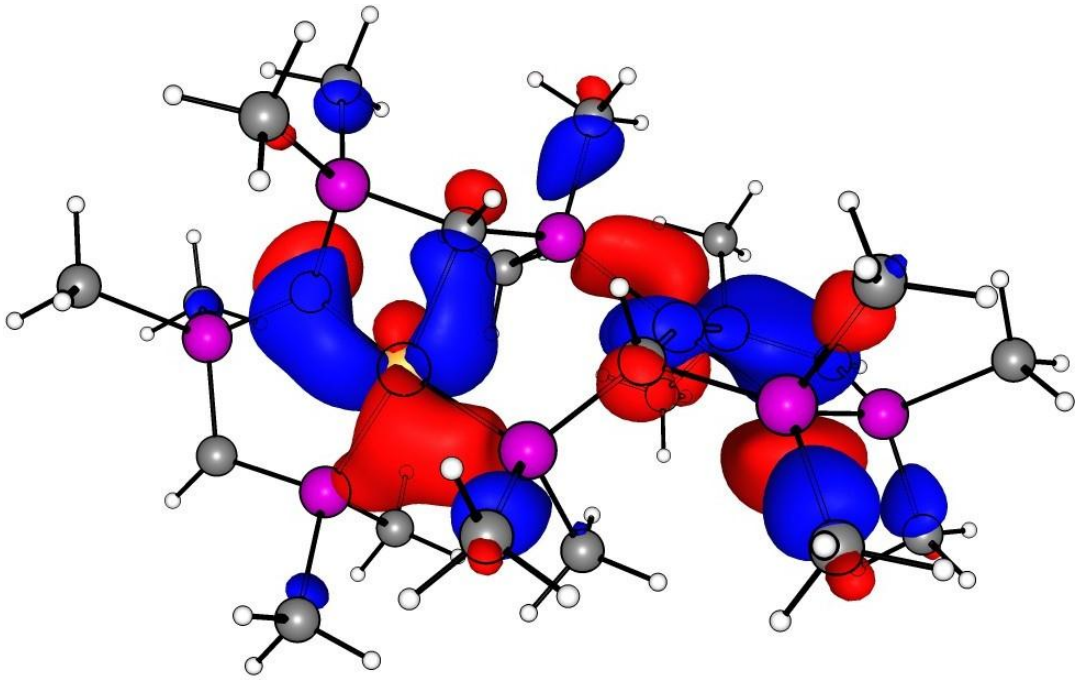
HOMO-8



HOMO-9

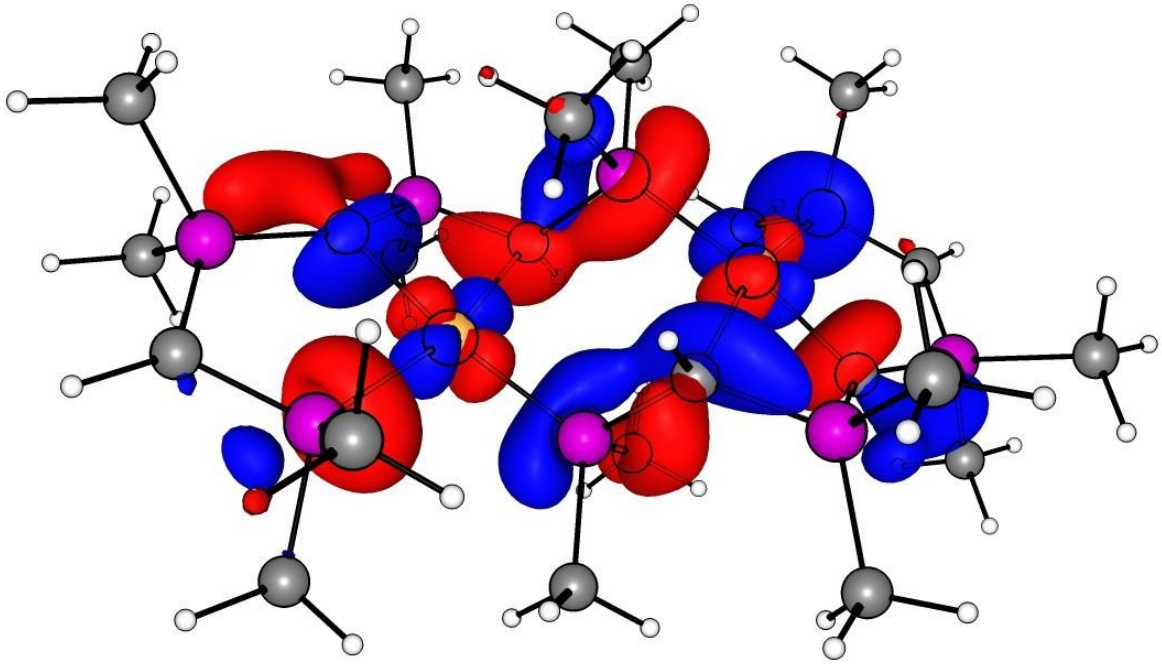


HOMO-10

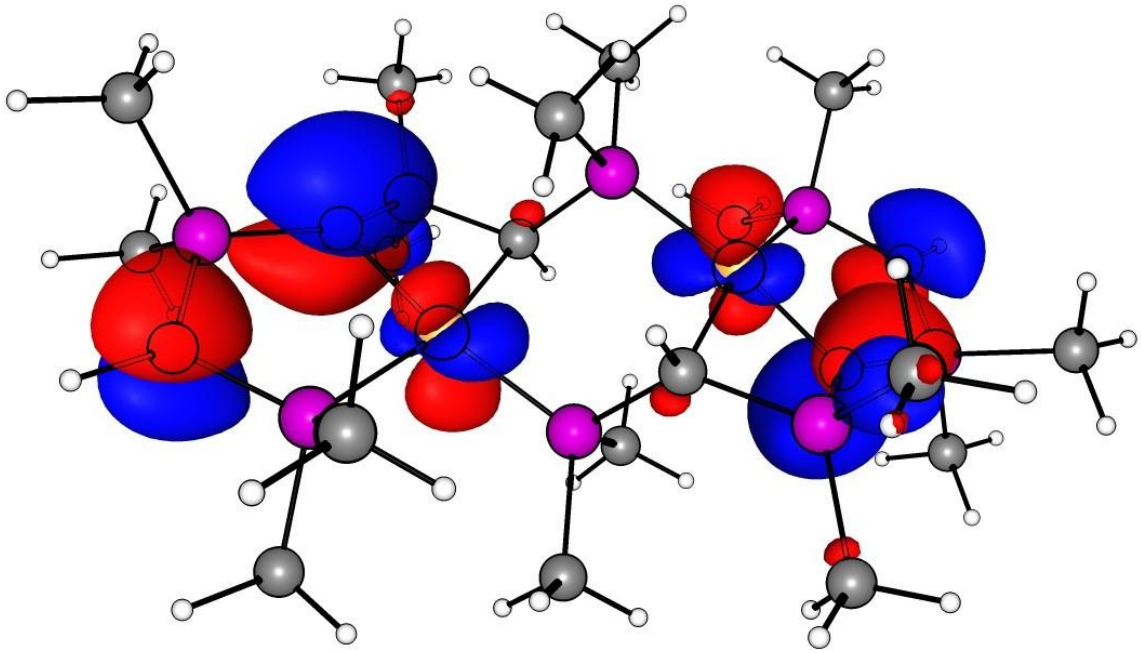


***trans*-5^{Me}**

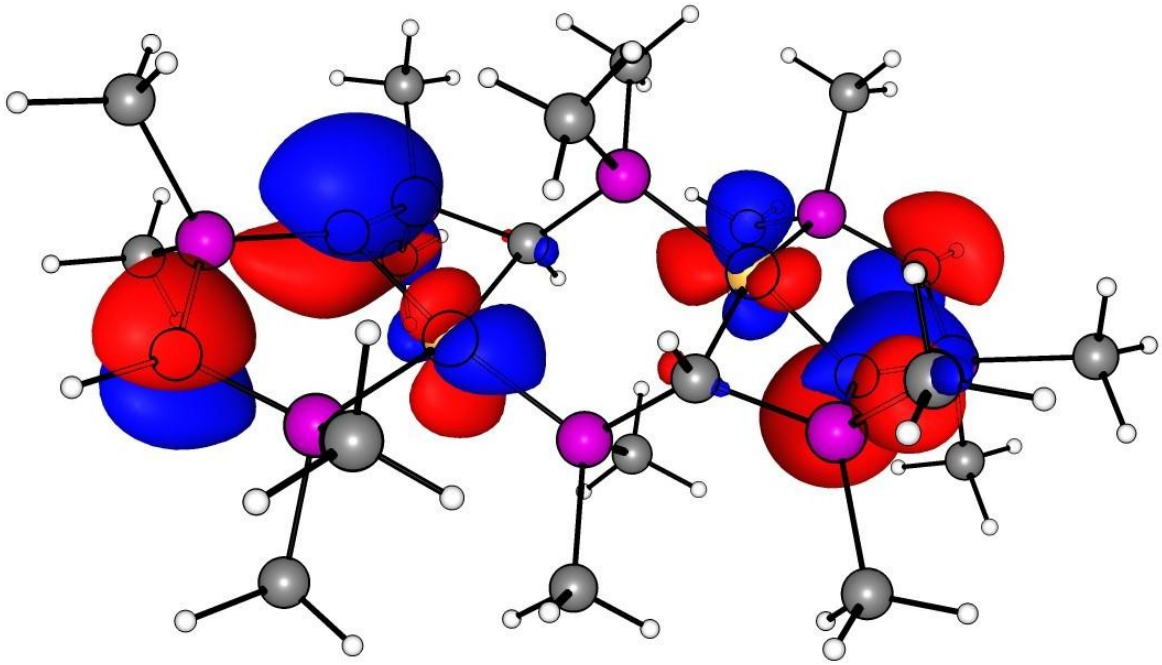
LUMO



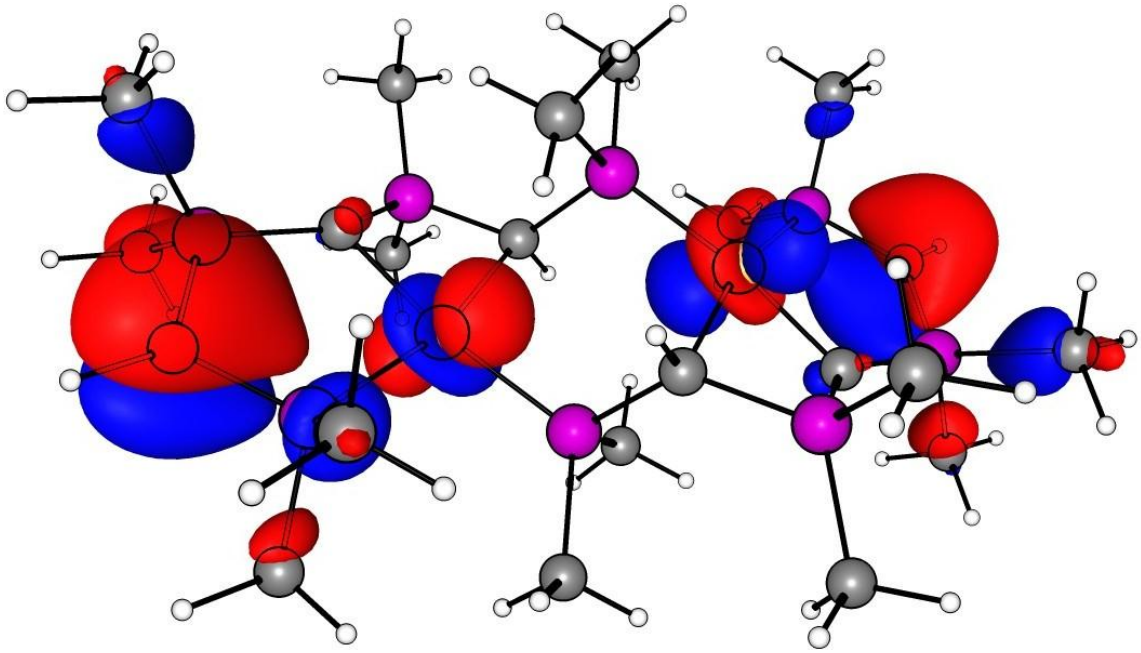
HOMO



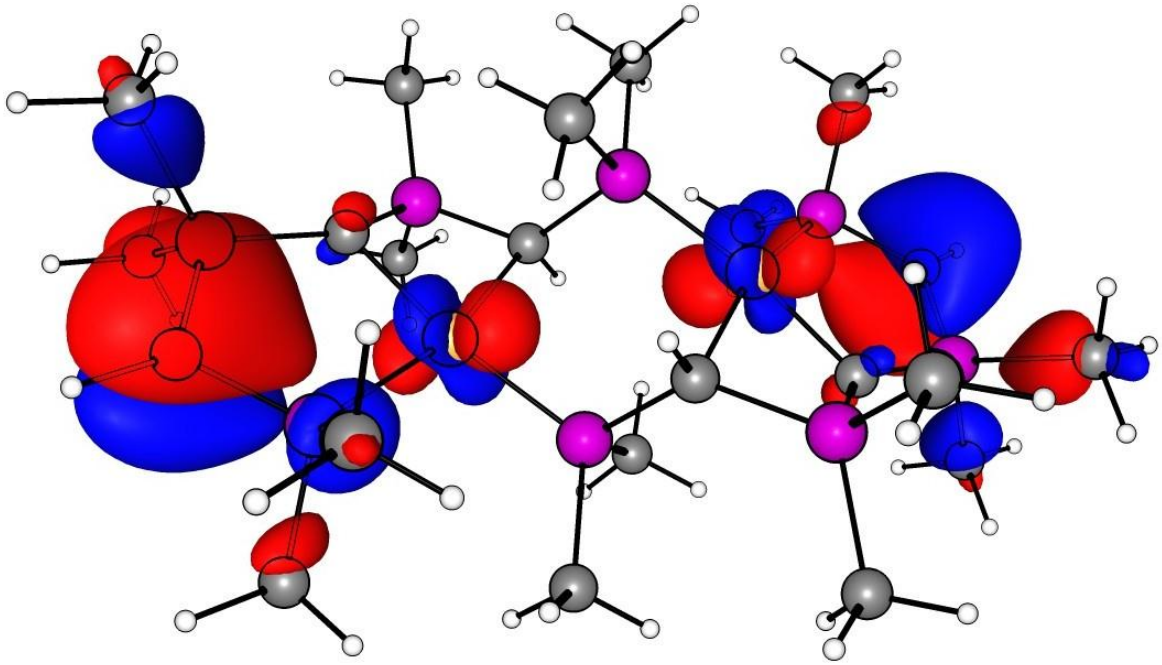
HOMO-1



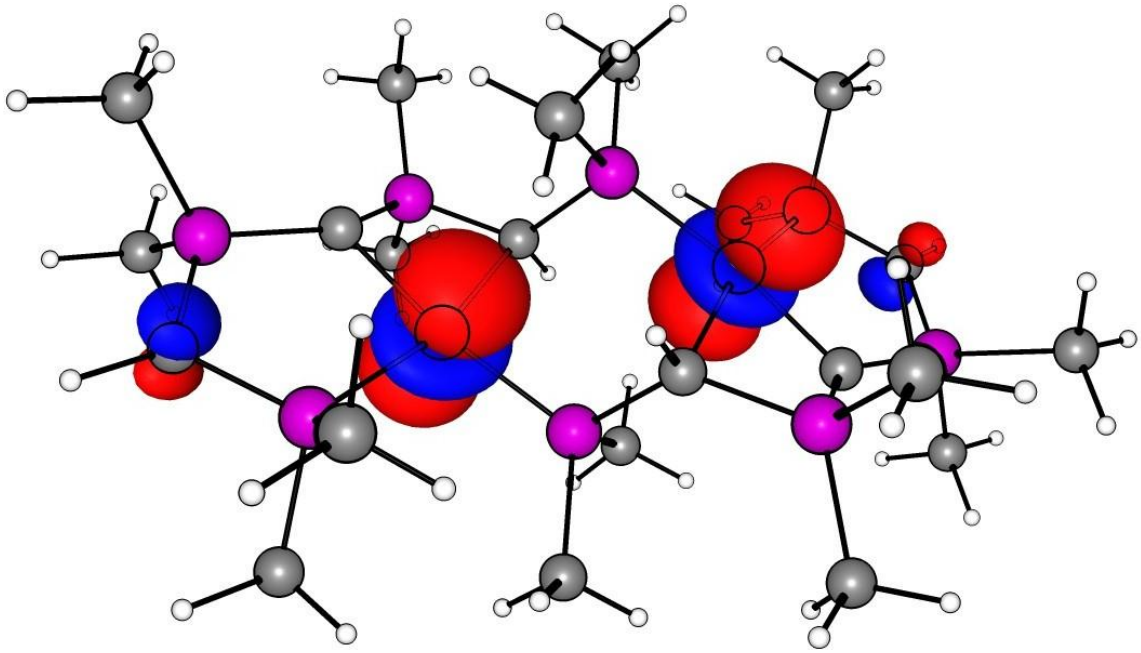
HOMO-2



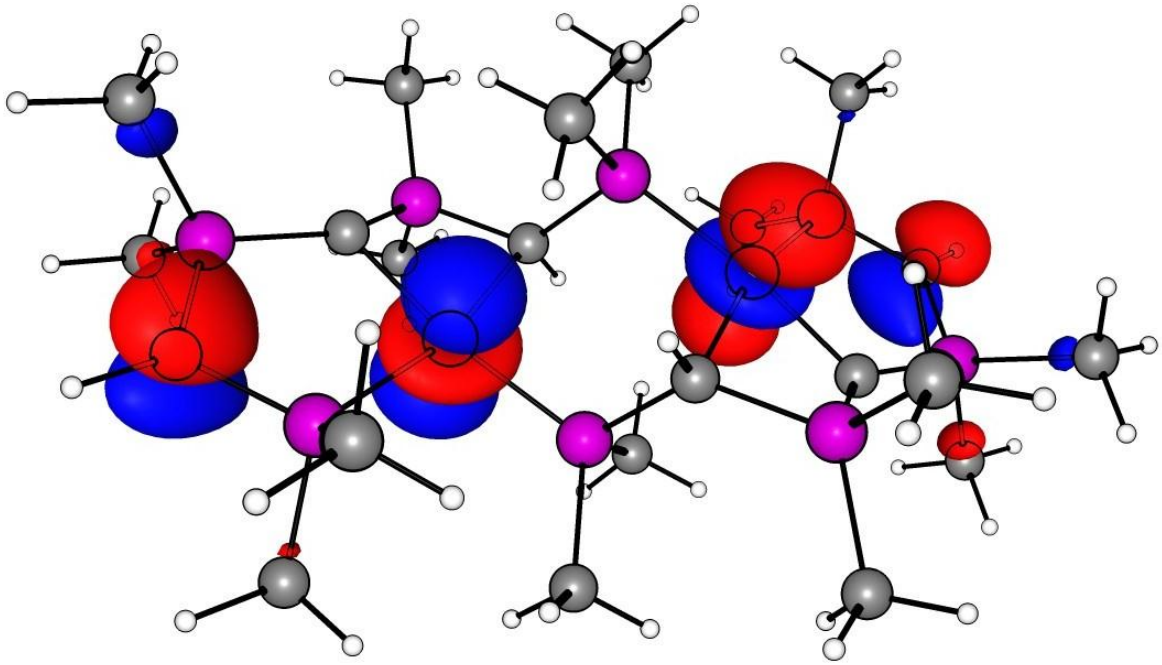
HOMO-3



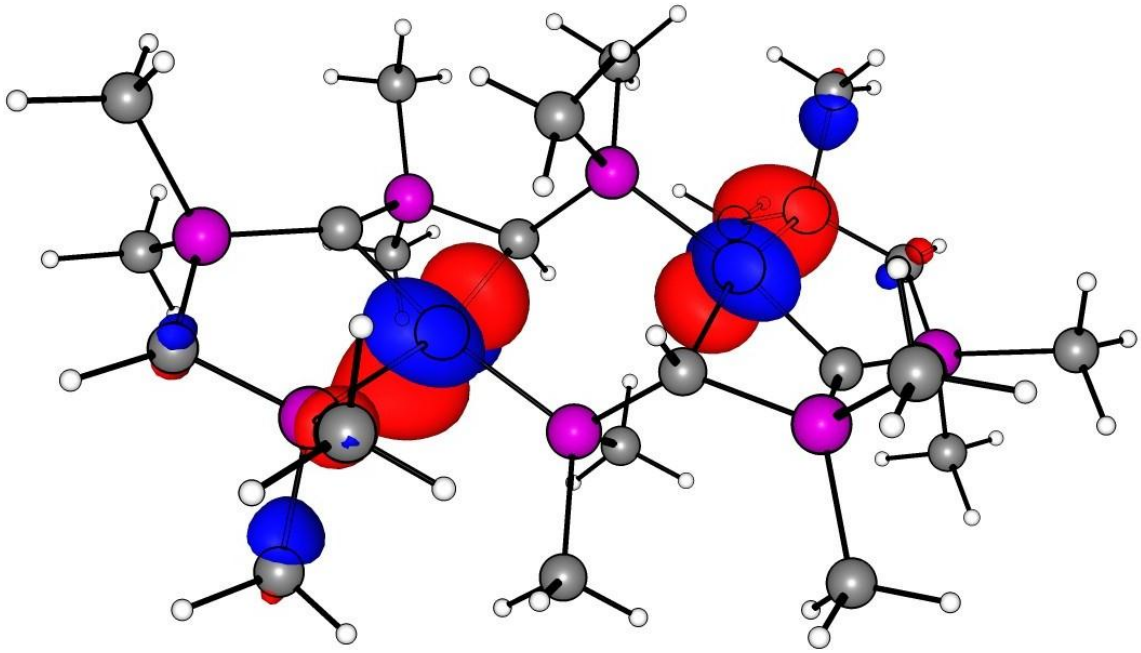
HOMO-4



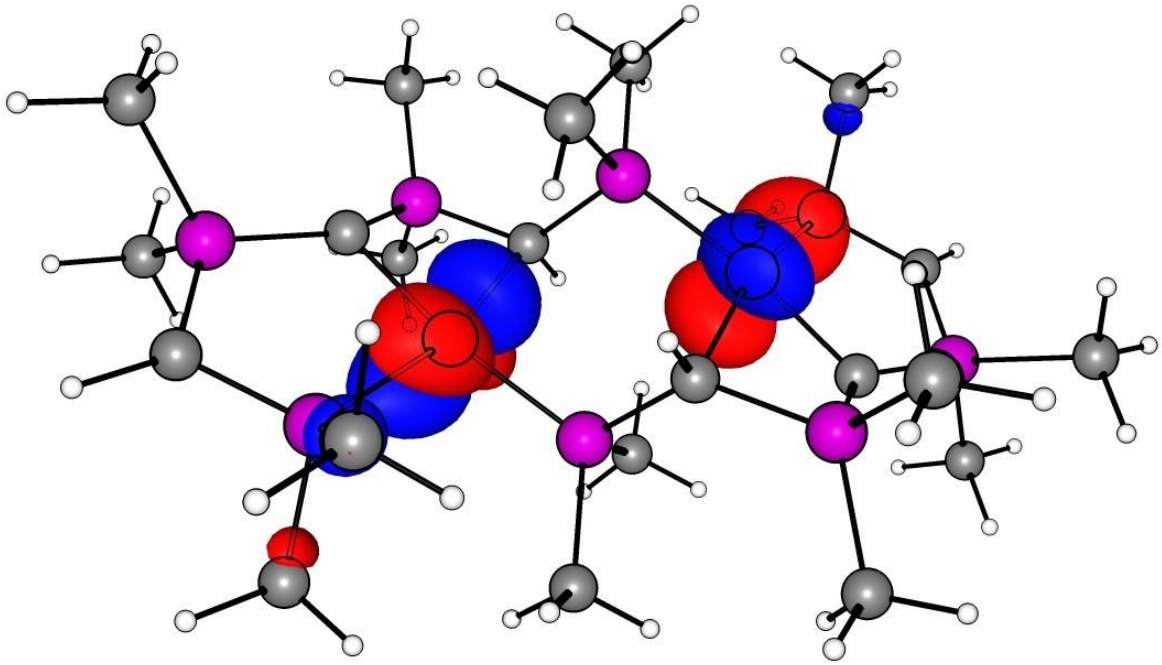
HOMO-5



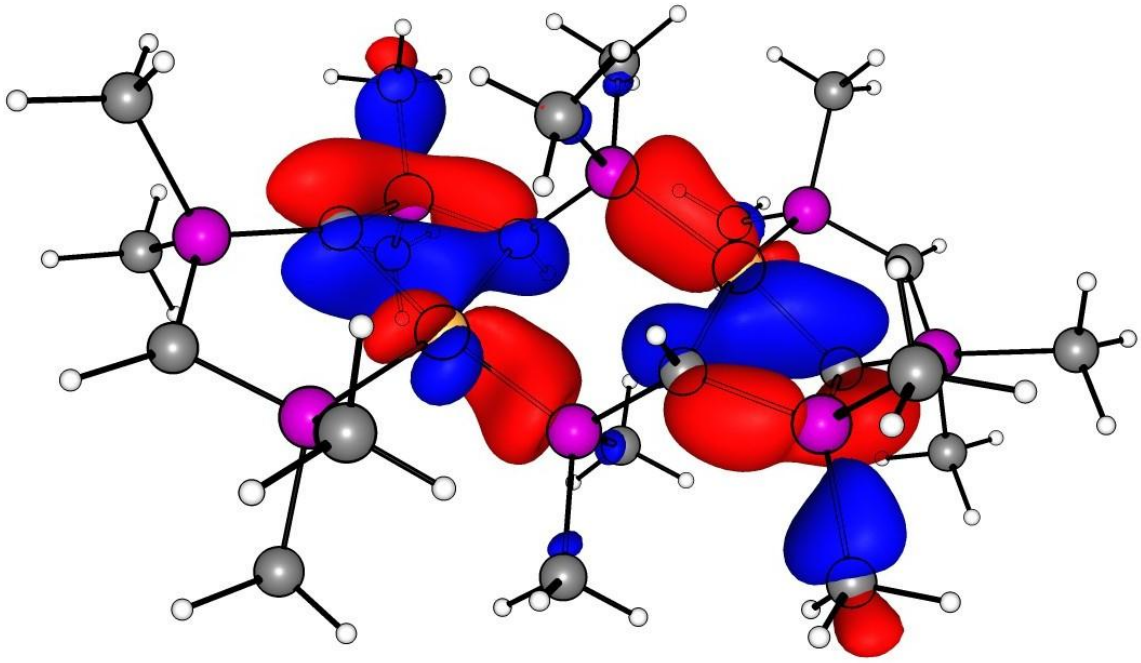
HOMO-6



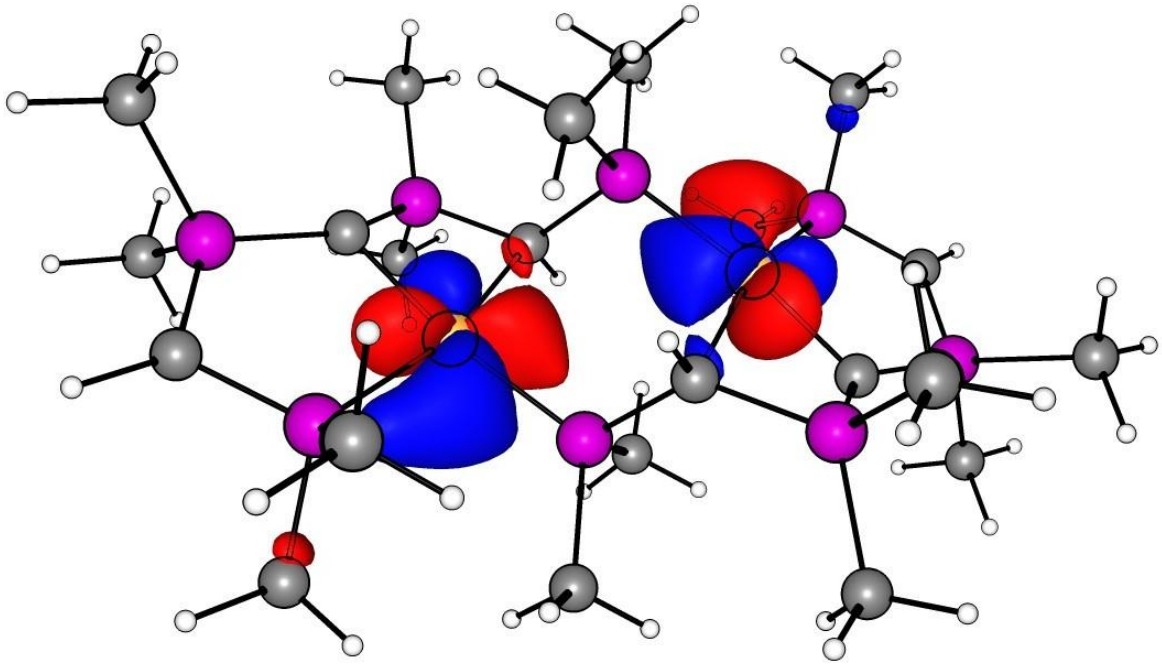
HOMO-7



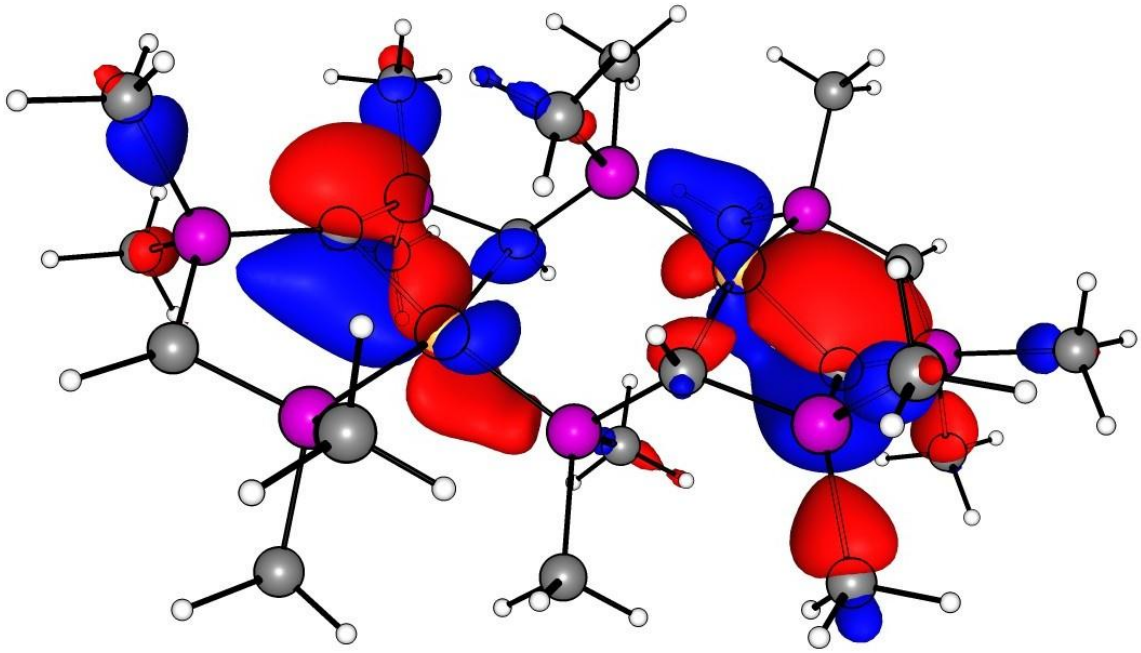
HOMO-8



HOMO-9

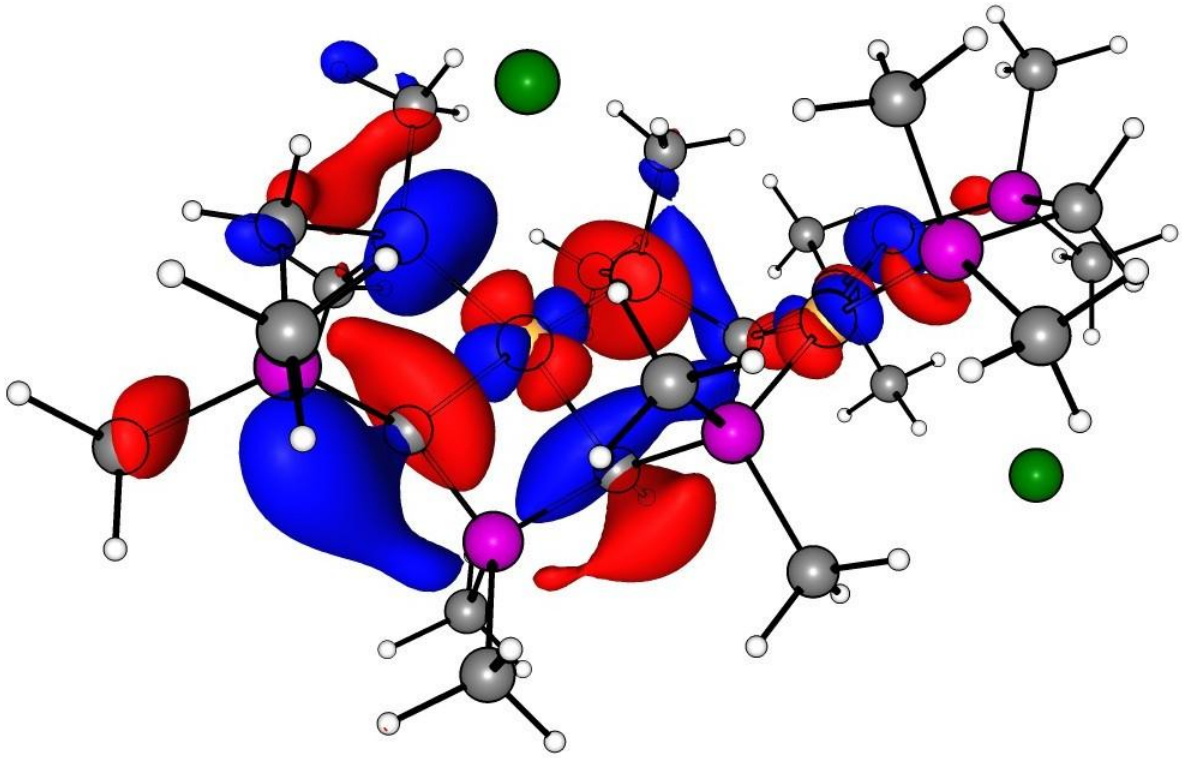


HOMO-10

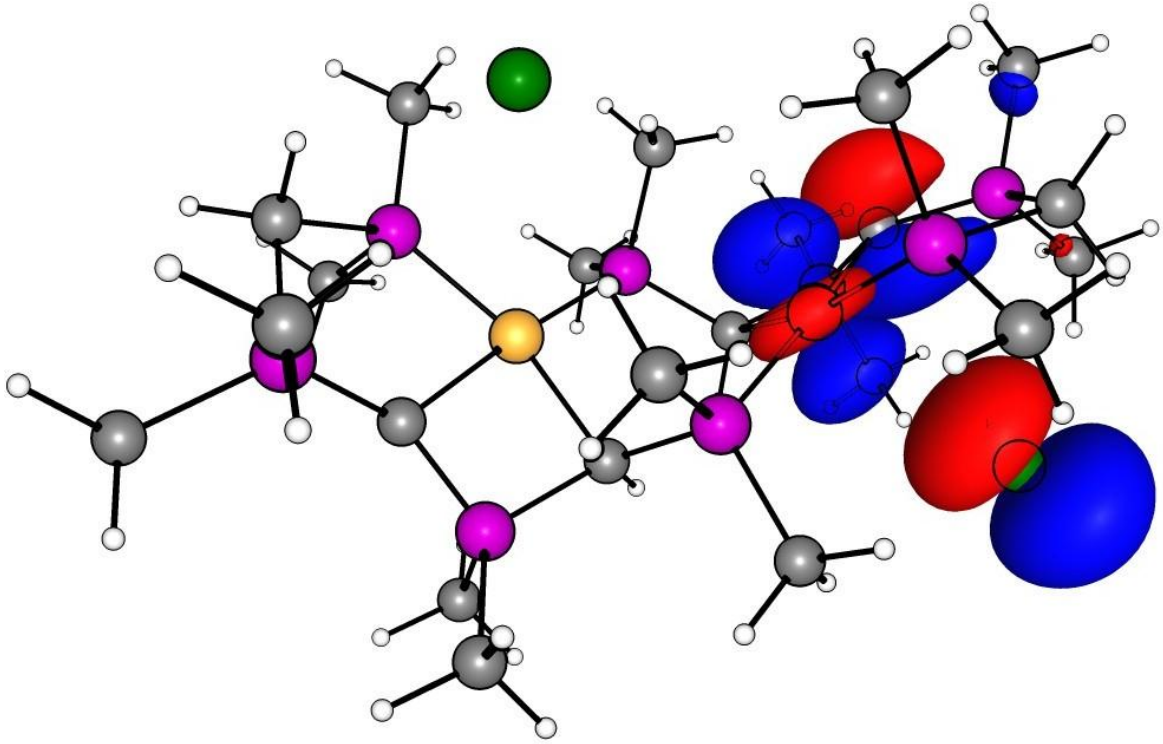


***cis*-6^{Me}**

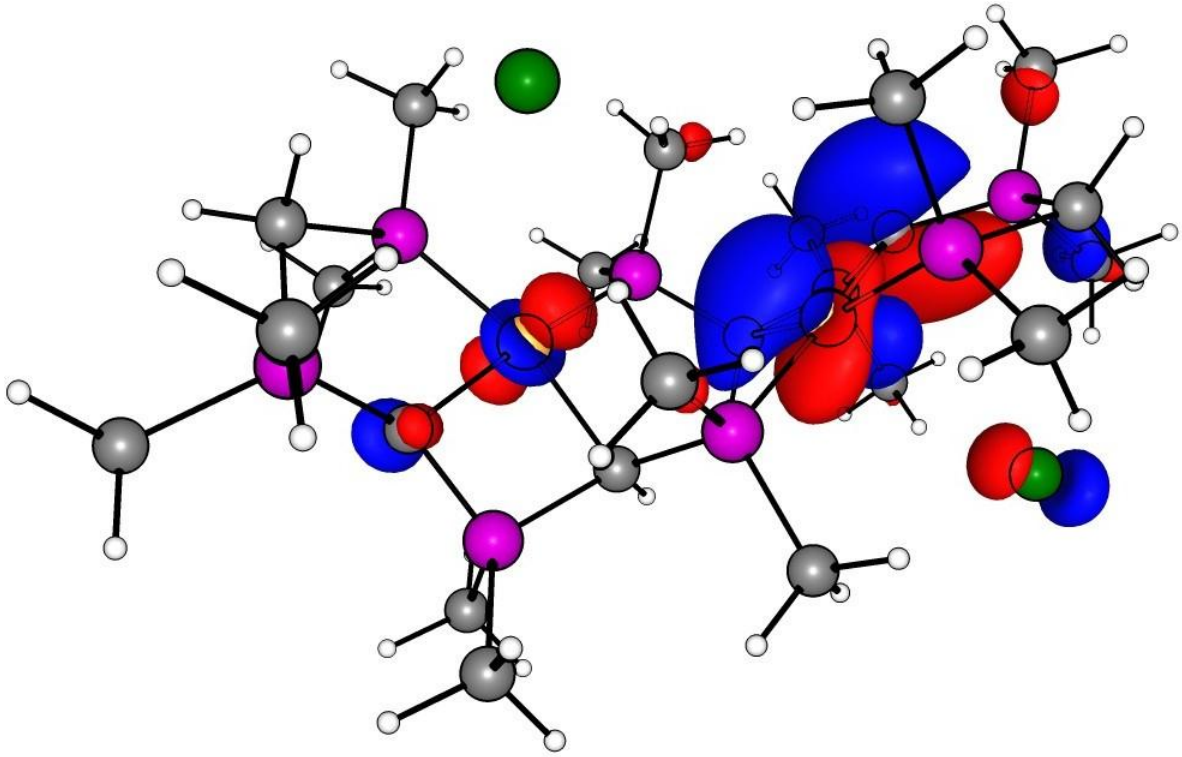
LUMO



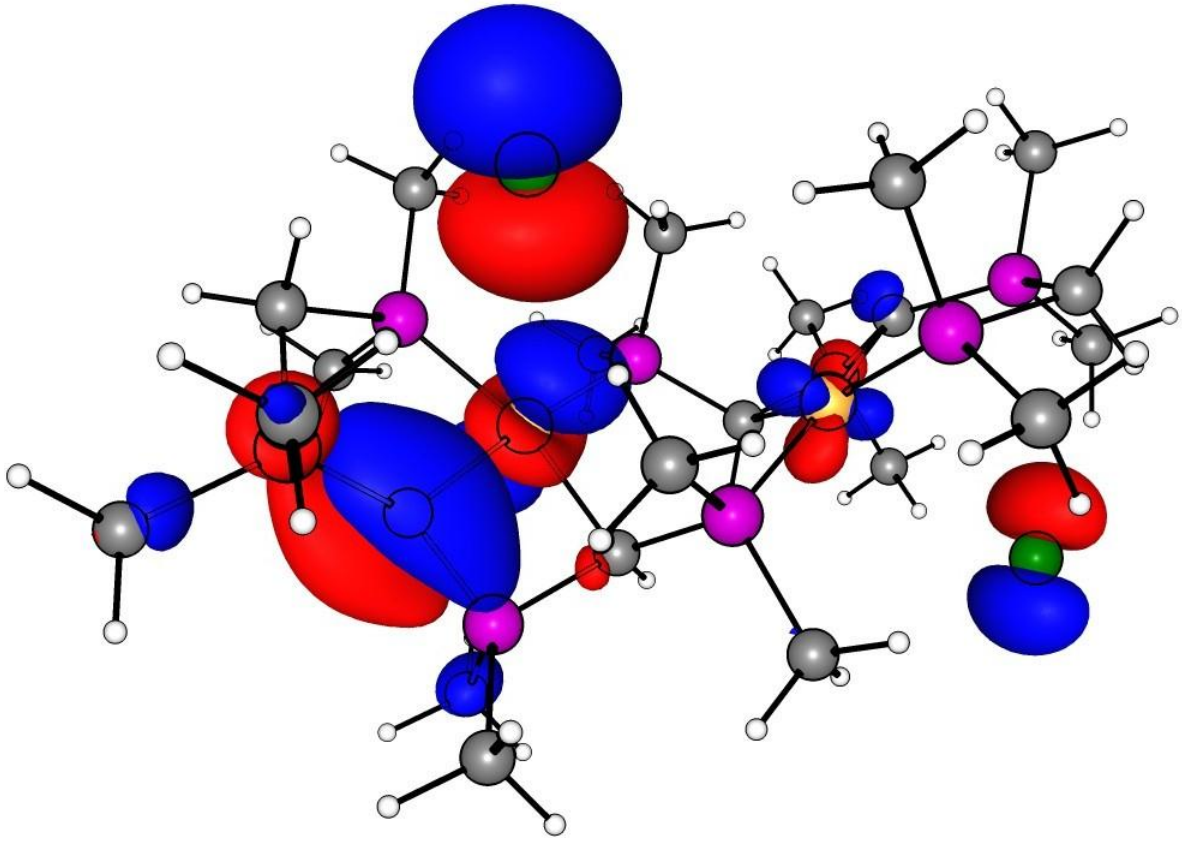
HOMO



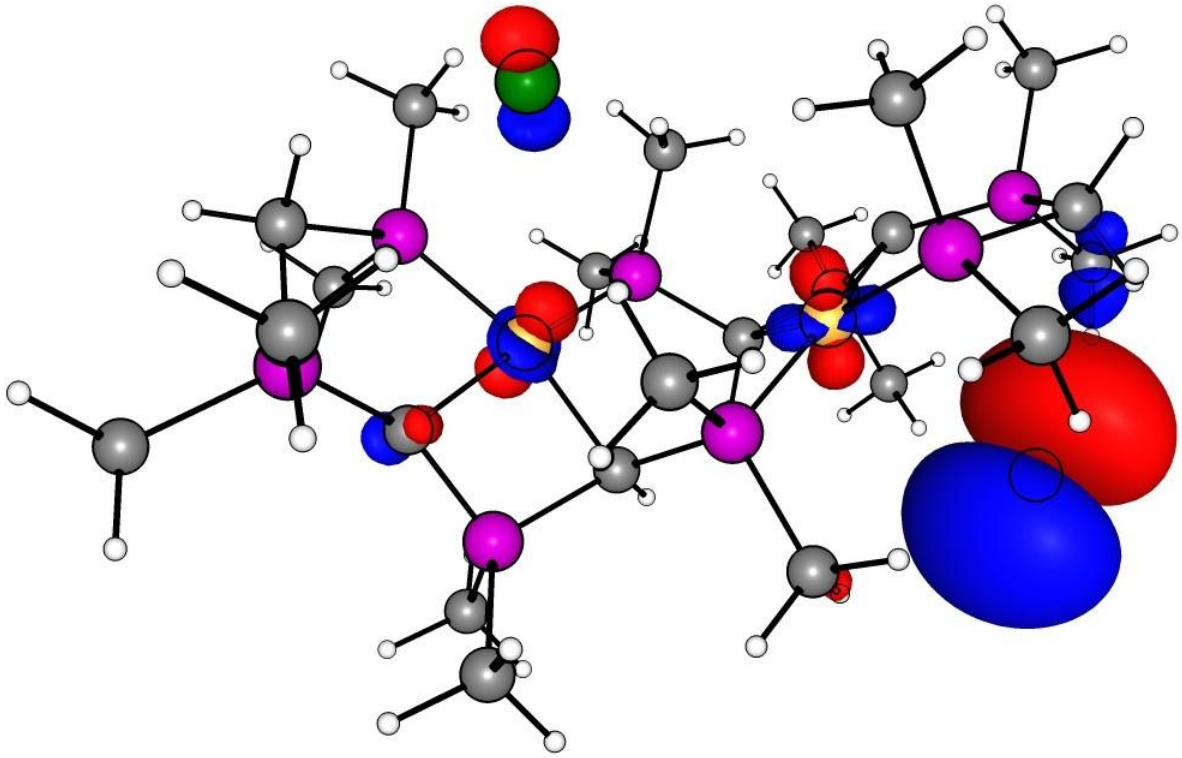
HOMO-1



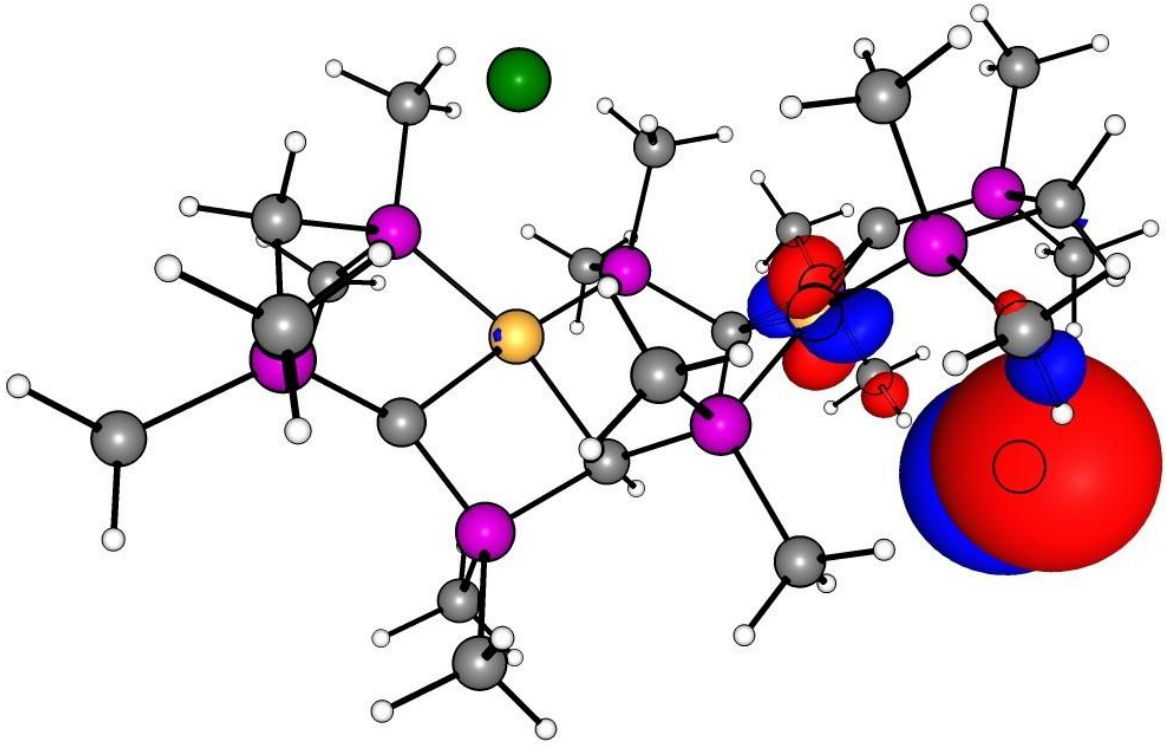
HOMO-2



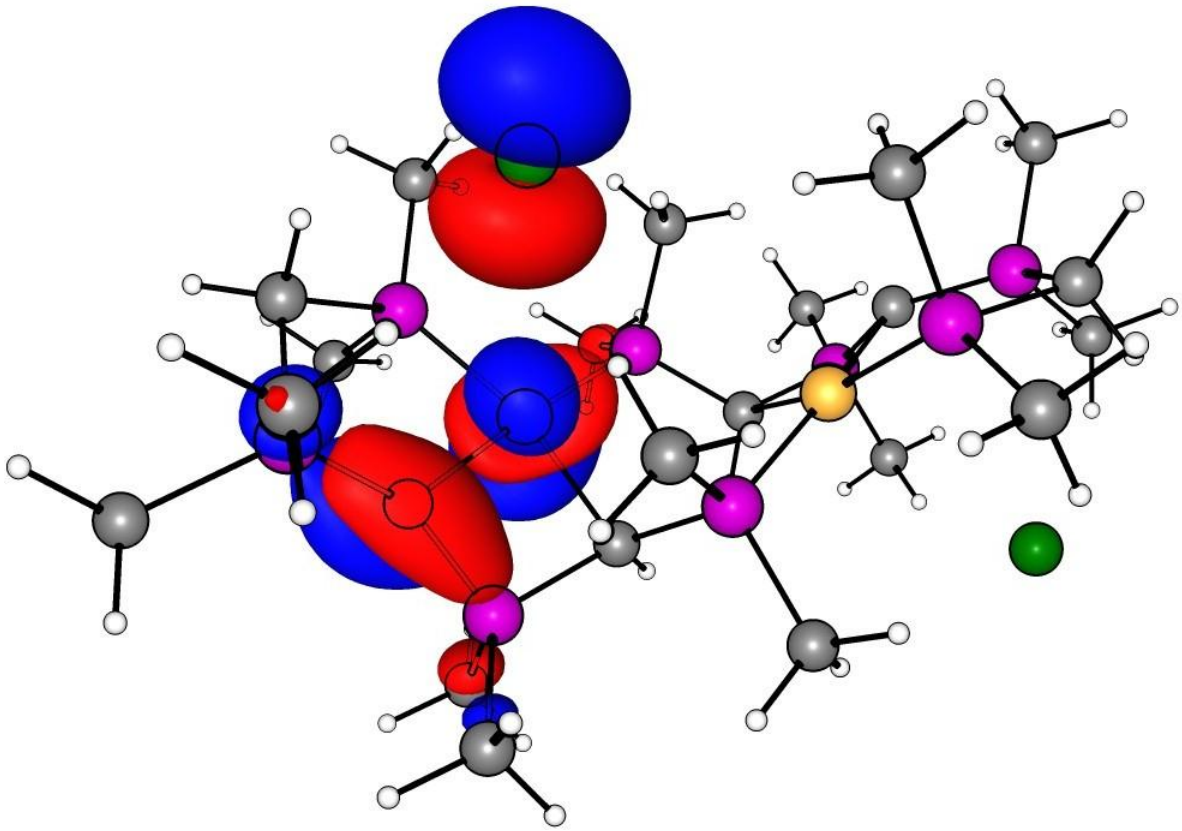
HOMO-3



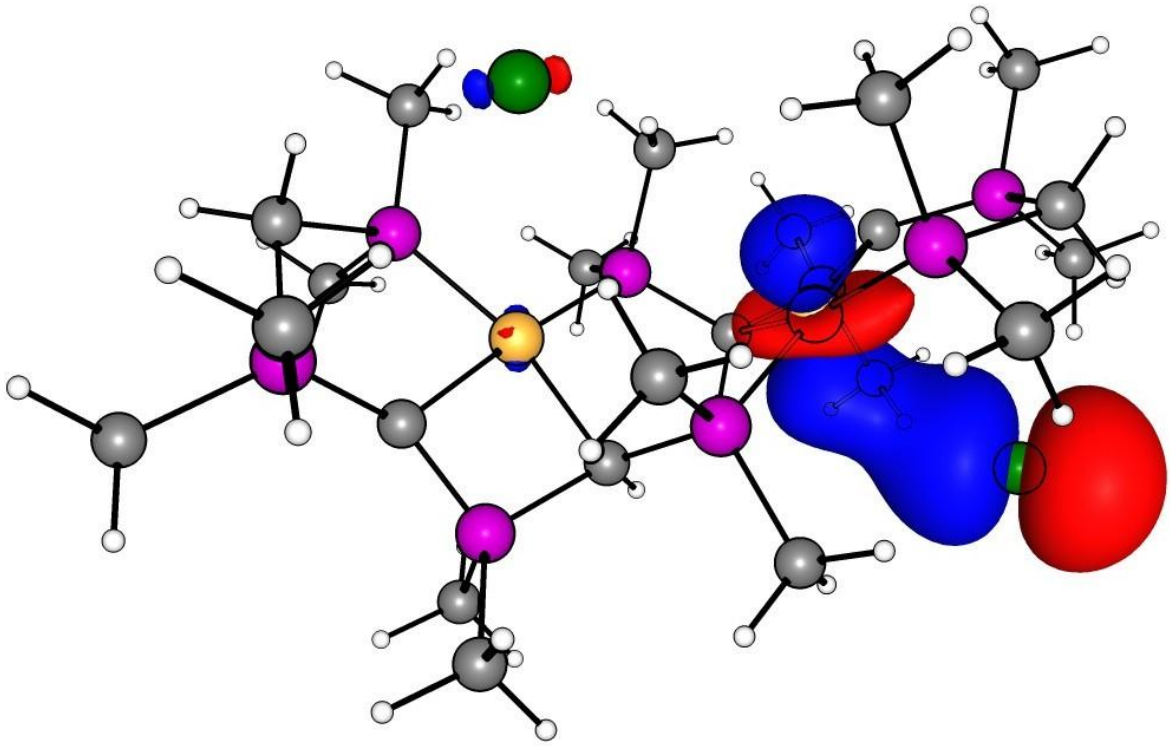
HOMO-4



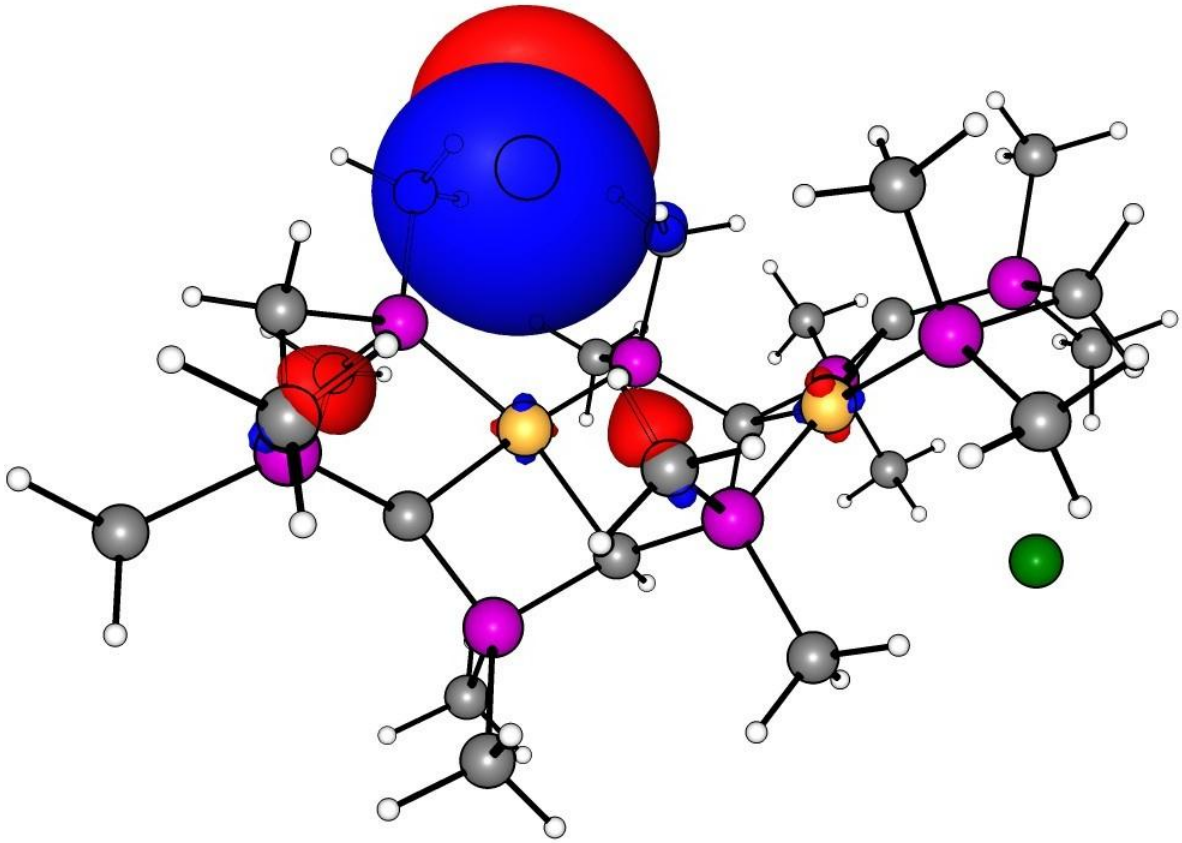
HOMO-5



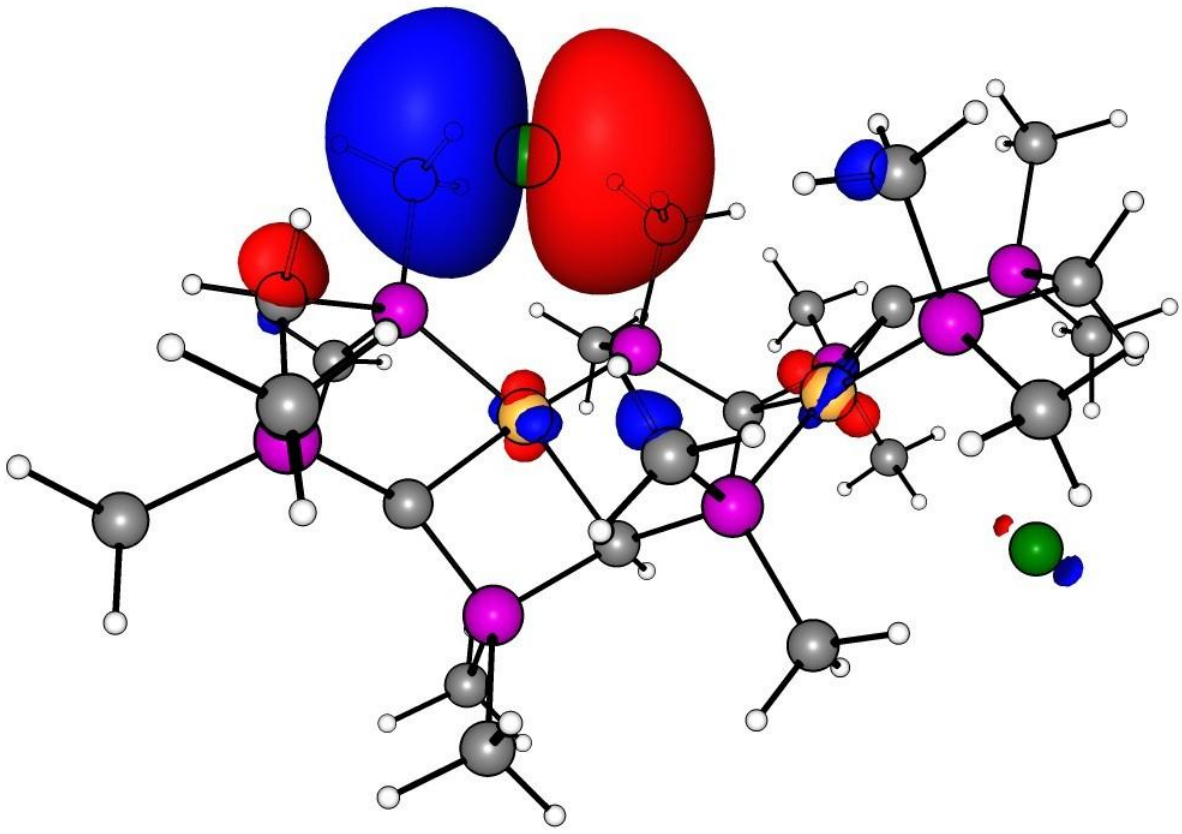
HOMO-6



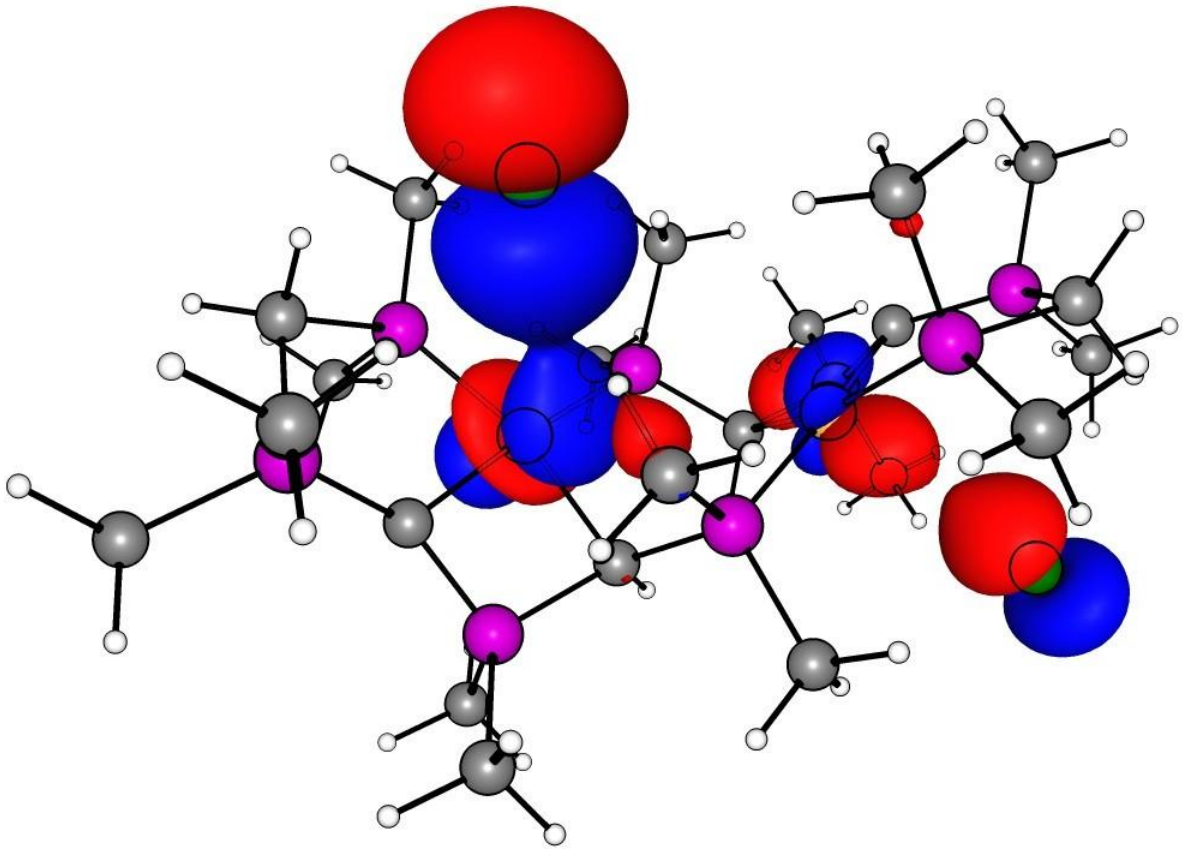
HOMO-7



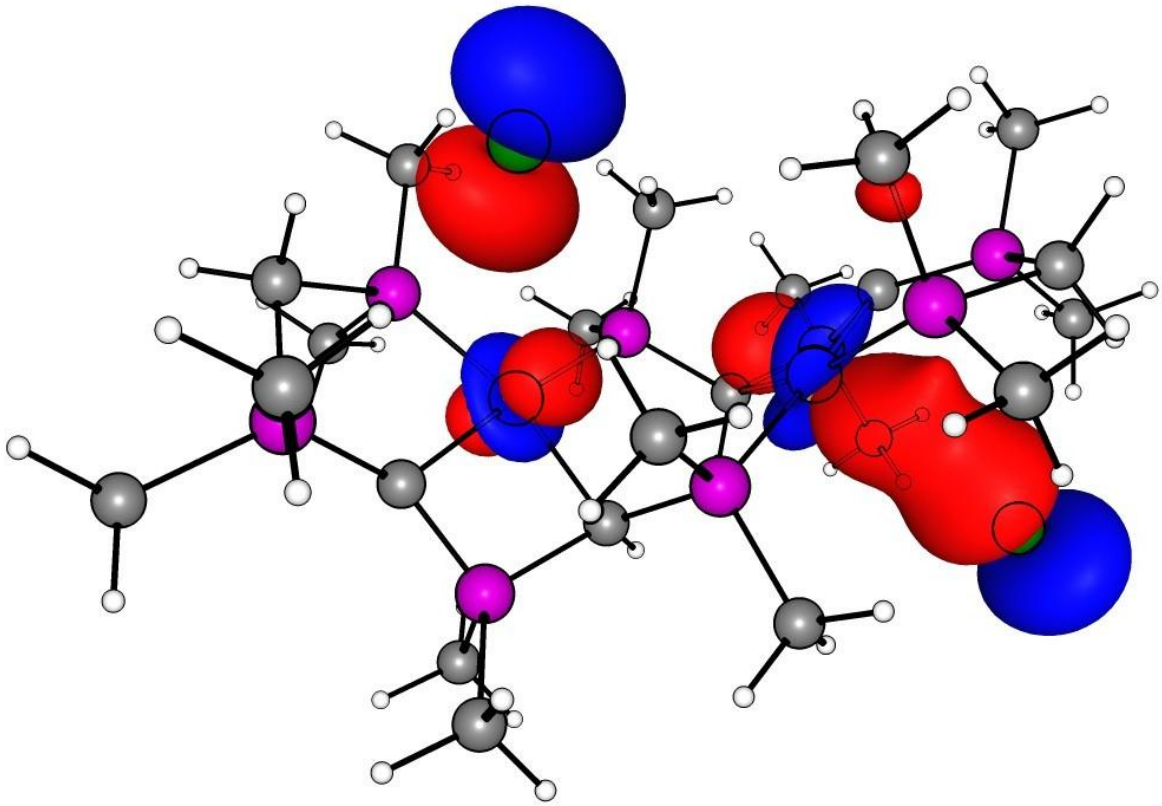
HOMO-8



HOMO-9

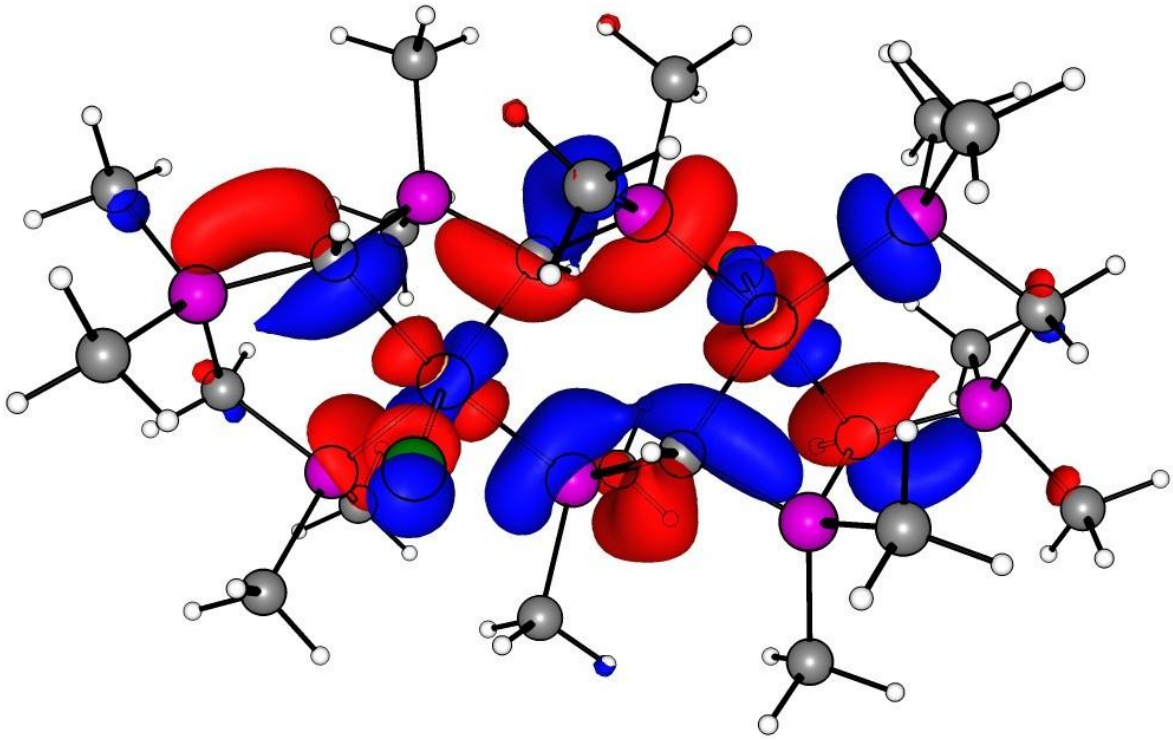


HOMO-10

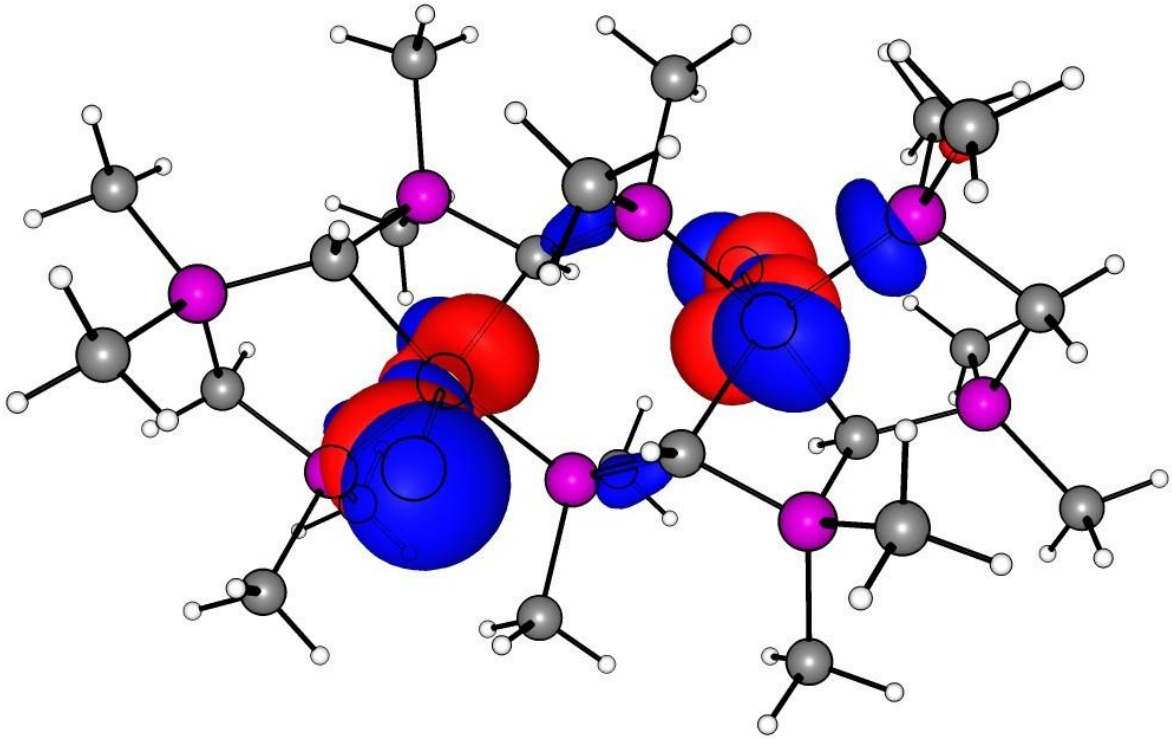


***trans*-8^{Me}**

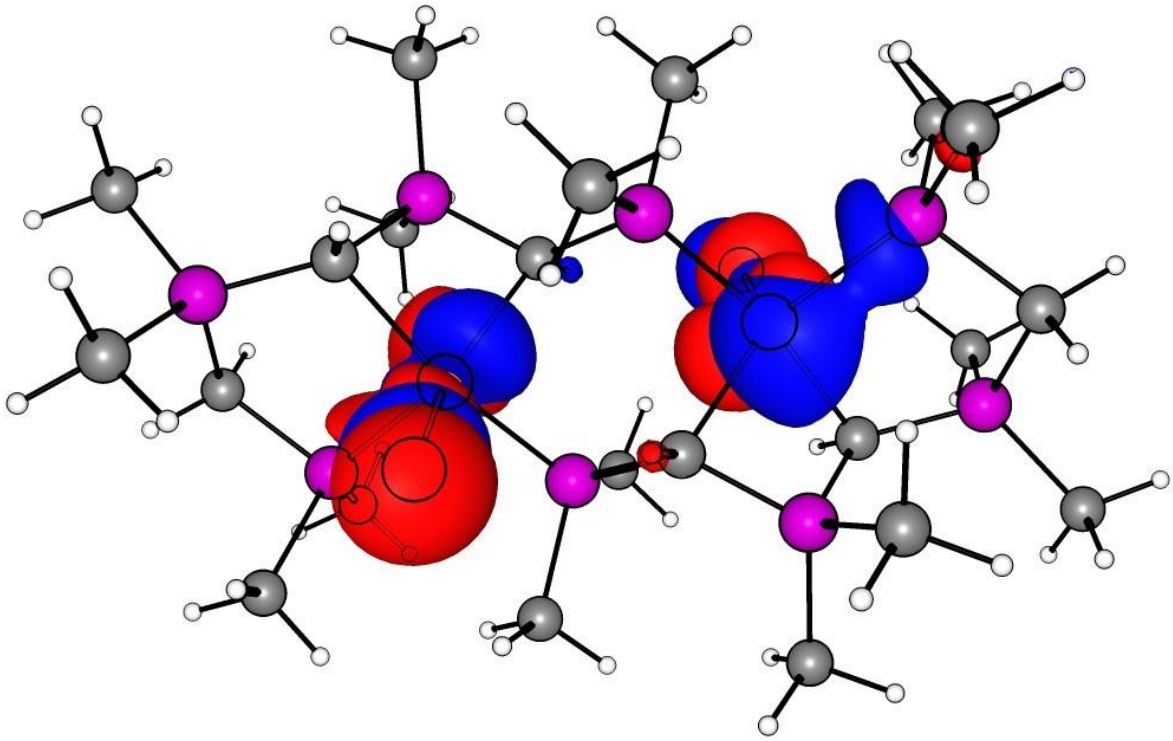
LUMO



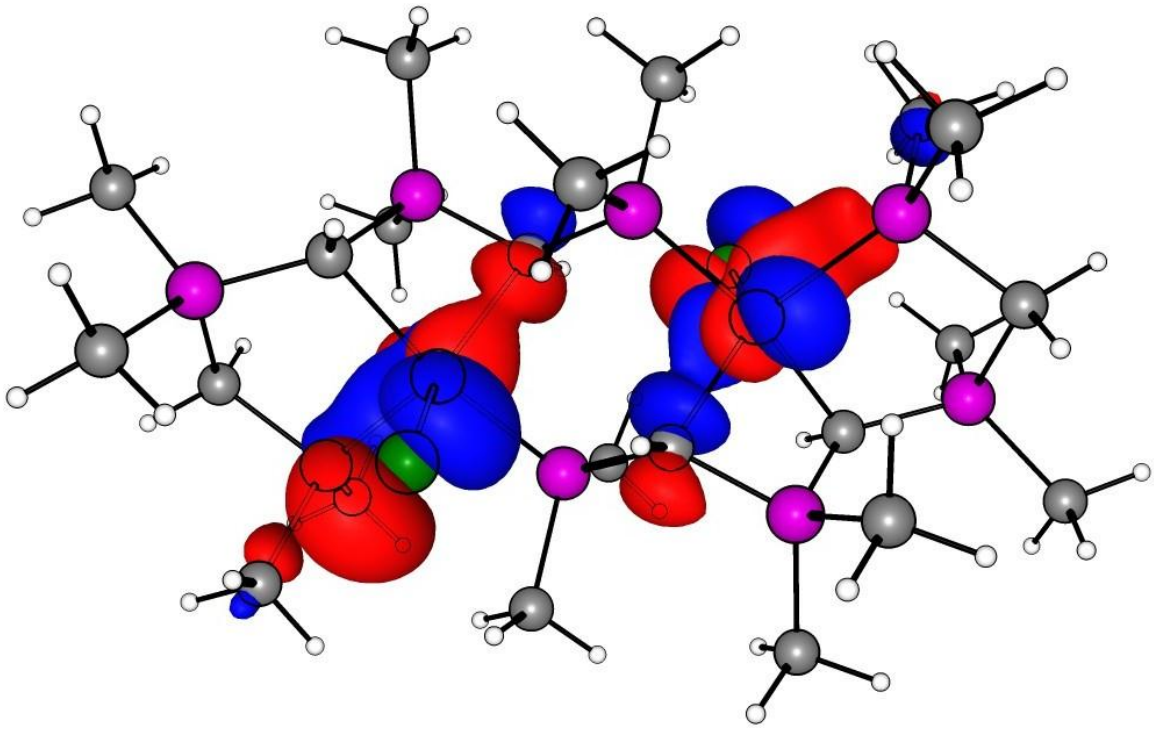
HOMO



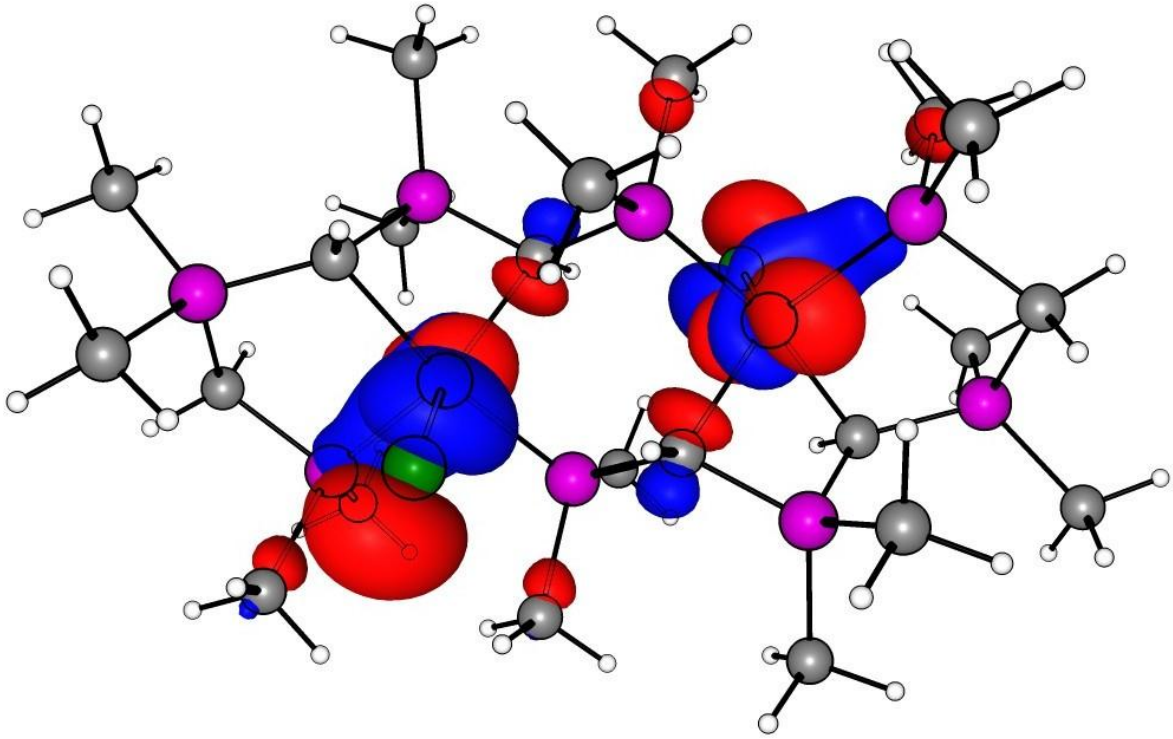
