

Supporting Information:

**A tetranuclear lanthanum-nickel hydrido complex supported by
arene-anchored bis(phosphinomethylamido) ligand**

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1. Experimental

General. All operations were performed under an inert atmosphere of nitrogen using standard Schlenk-line or glovebox techniques. THF, pentane, *n*-hexane, benzene, toluene, C₆D₆, and THF-*d*₈ were dried over K-Na alloy, followed by vacuum transfer, and stored in the glovebox. ¹H, ¹³C{¹H}, ³¹P{¹H} NMR and 2D NMR spectra were recorded on a Bruker Ascend™ 500 spectrometer. All chemical shifts were reported in δ units with references to the residual solvent resonance of the deuterated solvents for proton and carbon chemical shifts, to external H₃PO₄ for phosphorous chemical shifts. LaI₃(THF)₄,^[1] ¹Pr₂PCH₂OH,^[2] 1,3-bis(2-aminophenyl)benzene^[3] were prepared according to the literature procedure. IR spectra were measured on a SHIMADZU FTIR-8400S spectrometer. Elemental analyses were performed by the Microanalytical Laboratory of Soochow University.

Synthesis of *bis*-P-N^m-Ph. 1,3-bis(2-aminophenyl)benzene (2.0 g, 7.68 mmol) in 15 mL of toluene was added via a cannula to a solution of ¹Pr₂PCH₂OH (2.28 g, 15.36 mmol) in 15 mL of toluene at room temperature. The reaction mixture was then stirred at 120 °C for 24 h. After cooling the reaction mixture to room temperature, solid CaH₂ (1.5 equivalent) was slowly added to remove the byproduct water. The resulting slurry was filtered via a cannula, and the clear solution was evaporated to dryness under reduced pressure to afford *bis*-P-N^m-Ph as a pale-yellow oil. Yield: 3.68 g (92 %). ¹H NMR (C₆D₆, 500 MHz, 25°C): δ (ppm) = 7.65 (t, ⁴J_{HH} = 2.0 Hz, 1H, ArH), 7.36 (dd, ³J_{HH} = 8.0 Hz, ⁴J_{HH} = 2.0 Hz, 2H, ArH), 7.28 (td, ³J_{HH} = 8.0 Hz, ⁴J_{HH} = 1.5 Hz, 2H, ArH), 7.23 (dd, ³J_{HH} = 7.5 Hz, ⁴J_{HH} = 1.5 Hz, 2H, ArH), 7.19 (t, ³J_{HH} = 7.5 Hz, 1H, ArH), 6.85 (td, ³J_{HH} = 7.5 Hz, ⁴J_{HH} = 1.0 Hz, 2H, ArH), 6.78 (d, ³J_{HH} = 8.0 Hz, 2H, ArH), 4.23-4.21 (m, 2H, NH), 3.09 (m, 4H, PCH₂), 1.56 (sept.d, ³J_{HH} = 7.0 Hz, ²J_{PH} = 2.5 Hz, 4H, (CH₃)₂CH), 0.96 (d, ³J_{HH} = 7.0 Hz, 6H, (CH₃)₂CH), 0.94 (d, ³J_{HH} = 7.0 Hz, 6H, (CH₃)₂CH), 0.91 (d, ³J_{HH} = 7.0 Hz, 6H, (CH₃)₂CH), 0.90 (d, ³J_{HH} = 7.0 Hz, 6H, (CH₃)₂CH); ¹³C{¹H} NMR (C₆D₆, 126 MHz, 25°C): δ (ppm) = 146.09 (d, J_{PC} = 7.1 Hz, ArC), 140.71 (s, ArC), 131.00 (s, ArC), 130.43 (s, ArC), 129.65 (s, ArC), 129.26 (s, ArC), 128.39 (s, ArC), 128.35 (s, ArC), 127.79 (s, ArC), 117.59 (s, ArC), 111.02 (s, ArC), 38.53 (d, ¹J_{PC} = 17.6 Hz, PCH₂), 22.98 (d, ¹J_{PC} = 13.6 Hz, CH(CH₃)₂), 20.38 (s, CH(CH₃)₂), 20.25 (s, CH(CH₃)₂), 19.12 (s, CH(CH₃)₂), 19.05 (s, CH(CH₃)₂); ³¹P{¹H} NMR (C₆D₆, 202 MHz, 25°C): δ (ppm) = 3.35 (s, 2P); FT-IR (KBr pellets): ν_{NH} = 3410 cm⁻¹. Anal. calcd for C₃₂H₄₆N₂P₂ (520.68 g/mol): C, 73.82; H, 8.91; N, 5.38. Found: C, 74.02; H, 9.53; N, 5.61.

Synthesis of **1.** *bis*-P-N^m-Ph (100 mg, 0.19 mmol) in 2 mL of THF was slowly added to a slurry of KH (23 mg, 0.58 mmol) in 1 mL of THF at room temperature. The resulting orange solution was allowed to stir at room temperature for 2 h and filtered through a pad of Celite. After removal of the solvent under reduced pressure, an orange powder of **K₂P-N^m-Ph** was obtained and used in the next step. **K₂P-N^m-Ph** (100 mg, 0.17 mmol) in 2 mL of THF was slowly added to a slurry of LaI₃(THF)₄ (135 mg, 0.17 mmol) in 1 mL of THF at room temperature. The resulting orange solution was allowed to stir at room temperature for 24 h and then filtered through a pad of Celite. After removal of the volatiles under reduced pressure, the crude product was extracted with 6 mL of benzene. The benzene solution was layered with 4 mL of *n*-hexane and stored at room temperature overnight to afford compound **1** as orange crystals. Single crystals of **1** suitable for X-ray diffraction analysis were obtained from a benzene/pentane solution at room temperature. Yield: 113 mg (78 %). ¹H

NMR (C₆D₆, 500 MHz, 25°C): δ (ppm) = 7.75 (s, 2H, ArH), 7.64 (t, $^3J_{\text{HH}} = 7.3$ Hz, 2H, ArH), 7.40 (t, $^3J_{\text{HH}} = 7.8$ Hz, 4H, ArH), 7.24-7.21 (m, 6H, ArH), 7.00 (d, $^3J_{\text{HH}} = 5.5$ Hz, 4H, ArH), 6.77 (t, $^3J_{\text{HH}} = 7.3$ Hz, 3H, ArH), 6.47 (d, $^3J_{\text{HH}} = 8.5$ Hz, 3H, ArH), 3.65 (d, $^2J_{\text{HH}} = 13.0$ Hz, 4H, CH₂), 3.38 (d, $^2J_{\text{HH}} = 12.5$ Hz, 4H, CH₂), 1.88-1.83 (m, 4H, CH(CH₃)₂), 1.77-1.72 (m, 4H, CH(CH₃)₂), 1.24-1.19 (m, 12H, CH(CH₃)₂), 0.99-0.88 (m, 36H, CH(CH₃)₂); $^{31}\text{P}\{^1\text{H}\}$ NMR (C₆D₆, 202 MHz, 25°C): δ (ppm) = -22.04 ppm. Recrystallization by layering *n*-hexane into the THF solution of **1** led to the isolation of monomeric complex **1'**. ^1H NMR (THF-*d*₈, 500 MHz, 25°C): δ (ppm) = 8.22 (t, $^3J_{\text{HH}} = 7.5$ Hz, 1H, ArH), 8.15 (s, 1H, ArH), 7.50 (dd, $^3J_{\text{HH}} = 7.5$ Hz, $^4J_{\text{HH}} = 1.5$ Hz, 2H, ArH), 7.04 (td, $^3J_{\text{HH}} = 7.5$ Hz, $^4J_{\text{HH}} = 1.5$ Hz, 2H, ArH), 6.91 (dd, $^3J_{\text{HH}} = 7.5$ Hz, $^4J_{\text{HH}} = 1.5$ Hz, 2H, ArH), 6.40 (t, $^3J_{\text{HH}} = 7.5$ Hz, 2H, ArH), 6.30 (d, $^3J_{\text{HH}} = 8.5$ Hz, 2H, ArH), 3.46 and 3.41 (AB, $^2J_{\text{HH}} = 13.0$ Hz, 4H, PCH₂), 2.15-2.01 (m, 4H, (CH₃)₂CH), 1.28-1.20 (m, 12H, (CH₃)₂CH), 1.18-1.14 (m, 6H, (CH₃)₂CH), 1.08-1.02 (m, 6H, (CH₃)₂CH); $^{13}\text{C}\{^1\text{H}\}$ NMR (THF-*d*₈, 126 MHz, 25°C): δ (ppm) = 159.58 (d, $J_{\text{PC}} = 16.5$ Hz, ArC), 149.58 (s, ArC), 140.94 (s, ArC), 134.55 (s, ArC), 130.47 (d, $J_{\text{PC}} = 21.7$ Hz, ArC), 129.47 (s, ArC), 129.16 (s, ArC), 127.95 (s, ArC), 114.21 (s, ArC), 110.73 (s, ArC), 46.83 (m, PCH₂), 26.09 (s, (CH₃)₂CH), 24.74 (s, (CH₃)₂CH), 20.47 (d, $J_{\text{PC}} = 8.1$ Hz, (CH₃)₂CH), 20.07 (s, (CH₃)₂CH), 19.88 (s, (CH₃)₂CH); $^{31}\text{P}\{^1\text{H}\}$ NMR (THF-*d*₈, 202 MHz, 25°C): δ (ppm) = -19.49 (s, 2P). Anal. calcd for C₆₄H₈₈I₂La₂N₄P₄·2(C₆H₆) (1725.18 g/mol): C, 52.91; H, 5.84; N, 3.25. Found: C, 52.87; H, 5.59; N, 3.49.

Synthesis of 2. Complex **1** (50 mg, 0.03 mmol) in 2 mL of benzene was slowly added to a solution of Ni(COD)₂ (16 mg, 0.06 mmol) in 2 mL of benzene at room temperature. The reaction mixture was then stirred for 2 h. After evaporation of the solution to about 2 mL under reduced pressure, 3 mL of *n*-hexane was layered to afford **2** as yellow crystals. Yield: 49 mg (91 %). ^1H NMR (THF-*d*₈, 500 MHz, 25°C): δ (ppm) = 8.42 (t, $^4J_{\text{HH}} = 1.5$ Hz, 2H, ArH), 7.59 (t, $^3J_{\text{HH}} = 7.5$ Hz, 2H, ArH), 7.18 (dd, $^3J_{\text{HH}} = 7.5$, $^4J_{\text{HH}} = 1.8$ Hz, 4H, ArH), 7.01-6.99 (m, 4H, ArH), 6.74 (dd, $^3J_{\text{HH}} = 7.5$, $^4J_{\text{HH}} = 2.0$ Hz, 4H, ArH), 6.48 (d, $^3J_{\text{HH}} = 8.5$ Hz, 4H, ArH), 6.26 (t, $^3J_{\text{HH}} = 7.3$ Hz, 4H, ArH), 4.04 and 3.88 (AB, $^2J_{\text{HH}} = 14.0$ Hz, 8H, PCH₂), 2.28-2.21 (m, 8H, (CH₃)₂CH), 1.40-1.33 (m, 24H, (CH₃)₂CH), 1.29-1.25 (m, 12H, (CH₃)₂CH), 1.16-1.12 (m, 12H, (CH₃)₂CH); $^{13}\text{C}\{^1\text{H}\}$ NMR (THF-*d*₈, 126 MHz, 25°C): δ (ppm) = 159.69 (t, $J_{\text{PC}} = 6.3$ Hz, ArC), 148.76 (s, ArC), 133.27 (s, ArC), 130.46 (s, ArC), 130.42 (s, ArC), 130.24 (s, ArC), 129.64 (s, ArC), 129.19 (s, ArC), 128.89 (s, ArC), 112.63 (s, ArC), 110.15 (s, ArC), 51.78 (t, $^1J_{\text{PC}} = 16.8$ Hz, PCH₂), 28.14 (t, $^1J_{\text{PC}} = 8.1$ Hz, (CH₃)₂CH), 27.00 (t, $^1J_{\text{PC}} = 10.6$ Hz, (CH₃)₂CH), 21.46 (s, (CH₃)₂CH), 20.69 (s, (CH₃)₂CH), 20.51 (s, (CH₃)₂CH), 20.48 (s, (CH₃)₂CH); $^{31}\text{P}\{^1\text{H}\}$ NMR (THF-*d*₈, 202 MHz, 25°C): δ (ppm) = 1.62 (s, 4P). Anal. calcd for C₆₄H₈₈I₂La₂N₄Ni₂P₄ (1686.34 g/mol): C, 45.58; H, 5.26; N, 3.32. Found: C, 45.14; H, 5.40; N, 3.11.

Synthesis of 3. A solution of Li[HBET₃] (142 μL , 0.14 mmol, 1 M in THF) in 1 mL of toluene was slowly added to a solution of **2** (100 mg, 0.06 mmol) in 2 mL of toluene at room temperature. The reaction solution was stirred for about 1 minute, and then left for standing at room temperature overnight. The red crystals of **3** precipitated from the solution, which were collected. Yield: 42 mg (44 %). ^1H NMR (THF-*d*₈, 500 MHz, 25°C): δ (ppm) = 7.58-7.54 (m, 4H, ArH), 7.22-7.20 (m, 4H, ArH, partly overlapped with resonances of toluene), 7.07-7.04 (m, 4H, ArH), 6.72 (dd, $^3J_{\text{HH}} = 7.0$, $^4J_{\text{HH}} = 1.5$ Hz, 4H, ArH), 6.38 (d, $^3J_{\text{HH}} = 8.5$ Hz, 4H, ArH), 6.33 (t, $^3J_{\text{HH}} = 7.0$ Hz, 4H, ArH), 3.87 (s, 8H, PCH₂), 2.88 (t, $^2J_{\text{P-H}} = 11.5$ Hz, 2H, Ni-H-La), 2.25 (m, 4H, (CH₃)₂CH), 1.86 (m, 4H, (CH₃)₂CH), 1.28-1.19 (m, 36H, (CH₃)₂CH), 1.04-1.00 (m, 12H, (CH₃)₂CH); $^{31}\text{P}\{^1\text{H}\}$ NMR (THF-

d_8 , 202 MHz, 25°C): δ (ppm) = -2.04 (s, 4P). A satisfactory $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum was not obtained due to the poor solubility of **3** in common solvent. Anal. calcd for $\text{C}_{64}\text{H}_{90}\text{La}_2\text{N}_4\text{Ni}_2\text{P}_4\cdot 2(\text{C}_7\text{H}_8)$ (1618.83 g/mol): C, 57.87; H, 6.60; N, 3.46. Found: C, 57.38; H, 6.84; N, 3.35.