HOMO-1



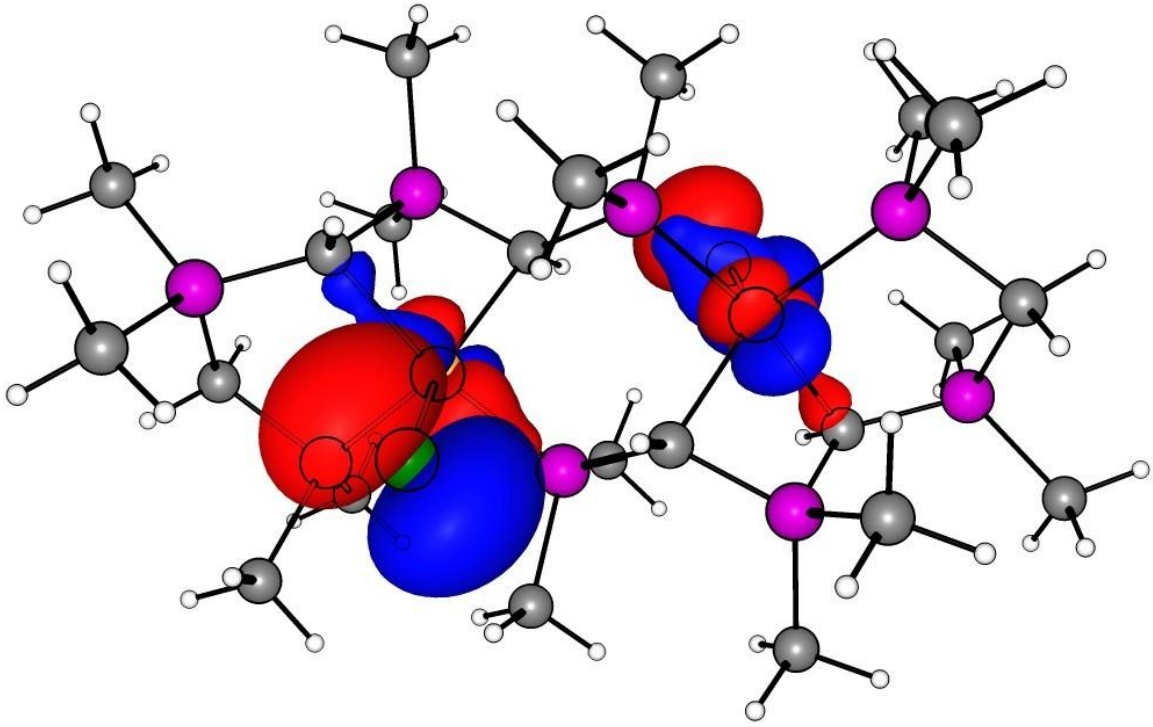
HOMO-2



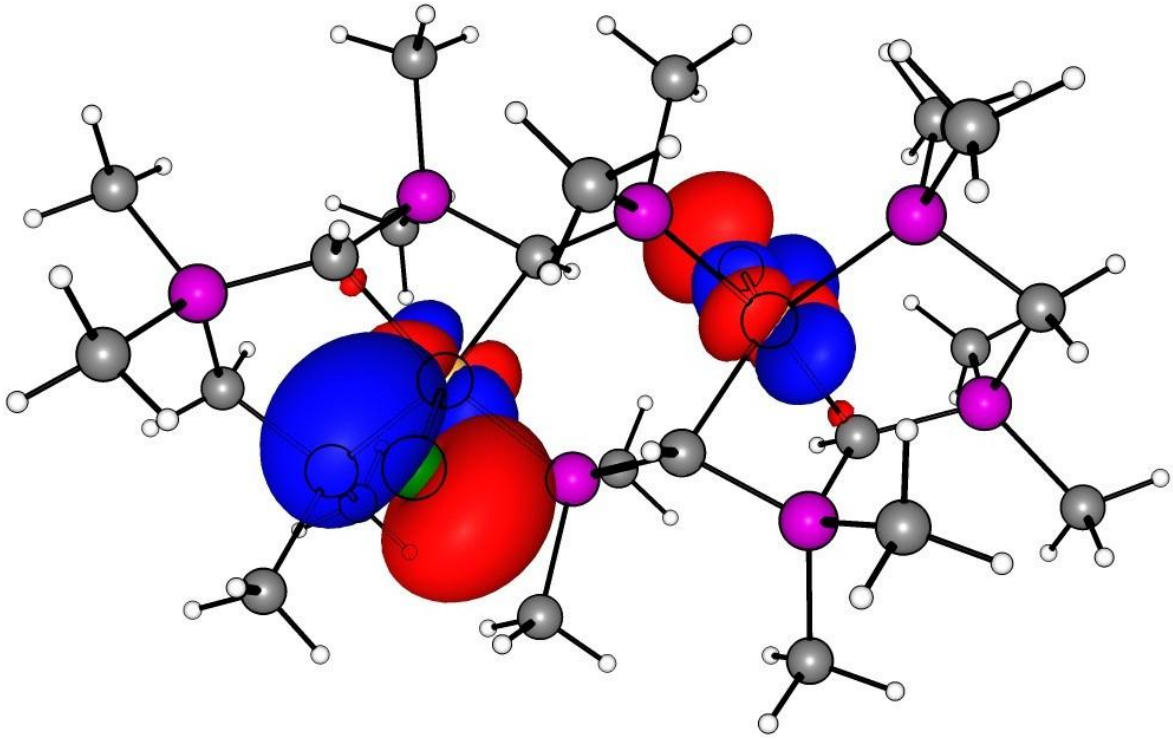
HOMO-3



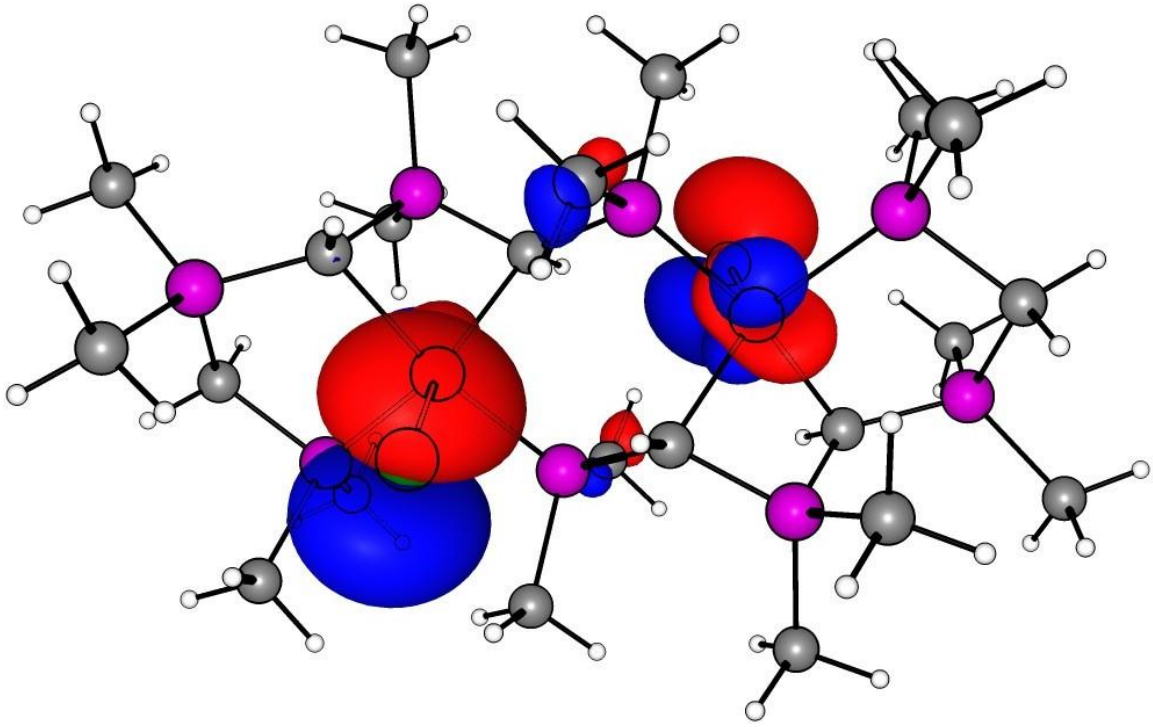
HOMO-4



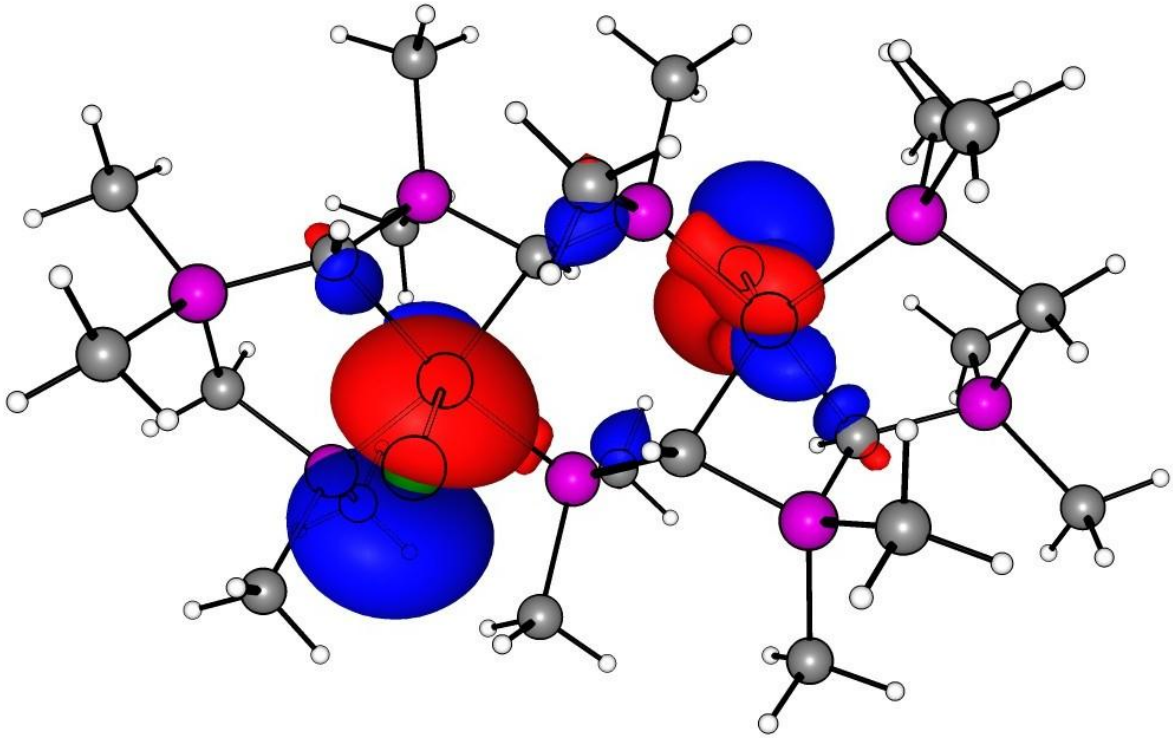
HOMO-5



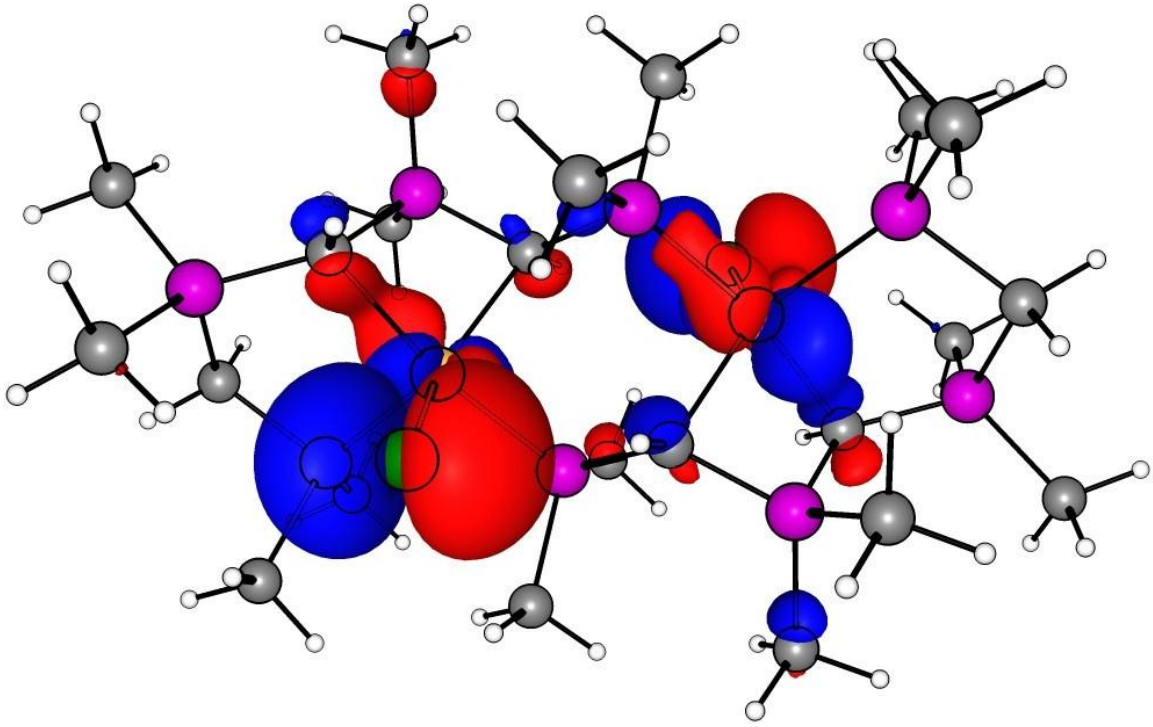
HOMO-6



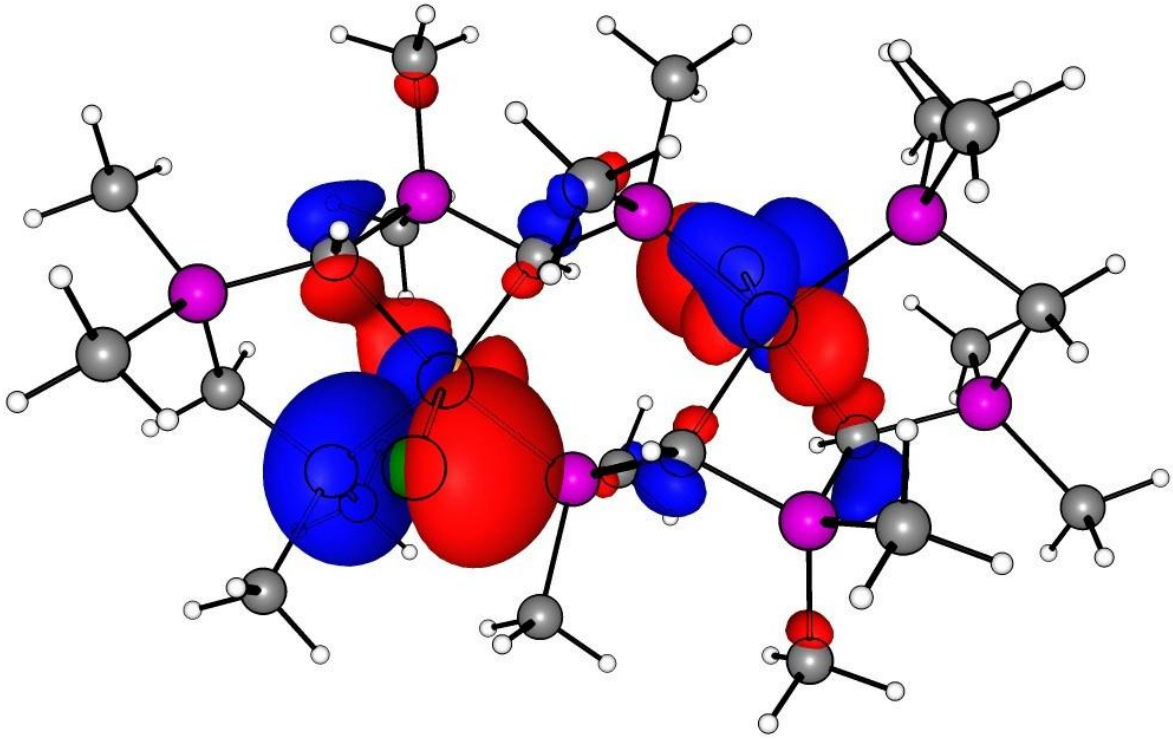
HOMO-7



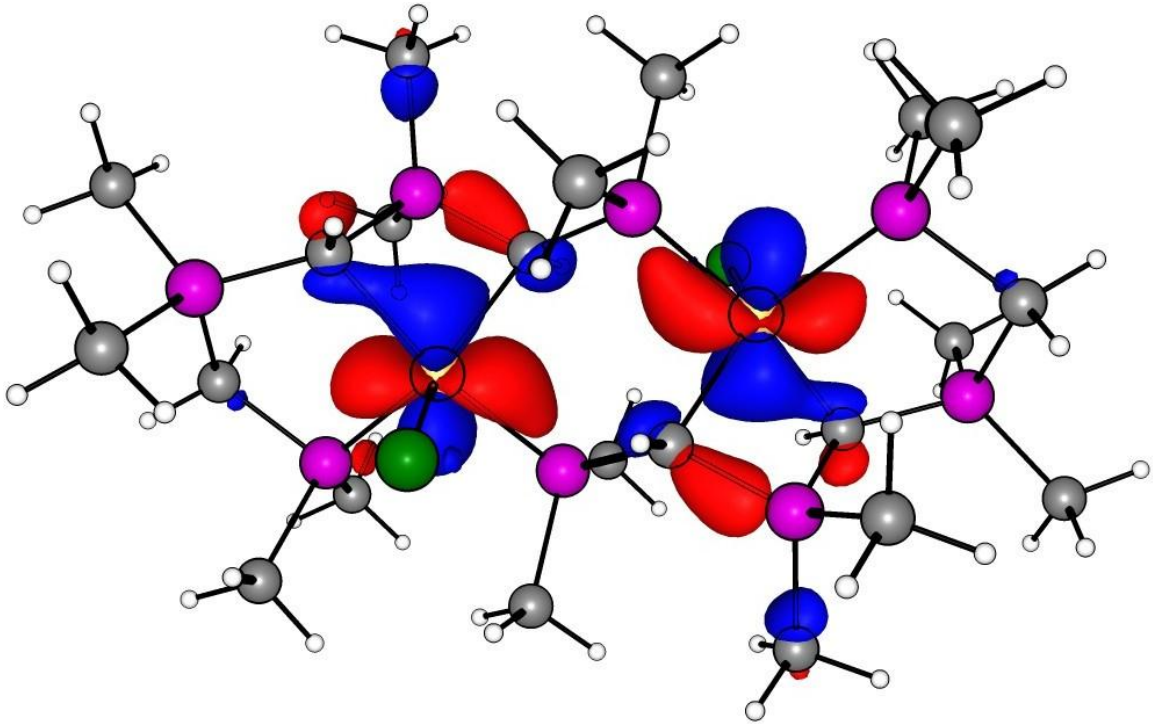
HOMO-8



HOMO-9



HOMO-10



3.2 Cartesian coordinates of all DFT-optimized geometries

1^{Me}

Ni	-1.161450	0.218978	0.009839
Cl	-3.368419	0.447311	-0.139963
P	-0.927795	1.902346	-1.358476
P	-1.460213	-1.463147	1.368012
C	0.791344	0.018530	0.137406
C	-1.679424	3.486358	-0.828778
C	-1.563147	1.625409	-3.052378
C	0.889558	2.282060	-1.569984
C	-2.412618	-2.877811	0.699380
C	-2.273189	-1.059058	2.956768
C	0.201586	-2.178283	1.833043
P	1.337231	-1.540774	0.541761
P	1.693322	1.429511	-0.158738
H	-2.747445	3.308093	-0.668195
H	-1.234014	3.812090	0.116844
H	-1.536684	4.263153	-1.589624
H	-1.072597	0.747933	-3.486417
H	-2.637556	1.428056	-2.976039
H	-1.386735	2.502280	-3.687309
H	1.248709	1.816209	-2.495218
H	1.102816	3.356633	-1.604104
H	-3.391554	-2.499041	0.388634
H	-1.903249	-3.290101	-0.177772
H	-2.535141	-3.662493	1.455604
H	-1.696868	-0.283745	3.472410
H	-3.269950	-0.666459	2.729990
H	-2.355891	-1.947154	3.595243
H	0.514339	-1.753005	2.793967
H	0.197732	-3.271821	1.907855
C	1.216191	-2.767733	-0.813756
C	3.048073	-1.714730	1.166063
C	1.658715	2.664856	1.194830
C	3.468486	1.237918	-0.559015
H	0.197817	-2.734642	-1.215230
H	1.912095	-2.489238	-1.613117
H	1.446499	-3.781030	-0.462842
H	3.763078	-1.448911	0.381554
H	3.196988	-1.064937	2.034583
H	3.224491	-2.755590	1.459848
H	0.613343	2.857696	1.458739
H	2.165947	2.249878	2.072974
H	2.145937	3.601732	0.898407
H	4.010872	0.854769	0.310762
H	3.588241	0.547479	-1.400191
H	3.889630	2.212623	-0.829870

2^{Me}

Ni	7.730152	15.712988	7.418858
P	8.263177	15.744453	9.563689
P	7.623069	15.894786	5.232888
Cl	7.453928	17.874381	7.510381
C	7.746740	13.660602	7.412980
C	6.941562	16.067345	10.779413
C	9.641140	16.860401	9.998217
C	8.914794	14.024354	9.960423
C	6.047522	16.433266	4.483761
C	7.975777	14.182121	4.542100
C	8.909966	16.947905	4.478853
P	9.200317	13.194329	8.365589
P	7.377510	12.989326	5.771931
H	6.884783	13.384706	8.041987
H	6.561312	17.077524	10.589566
H	6.121918	15.352857	10.649113
H	7.329247	16.007872	11.803420
H	10.520248	16.640920	9.383402
H	9.321714	17.886845	9.792869
H	9.895752	16.752538	11.059439
H	9.832084	14.040151	10.560392
H	8.158783	13.447475	10.508639
H	5.224036	15.775571	4.777776
H	5.837247	17.440121	4.861144
H	6.127943	16.459762	3.390458
H	7.529497	13.990991	3.558192
H	9.064101	14.069583	4.450330
H	8.739536	17.974580	4.818716
H	9.903008	16.627924	4.811554
H	8.851871	16.902186	3.384614
C	10.698284	13.849234	7.586694
C	9.442128	11.417640	8.666260
C	8.058010	11.345834	5.402007
C	5.572647	12.892364	5.665274
H	10.873073	13.346295	6.628339
H	10.566502	14.922675	7.414751
H	11.565160	13.673119	8.233828
H	8.532255	10.986553	9.098842
H	9.686692	10.898666	7.734410
H	10.270466	11.280189	9.371972
H	9.152931	11.372427	5.415200
H	7.695247	10.617109	6.134942