Synthesis of 4. *N,N'*-diisopropylcarbodiimide (6.2 mg, 0.05 mmol) in 1 mL of THF was added to a slurry of **3** (40 mg, 0.02 mmol) in 3 mL of THF at room temperature. The reaction mixture was then stirred at 60 °C for 2 h. After removal of the solvent under reduced pressure, the residue was extracted with 4 mL of toluene. The toluene solution was concentrated to about 2 mL under reduced pressure, slow diffusion of pentane into toluene solution at room temperature afforded red crystals of **4**. Yield: 37 mg (88 %). ^1H NMR (C_6D_6 , 500 MHz, 25°C): δ (ppm) = 8.26 (s, 1H, NCH), 7.64 (s, 1H, ArH), 7.47 (t, $^3J_{\text{HH}} = 7.8$ Hz, 2H, ArH), 7.10 (d, $^3J_{\text{HH}} = 7.5$ Hz, 2H, ArH), 7.02-6.97 (m, 3H, ArH), 6.75 (t, $^3J_{\text{HH}} = 7.5$ Hz, 2H, ArH), 6.72 (d, $^3J_{\text{HH}} = 8.0$ Hz, 2H, ArH), 4.04 and 3.90 (AB, $^2J_{\text{HH}} = 12.5$ Hz, 4H, PCH₂), 3.43-3.38 (m, 2H, (CH₃)₂CHN), 2.16-2.09 (br m, 4H, (CH₃)₂CH), 1.29-1.25 (m, 6H, (CH₃)₂CH), 1.11 (d, $^3J_{\text{HH}} = 6.0$ Hz, 12H, (CH₃)₂CHN), 1.09-1.03 (m, 18H, (CH₃)₂CH); $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 126 MHz, 25°C): δ (ppm) = 162.22 (s, ArC), 161.62 (t, $J_{\text{PC}} = 9.3$ Hz, ArC), 152.30 (s, ArC), 137.81 (s, ArC), 133.91 (s, ArC), 130.64 (d, $J_{\text{PC}} = 16.4$ Hz, ArC), 127.22 (s, ArC), 112.44 (s, ArC), 109.18 (s, ArC), 59.70 (t, $^1J_{\text{PC}} = 19.5$ Hz, PCH₂), 28.37 (t, $^1J_{\text{PC}} = 9.6$ Hz, (CH₃)₂CH), 27.37 (t, $^1J_{\text{PC}} = 7.5$ Hz, (CH₃)₂CH), 25.57 (s, (CH₃)₂CHN), 20.88 (s, (CH₃)₂CH), 20.27 (s, (CH₃)₂CH), 19.36 (s, (CH₃)₂CH), 18.75 (s, (CH₃)₂CH); $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6 , 202 MHz, 25°C): δ (ppm) = -13.04 (s, 2P). Anal. calcd for $\text{C}_{39}\text{H}_{59}\text{LaN}_4\text{NiP}_2$ (843.48 g/mol): C, 55.54; H, 7.05; N, 6.64. Found: C, 55.89; H, 7.42; N, 6.28.

Synthesis of 5. *tert*-butyl isocyanide (8.2 mg, 0.1 mmol) in 1 mL of THF was added to a slurry of **3** (40 mg, 0.02 mmol) in 3 mL of THF at room temperature. The reaction mixture was then stirred at 60 °C for 0.5 h. After removal of the solvent under reduced pressure, the residue was extracted with 4 mL of benzene. The benzene solution was concentrated to about 2 mL under reduced pressure and 2 mL of *n*-hexane was layered to afford **5** as yellow crystals. Yield: 38 mg (87 %). ^1H NMR (C_6D_6 , 500 MHz, 25°C): δ (ppm) = 11.92 (s, 1H, N=CH), 7.67 (s, 1H, ArH), 7.47 (t, $^3J_{\text{HH}} = 7.4$ Hz, 2H, ArH), 7.22 (d, $^3J_{\text{HH}} = 7.5$ Hz, 2H, ArH), 7.05 (d, $^3J_{\text{HH}} = 7.0$ Hz, 2H, ArH), 6.75 (t, $^3J_{\text{HH}} = 7.5$ Hz, 2H, ArH), 6.72 (d, $^3J_{\text{HH}} = 8.5$ Hz, 2H, ArH), 3.76 (dd, $^2J_{\text{HH}} = 13.0$, $^2J_{\text{PH}} = 3.0$ Hz, 2H, PCH₂), 3.38 (dd, $^2J_{\text{HH}} = 13.0$, $^2J_{\text{PH}} = 3.0$ Hz, 2H, PCH₂), 2.00-1.96 (m, 2H, (CH₃)₂CH), 1.95-1.91 (m, 2H, (CH₃)₂CH), 1.36-1.31 (m, 6H, (CH₃)₂CH), 1.17-1.13 (m, 6H, (CH₃)₂CH), 1.12-1.11 (m, 6H, (CH₃)₂CH), 1.09 (s, 9H, (CH₃)₃C), 1.08 (s, 9H, (CH₃)₃C), 1.07-1.04 (m, 6H, (CH₃)₂CH); $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 126 MHz, 25°C): δ (ppm) = 233.18 (s, N=CH), 168.23 (s, NC), 162.30 (t, $J_{\text{PC}} = 8.2$ Hz, ArC), 153.56 (s, ArC), 138.73 (s, ArC), 132.08 (s, ArC), 130.99 (s, ArC), 130.50 (s, ArC), 128.59 (s, ArC), 126.71 (s, ArC), 112.10 (s, ArC), 109.09 (s, ArC), 59.17 (s, (CH₃)₃C), 53.97 (s, (CH₃)₃C), 50.20 (m, PCH₂), 30.79 (s, (CH₃)₃C), 30.68 (s, (CH₃)₃C), 29.60 (t, $^1J_{\text{PC}} = 14.5$ Hz, (CH₃)₂CH), 28.19 (t, $^1J_{\text{PC}} = 8.8$ Hz, (CH₃)₂CH), 19.17 (s, (CH₃)₂CH), 18.50 (s, (CH₃)₂CH), 18.24 (s, (CH₃)₂CH), 17.05 (s, (CH₃)₂CH); $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6 , 202 MHz, 25°C): δ (ppm) = 10.06 (s, 2P); FT-IR (KBr pellets): $\nu_{\text{NH}} = 2037\text{ cm}^{-1}$. Anal. calcd for $\text{C}_{42}\text{H}_{63}\text{LaN}_4\text{NiP}_2$ (883.54 g/mol): C, 57.10; H, 7.19; N, 6.34. Found: C, 57.20; H, 7.24; N, 6.26.

Synthesis of 6. *p*-Tolunitrile (7.2 mg, 0.06 mmol) in 1 mL of THF was added to a slurry of **3** (40

mg, 0.02 mmol) in 4 mL of THF at room temperature. The solution was stirred at 60 °C for 12 days. The color of the solution changed from deep red to yellow, with concomitant formation of yellow precipitate. After removal of the volatiles under reduced pressure, the residue was extracted with 4 mL of benzene. The benzene solution was concentrated to about 2 mL under reduced pressure and 2 mL of *n*-hexane was layered to afford **6** as yellow crystals. Yield: 37 mg (80 %). ¹H NMR (THF-*d*₈, 500 MHz, 25°C): δ (ppm) = 7.73 (t, ³*J*_{HH} = 7.5 Hz, 2H, ArH), 7.57 (t, ⁴*J*_{HH} = 1.5 Hz, 2H, ArH), 7.31-7.29 (m, 4H, ArH), 7.07-7.04 (m, 4H, ArH), 6.74 (dd, ³*J*_{HH} = 7.0 Hz, ⁴*J*_{HH} = 2.0 Hz, 4H, ArH), 6.41 (d, ³*J*_{HH} = 8.5 Hz, 4H, ArH), 6.32 (t, ³*J*_{HH} = 7.3 Hz, 4H, ArH), 3.85 and 3.81 (AB, ²*J*_{HH} = 12.8 Hz, 8H, PCH₂), 2.15-2.11 (m, 4H, (CH₃)₂CH), 2.09-2.04 (m, 4H, (CH₃)₂CH), 1.31-1.27 (m, 12H, (CH₃)₂CH), 1.18-1.10 (m, 24H, (CH₃)₂CH), 1.10-1.05 (m, 12H, (CH₃)₂CH); ³¹P{¹H} NMR (THF-*d*₈, 202 MHz, 25°C): δ (ppm) = 0.51 (s, 4P). FT-IR (KBr pellets): ν_{CN} = 2036 cm⁻¹. A satisfactory ¹³C{¹H} NMR spectrum was not obtained due to the poor solubility of **6** in common solvent. Anal. calcd for C₆₆H₈₈La₂N₆Ni₂P₄ (1484.56 g/mol): C, 53.40; H, 5.98; N, 5.66. Found: C, 53.27; H, 5.88; N, 5.36.

In-situ characterization of 6'. *p*-Tolunitrile (3.6 mg, 0.03 mmol) and **3** (20 mg, 0.01 mmol) were mixed in 0.6 mL of THF-*d*₈ in a J-Young NMR tube at room temperature. The process of the reaction was monitored by ¹H and ³¹P{¹H} NMR spectra. After 3h, ¹H and ³¹P{¹H} NMR spectra showed the intermediate product **6'** was formed. However, it is also noted that a large amount of precipitants in the bottom of NMR tube, which were attributed to unreacted **3**, and product **6** due to their poor solubility. This was further confirmed by several up-scaled reactions, which readily formed mixtures of **6** and **6'**. Attempts to isolate **6'** out of the mixture via multiple recrystallizations always led to **6**, due to the lower solubility of the latter. ¹H NMR (THF-*d*₈, 500 MHz, 25°C): δ (ppm) = 9.32 (s, 1H, LaH), 8.52 (t, ⁴*J*_{HH} = 1.5 Hz, 1H, ArH), 7.67 (t, ³*J*_{HH} = 7.8 Hz, 1H, ArH), 7.28 (dd, ³*J*_{HH} = 7.8 Hz, ⁴*J*_{HH} = 1.8 Hz, 2H, ArH), 7.10 (d, ³*J*_{HH} = 8.5 Hz, 2H, ArH), 6.96-6.93 (m, 2H, ArH), 6.77 (dd, ³*J*_{HH} = 7.3 Hz, ⁴*J*_{HH} = 1.8 Hz, 2H, ArH), 6.72 (d, ³*J*_{HH} = 7.5 Hz, 2H, ArH), 6.39 (d, ³*J*_{HH} = 8.5 Hz, 2H, ArH), 6.20 (t, ³*J*_{HH} = 7.0 Hz, 2H, ArH), 3.79 (d, ³*J*_{HH} = 13.5 Hz, 2H, PCH₂), 3.36 (d, ³*J*_{HH} = 13.5 Hz, 2H, PCH₂), 2.22 (s, 3H, ArCH₃), 2.13-2.07 (m, 2H, (CH₃)₂CH), 1.84-1.80 (m, 2H, (CH₃)₂CH), 1.41-1.37 (m, 6H, (CH₃)₂CH), 1.30-1.27 (m, 6H, (CH₃)₂CH), 1.06-1.02 (m, 6H, (CH₃)₂CH), 0.68-0.63 (m, 6H, (CH₃)₂CH); ³¹P{¹H} NMR (THF-*d*₈, 202 MHz, 25°C): δ (ppm) = 15.27 (s, 2P).

Synthesis of 6 from acetonitrile. Acetonitrile (3.0 mg, 0.07 mmol) in 1 mL of THF was added to a slurry of **3** (40 mg, 0.02 mmol) in 4 mL of THF at room temperature. The reaction mixture was stirred at room temperature for 24 h, during the time the color of solution changed from dark red to yellow, with concomitant formation of an yellow precipitate. After removal of the volatiles under reduced pressure, the residue was extracted with 4 mL of benzene. The benzene solution was concentrated to about 2 mL under reduced pressure and 2 mL of *n*-hexane was layered to afford **6** as yellow crystals. Yield: 18 mg (40 %). ¹H NMR and ³¹P{¹H} NMR spectra were consistent with compound **6**.