H	7.728904	11.037868	4.402286
H	5.209474	12.103284	6.333329
H	5.139273	13.849929	5.970777
H	5.272019	12.660854	4.637498

3^{Me}

Ni	-1.327645	-0.006321	0.150559
Cl	-3.580851	0.164109	0.071349
P	-1.474409	-1.576014	-1.327066
P	-1.176650	1.547311	1.711724
C	0.622844	-0.165690	0.183647
C	-2.141314	-1.111913	-2.978095
C	-2.464099	-3.059103	-0.879970
C	0.223835	-2.254116	-1.698663
C	-2.199805	1.135665	3.193335
C	-1.953357	3.137518	1.177755
C	0.480729	1.779507	2.179781
P	1.562687	0.838926	1.263016
P	1.350348	-0.919231	-1.144491
H	-3.136333	-0.684337	-2.815292
H	-1.503435	-0.344599	-3.429774
H	-2.207444	-1.978011	-3.649263
H	-2.053707	-3.498234	0.035768
H	-3.486102	-2.721421	-0.678597
H	-2.461293	-3.805658	-1.684922
H	0.402327	-3.127349	-1.060706
H	0.370752	-2.536352	-2.748155
H	-3.248826	1.034704	2.894603
H	-1.847784	0.188152	3.614311
H	-2.100294	1.924844	3.951578
H	-1.425976	3.509296	0.292826
H	-3.005082	2.960526	0.926930
H	-1.879193	3.884070	1.980561
H	0.813240	2.431938	2.983821
C	2.692718	-0.162874	2.334767
C	2.816739	1.875719	0.360887
C	1.648830	0.065250	-2.687814
C	2.997830	-1.695820	-0.868706
H	2.087855	-0.912567	2.855008
H	3.472089	-0.662527	1.747150
H	3.172792	0.490951	3.074627
H	3.556456	1.266101	-0.175997
H	2.284059	2.516913	-0.349243
H	3.351157	2.511168	1.079088
H	0.700836	0.526560	-2.985199
H	2.364356	0.863521	-2.462111
H	2.037374	-0.551541	-3.509318
H	3.730692	-0.927005	-0.602160
H	2.923019	-2.416552	-0.048633
H	3.336236	-2.202816	-1.780116

***cis*-5^{Me}**

Ni	-2.291904	7.482863	8.092790
P	-3.167491	5.501956	7.748392