2. Spectroscopic Data

NMR spectra

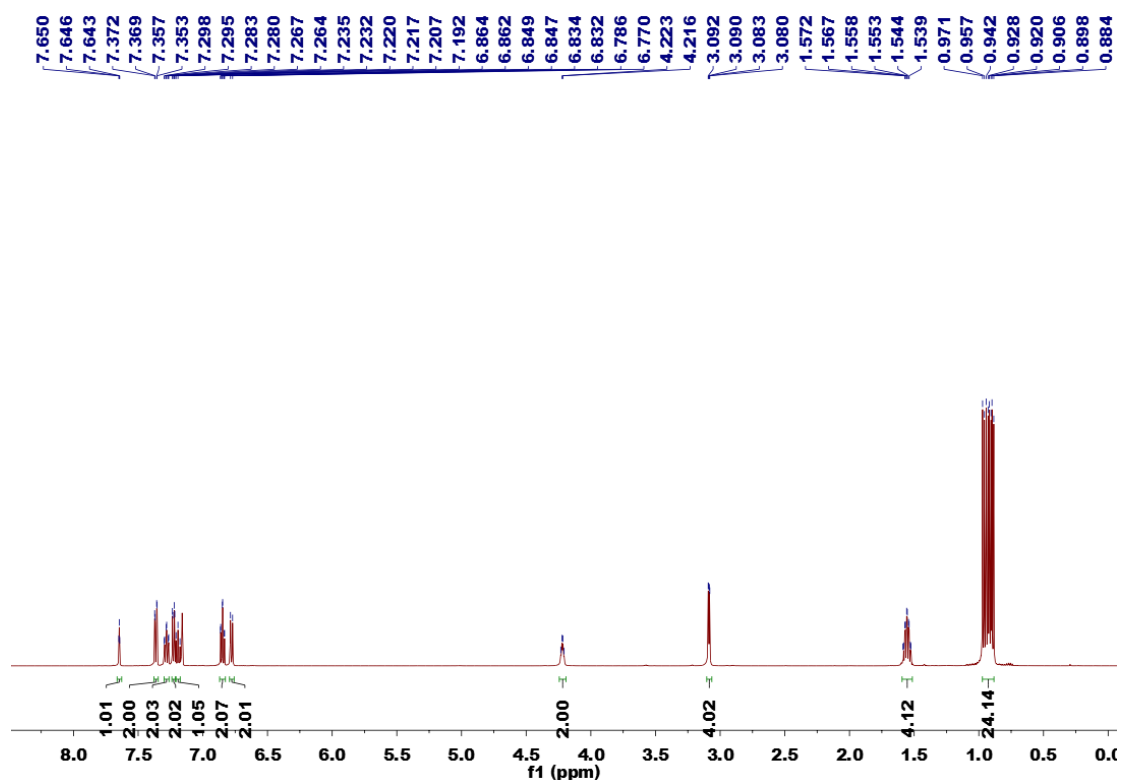


Figure S1. ¹H NMR spectrum of *bis*-P-N^m-Ph in C₆D₆ at 25°C.

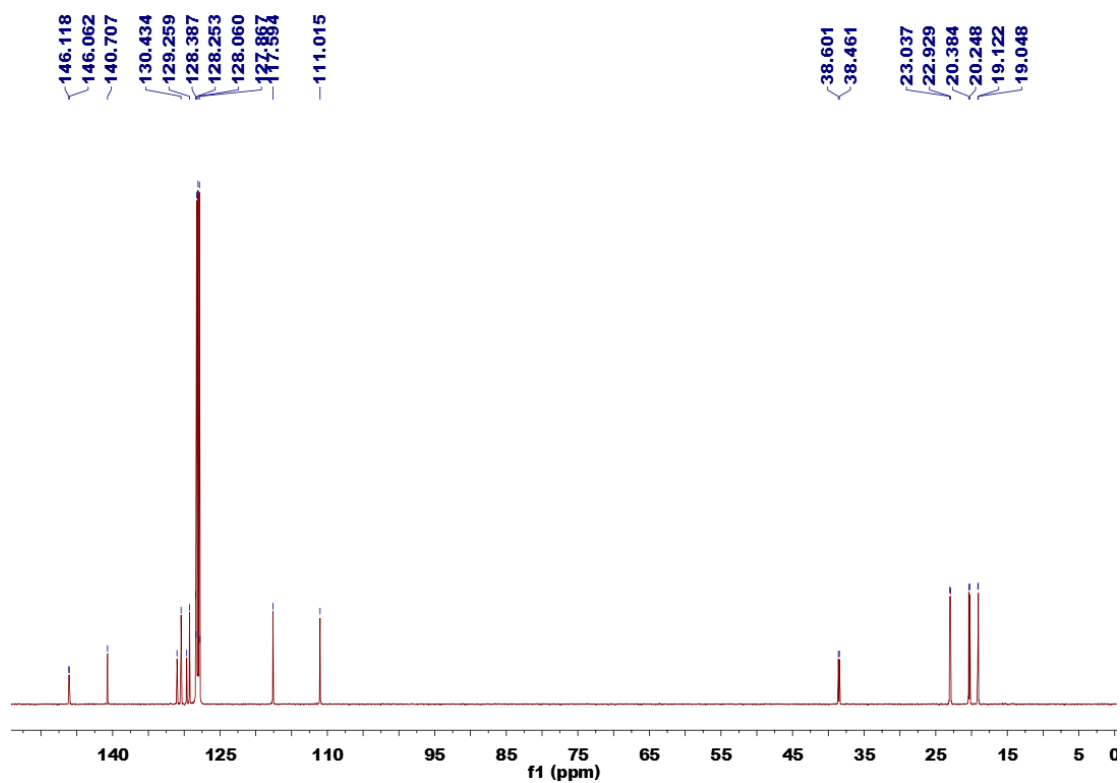


Figure S2. ¹³C{¹H} NMR spectrum of *bis*-P-N^m-Ph in C₆D₆ at 25°C.

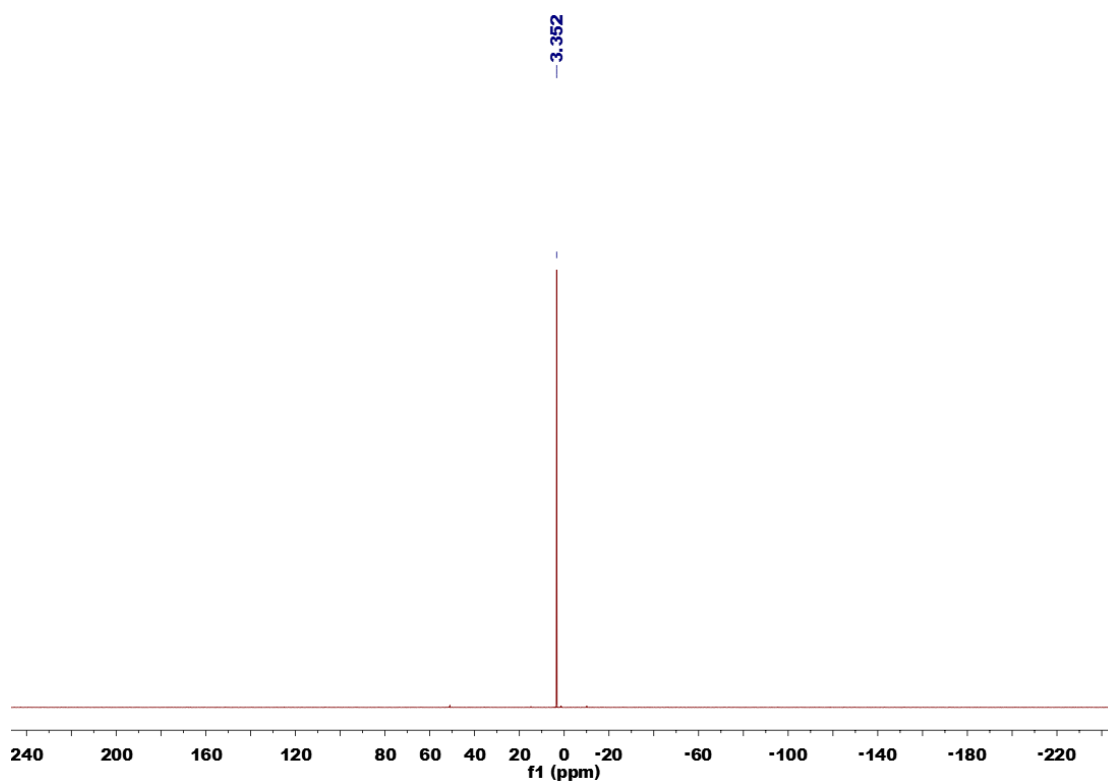


Figure S3. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *bis*-P-N^m-Ph in C₆D₆ at 25°C.

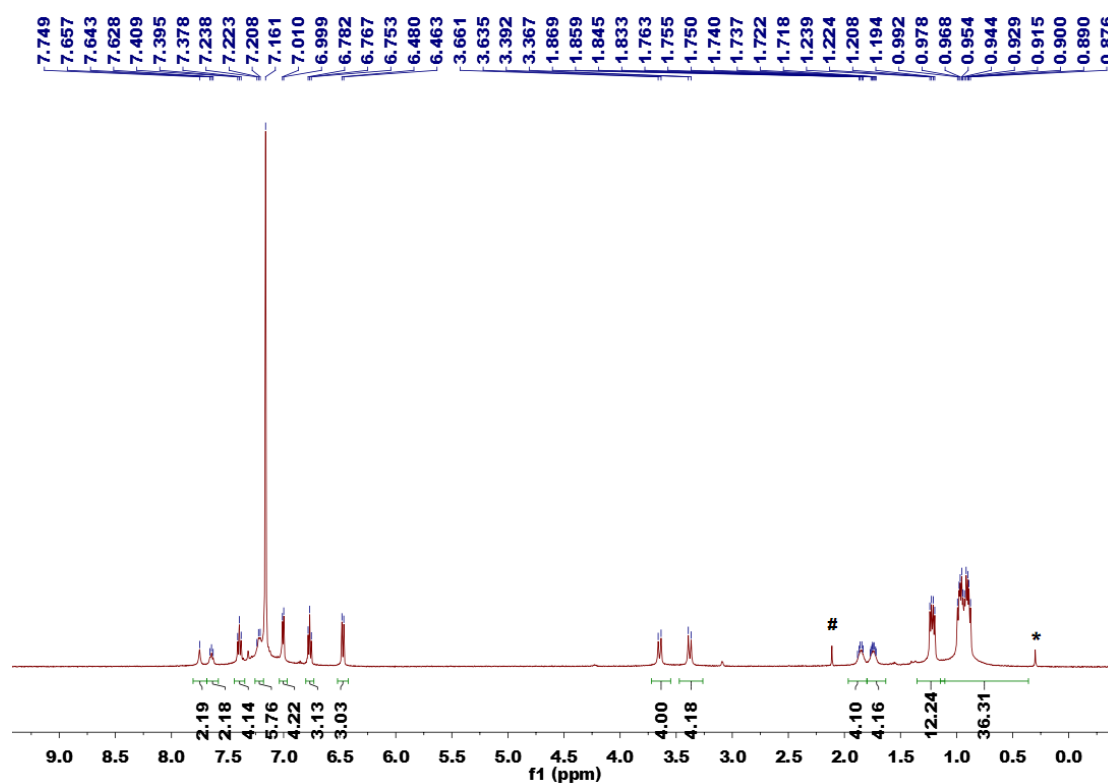


Figure S4. ^1H NMR spectrum of **1** in C₆D₆ at 25°C (# and * denote to small amount of toluene and silicone grease, respectively).

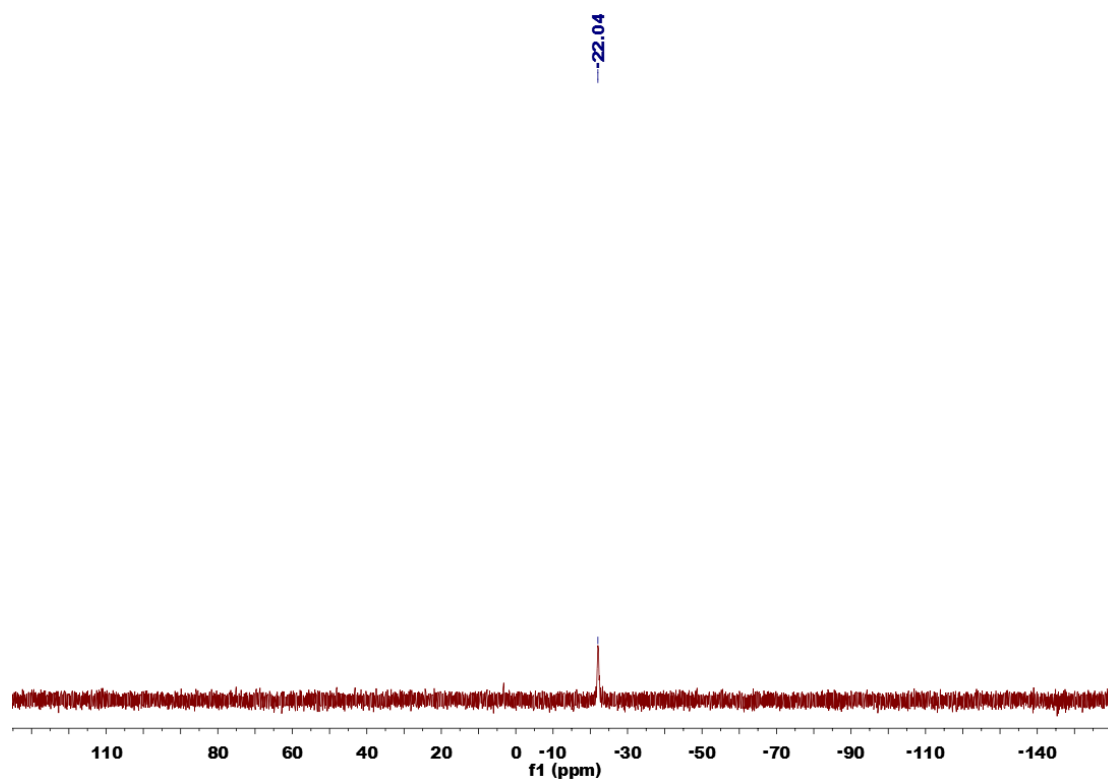


Figure S5. ³¹P {¹H} NMR spectrum of **1** in C₆D₆ at 25°C.

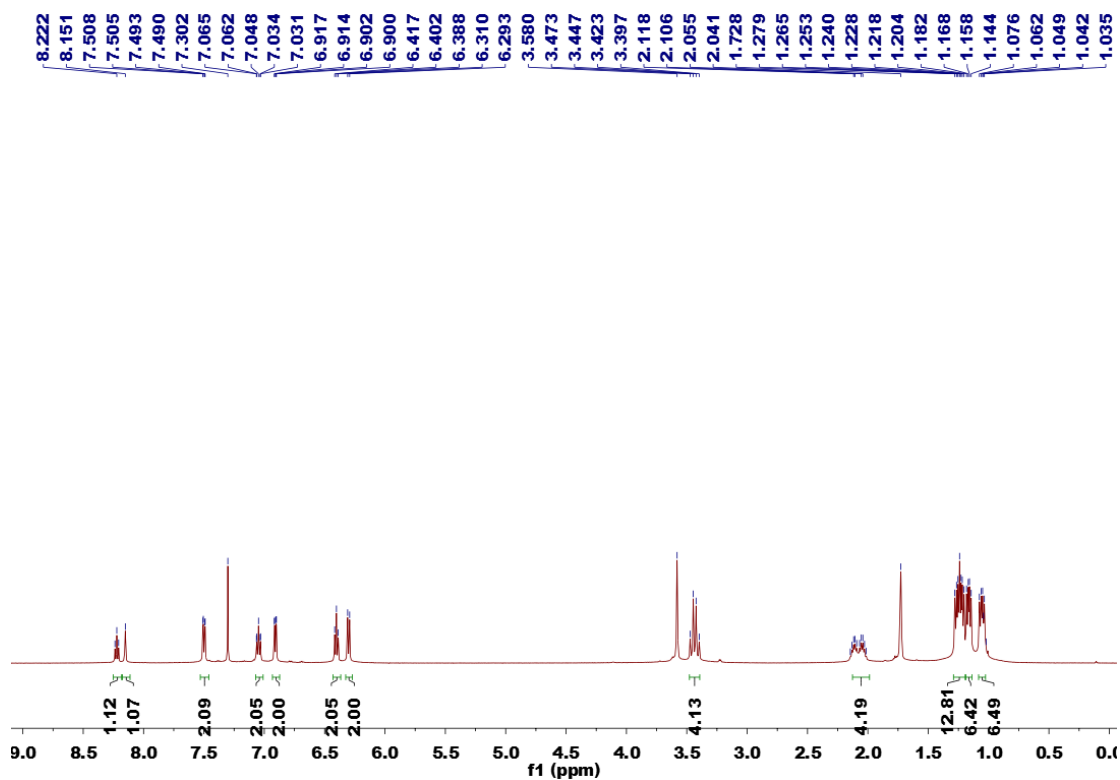


Figure S6. ¹H NMR spectrum of **1'** in THF-*d*₈ at 25°C.

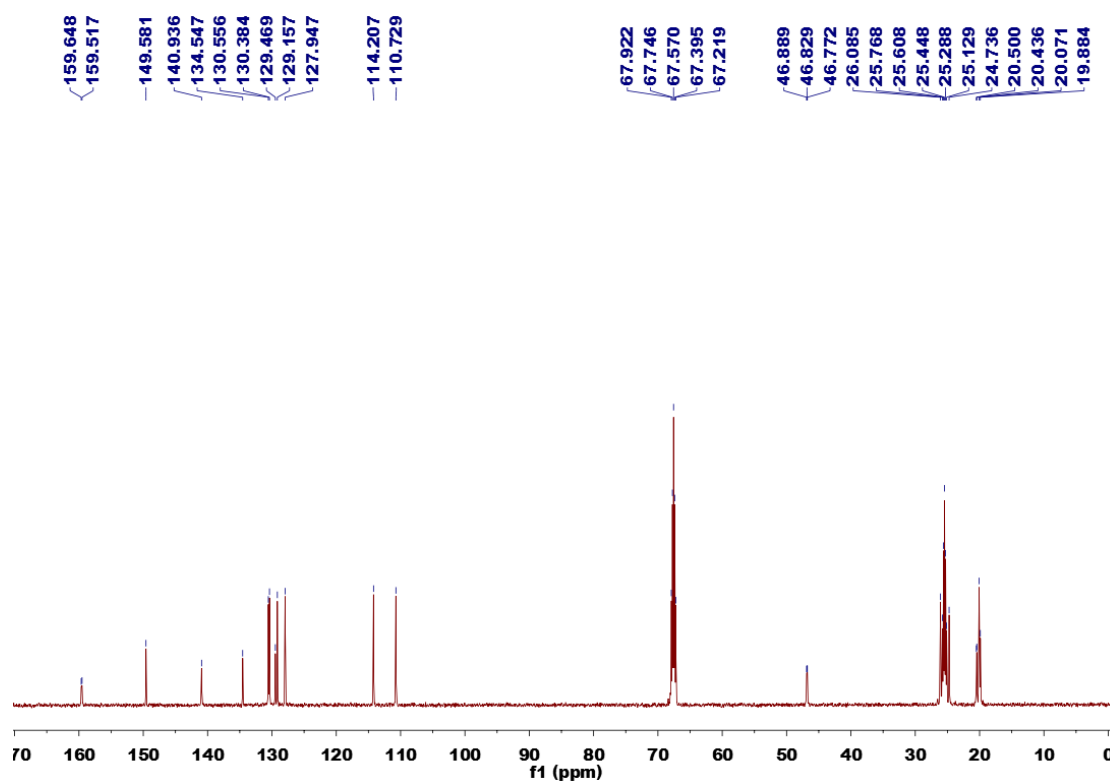


Figure S7. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1'** in $\text{THF-}d_8$ at 25°C .

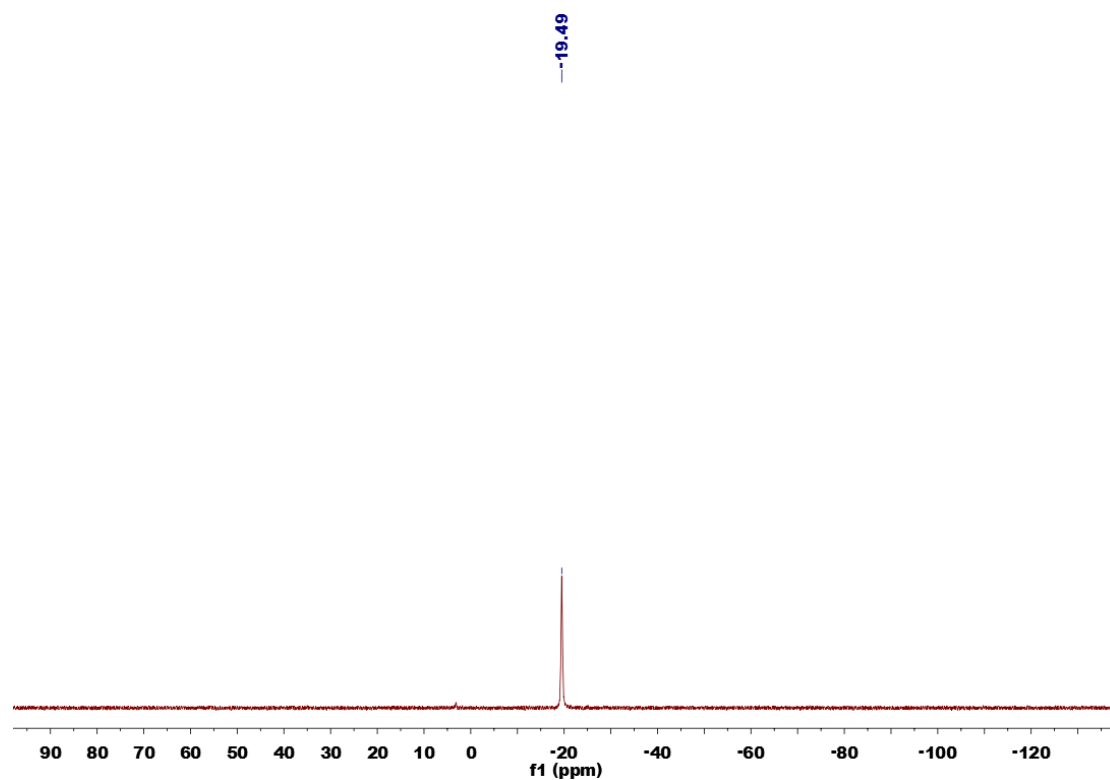


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1'** in $\text{THF-}d_8$ at 25°C .

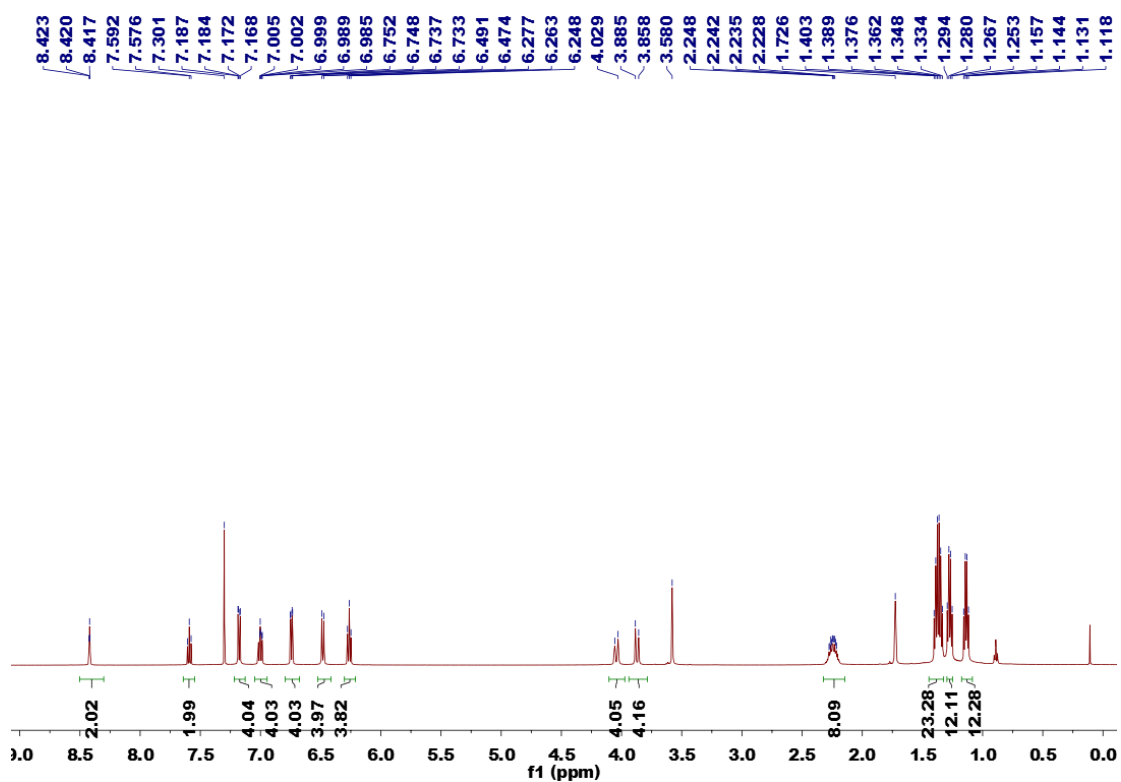


Figure S9. ¹H NMR spectrum of **2** in THF-*d*₈ at 25°C.

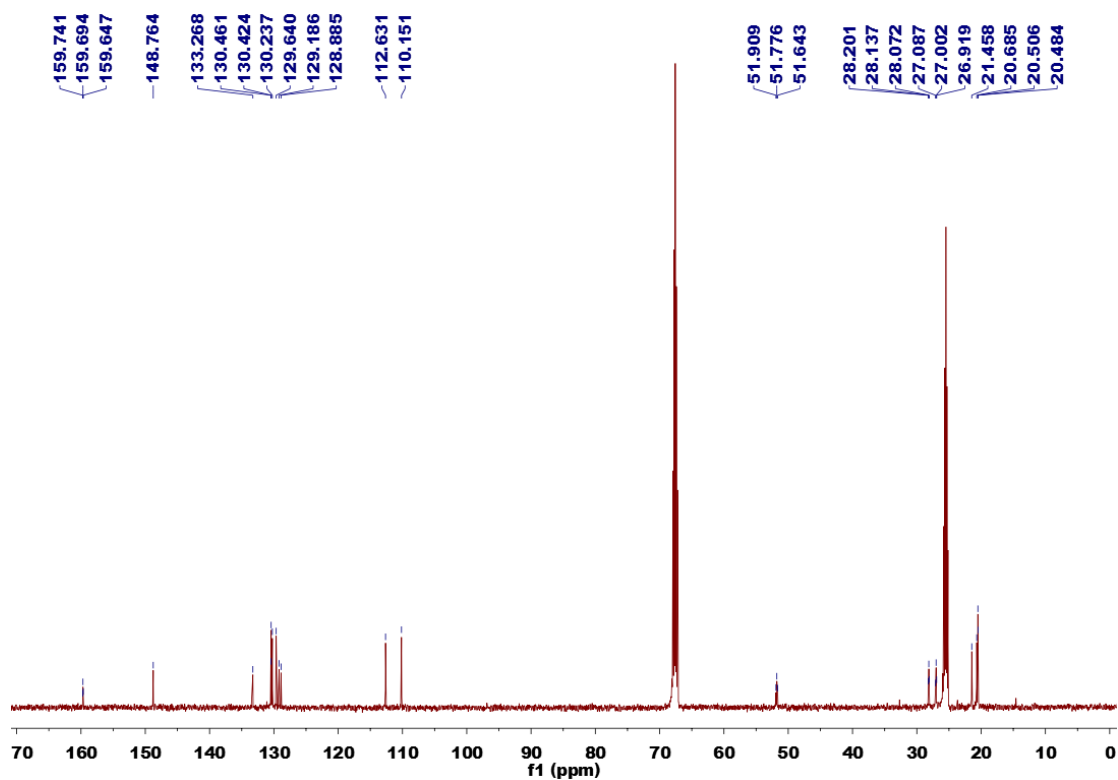


Figure S10. ¹³C{¹H} NMR spectrum of **2** in THF-*d*₈ at 25°C.