P	-3.160616	9.201477	9.868334
P	-0.486900	7.335714	6.879568
C	-2.025655	9.485707	8.534786
C	-3.825155	7.780348	9.286657
C	-2.088145	4.006961	7.549244
C	-3.991374	5.529643	6.076498
C	-4.326768	5.108541	8.986746
C	-4.314277	10.583656	10.307965
C	-2.123677	9.145193	11.402155
C	0.348102	8.925512	6.672429
C	0.781523	6.170126	7.580586
C	-0.688438	6.688007	5.162369
P	-2.393606	10.366631	7.000161
H	-1.021457	9.738148	8.883675
P	-4.764216	6.485220	9.907815
H	-1.429006	4.101939	6.678901
H	-1.482196	3.877121	8.452008
H	-2.719287	3.117821	7.417851
H	-4.742262	6.326861	6.093000
H	-3.271885	5.734207	5.275763
H	-4.493615	4.571748	5.881912
H	-4.883416	4.173956	9.009161
H	-4.950225	10.827334	9.452017
H	-4.955245	10.261228	11.139802
H	-3.754629	11.476026	10.615696
H	-2.742548	8.830904	12.250853
H	-1.331002	8.405878	11.246838
H	-1.682810	10.126380	11.622903
Ni	-0.897992	10.042683	5.451291
P	1.613496	9.295308	5.485485
H	0.541329	9.378310	7.647799
H	1.090083	6.543882	8.563700
H	0.345395	5.174396	7.709516
H	1.661964	6.102970	6.929929
H	-1.003446	5.639660	5.202087
H	-1.450969	7.285997	4.656023
H	0.238046	6.776055	4.586087
C	-2.588926	12.157157	7.462632
C	-4.126898	9.891863	6.581141
C	-4.559102	6.228447	11.732520
C	-6.575316	6.859015	9.831721
P	-1.923281	10.907502	3.714979
C	0.607564	9.740283	4.226757
C	2.880549	7.981879	5.158668
C	2.678184	10.586243	6.280235
H	-3.377383	12.289186	8.213544
H	-1.637609	12.514245	7.873338
H	-2.826475	12.749813	6.573731
H	-4.130117	8.850350	6.248676
H	-4.792995	9.966974	7.446351
H	-4.488268	10.539121	5.775038
H	-3.499099	6.041737	11.933034