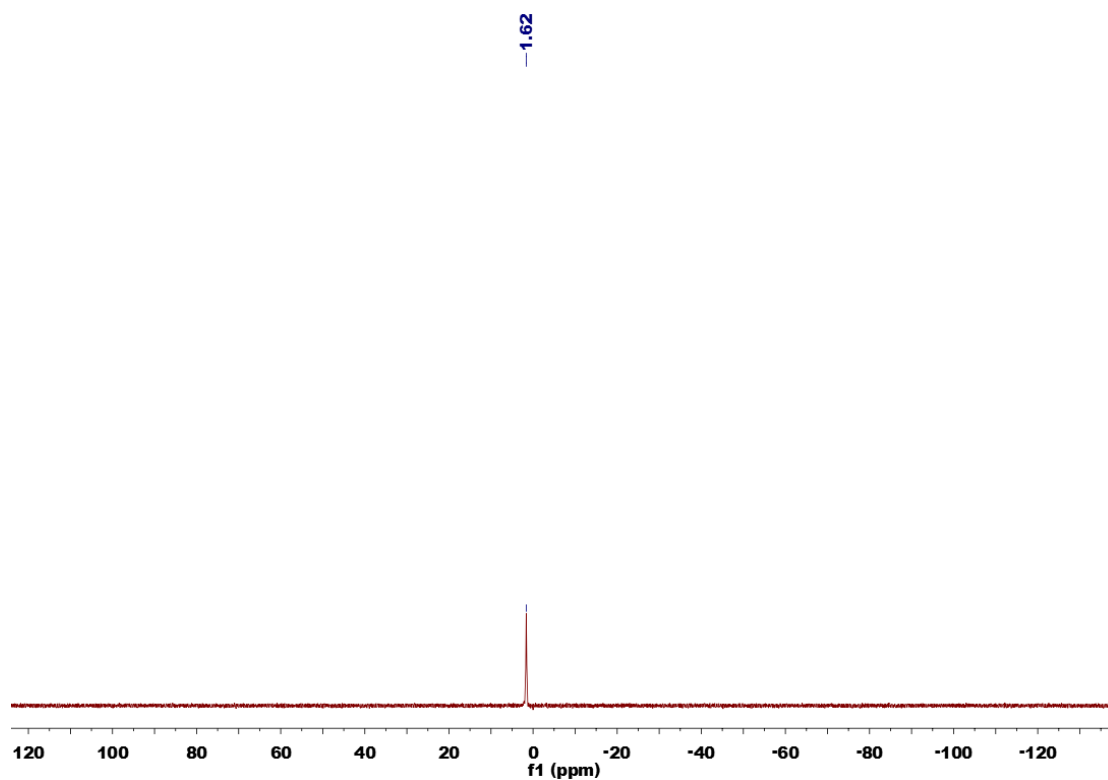


Figure S11. ³¹P {¹H} NMR spectrum of **2** in THF-*d*₈ at 25°C.

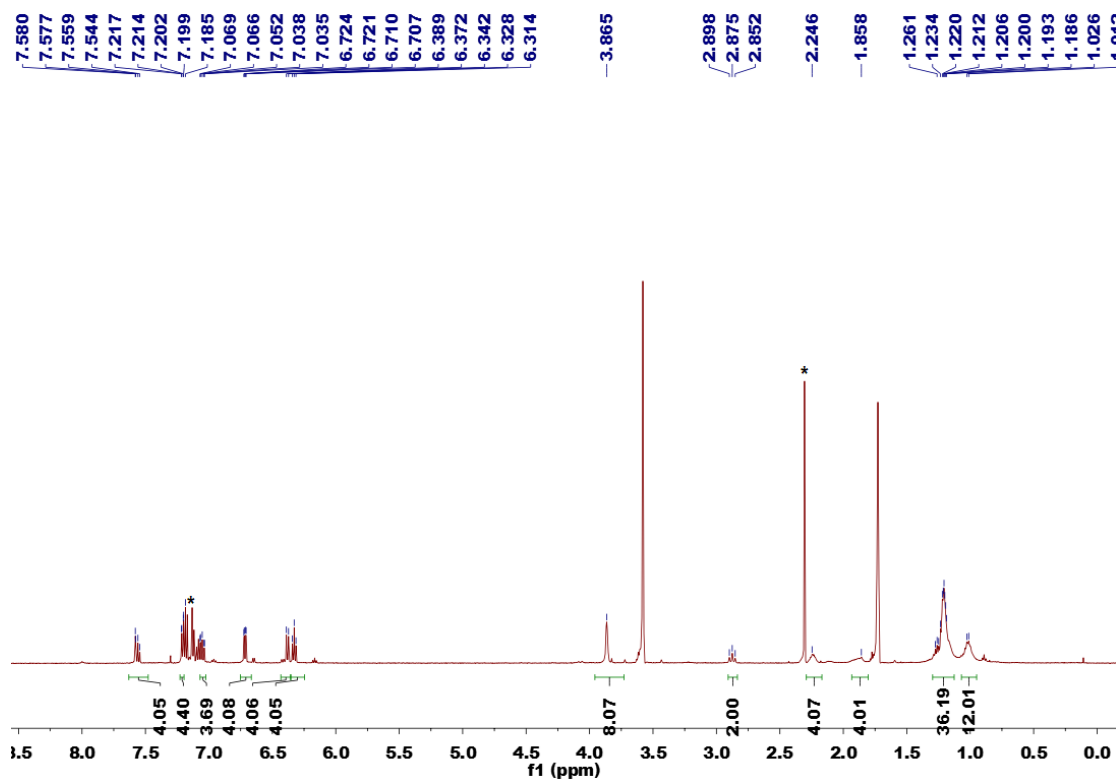


Figure S12. ¹H NMR spectrum of **3** in THF-*d*₈ at 25°C (* denotes co-crystallized toluene).

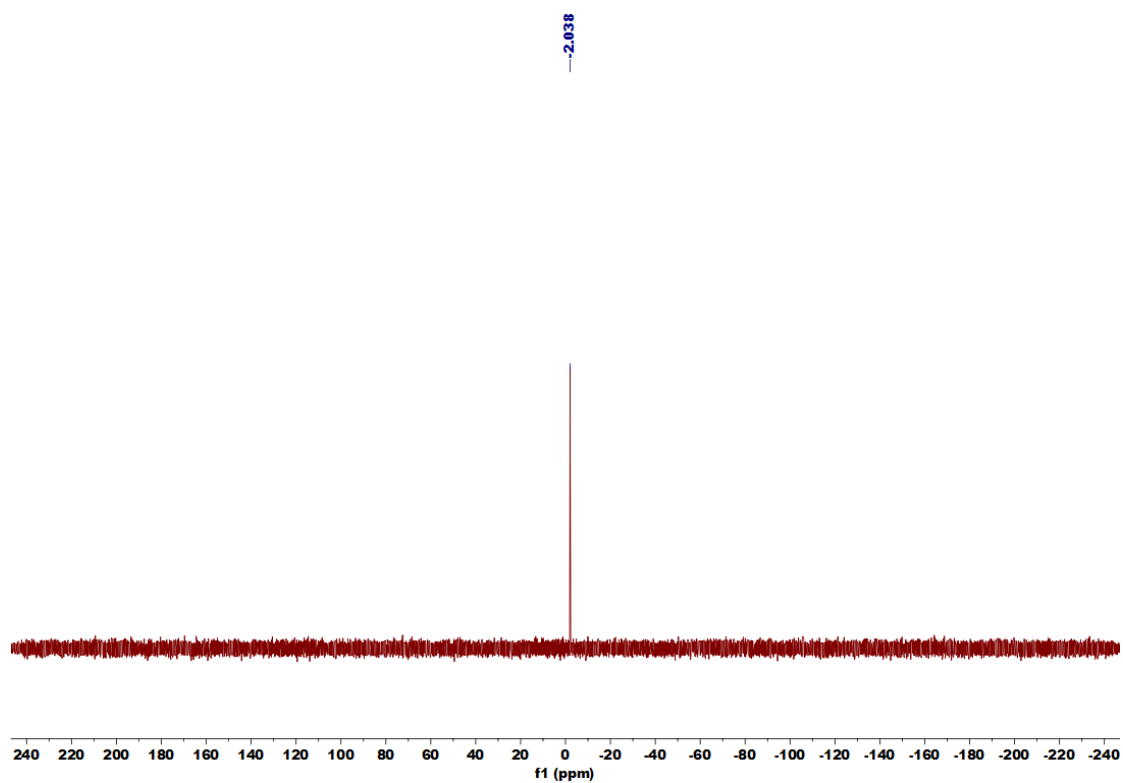


Figure S13. ^{31}P $\{^1\text{H}\}$ NMR spectrum of **3** in $\text{THF-}d_8$ at 25°C .

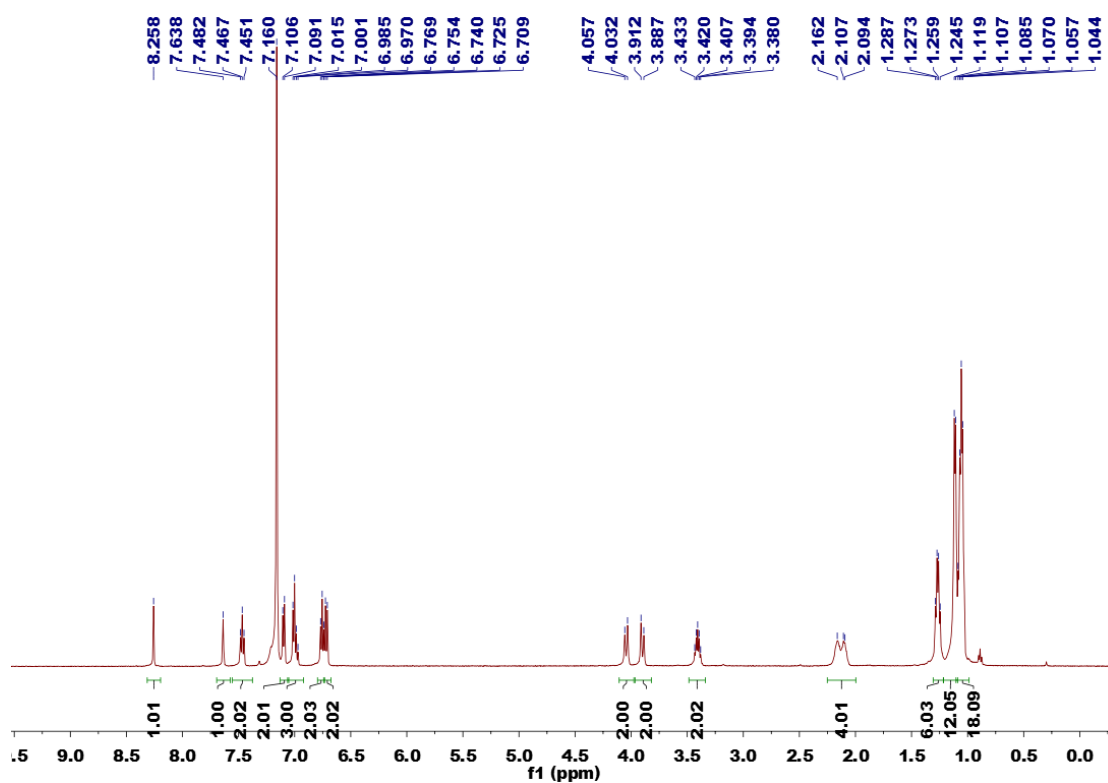


Figure S14. ^1H NMR spectrum of **4** in C_6D_6 at 25°C .

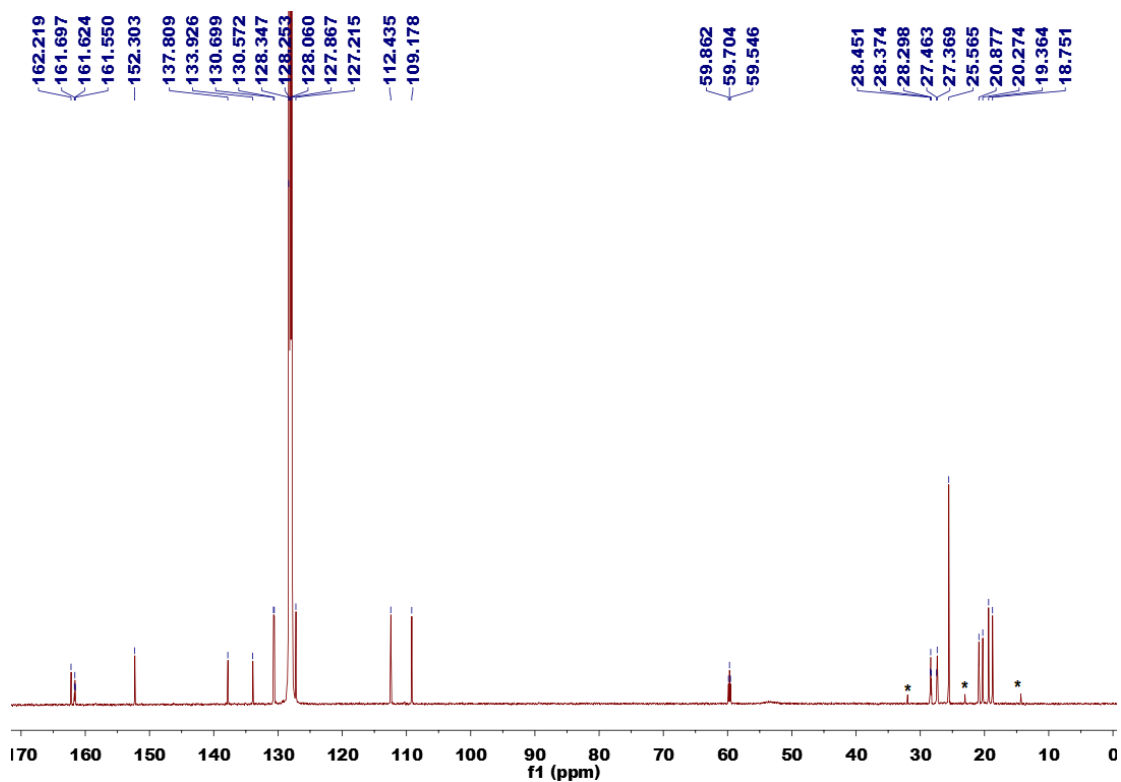


Figure S15. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** in C_6D_6 at 25°C (* denotes small amount of *n*-hexane).