H	-4.891227	7.112570	12.293642
H	-5.145596	5.361154	12.063064
H	-6.818392	7.718531	10.469986
H	-6.833392	7.092125	8.793634
H	-7.160046	5.991942	10.165911
C	-2.990625	12.414419	3.906939
C	-3.201497	9.691792	3.107062
C	-0.792515	11.262012	2.438883
P	0.735552	10.539134	2.715322
H	3.425423	7.725062	6.076042
H	2.396981	7.086641	4.756455
H	3.596106	8.356778	4.414186
H	2.026649	11.403983	6.605732
H	3.227299	10.180042	7.140051
H	3.395027	10.973026	5.545968
H	-3.840734	12.226405	4.573467
H	-2.386027	13.233100	4.310937
H	-3.376057	12.714343	2.923218
H	-2.689062	8.747607	2.892768
H	-3.986247	9.511206	3.850882
H	-3.659139	10.063546	2.179651
H	-1.086969	11.685787	1.480984
C	1.237254	9.374379	1.367159
C	2.132855	11.754810	2.637458
H	2.237915	8.966312	1.561161
H	0.510027	8.556500	1.336779
H	1.245390	9.889870	0.397837
H	1.975339	12.503003	3.420995
H	3.098303	11.254097	2.792064
H	2.148150	12.255646	1.660506

***trans*-5^{Me}**

Ni	-3.447788	-3.755352	19.981523
P	-2.936084	-3.140970	22.463704
P	-4.931933	-5.250896	19.356697
P	-2.458550	-3.287394	18.097600
C	-2.363137	-2.281997	21.014890
C	-4.249152	-3.900434	21.759621
C	-1.487770	-4.157486	23.014859
C	-3.264304	-2.183704	24.018690
C	-6.121582	-4.470288	18.152122
C	-5.810575	-5.879523	20.722571
C	-4.402278	-6.735058	18.370312
C	-3.028040	-1.658712	17.537023
C	-2.593871	-4.451734	16.656016
C	-0.619144	-3.166480	18.184164
P	-2.932623	-0.653314	20.454312
H	-1.280095	-2.350491	20.885777
P	-5.359082	-5.135410	22.192942
H	-1.810641	-4.857224	23.794955
H	-1.129733	-4.727418	22.151142
H	-0.677969	-3.528286	23.408041
H	-2.397464	-1.577196	24.308584
H	-4.137085	-1.538683	23.880131
H	-3.482387	-2.899467	24.823307
H	-6.596977	-3.618850	18.650823
H	-5.601473	-4.113415	17.254089
H	-6.898919	-5.189313	17.858673
H	-6.580105	-6.643475	20.639531
H	-4.144501	-6.483048	17.337718
H	-3.540699	-7.203640	18.858337
H	-5.231799	-7.454627	18.363609
Ni	-1.943386	-0.185357	18.570389
P	-2.455098	-0.799738	16.088208
H	-4.111081	-1.590219	17.666139
H	-2.243675	-5.442674	16.964125
H	-3.634981	-4.534948	16.329625
H	-1.982122	-4.103215	15.818522
H	-0.336902	-2.483782	18.988990
H	-0.203597	-4.164171	18.374742
H	-0.222380	-2.755540	17.249079
C	-2.797298	0.511027	21.895895
C	-4.772029	-0.774224	20.367750
C	-4.679599	-6.325811	23.443369
C	-6.799550	-4.456041	23.132326
P	-0.459231	1.310175	19.195217
C	-1.142031	-0.040269	16.792288
C	-3.903417	0.216772	15.537055
C	-2.126877	-1.757003	14.533221
H	-3.409045	0.162511	22.733391
H	-1.756187	0.594241	22.222284
H	-3.147493	1.501967	21.587784
H	-5.054273	-1.456923	19.562925
H	-5.168794	-1.185161	21.302835
H	-5.187573	0.223468	20.177169
H	-3.779945	-6.784612	23.020190

H	-4.424530	-5.808215	24.378257
H	-5.413143	-7.112025	23.665882
H	-6.468249	-4.015881	24.081866
H	-7.271718	-3.683908	22.516468
H	-7.528504	-5.249589	23.342575
C	0.730411	0.529558	20.399791
C	0.419419	1.938795	17.829343
C	-0.988876	2.794341	20.181601
P	-0.032097	1.194704	16.358968
H	-4.713216	-0.412433	15.143877
H	-4.261454	0.786704	16.400772
H	-3.580552	0.916510	14.756957
H	-1.254093	-2.402022	14.671779
H	-2.993715	-2.363514	14.243328
H	-1.908797	-1.041239	13.728604
H	0.210299	0.172686	21.297823
H	1.205800	-0.321884	19.901088
H	1.507754	1.248576	20.693241
H	1.188939	2.702757	17.912381
H	-1.850450	3.262929	19.693575
H	-1.246657	2.542332	21.214195
H	-0.159350	3.513904	20.188307
C	-0.711587	2.385126	15.108564
C	1.408355	0.515335	15.419560
H	-0.966668	1.867543	14.173672
H	-1.611234	2.843925	15.531760
H	0.021959	3.171339	14.886055
H	1.880524	-0.256809	16.035402
H	1.077038	0.075189	14.470018
H	2.137312	1.308880	15.209311

***cis*-6^{Me}**

Ni	-2.025679	0.597417	-0.549669
P	-0.263571	1.865515	-0.681784
P	-2.800632	-1.615865	-1.699488
P	-3.394035	1.949829	0.434266
C	-3.580286	-0.641854	-0.572033
C	-1.150138	-0.989772	-1.517856
C	1.154263	1.041668	-1.434796
C	-0.583680	3.400430	-1.683882
C	0.300901	2.524099	0.940198
C	-3.063082	-3.444198	-1.625500
C	-3.277748	-1.259842	-3.440041
C	-2.951913	3.346384	1.544565
C	-4.487337	2.761291	-0.816086
C	-4.599101	0.973936	1.459236
P	-4.656268	-0.699339	0.714996
P	0.110873	-1.704725	-0.420074
H	-0.692770	-0.716429	-2.472711
Ni	1.785511	-0.363510	-0.084820
P	2.817154	1.661294	-1.367362
H	0.893522	0.621344	-2.408987
H	-0.826659	3.112484	-2.713192
H	-1.439578	3.941520	-1.263141
H	0.289150	4.063677	-1.693108
H	-0.117585	3.525110	1.093195
H	-0.070925	1.861212	1.731195
H	1.394807	2.553461	0.978360
H	-2.508796	-3.940432	-2.431098
H	-2.735050	-3.846173	-0.663701
H	-4.134897	-3.647800	-1.752242
H	-4.341252	-1.485269	-3.582241
H	-3.109940	-0.193414	-3.621901
H	-2.679029	-1.856314	-4.139918
H	-2.385307	2.933683	2.386486
H	-2.337173	4.068275	0.995842
H	-3.858823	3.849479	1.904329
H	-3.886931	3.419459	-1.454528
H	-4.930861	1.980201	-1.441757
H	-5.276363	3.351462	-0.331616
H	-4.154368	0.895739	2.460959
H	-5.589743	1.443702	1.506388
C	-6.409110	-1.042505	0.264295
C	-4.320580	-1.872715	2.079865
C	-0.811008	-2.211446	1.081060
C	0.620999	-3.294608	-1.202260
P	2.676237	-1.386337	1.593643
C	3.243815	1.002695	0.129248
C	3.674713	1.029943	-2.858859
C	2.998212	3.493215	-1.527834
H	-6.745046	-0.300693	-0.467989
H	-6.471960	-2.039663	-0.188049
H	-7.056506	-1.013299	1.149067
H	-4.240142	-2.890307	1.679420
H	-3.376044	-1.564936	2.547144
H	-5.124961	-1.837087	2.825743

H	-1.148769	-1.316020	1.620364
H	-1.673918	-2.839719	0.839622
H	-0.144866	-2.776005	1.739208
H	-0.249591	-3.934723	-1.393443
H	1.160014	-3.077126	-2.129509
H	1.331035	-3.806962	-0.546856
C	2.030840	-0.742795	3.192157
C	4.498532	-1.012025	1.648739
C	2.725256	-3.214497	1.801373
P	4.741095	0.580460	0.786663
H	3.700572	-0.066721	-2.790065
H	3.153067	1.358194	-3.767191
H	4.702107	1.412143	-2.880456
H	2.620985	3.843981	-2.496913
H	2.449708	3.982942	-0.717254
H	4.061811	3.754294	-1.442919
H	2.241443	0.331293	3.234770
H	0.940091	-0.853721	3.236563
H	2.497659	-1.247174	4.048807
H	4.910313	-1.024485	2.665937
H	4.970521	-1.782659	1.026713
H	1.718990	-3.631450	1.894320
H	3.213200	-3.615986	0.905417
H	3.300974	-3.475699	2.698678
C	6.158700	0.350359	-0.349914
C	5.367827	1.767270	2.047127
H	5.877975	-0.455247	-1.041388
H	6.344766	1.281685	-0.898201
H	7.062920	0.075688	0.207920
H	5.516537	2.744546	1.572747
H	4.615801	1.873608	2.836130
H	6.317257	1.427982	2.480014
Cl	-1.716622	0.446448	3.215420
Cl	4.021395	-2.358434	-1.480874

7^{Me}

Ni	0.875232	0.007883	-0.007592
P	0.931393	-2.203042	-0.169116
P	0.889370	2.214983	0.169822
C	-1.014957	-0.007056	-0.020575
C	2.057662	-2.976497	1.092209
C	1.738834	-2.807191	-1.730431
C	-0.677117	-2.800128	-0.009028
C	2.016155	3.013951	-1.074620
C	1.676380	2.813635	1.743773
C	-0.725962	2.790469	0.001427
P	-1.845013	1.509230	-0.207501
P	-1.815101	-1.534883	0.196511
H	3.094422	-2.642855	0.950005
H	1.719814	-2.690816	2.093807
H	2.028062	-4.071650	1.003559
H	1.178293	-2.415240	-2.585433
H	2.781057	-2.466010	-1.792982
H	1.723212	-3.905654	-1.763958
H	-0.948216	-3.846474	0.105510
H	3.055605	2.691291	-0.926501
H	1.689995	2.733532	-2.081541
H	1.972760	4.107776	-0.976149
H	1.115223	2.404572	2.590301
H	2.722751	2.486411	1.810635
H	1.645057	3.911363	1.788880
H	-1.013489	3.834126	-0.095411
C	-2.718873	1.659465	-1.835482
C	-3.288471	1.656596	0.943346
C	-2.675004	-1.690549	1.832189
C	-3.263352	-1.714821	-0.943832
H	-1.973638	1.522579	-2.625712
H	-3.506478	0.905038	-1.942418
H	-3.164862	2.659054	-1.927060
H	-4.040522	0.884995	0.738867
H	-2.929488	1.558879	1.972197
H	-3.754680	2.641319	0.811082
H	-1.926951	-1.533946	2.616169
H	-3.477332	-0.952106	1.941207
H	-3.099382	-2.698577	1.933774
H	-4.030956	-0.958736	-0.738340
H	-2.912282	-1.614302	-1.975150
H	-3.707384	-2.708671	-0.804051

***trans*-8^{Me}**

Ni	-3.911916	-3.650354	19.862321
P	-2.936658	-3.466810	22.251409
P	-4.592434	-5.720449	19.440938
P	-3.040010	-3.194207	17.931412
C	-2.391248	-2.579294	20.829339
C	-4.632232	-3.693595	21.827328
C	-2.030470	-5.043960	22.318738
C	-2.693463	-2.741312	23.917352
C	-6.123507	-5.978444	18.456083
C	-5.060667	-6.444115	21.114641
C	-3.462728	-7.031613	18.800677
C	-3.012428	-1.388666	17.764005
C	-4.038247	-3.866304	16.537241
C	-1.352467	-3.797975	17.567685
P	-2.363663	-0.773752	20.661938
H	-1.400968	-2.925939	20.517916
P	-5.660711	-5.085664	22.165219
H	-2.090519	-5.531053	21.342708
H	-0.982050	-4.827652	22.552290
H	-2.434588	-5.695205	23.101562
H	-3.257430	-1.807346	24.007881
H	-3.059522	-3.447552	24.673396
H	-1.630108	-2.543192	24.095467
H	-6.854193	-5.209110	18.721444
H	-5.884892	-5.851689	17.395836
H	-6.532714	-6.983594	18.612145
H	-5.799257	-7.252267	21.046213
H	-4.152584	-6.848649	21.578679
H	-3.187376	-6.790706	17.768107
H	-2.547195	-7.066664	19.401670
H	-3.943059	-8.017556	18.812280
Ni	-1.491769	-0.317587	18.731031
P	-2.467024	-0.501147	16.341936
H	-4.002709	-1.042022	18.075432
H	-3.984480	-4.960254	16.548111
H	-5.075833	-3.548479	16.672837
H	-3.654113	-3.519097	15.574073
H	-0.634349	-3.344180	18.259295
H	-1.324937	-4.888850	17.661217
H	-1.071181	-3.537642	16.538673
C	-1.365417	-0.101666	22.056107
C	-4.051204	-0.169982	21.025675
C	-5.681915	-5.666936	23.891629
C	-7.346748	-4.643603	21.690084
P	-0.811306	1.752521	19.152424
C	-0.771456	-0.274316	16.766021
C	-3.373249	1.075980	16.274592
C	-2.710187	-1.226672	14.676001
H	-1.749535	-0.448893	23.019273
H	-0.327829	-0.419480	21.920494
H	-1.419193	0.992283	22.045256
H	-4.769329	-0.623798	20.334087
H	-4.332471	-0.430286	22.054700
H	-4.078740	0.920890	20.932111

H	-4.673944	-5.965888	24.199000
H	-6.033184	-4.857163	24.540866
H	-6.355656	-6.525669	23.994275
H	-7.757663	-3.955233	22.437046
H	-7.309766	-4.131170	20.720541
H	-7.971514	-5.542068	21.643217
C	0.719776	2.010536	20.137263
C	-0.343102	2.476212	17.478725
C	-1.941030	3.063653	19.792716
P	0.256984	1.117783	16.428142
H	-4.421673	0.859639	16.041084
H	-3.313181	1.563102	17.250607
H	-2.969175	1.727213	15.491736
H	-2.146210	-2.160634	14.585498
H	-3.773537	-1.424805	14.497872
H	-2.344122	-0.520442	13.919952
H	0.481173	1.883792	21.197514
H	1.450460	1.241200	19.871902
H	1.128979	3.015685	19.981187
H	0.395463	3.284387	17.547156
H	-1.251197	2.880719	17.014687
H	-2.856579	3.098683	19.191746
H	-2.216350	2.822735	20.825292
H	-1.460724	4.049608	19.781105
C	0.278185	1.699069	14.701736
C	1.943029	0.675760	16.903284
H	0.629440	0.889297	14.052491
H	-0.729783	1.998038	14.394373
H	0.951938	2.557794	14.599095
H	1.906046	0.163271	17.872798
H	2.353986	-0.012550	16.156290
H	2.567761	1.574246	16.950216
H	-0.197952	-1.203200	16.701456
H	-5.205706	-2.764693	21.891892
Cl	0.609381	-1.513691	19.475935
Cl	-6.013060	-2.454236	19.117391

2-2-2

C	5.264874000	-0.471342000	-0.183858000
P	4.024924000	0.809909000	-0.696983000
H	6.250318000	-0.135832000	-0.529313000
H	5.299821000	-0.602567000	0.904831000
H	5.059303000	-1.433389000	-0.666778000
C	4.450611000	2.192963000	0.461204000
C	2.482877000	0.132339000	0.259447000
H	4.535880000	1.856714000	1.501579000
H	5.416984000	2.602111000	0.142261000
H	3.707163000	2.994547000	0.384134000
P	1.370808000	-0.697494000	-0.888981000
H	2.766875000	-0.556490000	1.066784000
H	1.954473000	0.988533000	0.694957000
C	0.694747000	0.495776000	-2.066310000
C	2.249355000	-1.994860000	-1.792078000
C	-0.000829000	-1.577305000	-0.015975000
H	0.197063000	1.315458000	-1.538252000
H	1.533403000	0.905539000	-2.641679000
H	-0.010863000	0.003845000	-2.744617000
H	3.069810000	-1.528603000	-2.349710000
H	2.654978000	-2.731443000	-1.089779000
H	1.570105000	-2.490427000	-2.494694000
P	-1.368475000	-0.700854000	0.866561000
H	0.477615000	-2.239625000	0.719554000
H	-0.482412000	-2.229218000	-0.758743000
C	-0.687861000	0.479838000	2.053921000
C	-2.249867000	-2.003542000	1.759260000
C	-2.479122000	0.142795000	-0.273245000
H	0.015849000	-0.020276000	2.728224000
H	-0.187291000	1.302246000	1.532909000
H	-1.525153000	0.887696000	2.632646000
H	-2.658000000	-2.733214000	1.051218000
H	-1.570972000	-2.506543000	2.456926000
H	-3.068506000	-1.540001000	2.321792000
P	-4.016788000	0.817895000	0.691900000
H	-2.766949000	-0.538300000	-1.085735000
H	-1.948148000	1.000538000	-0.702557000
C	-5.263370000	-0.451936000	0.166720000
C	-4.437594000	2.215171000	-0.450899000
H	-5.302105000	-0.569282000	-0.923439000
H	-5.059810000	-1.420715000	0.636881000
H	-6.246466000	-0.117132000	0.519455000
H	-3.690354000	3.012486000	-0.366586000
H	-4.525990000	1.890140000	-1.494563000
H	-5.401608000	2.625353000	-0.126191000

2-1-2

C	-5.309071000	-0.717672000	-0.457123000
P	-4.221834000	0.044836000	0.847498000
H	-6.319412000	-0.827064000	-0.045594000
H	-5.360441000	-0.096951000	-1.361261000
H	-4.948586000	-1.717058000	-0.724522000
C	-4.941503000	1.760172000	0.888342000
C	-2.687081000	0.419600000	-0.206019000
H	-5.027938000	2.197099000	-0.114771000
H	-5.939259000	1.708333000	1.339994000
H	-4.319250000	2.408494000	1.516212000
P	-1.333947000	-0.816438000	-0.107394000
H	-2.942989000	0.553279000	-1.266288000
H	-2.258313000	1.367576000	0.146465000
C	-0.840160000	-0.819373000	1.646347000
C	-2.081233000	-2.431806000	-0.474380000
C	-0.005171000	-0.556111000	-1.160333000
H	-0.360457000	0.132699000	1.899229000
H	-1.733135000	-0.937847000	2.270155000
H	-0.137612000	-1.638198000	1.828167000
H	-2.933868000	-2.601504000	0.191606000
H	-2.425363000	-2.443765000	-1.514382000
H	-1.333696000	-3.218031000	-0.331992000
P	1.334629000	0.489698000	-0.916901000
H	-0.061847000	-1.033331000	-2.134931000
C	0.887413000	2.181293000	-0.394224000
C	2.221144000	0.633464000	-2.495776000
C	2.539165000	-0.068600000	0.346930000
H	0.278672000	2.651509000	-1.173140000
H	0.306729000	2.136661000	0.534413000
H	1.795708000	2.767965000	-0.214861000
H	2.569010000	-0.356032000	-2.809849000
H	1.543324000	1.038593000	-3.253601000
H	3.079321000	1.302135000	-2.373746000
P	4.134711000	0.955824000	0.448108000
H	2.749135000	-1.131885000	0.169113000
H	2.028904000	0.009244000	1.316006000
C	5.235053000	-0.103400000	-0.616389000
C	4.699230000	0.394366000	2.130144000
H	5.195237000	-1.159735000	-0.319741000
H	4.954461000	-0.013372000	-1.671355000
H	6.266241000	0.254600000	-0.513521000
H	4.047751000	0.820910000	2.901770000
H	4.705064000	-0.699650000	2.220041000
H	5.715269000	0.769873000	2.300055000

2-2-1

C	1.513654000	-0.909141000	-2.343901000
P	2.582139000	-0.772162000	-0.813482000
H	2.137887000	-0.751287000	-3.232046000
H	1.036390000	-1.895869000	-2.422853000
H	0.738649000	-0.133074000	-2.340691000
C	3.767768000	-2.159387000	-1.188217000
C	1.543311000	-1.467525000	0.480375000
H	3.235577000	-3.101526000	-1.375367000
H	4.364804000	-1.904234000	-2.072637000
H	4.444573000	-2.295983000	-0.337547000
P	1.346126000	-0.725800000	1.969787000
H	1.047865000	-2.435592000	0.370806000
C	1.149142000	-1.890448000	3.359225000
C	2.665817000	0.454889000	2.395320000
C	-0.234402000	0.350469000	2.255999000
H	0.364973000	-2.614573000	3.110653000
H	2.093446000	-2.426523000	3.498634000
H	0.878646000	-1.364919000	4.282336000
H	3.593989000	-0.105008000	2.547584000
H	2.820299000	1.147800000	1.563364000
H	2.411288000	1.003932000	3.308321000
P	-0.846175000	1.199552000	0.775347000
H	-0.061893000	1.088551000	3.050540000
H	-1.038860000	-0.319457000	2.587011000
C	0.471729000	2.153681000	-0.008072000
C	-2.154909000	2.356791000	1.264329000
C	-1.505615000	-0.023847000	-0.374631000
H	0.829217000	2.920977000	0.687653000
H	1.302237000	1.490640000	-0.289615000
H	0.065990000	2.630411000	-0.907198000
H	-2.984510000	1.812777000	1.727965000
H	-1.755811000	3.087550000	1.976019000
H	-2.515925000	2.880410000	0.372170000
P	-2.221185000	0.719491000	-1.971088000
H	-2.245041000	-0.637792000	0.159324000
H	-0.646835000	-0.663566000	-0.622058000
C	-4.013145000	0.829495000	-1.477772000
C	-2.262367000	-0.846769000	-2.968862000
H	-4.379858000	-0.111722000	-1.047460000
H	-4.171314000	1.642484000	-0.760602000
H	-4.601431000	1.059584000	-2.373993000
H	-1.240304000	-1.147625000	-3.221136000
H	-2.764243000	-1.662978000	-2.434120000
H	-2.803392000	-0.645776000	-3.900917000