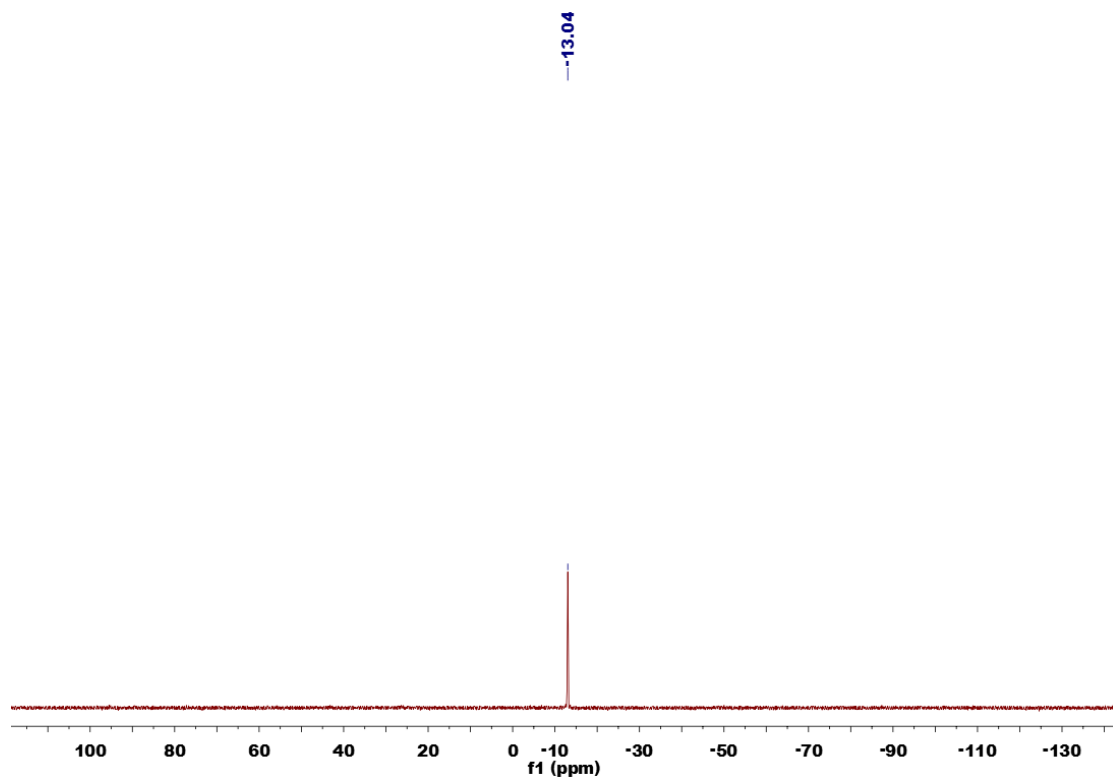


Figure S16. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **4** in C_6D_6 at 25°C .

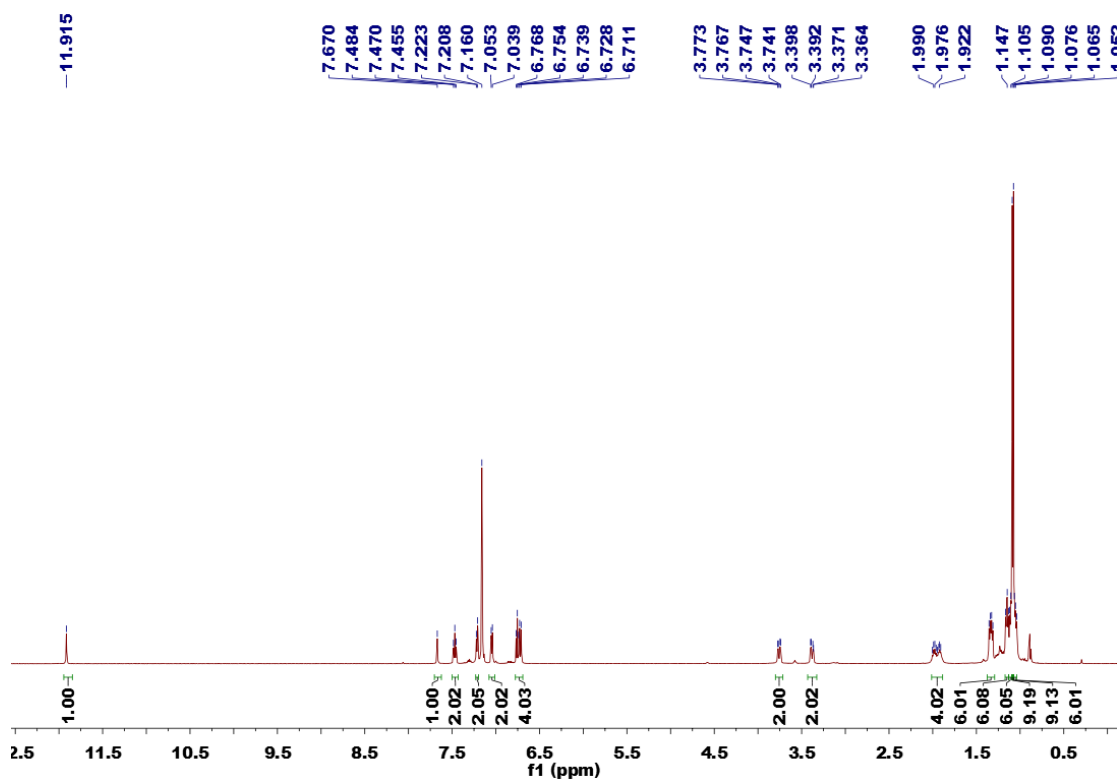


Figure S17. ¹H NMR spectrum of **5** in C₆D₆ at 25°C.

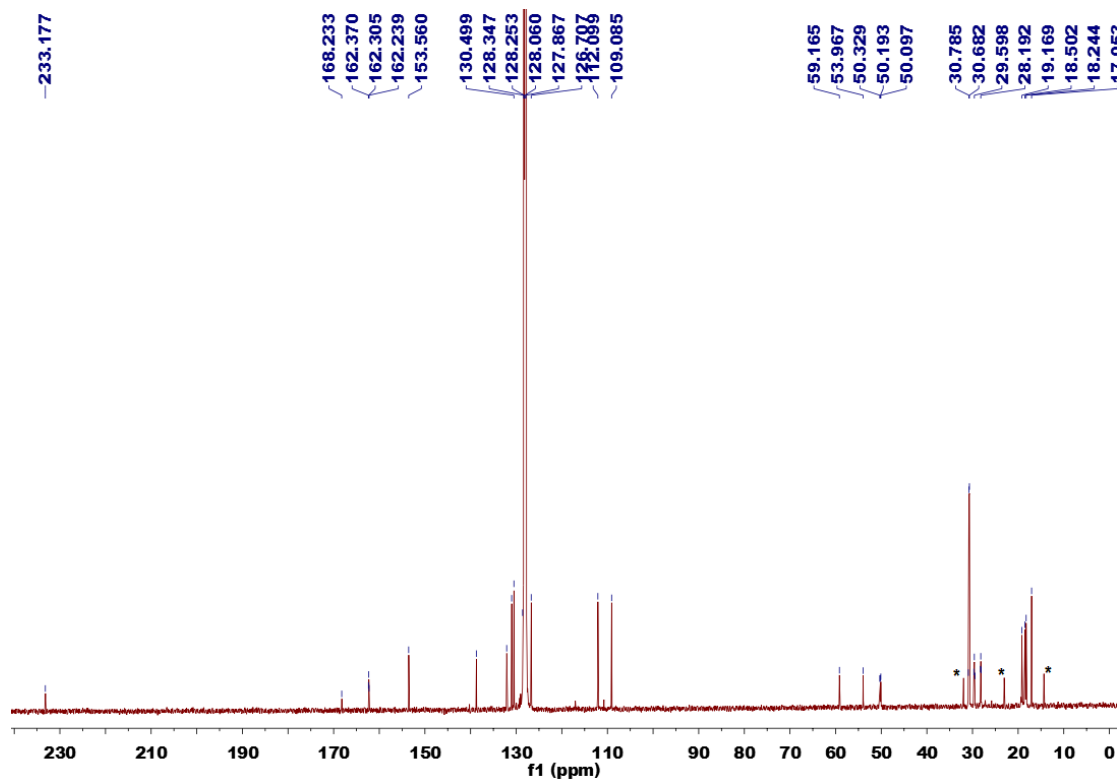


Figure S18. ¹³C{¹H} NMR spectrum of **5** in C₆D₆ at 25°C (* denotes small amount of *n*-hexane).

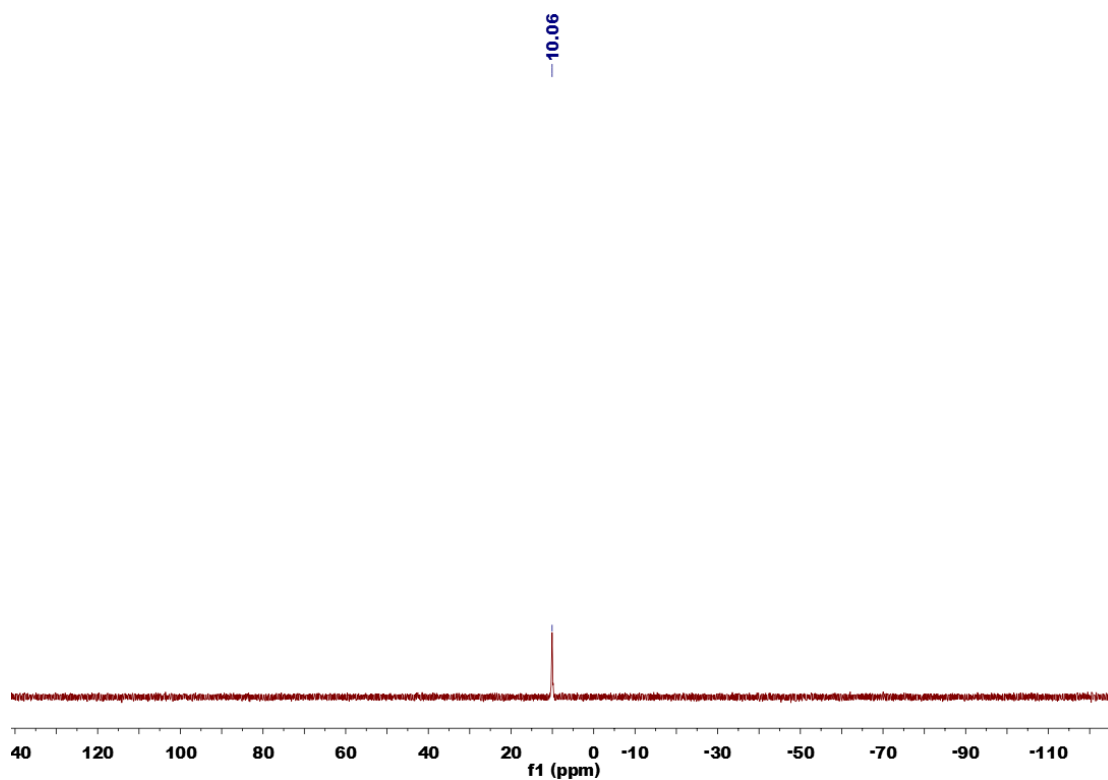


Figure S19. ³¹P {¹H} NMR spectrum of **5** in C₆D₆ at 25°C.

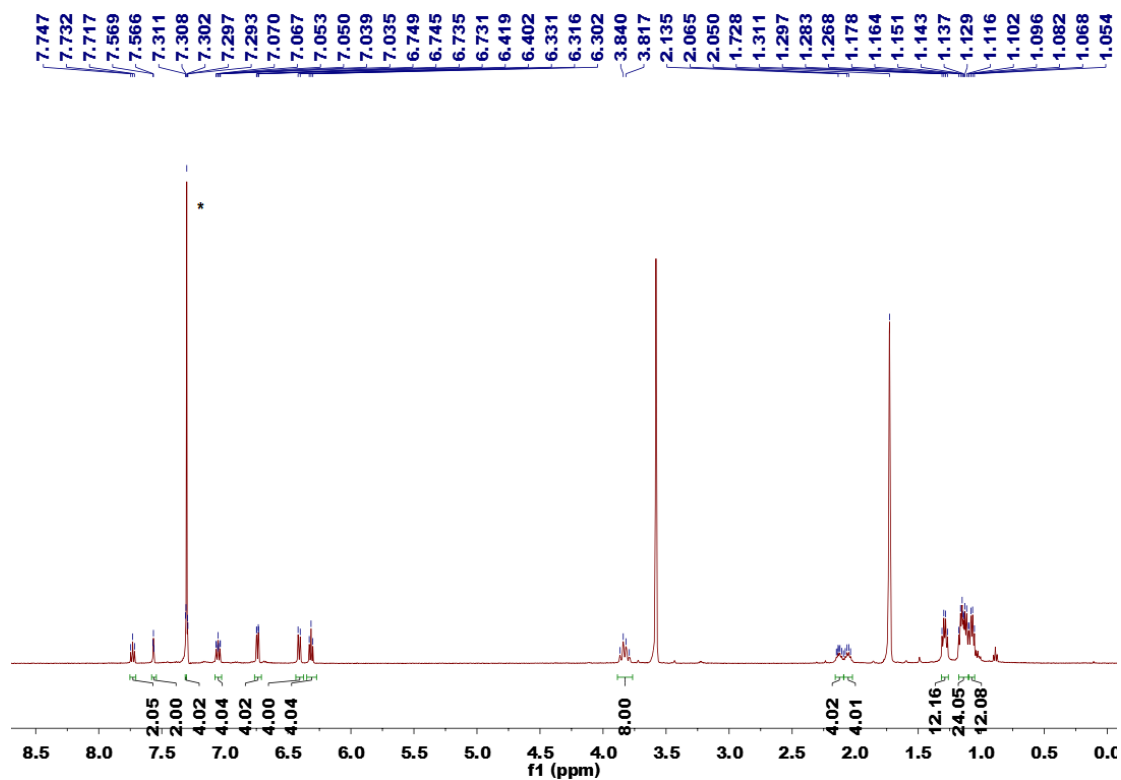


Figure S20. ¹H NMR spectrum of **6** in THF-*d*₈ at 25°C (* denotes co-crystallized benzene).

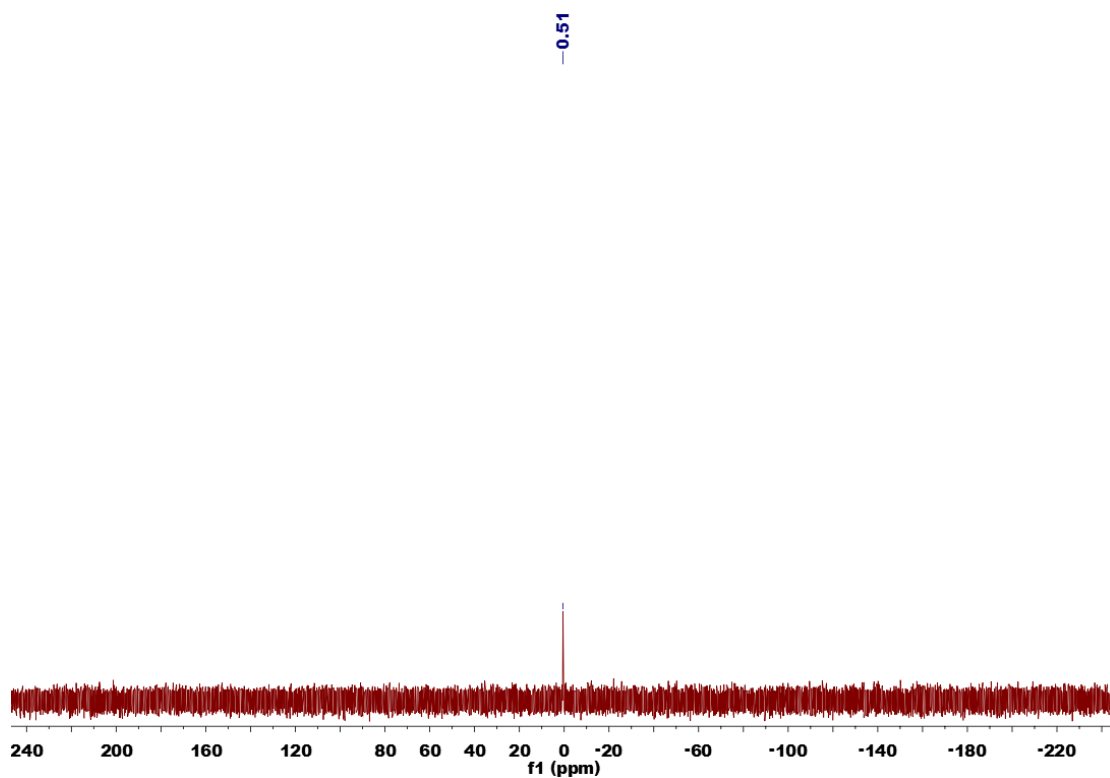


Figure S21. ³¹P {¹H} NMR spectrum of **6** in THF-*d*₈ at 25°C.

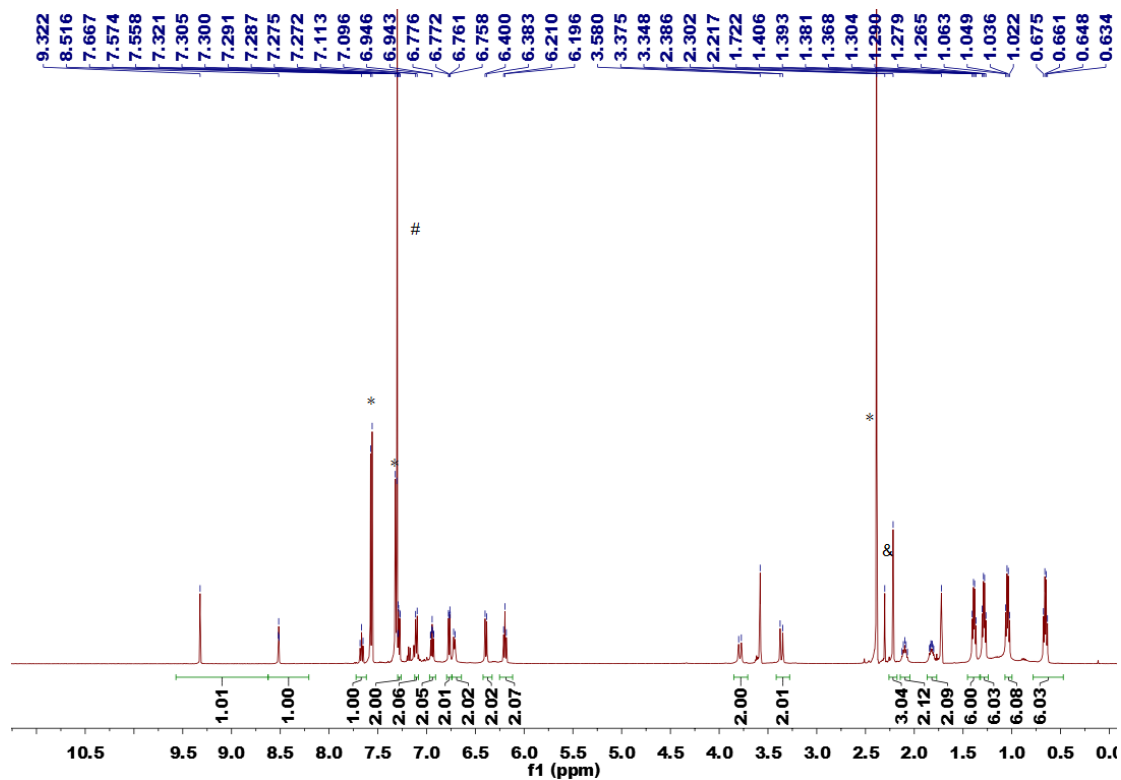


Figure S22. In-situ ¹H NMR spectrum of the intermediate **6'** in THF-*d*₈ at 25°C (* denotes excess amount of *p*-Tolunitrile, # denotes co-crystallized benzene from the starting material **3**, & denotes the toluene produced during the reaction).

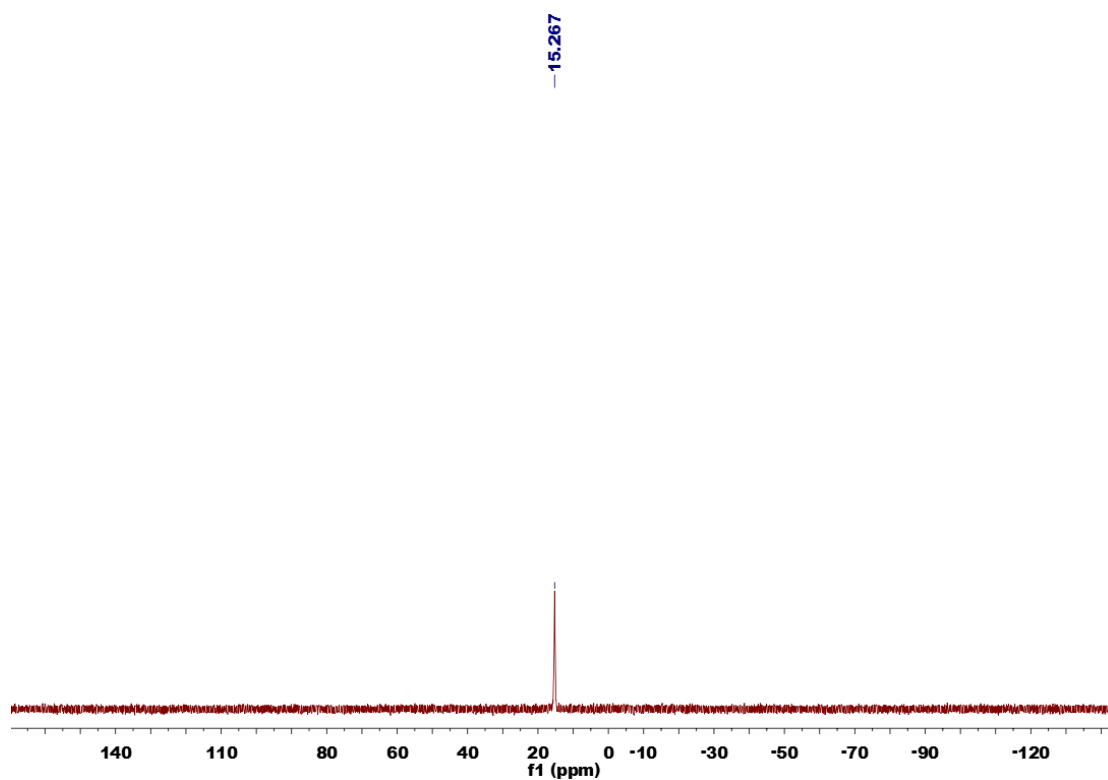


Figure S23. In-situ ^{31}P $\{^1\text{H}\}$ NMR spectrum of the intermediate **6'** in $\text{THF-}d_8$ at 25 °C.

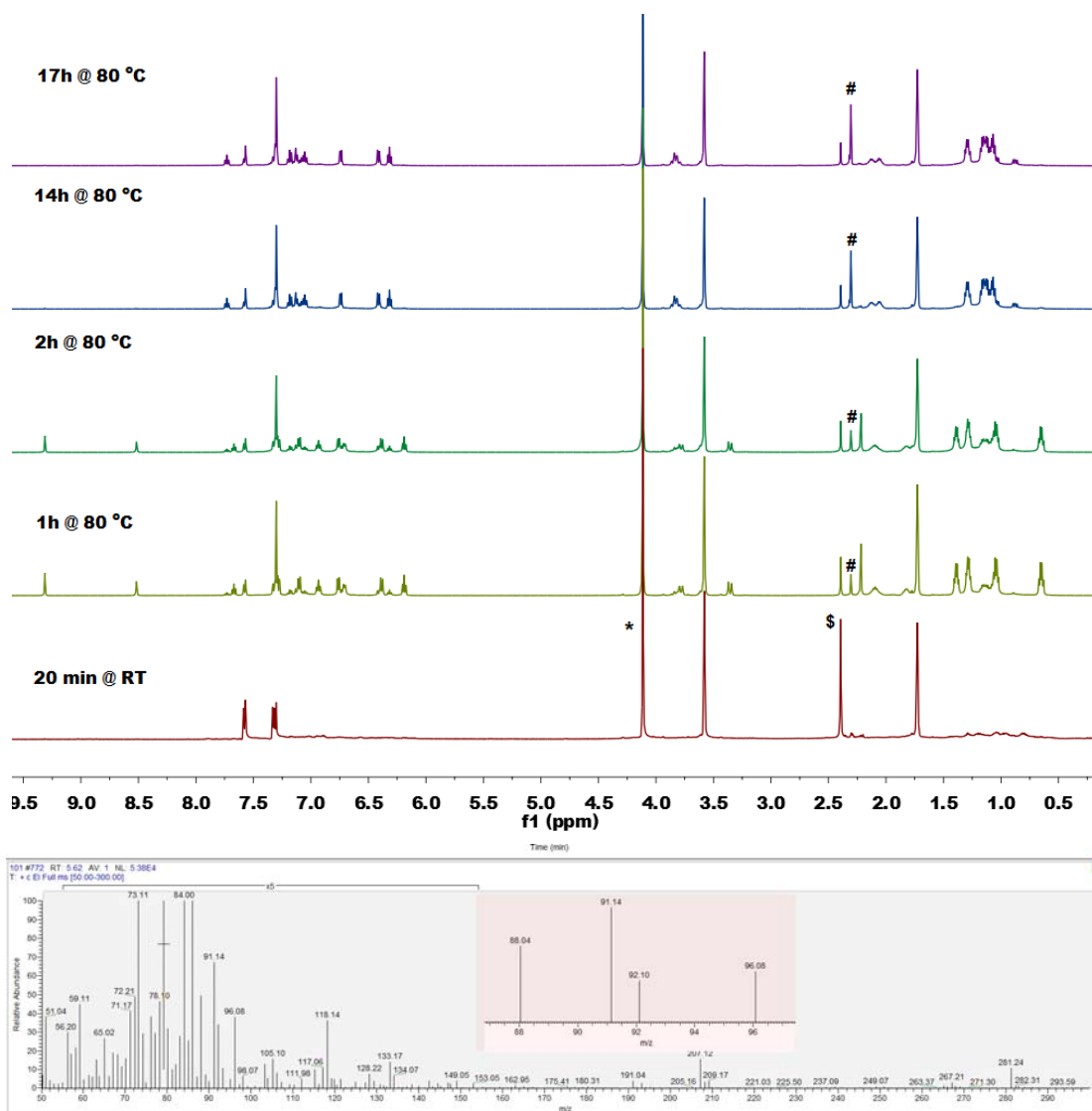


Figure S24. In-situ ^1H NMR reaction of complex **3** (10 mg, 0.006 mmol), p-tolunitrile (2.7 mg, 0.023 mmol) and ferrocene (internal standard, 2.9 mg, 0.015 mmol) in 0.5 mL of THF- d_8 . Note that to accelerate the process, the J-Young NMR tube was heat at 80°C. \$ denotes to methyl group of p-tolunitrile, * denotes to ferrocene and # denotes to the methyl group of toluene. After 17 h, the yield of toluene was ca. 80 %. This reaction solution was used for GC-MS measurement, which confirmed the formation of toluene.