2-1-1

C	-4.344678000	0.689660000	-0.249316000
P	-2.818053000	1.469850000	0.489940000
H	-5.182447000	1.393513000	-0.172438000
H	-4.192825000	0.430626000	-1.306261000
H	-4.612064000	-0.217100000	0.304668000
C	-2.503574000	2.775433000	-0.803989000
C	-1.532384000	0.221582000	-0.075601000
H	-2.493837000	2.352173000	-1.817423000
H	-3.286978000	3.540902000	-0.743108000
H	-1.537492000	3.254787000	-0.608126000
P	-1.085470000	-1.121904000	1.094887000
H	-1.825488000	-0.248456000	-1.023926000
H	-0.575690000	0.736653000	-0.241903000
C	-0.575538000	-0.218013000	2.606999000
C	-2.631160000	-1.973534000	1.570359000
C	0.000319000	-2.267223000	0.465345000
H	0.335879000	0.337763000	2.367463000
H	-1.359504000	0.477006000	2.930758000
H	-0.358462000	-0.946526000	3.395918000
H	-3.318028000	-1.263288000	2.042330000
H	-3.099800000	-2.407632000	0.681554000
H	-2.394259000	-2.773456000	2.280113000
P	1.426789000	-1.750347000	-0.401030000
H	-0.269212000	-3.317031000	0.554985000
C	1.147674000	-1.708738000	-2.220332000
C	2.594808000	-3.182846000	-0.251788000
C	1.963391000	-0.217073000	0.122476000
H	0.756440000	-2.684294000	-2.532382000
H	0.419740000	-0.927528000	-2.458724000
H	2.080127000	-1.489545000	-2.751817000
H	2.912984000	-3.267837000	0.793055000
H	2.114205000	-4.121718000	-0.558735000
H	3.472501000	-2.999081000	-0.882690000
P	2.633286000	1.029132000	-0.958848000
H	2.145669000	-0.155380000	1.199731000
C	4.392068000	1.274958000	-0.341110000
C	1.924792000	2.604057000	-0.213536000
H	4.416634000	1.401599000	0.751564000
H	4.991272000	0.394655000	-0.604572000
H	4.845983000	2.159075000	-0.810460000
H	0.847830000	2.653820000	-0.417514000
H	2.078003000	2.638146000	0.875616000
H	2.400950000	3.485761000	-0.664034000

1-2-1

C	-3.966200000	-1.957632000	0.620799000
P	-2.211728000	-1.564901000	0.090334000
H	-4.132064000	-3.043104000	0.589918000
H	-4.168647000	-1.599609000	1.640960000
H	-4.670926000	-1.475778000	-0.067431000
C	-1.336973000	-2.401983000	1.520433000
C	-2.076092000	0.173783000	0.482007000
H	-1.677396000	-2.006055000	2.488955000
H	-1.537559000	-3.481832000	1.494294000
H	-0.254193000	-2.251335000	1.427768000
P	-1.478271000	1.316441000	-0.597805000
H	-2.413737000	0.566858000	1.445955000
C	-0.939754000	0.604113000	-2.179910000
C	-2.645347000	2.678823000	-1.040965000
C	-0.036044000	2.332835000	0.005226000
H	-0.053680000	-0.008987000	-1.997457000
H	-1.744255000	-0.013411000	-2.589615000
H	-0.694518000	1.418448000	-2.871466000
H	-3.497934000	2.242351000	-1.573542000
H	-3.012489000	3.144634000	-0.118620000
H	-2.165968000	3.443312000	-1.665931000
P	1.438622000	1.361491000	0.604997000
H	-0.398042000	2.976807000	0.819421000
H	0.305032000	2.992332000	-0.805678000
C	0.923188000	0.626633000	2.184495000
C	2.559649000	2.760367000	1.053665000
C	2.072000000	0.242707000	-0.479381000
H	0.648170000	1.430029000	2.877681000
H	0.059706000	-0.017147000	1.999258000
H	1.748421000	0.037107000	2.594197000
H	2.914189000	3.238723000	0.132808000
H	2.053407000	3.508321000	1.677563000
H	3.424328000	2.351502000	1.588688000
P	2.274417000	-1.489652000	-0.089962000
H	2.393563000	0.649430000	-1.443138000
C	4.043407000	-1.815575000	-0.618860000
C	1.432665000	-2.355267000	-1.522521000
H	4.234192000	-1.448467000	-1.638081000
H	4.728837000	-1.309111000	0.071255000
H	4.249807000	-2.894150000	-0.589608000
H	0.345124000	-2.245645000	-1.429579000
H	1.757595000	-1.943402000	-2.489677000
H	1.673770000	-3.426825000	-1.499759000

2-0-2

C	5.143258000	0.019338000	0.618367000
P	4.096022000	-0.445716000	-0.854340000
H	6.197800000	-0.172273000	0.384787000
H	5.022230000	1.080261000	0.877621000
H	4.867201000	-0.591868000	1.483468000
C	4.638151000	0.915952000	-2.014584000
C	2.451183000	0.285467000	-0.315444000
H	4.553900000	1.906098000	-1.545793000
H	5.681594000	0.749856000	-2.311005000
H	4.019125000	0.895264000	-2.919618000
P	1.255770000	-0.779835000	0.649859000
H	2.604903000	1.201951000	0.271358000
H	1.906667000	0.571142000	-1.226094000
C	0.913575000	-2.132719000	-0.572638000
C	2.303835000	-1.636704000	1.890901000
C	-0.002339000	-0.000492000	1.370788000
H	0.363468000	-1.713184000	-1.423468000
H	1.843222000	-2.590401000	-0.934330000
H	0.287059000	-2.891010000	-0.089944000
H	3.137233000	-2.167154000	1.415219000
H	2.685132000	-0.899395000	2.604998000
H	1.670543000	-2.349257000	2.430290000
P	-1.258018000	0.779423000	0.646268000
C	-0.911805000	2.133049000	-0.574274000
C	-2.310160000	1.635747000	1.884248000
C	-2.450268000	-0.285275000	-0.323532000
H	-0.286604000	2.890859000	-0.089134000
H	-0.359218000	1.713967000	-1.423707000
H	-1.840238000	2.591199000	-0.938491000
H	-2.693876000	0.898187000	2.596790000
H	-1.678706000	2.348134000	2.426006000
H	-3.141922000	2.166382000	1.405919000
P	-4.092876000	0.446352000	-0.868562000
H	-2.606380000	-1.201842000	0.262492000
H	-1.902396000	-0.570911000	-1.232176000
C	-5.146023000	-0.019865000	0.599568000
C	-4.630226000	-0.914401000	-2.032129000
H	-5.026357000	-1.081093000	0.858180000
H	-4.873019000	0.590343000	1.466347000
H	-6.199584000	0.172402000	0.362146000
H	-4.007527000	-0.892866000	-2.934623000
H	-4.547761000	-1.904954000	-1.563878000
H	-5.672469000	-0.748157000	-2.332659000

2-2-0

C	-3.246686000	1.290204000	-1.712471000
P	-2.620103000	1.899720000	-0.043714000
H	-3.642535000	2.137586000	-2.288835000
H	-2.462171000	0.799945000	-2.304595000
H	-4.063243000	0.577495000	-1.546464000
C	-1.222826000	2.999058000	-0.633467000
C	-1.853458000	0.633593000	0.845696000
H	-0.492046000	2.454725000	-1.246034000
H	-1.634133000	3.827901000	-1.224247000
H	-0.710852000	3.413152000	0.242177000
P	-1.881244000	-0.987294000	0.895277000
C	-1.410416000	-1.747620000	2.497528000
C	-3.240081000	-2.063919000	0.239222000
C	0.177796000	-2.642884000	-0.267417000
H	-0.512375000	-1.244975000	2.869131000
H	-2.215781000	-1.623927000	3.232518000
H	-1.201593000	-2.813116000	2.350678000
H	-4.123807000	-2.007366000	0.887984000
H	-3.509643000	-1.719054000	-0.763850000
H	-2.892081000	-3.102368000	0.183756000
P	1.194765000	-1.393909000	-0.828688000
H	-0.341839000	-3.211492000	-1.038086000
H	0.542732000	-3.224714000	0.577858000
C	0.307481000	-0.408720000	-2.072933000
C	2.811623000	-1.796119000	-1.635163000
C	1.612742000	-0.260723000	0.539904000
H	-0.021129000	-1.063582000	-2.887478000
H	-0.563666000	0.031997000	-1.578766000
H	0.955323000	0.380697000	-2.466556000
H	3.437369000	-2.353145000	-0.928284000
H	2.620963000	-2.430165000	-2.508787000
H	3.336705000	-0.885257000	-1.952095000
P	2.693546000	1.214614000	0.108049000
H	2.044534000	-0.849483000	1.361695000
H	0.645980000	0.145328000	0.877871000
C	4.358760000	0.571192000	0.654167000
C	2.266402000	2.258246000	1.590048000
H	4.311528000	0.138373000	1.663099000
H	4.716972000	-0.191519000	-0.046472000
H	5.080745000	1.397024000	0.655840000
H	1.208542000	2.537675000	1.529567000
H	2.437954000	1.716895000	2.530208000
H	2.875072000	3.170574000	1.583629000

2-1-0

C	3.712258000	6.636720000	6.949356000
P	5.494234000	6.161590000	7.282244000
H	3.042468000	6.032878000	7.576717000
H	3.536836000	7.701363000	7.161777000
H	3.467503000	6.443072000	5.898692000
C	5.635628000	6.830182000	9.022637000
C	6.381389000	7.547025000	6.403994000
H	5.297048000	7.874178000	9.079604000
H	5.036739000	6.218323000	9.710815000
H	6.686589000	6.790710000	9.331827000
P	6.915757000	7.320638000	4.648979000
H	5.797487000	8.477912000	6.442338000
H	7.348200000	7.746958000	6.894220000
C	7.940300000	5.793926000	4.694486000
C	5.394150000	6.777259000	3.757754000
C	7.507375000	8.694903000	3.867009000
H	8.898212000	6.111326000	5.126355000
H	7.466790000	5.012681000	5.305384000
H	8.078783000	5.439513000	3.664369000
H	5.024702000	5.837492000	4.184275000
H	4.620755000	7.548441000	3.841603000
H	5.635930000	6.623775000	2.699811000
P	8.936991000	9.447246000	4.605627000
H	7.052401000	8.987372000	2.919941000
C	8.503800000	11.266730000	4.833221000
C	10.138858000	9.653191000	3.164902000
C	9.432012000	8.546206000	5.906604000
H	8.209078000	11.745772000	3.887156000
H	7.674838000	11.329475000	5.547906000
H	9.374351000	11.786051000	5.255587000
H	10.512457000	8.655292000	2.905177000
H	9.670249000	10.112642000	2.279305000
H	10.983377000	10.275050000	3.493969000
P	10.230639000	9.258330000	7.285242000
C	11.802861000	8.208492000	7.521024000
C	9.341622000	8.454292000	8.769198000
H	11.553128000	7.135827000	7.452402000
H	12.513593000	8.448335000	6.718158000
H	12.282780000	8.413365000	8.493139000
H	8.337261000	8.889189000	8.868618000
H	9.239826000	7.366921000	8.602270000
H	9.890946000	8.624360000	9.709404000

2-0-1

C	4.598700000	1.091031000	1.071685000
P	3.179231000	1.260005000	-0.179418000
H	5.352217000	1.884192000	0.938927000
H	4.215521000	1.136150000	2.104188000
H	5.084411000	0.117255000	0.925950000
C	2.572013000	2.921540000	0.490726000
C	1.935719000	0.134197000	0.365780000
H	2.296860000	2.835631000	1.554335000
H	3.345522000	3.698661000	0.386369000
H	1.682037000	3.228784000	-0.073311000
P	1.422020000	-1.276528000	-0.525436000
H	1.726002000	0.066414000	1.438725000
C	1.330079000	-0.740811000	-2.307946000
C	2.787165000	-2.541765000	-0.683934000
C	0.037904000	-2.118480000	-0.014570000
H	0.502670000	-0.029669000	-2.409896000
H	2.263028000	-0.248671000	-2.613926000
H	1.135229000	-1.620251000	-2.935298000
H	3.685114000	-2.069826000	-1.106023000
H	3.014202000	-2.920353000	0.319951000
H	2.467369000	-3.380220000	-1.318185000
P	-1.212915000	-1.257521000	0.608276000
C	-1.118667000	-0.585931000	2.348637000
C	-2.759536000	-2.265810000	0.707019000
C	-1.747007000	0.307795000	-0.303339000
H	-0.898918000	-1.420130000	3.026025000
H	-0.284184000	0.123656000	2.377477000
H	-2.044588000	-0.079848000	2.657420000
H	-3.084628000	-2.519266000	-0.308290000
H	-2.517146000	-3.194020000	1.237422000
H	-3.560900000	-1.733002000	1.235984000
P	-3.264811000	1.272574000	0.183860000
H	-1.797220000	0.042564000	-1.369739000
H	-0.866265000	0.956163000	-0.171986000
C	-4.561807000	0.359779000	-0.811830000
C	-3.060428000	2.741274000	-0.964574000
H	-4.236548000	0.221147000	-1.853526000
H	-4.745784000	-0.624586000	-0.368753000
H	-5.501710000	0.927694000	-0.802686000
H	-2.207320000	3.343160000	-0.628547000
H	-2.874275000	2.413403000	-1.997469000
H	-3.960619000	3.371288000	-0.943862000

1-1-1

C	4.847801000	-0.861875000	0.037237000
P	3.115279000	-1.046748000	0.776571000
H	5.503120000	-1.688911000	0.352371000
H	4.804439000	-0.845225000	-1.063416000
H	5.284642000	0.084410000	0.381982000
C	2.694209000	-2.641272000	-0.139272000
C	2.152626000	0.165312000	-0.075170000
H	2.793463000	-2.505948000	-1.227847000
H	3.352768000	-3.464426000	0.177572000
H	1.654550000	-2.910211000	0.083402000
P	1.248042000	1.417969000	0.670000000
H	2.219686000	0.258513000	-1.162112000
C	0.666786000	0.801565000	2.311908000
C	2.235937000	2.914157000	1.195196000
C	-0.006593000	2.100619000	-0.303764000
H	-0.128118000	0.073921000	2.119116000
H	1.490560000	0.313056000	2.847775000
H	0.266829000	1.638238000	2.898445000
H	3.036208000	2.583652000	1.869101000
H	2.686200000	3.363197000	0.301910000
H	1.607212000	3.658661000	1.703786000
P	-1.242269000	1.164141000	-1.066906000
H	-0.005603000	3.175924000	-0.460700000
C	-0.639373000	0.144000000	-2.485317000
C	-2.245600000	2.451040000	-1.976979000
C	-2.137018000	0.141178000	-0.020682000
H	-0.233301000	0.803602000	-3.262577000
H	0.154419000	-0.504247000	-2.100694000
H	-1.453481000	-0.471595000	-2.888487000
H	-2.704538000	3.119559000	-1.238885000
H	-1.623436000	3.037466000	-2.667751000
H	-3.038986000	1.940388000	-2.536864000
P	-3.024940000	-1.305108000	-0.510480000
H	-2.216600000	0.517425000	1.002317000
C	-4.766418000	-1.025196000	0.173952000
C	-2.519392000	-2.579818000	0.786650000
H	-4.729135000	-0.704371000	1.227257000
H	-5.259445000	-0.237848000	-0.411035000
H	-5.368923000	-1.944433000	0.106360000
H	-1.464212000	-2.836838000	0.633586000
H	-2.633962000	-2.172982000	1.803698000
H	-3.126330000	-3.494141000	0.699147000

1-2-0

C	2.564250000	7.740101000	5.717880000
P	4.077011000	6.973685000	6.534337000
H	1.661440000	7.536511000	6.312312000
H	2.682367000	8.829678000	5.614363000
H	2.436683000	7.306095000	4.718637000
C	4.012519000	8.021020000	8.102733000
C	5.411891000	7.660314000	5.592456000
H	4.022659000	9.094443000	7.859278000
H	3.107603000	7.797993000	8.688037000
H	4.892887000	7.797107000	8.717728000
P	6.826647000	6.757560000	5.293950000
H	5.528229000	8.740792000	5.493502000
C	7.913092000	6.339532000	6.718786000
C	6.394914000	5.085051000	4.658339000
C	7.897979000	7.561656000	4.072659000
H	8.284658000	7.258642000	7.186492000
H	7.314259000	5.767998000	7.440425000
H	8.783348000	5.755086000	6.398325000
H	5.677269000	4.628688000	5.351179000
H	5.923220000	5.189556000	3.675584000
H	7.293009000	4.459828000	4.582802000
P	9.154950000	8.938356000	4.685312000
H	7.244950000	7.934527000	3.272807000
H	8.573071000	6.799805000	3.661309000
C	7.941070000	10.162068000	5.441528000
C	9.393221000	9.698471000	3.003908000
C	10.543107000	8.466504000	5.383529000
H	7.035583000	10.289570000	4.831833000
H	7.657409000	9.809198000	6.439235000
H	8.455348000	11.125554000	5.544606000
H	9.955496000	8.992458000	2.381869000
H	8.436978000	9.946531000	2.520232000
H	9.995714000	10.605971000	3.129658000
P	10.841507000	8.466817000	7.110636000
C	12.461479000	9.440509000	7.268757000
C	11.661319000	6.782511000	7.417883000
H	13.191089000	9.082105000	6.524566000
H	12.258547000	10.501909000	7.073265000
H	12.884938000	9.339427000	8.281245000
H	10.903847000	5.989815000	7.356298000
H	12.428117000	6.593252000	6.649252000
H	12.123227000	6.747006000	8.417569000

2-0-0

C	-4.499469000	0.542371000	-0.774433000
P	-3.143021000	1.219878000	0.340950000
H	-5.418018000	1.141048000	-0.670643000
H	-4.179552000	0.557109000	-1.828297000
H	-4.721183000	-0.494290000	-0.494315000
C	-2.907440000	2.852902000	-0.572584000
C	-1.681706000	0.283512000	-0.292454000
H	-2.752184000	2.680947000	-1.648510000
H	-3.777707000	3.514509000	-0.434575000
H	-2.014575000	3.350109000	-0.172967000
P	-1.147423000	-1.418779000	0.369250000
H	-1.748406000	0.177183000	-1.386906000
H	-0.740986000	0.840607000	-0.079974000
C	-1.047742000	-0.993344000	2.192306000
C	-2.725266000	-2.403417000	0.324906000
C	0.078207000	-2.178618000	-0.409273000
H	-0.164786000	-0.341732000	2.267646000
H	-1.946579000	-0.480328000	2.572614000
H	-0.872380000	-1.921723000	2.753777000
H	-3.526896000	-1.893890000	0.881011000
H	-3.027347000	-2.547681000	-0.720123000
H	-2.526777000	-3.386133000	0.772446000
P	1.574945000	-1.284133000	-0.458195000
C	2.188322000	-1.439297000	-2.249839000
C	2.872795000	-2.453383000	0.299485000
C	1.644435000	0.287151000	0.170082000
H	2.231705000	-2.491878000	-2.574214000
H	1.474139000	-0.896311000	-2.882745000
H	3.178941000	-0.967012000	-2.334165000
H	2.679294000	-2.490870000	1.379923000
H	2.801875000	-3.471418000	-0.119419000
H	3.879133000	-2.038866000	0.129219000
P	3.027727000	1.291996000	-0.102750000
C	3.588098000	1.878682000	1.647636000
C	2.285718000	3.017634000	-0.512891000
H	2.699905000	2.195285000	2.226218000
H	4.052433000	1.028703000	2.169488000
H	4.317090000	2.711361000	1.600346000
H	1.834287000	2.973952000	-1.514799000
H	1.487148000	3.250868000	0.216764000
H	3.049298000	3.818857000	-0.495919000

1-1-0

C	4.504270000	-1.364213000	-0.503872000
C	3.149398000	-0.766291000	-0.808083000
H	4.562768000	-2.417507000	-0.841699000
H	5.394287000	-0.858856000	-0.964000000
H	4.707700000	-1.384594000	0.579557000
P	2.456340000	0.560939000	0.011682000
H	2.752257000	-0.915231000	-1.812598000
C	3.026207000	0.368911000	1.807687000
C	3.239572000	2.278501000	-0.254297000
C	0.793173000	0.858721000	-0.238566000
H	2.569404000	-0.539980000	2.215877000
H	4.122529000	0.300595000	1.901395000
H	2.668179000	1.237579000	2.375542000
H	4.325787000	2.214700000	-0.090377000
H	3.045637000	2.583800000	-1.290185000
H	2.814432000	3.030363000	0.429089000
P	-0.597591000	-0.243919000	-0.095142000
H	0.497888000	1.906053000	-0.192999000
C	-0.078309000	-1.497281000	1.231550000
C	-0.453413000	-1.429639000	-1.563551000
C	-2.045621000	0.539259000	0.166676000
H	0.944473000	-1.869135000	1.055942000
H	-0.139149000	-0.990177000	2.203144000
H	-0.791228000	-2.335680000	1.220205000
H	-0.574010000	-0.838396000	-2.480001000
H	0.533882000	-1.912919000	-1.562471000
H	-1.258346000	-2.177417000	-1.509914000
P	-3.548131000	-0.177080000	-0.305332000
C	-4.625656000	1.337652000	-0.793051000
C	-4.543175000	-0.429086000	1.335035000
H	-4.515781000	2.126733000	-0.025849000
H	-4.257325000	1.735125000	-1.750425000
H	-5.693492000	1.068335000	-0.901576000
H	-4.104007000	-1.275046000	1.885251000
H	-4.449860000	0.476904000	1.963187000
H	-5.613970000	-0.643567000	1.147625000

1-0-1

C	5.343584000	0.237824000	-0.020485000
P	3.765269000	-0.557304000	-0.774029000
H	6.244879000	0.028784000	-0.625762000
H	5.223147000	1.331437000	0.067846000
H	5.491305000	-0.174130000	0.987472000
C	3.859921000	0.491317000	-2.363163000
C	2.408348000	0.103231000	0.101850000
H	3.804808000	1.565924000	-2.119560000
H	4.792289000	0.303200000	-2.924433000
H	3.001013000	0.239721000	-2.998914000
P	1.237361000	-0.817471000	1.057233000
H	2.338207000	1.182343000	0.268786000
C	0.746405000	-2.267518000	-0.036150000
C	2.198868000	-1.787726000	2.345315000
C	-0.000217000	-0.024071000	1.852397000
H	0.062831000	-1.881340000	-0.801377000
H	1.629811000	-2.715673000	-0.516556000
H	0.219130000	-3.019377000	0.569153000
H	3.032003000	-2.322175000	1.864840000
H	2.596050000	-1.066816000	3.071187000
H	1.537452000	-2.497016000	2.865234000
P	-1.231289000	0.787373000	1.065372000
C	-0.731160000	2.259585000	0.006789000
C	-2.200301000	1.731299000	2.367302000
C	-2.396518000	-0.110977000	0.082100000
H	-0.206569000	2.997062000	0.631759000
H	-0.043251000	1.888617000	-0.762056000
H	-1.610959000	2.719436000	-0.469156000
H	-2.606181000	0.995529000	3.073195000
H	-1.540631000	2.425973000	2.908657000
H	-3.027268000	2.279726000	1.891897000
P	-3.746173000	0.570180000	-0.789523000
H	-2.332835000	-1.193106000	0.231644000
C	-5.334319000	-0.221790000	-0.052028000
C	-3.841478000	-0.459233000	-2.390487000
H	-5.223496000	-1.317453000	0.022386000
H	-5.482411000	0.178122000	0.960724000
H	-6.231596000	0.003024000	-0.657683000
H	-2.978508000	-0.206372000	-3.020173000
H	-3.794629000	-1.536776000	-2.158531000
H	-4.770494000	-0.258385000	-2.952774000

0-2-0

C	5.298710000	0.138840000	-0.914505000
P	4.021057000	-0.333316000	0.440363000
H	6.327211000	-0.148670000	-0.627846000
H	5.026910000	-0.353493000	-1.864895000
H	5.267473000	1.227319000	-1.068495000
C	4.402791000	-2.192922000	0.293654000
C	2.464285000	-0.202077000	-0.331560000
H	4.198932000	-2.533665000	-0.736200000
H	5.453203000	-2.409052000	0.556024000
H	3.742924000	-2.745444000	0.976655000
P	1.440136000	1.031074000	0.035456000
C	1.209232000	1.603156000	1.825442000
C	1.812121000	2.739571000	-0.710721000
C	-0.322730000	0.843447000	-0.534532000
H	0.729674000	0.799620000	2.393400000
H	2.209634000	1.782083000	2.240552000
H	0.601935000	2.517712000	1.903143000
H	2.753771000	3.104610000	-0.274940000
H	1.955692000	2.604918000	-1.790353000
H	1.012059000	3.476702000	-0.531787000
P	-1.395352000	-0.713694000	-0.274607000
H	-0.335199000	1.000421000	-1.622331000
H	-0.899923000	1.667929000	-0.091096000
C	-0.834430000	-1.241785000	1.438118000
C	-0.454631000	-1.905618000	-1.319284000
C	-2.992929000	-0.606509000	-0.673260000
H	0.262939000	-1.273327000	1.495240000
H	-1.240919000	-0.537764000	2.174582000
H	-1.257129000	-2.235613000	1.635471000
H	-0.723432000	-1.716938000	-2.366153000
H	0.626186000	-1.757358000	-1.163288000
H	-0.763000000	-2.926587000	-1.055385000
P	-4.166625000	0.050393000	0.435361000
C	-5.706133000	-1.035528000	0.110665000
C	-4.921156000	1.553704000	-0.488588000
H	-5.859175000	-1.142957000	-0.978187000
H	-5.529049000	-2.034628000	0.534043000
H	-6.612126000	-0.604962000	0.573937000
H	-4.186573000	2.371808000	-0.492741000
H	-5.132383000	1.273405000	-1.536112000
H	-5.848667000	1.911418000	-0.004381000

10^{Me}

Ni	-0.007599000	-1.016766000	-0.042566000
P	2.129808000	-0.998869000	-0.131474000
P	-2.145123000	-0.966221000	-0.133941000
P	1.609021000	1.864765000	-0.053630000
P	-1.580361000	1.889378000	-0.049159000
B	0.007076000	0.975142000	-0.228820000
C	2.897556000	0.651761000	-0.543773000
C	-2.888159000	0.697340000	-0.539871000
H	3.864121000	0.814355000	-0.049952000
H	3.035427000	0.714542000	-1.629193000
H	-3.027561000	0.765777000	-1.624770000
H	-3.851096000	0.873155000	-0.043491000
C	-1.851175000	3.428849000	-1.045828000
H	-1.125794000	4.191661000	-0.738892000
H	-1.692115000	3.199757000	-2.104226000
H	-2.862123000	3.828316000	-0.895194000
C	-2.155973000	2.484822000	1.624487000
H	-3.166541000	2.916621000	1.596899000
H	-2.131275000	1.635109000	2.314706000
H	-1.451142000	3.241853000	1.989893000
C	-2.903207000	-2.091561000	-1.381184000
H	-2.542607000	-1.811633000	-2.377009000
H	-2.559724000	-3.106882000	-1.156486000
H	-4.000104000	-2.043679000	-1.354351000
C	-3.023310000	-1.458231000	1.413251000
H	-4.109820000	-1.515893000	1.265625000
H	-2.631740000	-2.438272000	1.706391000
H	-2.796422000	-0.740047000	2.208328000
C	2.874500000	-2.140642000	-1.371960000
H	3.971895000	-2.107361000	-1.343295000
H	2.516986000	-3.150153000	-1.143131000
H	2.519620000	-1.860793000	-2.369862000
C	2.998690000	-1.495976000	1.419422000
H	2.782143000	-0.770122000	2.210385000
H	2.592115000	-2.468410000	1.717462000
H	4.084330000	-1.570952000	1.273114000
C	1.902266000	3.397853000	-1.053801000
H	2.918538000	3.783735000	-0.903486000
H	1.740626000	3.168672000	-2.111811000
H	1.187114000	4.171102000	-0.749154000
C	2.196219000	2.454520000	1.617977000
H	1.504767000	3.224473000	1.981947000
H	2.157349000	1.607075000	2.310306000
H	3.214040000	2.868756000	1.588454000
Cl	-0.026365000	-3.307955000	0.321029000

10^{Me}+H^+

Ni	0.001072000	-0.936694000	-0.079415000
P	2.169019000	-0.989887000	-0.171802000
P	-2.166722000	-0.994454000	-0.171279000
P	1.639146000	1.880673000	-0.082644000
P	-1.643354000	1.877383000	-0.083464000
B	-0.001159000	1.065707000	-0.666411000
C	2.912257000	0.676970000	-0.600670000
C	-2.913593000	0.670523000	-0.601190000
H	3.892856000	0.864805000	-0.148351000
H	3.005606000	0.745867000	-1.691794000
H	-3.006602000	0.738614000	-1.692397000
H	-3.894822000	0.856321000	-0.149416000
C	-2.112368000	3.515084000	-0.758958000
H	-1.394923000	4.270777000	-0.418467000
H	-2.084614000	3.471152000	-1.853090000
H	-3.117180000	3.805057000	-0.430901000
C	-1.795781000	2.032369000	1.731042000
H	-2.830611000	2.255192000	2.013225000
H	-1.478624000	1.093842000	2.195253000
H	-1.151385000	2.841615000	2.089404000
C	-2.840030000	-2.126248000	-1.445480000
H	-2.456232000	-1.838419000	-2.429892000
H	-2.482460000	-3.133609000	-1.208608000
H	-3.936724000	-2.105745000	-1.452255000
C	-3.031696000	-1.487447000	1.370177000
H	-4.115087000	-1.546498000	1.210212000
H	-2.640442000	-2.467489000	1.661499000
H	-2.818831000	-0.774318000	2.172871000
C	2.844100000	-2.119373000	-1.447104000
H	3.940751000	-2.096767000	-1.454244000
H	2.488561000	-3.127608000	-1.210865000
H	2.459403000	-1.831536000	-2.431161000
C	3.035484000	-1.482383000	1.368966000
H	2.821155000	-0.770544000	2.172416000
H	2.646514000	-2.463586000	1.659427000
H	4.118970000	-1.538820000	1.208714000
C	2.104873000	3.519819000	-0.756929000
H	3.109470000	3.811121000	-0.429394000
H	2.076330000	3.476866000	-1.851080000
H	1.386513000	4.274052000	-0.415138000
C	1.790930000	2.034686000	1.731999000
H	1.144418000	2.841932000	2.091041000
H	1.476191000	1.094937000	2.195386000
H	2.825163000	2.259956000	2.014433000
H	-0.000871000	1.084908000	-1.884531000
Cl	0.003346000	-3.129584000	0.477064000

11^{Me}

Ni	0.000000000	-0.257344000	-0.126652000
P	2.153353000	-0.093888000	0.008646000
P	-2.153352000	-0.093881000	0.008648000
C	1.193223000	2.394215000	0.022139000
C	-1.193211000	2.394218000	0.022140000
N	0.000005000	1.654734000	-0.387793000
C	2.451648000	1.663457000	-0.463187000
C	-2.451640000	1.663465000	-0.463185000
Cl	-0.000012000	-2.492138000	-0.018429000
H	3.374484000	2.080365000	-0.040849000
H	2.505838000	1.703927000	-1.557944000
H	-2.505830000	1.703935000	-1.557942000
H	-3.374472000	2.080379000	-0.040847000
C	-3.238932000	-1.158025000	-1.014603000
H	-3.011503000	-0.985710000	-2.072222000
H	-3.007701000	-2.202266000	-0.777301000
H	-4.301017000	-0.954696000	-0.827053000
C	-2.820859000	-0.273752000	1.712404000
H	-3.905490000	-0.106360000	1.740671000
H	-2.592408000	-1.283787000	2.069880000
H	-2.322713000	0.450235000	2.366879000
C	3.238934000	-1.158037000	-1.014598000
H	4.301018000	-0.954709000	-0.827045000
H	3.007702000	-2.202277000	-0.777292000
H	3.011508000	-0.985727000	-2.072219000
C	2.820857000	-0.273757000	1.712405000
H	2.322716000	0.450235000	2.366877000
H	2.592399000	-1.283790000	2.069884000
H	3.905490000	-0.106373000	1.740672000
H	-1.256903000	2.534055000	1.124275000
H	1.256917000	2.534053000	1.124274000
H	-1.157657000	3.411585000	-0.409555000
H	1.157671000	3.411582000	-0.409557000

11^{Me}+H^+

Ni	0.011756000	-0.260668000	-0.241719000
P	-2.156394000	-0.191158000	0.092109000
P	2.185605000	-0.077497000	0.007119000
C	-1.391973000	2.391079000	-0.307162000
C	1.018356000	2.362843000	0.468951000
N	-0.026291000	1.747719000	-0.423618000
C	-2.309410000	1.584816000	0.612947000
C	2.386125000	1.772179000	0.105951000
Cl	0.103907000	-2.421992000	-0.164823000
H	-3.338424000	1.961120000	0.564063000
H	-1.973589000	1.650786000	1.655149000
H	3.149289000	2.071012000	0.832825000
H	2.702403000	2.138042000	-0.879840000
C	2.744803000	-0.742701000	1.614967000
H	2.170648000	-0.281773000	2.425888000
H	2.553600000	-1.820662000	1.622357000
H	3.813758000	-0.547635000	1.764473000
C	3.367736000	-0.710913000	-1.231070000
H	4.401907000	-0.501499000	-0.931996000
H	3.221401000	-1.793869000	-1.311070000
H	3.166886000	-0.257022000	-2.207284000
C	-2.842715000	-1.219423000	1.431076000
H	-3.904187000	-0.995277000	1.591801000
H	-2.721801000	-2.270931000	1.150436000
H	-2.281106000	-1.041775000	2.353922000
C	-3.271804000	-0.427028000	-1.339809000
H	-3.002801000	0.262648000	-2.146913000
H	-3.147540000	-1.452245000	-1.705897000
H	-4.318365000	-0.266290000	-1.053396000
H	1.009029000	3.453469000	0.342840000
H	-1.813245000	2.420998000	-1.317419000
H	0.744654000	2.129501000	1.502409000
H	-1.278012000	3.425245000	0.039647000
H	0.289046000	1.919423000	-1.380070000

12^{Me}

Ni	0.000000000	1.134729000	-0.000002000
C	-0.000001000	-0.849949000	-0.000004000
Cl	0.000005000	3.447600000	-0.000021000
C	2.728467000	-3.454298000	0.646654000
C	1.462123000	-2.897055000	0.539908000
C	3.901187000	-2.712087000	0.392003000
H	0.606784000	-3.505907000	0.812025000
H	4.885720000	-3.166916000	0.475514000
C	1.259051000	-1.523842000	0.151550000
C	3.751009000	-1.354923000	0.080585000
H	4.633678000	-0.731217000	-0.070977000
C	2.485244000	-0.781469000	-0.015010000
H	2.813522000	-4.496322000	0.959115000
P	2.120950000	0.955289000	-0.272556000
C	-1.259056000	-1.523838000	-0.151555000
C	-1.462132000	-2.897049000	-0.539921000
C	-2.485247000	-0.781464000	0.015017000
C	-2.728478000	-3.454289000	-0.646665000
C	-3.751014000	-1.354916000	-0.080576000
C	-3.901195000	-2.712078000	-0.392003000
H	-0.606795000	-3.505899000	-0.812049000
H	-2.813536000	-4.496310000	-0.959133000
H	-4.633681000	-0.731210000	0.070995000
H	-4.885729000	-3.166904000	-0.475511000
P	-2.120947000	0.955291000	0.272567000
C	-3.194001000	1.919850000	-0.877015000
H	-2.970330000	1.611088000	-1.903612000
H	-4.259752000	1.750957000	-0.669939000
H	-2.946137000	2.981541000	-0.762806000
C	-2.788954000	1.456189000	1.921383000
H	-2.289911000	0.861441000	2.693755000
H	-2.559129000	2.516737000	2.080078000
H	-3.874236000	1.294024000	1.978905000
C	2.788974000	1.456185000	-1.921366000
H	2.559155000	2.516734000	-2.080064000
H	3.874256000	1.294015000	-1.978877000
H	2.289936000	0.861438000	-2.693741000
C	3.193996000	1.919841000	0.877038000
H	2.946142000	2.981534000	0.762826000
H	2.970311000	1.611081000	1.903633000
H	4.259748000	1.750940000	0.669975000

12^{Me}+H^+

Ni	0.240931000	-1.157810000	-0.210325000
C	-0.129748000	0.788074000	-0.664157000
Cl	0.614392000	-3.327750000	0.232085000
H	0.109186000	0.790010000	-1.742476000
C	1.721631000	3.642061000	1.178189000
C	0.668421000	2.895302000	0.635167000
C	3.037505000	3.179441000	1.113099000
H	-0.343337000	3.282744000	0.699771000
H	3.849738000	3.764558000	1.537247000
C	0.908510000	1.657776000	0.019605000
C	3.292978000	1.931025000	0.533019000
H	4.306055000	1.533220000	0.525156000
C	2.240127000	1.173109000	0.019375000
H	1.506620000	4.594720000	1.657863000
P	2.325475000	-0.571178000	-0.507055000
C	-1.577169000	1.233289000	-0.540493000
C	-2.023889000	2.481986000	-1.008905000
C	-2.529343000	0.352102000	-0.002679000
C	-3.368456000	2.844248000	-0.908468000
C	-3.880511000	0.711806000	0.102933000
C	-4.301057000	1.964627000	-0.343268000
H	-1.310818000	3.168229000	-1.459362000
H	-3.694873000	3.813279000	-1.279848000
H	-4.602330000	0.011531000	0.519122000
H	-5.347563000	2.250318000	-0.268346000
P	-1.806336000	-1.265413000	0.405778000
C	-2.032828000	-1.522462000	2.212419000
H	-1.490137000	-0.741840000	2.755176000
H	-3.094832000	-1.491422000	2.487186000
H	-1.606260000	-2.498489000	2.469033000
C	-2.903778000	-2.535406000	-0.341081000
H	-2.952142000	-2.377674000	-1.423404000
H	-2.454984000	-3.515050000	-0.143853000
H	-3.915220000	-2.491565000	0.082145000
C	3.584872000	-1.375589000	0.556395000
H	3.603401000	-2.442001000	0.307608000
H	4.579336000	-0.935399000	0.412626000
H	3.279677000	-1.272704000	1.602344000
C	3.101711000	-0.599808000	-2.180420000
H	3.187408000	-1.640630000	-2.514032000
H	2.462536000	-0.054730000	-2.883164000
H	4.096884000	-0.137268000	-2.162334000

13^{Me}

Ni	-0.000007000	-1.131536000	-0.000088000
N	0.000029000	0.819822000	-0.000034000
Cl	-0.000040000	-3.335223000	-0.000251000
C	-2.599293000	3.386635000	0.861286000
C	-1.343816000	2.809959000	0.692053000
C	-3.777276000	2.685715000	0.566355000
H	-0.461764000	3.374253000	0.971368000
H	-4.750233000	3.150030000	0.700268000
C	-1.207811000	1.485955000	0.199499000
C	-3.670208000	1.361588000	0.140981000
H	-4.569069000	0.775538000	-0.043791000
C	-2.416605000	0.765882000	-0.023930000
H	-2.658928000	4.401778000	1.248893000
P	-2.133921000	-0.980894000	-0.374101000
C	1.207901000	1.485909000	-0.199547000
C	1.343966000	2.809893000	-0.692133000
C	2.416659000	0.765788000	0.023915000
C	2.599472000	3.386500000	-0.861394000
C	3.670291000	1.361422000	-0.141028000
C	3.777421000	2.685529000	-0.566454000
H	0.461942000	3.374220000	-0.971466000
H	2.659156000	4.401626000	-1.249037000
H	4.569123000	0.775335000	0.043762000
H	4.750401000	3.149788000	-0.700394000
P	2.133867000	-0.980949000	0.374198000
C	3.250510000	-1.948805000	-0.709797000
H	3.038960000	-1.695607000	-1.753340000
H	4.303517000	-1.736431000	-0.486984000
H	3.038859000	-3.011962000	-0.552572000
C	2.726093000	-1.362160000	2.070949000
H	2.167078000	-0.755520000	2.790533000
H	2.537703000	-2.422853000	2.272973000
H	3.798426000	-1.150388000	2.169229000
C	-2.726673000	-1.362311000	-2.070617000
H	-2.538385000	-2.423036000	-2.272562000
H	-3.799032000	-1.150519000	-2.168573000
H	-2.167875000	-0.755783000	-2.790464000
C	-3.250281000	-1.948588000	0.710342000
H	-3.038655000	-3.011770000	0.553245000
H	-3.038478000	-1.695206000	1.753789000
H	-4.303345000	-1.736261000	0.487750000

13^{Me}+H^+

Ni	0.261952000	-1.133383000	-0.218972000
N	-0.147524000	0.807686000	-0.662397000
Cl	0.660249000	-3.202617000	0.258000000
H	0.086260000	0.875788000	-1.655749000
C	1.566438000	3.590023000	1.288090000
C	0.540279000	2.846190000	0.689230000
C	2.889782000	3.152880000	1.236132000
H	-0.481369000	3.203446000	0.740068000
H	3.678658000	3.738104000	1.699684000
C	0.854283000	1.652348000	0.048459000
C	3.192653000	1.937377000	0.614385000
H	4.215059000	1.568729000	0.616220000
C	2.178279000	1.170085000	0.033226000
H	1.318508000	4.517631000	1.796345000
P	2.374414000	-0.550753000	-0.558215000
C	-1.569137000	1.200599000	-0.558995000
C	-2.006803000	2.412992000	-1.096248000
C	-2.471806000	0.304478000	0.023361000
C	-3.357952000	2.754950000	-1.003419000
C	-3.824452000	0.663648000	0.121532000
C	-4.263820000	1.888985000	-0.381086000
H	-1.300248000	3.085353000	-1.575328000
H	-3.702852000	3.696405000	-1.421482000
H	-4.537262000	-0.024130000	0.569318000
H	-5.313410000	2.159662000	-0.309077000
P	-1.791561000	-1.334867000	0.451018000
C	-2.006466000	-1.589887000	2.247889000
H	-1.458728000	-0.816946000	2.796070000
H	-3.067875000	-1.553767000	2.521130000
H	-1.591367000	-2.571520000	2.501163000
C	-2.859349000	-2.578466000	-0.354366000
H	-2.878368000	-2.401483000	-1.434209000
H	-2.423587000	-3.564595000	-0.161070000
H	-3.879515000	-2.537932000	0.045242000
C	3.645621000	-1.333705000	0.488897000
H	3.708337000	-2.390470000	0.208144000
H	4.622606000	-0.855804000	0.353817000
H	3.336225000	-1.271384000	1.536384000
C	3.102672000	-0.498639000	-2.243177000
H	3.223781000	-1.526801000	-2.603394000
H	2.435469000	0.036104000	-2.927859000
H	4.079353000	0.000172000	-2.228898000

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