IR spectra

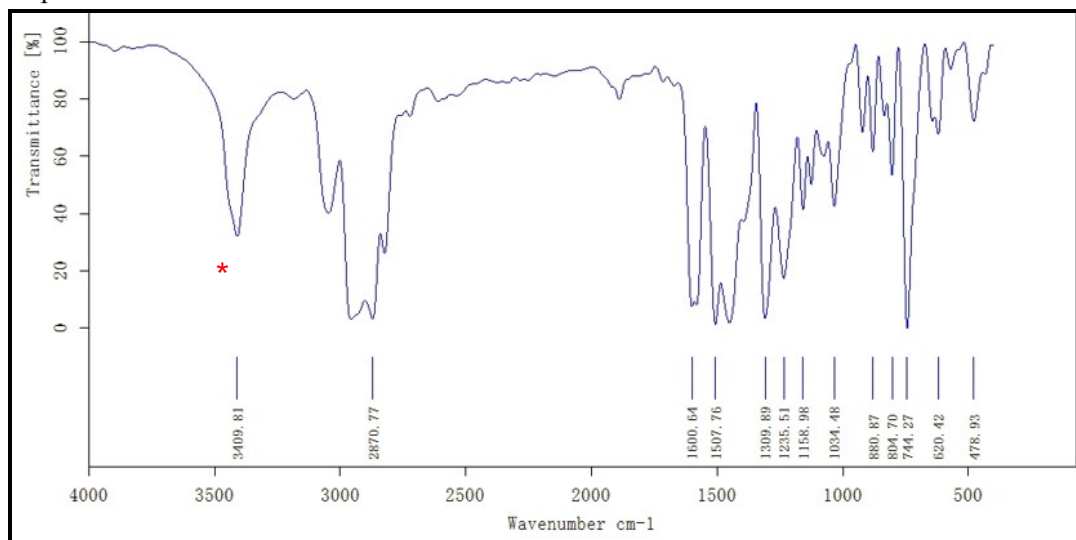


Figure S25. IR spectrum of *bis-P-N^m-Ph*. (* denotes the stretching vibrational peak of N-H bond)

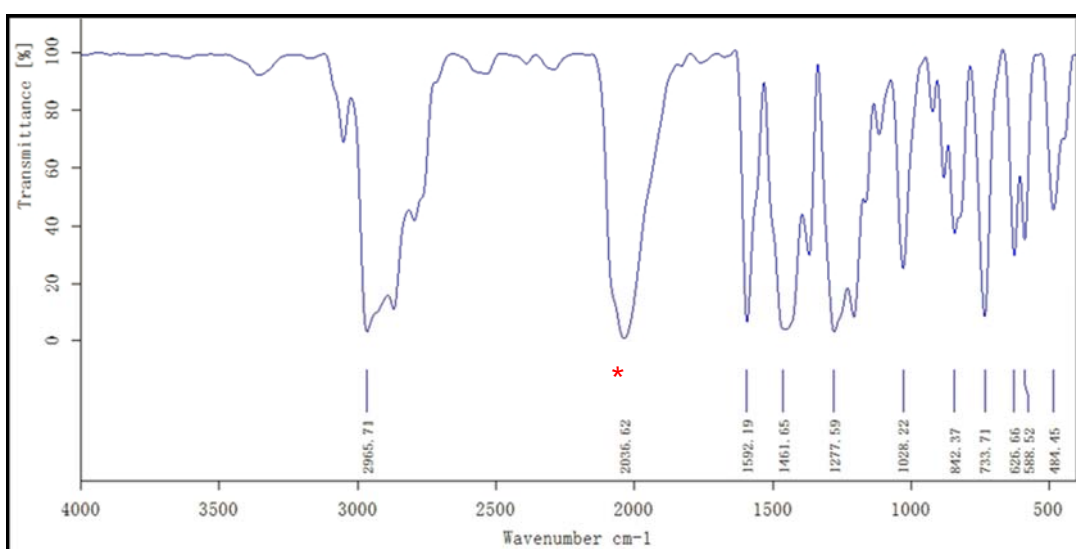


Figure S26. IR spectrum of **5**. (* denotes the stretching vibrational peak of C≡N bond)

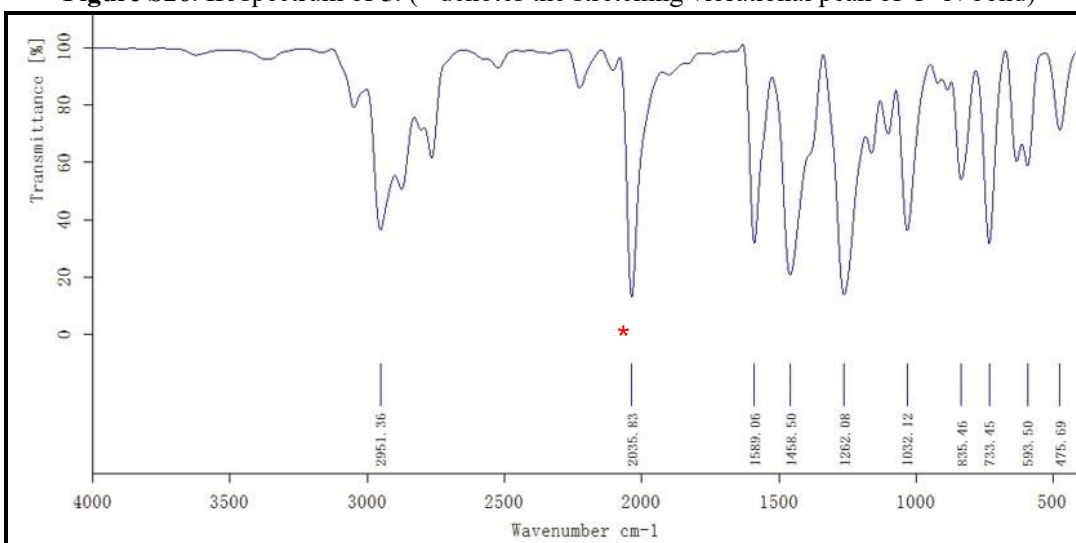


Figure S27. IR spectrum of **6**. (* denotes the stretching vibrational peak of C≡N bond)

3. X-ray Crystallography

X-ray Crystallography. Diffraction was performed on a Bruker SMART APEX II CCD area detector diffractometer using graphite-monochromated Mo K α radiation ($\lambda = 0.71073$ Å) at 300 K, with ϕ and ω scan technique. An empirical absorption correction was applied using the SADABS program.^[4] All structures were solved by direct methods, completed by subsequent difference Fourier syntheses, and refined anisotropically for all nonhydrogen atoms by full-matrix least-squares calculations based on F² using the SHELXTL program package^[5] and Olex 2 program.^[6] The hydrogen atom coordinates were calculated with SHELXTL by using an appropriate riding model with varied thermal parameters. The residual electron densities of solvent were squeezed by using PLATON.^[7] Crystal parameters and refinement results are given in Table S1-S2.

Table S1. Crystallographic and Refinement Data ^{a,b} for **1-3**.

	1	1'	2	3
formula	C ₆₄ H ₈₈ I ₂ La ₂ N ₄ P ₄ •2(C ₆ H ₆)	C ₃₆ H ₅₂ ILa ₂ N ₂ OP ₂	C ₆₄ H ₈₈ I ₂ La ₂ N ₄ Ni ₂ P ₄ •2(C ₆ H ₆)	C ₆₄ H ₉₀ La ₂ N ₄ Ni ₂ P ₄ •2(C ₇ H ₈)
Fw, g•mol ⁻¹	1725.09	856.54	1842.51	1618.78
cryst size, mm	0.09 × 0.1 × 0.13	0.13 × 0.15 × 0.18	0.1 × 0.12 × 0.13	0.11 × 0.12 × 0.13
cryst. syst.	triclinic	monoclinic	triclinic	monoclinic
space group	P -1	P 1 21/n 1	P -1	P 1 21/n 1
T, K	293.15	296.15	296.15	150.00
a, Å	10.2900(15)	11.0776(7)	11.364(14)	12.8479(5)
b, Å	11.7435(17)	17.6945(12)	13.293(15)	20.5016(7)
c, Å	16.775(2)	19.5440(11)	14.600(16)	14.9962(6)
α , °	77.377(2)	90	79.748(13)	90
β , °	84.430(2)	91.566(2)	71.941(15)	112.0530(10)
γ , °	84.471(2)	90	67.907(14)	90
V, Å ³	1962.9(5)	3829.4(4)	1938(4)	3661.0(2)
Z	1	4	1	2
D _{calcd} , Kg•m ⁻³	1.459	1.486	1.579	1.468
F(000)	864	1720	920	1664
μ , mm ⁻¹	1.983	2.034	2.479	1.782
θ range /°	1.248-24.846	2.527-30.559	1.471-28.088	2.044-27.523
refns collected	14147	175506	17472	123124
indep reflns (R_{int})	6756(0.0698)	11658 (0.0598)	8900(0.0376)	8413(0.0810)
reflns obsd [$I > 2\sigma(I)$]	3979	8536	6703	7352
data/restrnts/params	6756/569/578	11658/377/532	8900/536/597	8413/239/460
R1, wR2 ($I > 2\sigma(I)$)	0.0557, 0.0813	0.0385, 0.0749	0.0461, 0.1192	0.0239, 0.0582
R1, wR2 (all data)	0.1203, 0.0972	0.0619, 0.0840	0.0647, 0.1295	0.0301, 0.0613
GOF on F ²	1.006	1.103	0.969	1.042
$\Delta\rho_{max, min}$, e•Å ⁻³	0.848/-0.671	0.799/-0.670	1.929/-1.172	0.527/-0.775

$$^a R1 = \Sigma|F_o| - |F_c|/\Sigma|F_o|. \quad ^b wR2 = \{\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2\}^{1/2}.$$

Table S2. Crystallographic and Refinement Data ^{a,b} for **4-6**.

	4	5	6
formula	C ₃₉ H ₅₉ LaNaNiP ₂	C ₄₂ H ₆₃ LaNaNiP ₂ •C ₆ H ₆	C ₆₆ H ₈₈ La ₂ N ₆ Ni ₂ P ₄ •2(C ₄ H ₈ O)
Fw, g·mol ⁻¹	843.46	961.63	1628.75
cryst size, mm	0.25 × 0.3 × 0.4	0.25 × 0.25 × 0.3	0.25 × 0.255 × 0.3
cryst. syst.	triclinic	triclinic	triclinic
space group	P -1	P -1	P -1
T, K	298(2)	298(2)	298(2)
<i>a</i> , Å	10.7419(16)	10.1638(14)	11.5616(12)
<i>b</i> , Å	12.0017(17)	12.7284(17)	11.8002(12)
<i>c</i> , Å	17.493(3)	20.816(4)	16.2436(17)
<i>α</i> , °	98.310(2)	104.653(3)	75.419(2)
<i>β</i> , °	91.120(2)	104.046(3)	70.756(2)
<i>γ</i> , °	113.988(2)	96.320(2)	66.803(2)
<i>V</i> , Å ³	2031.2(5)	2484.9(6)	1904.1(3)
<i>Z</i>	2	2	1
<i>D</i> _{calcd} , Kg·m ⁻³	1.379	1.285	1.420
<i>F</i> (000)	872	1000	836
<i>μ</i> , mm ⁻¹	1.610	1.325	1.716
<i>θ</i> range /°	1.181-30.047	1.054-31.180	2.163-25.345
refns collected	13736	11978	6865
indep reflns (<i>R</i> _{int})	10288 (0.0216)	11978(0.0628)	6865(0.0634)
reflns obsd [<i>I</i> > 2σ(<i>I</i>)]	8357	9844	4669
data/restrnts/params	10288/0/436	11978/523/696	6865/162/460
<i>R</i> ₁ , <i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0406, 0.1020	0.0553, 0.1663	0.0583, 0.1484
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0537, 0.1072	0.0680, 0.1737	0.0886, 0.1630
GOF on <i>F</i> ²	1.072	1.075	1.114
Δρ _{max, min} , e·Å ⁻³	0.976/-0.812	1.002/-1.116	1.100/-1.203

^a $R1 = \Sigma |F_o| - |F_c| / \Sigma |F_o|$. ^b $wR2 = \{\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)\}^{1/2}$.

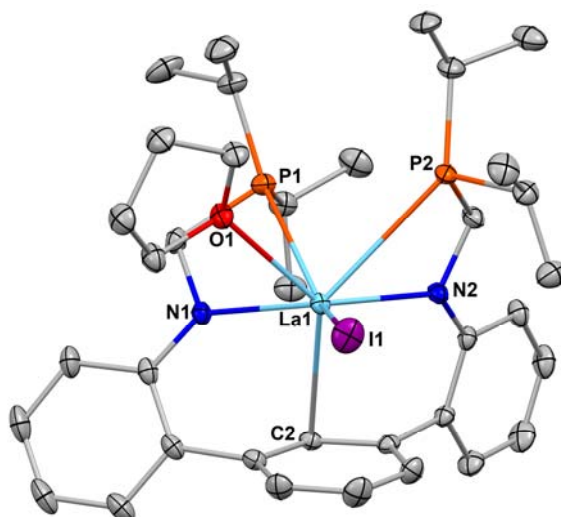


Figure S28. Molecular structure of **1'**. Disordered part and hydrogen atoms were omitted. Selected bond lengths (Å): La1-I1 3.236(3), La1-O1 2.618(2), La1-N1 2.459(2), La1-N2 2.450(3), La1-P1 3.2115(9), La1-P2 3.1712(9), La1-C2 2.938(3).

4. Computational Details

All density functional theory (DFT) calculations were performed using the ORCA program package, version 6.0.1.^[8] Geometry optimizations were conducted at BP/def2-SVP level of theory.^[9] ^[10] For the lanthanum and iodine atoms, the Def2 effective core potentials (ECPs) were employed, which replace 46 and 28 core electrons for La and I, respectively.^[11, 12] The resolution of the identity (RI) approximation was applied to accelerate the calculations, using the def2/J auxiliary basis set^[13]. ^[14] Empirical dispersion corrections were included using the atom-pairwise dispersion correction with Becke–Johnson damping (D3BJ).^[15–17] Natural Bond Orbital (NBO) and Natural Localized Molecular Orbital (NLMO) analyses were conducted using the NBO 7.0 program.^[18] The Quantum Theory of Atoms in Molecules (QTAIM)^[19, 20] analysis was performed using the Multiwfn program (version 3.7)^[21] based on single-point calculations. These single-point energy calculations were performed at the BP level with the ZORA-def2-SVP^[22] basis set for all atoms except lanthanum and iodine atoms, for which the SARC-ZORA-TZVP basis set was used to account for scalar relativistic effects.^[23, 24] The RI approximation with the SARC/J^[23, 24] auxiliary basis set and D3BJ dispersion correction were also applied in these single-point calculations.

Table S3. Experimental (Exp.; XRD) vs. calculated (Cal.; using BP functionals) selected bond lengths [Å] for complexes **2–4**, with associated deviations.

Bond lengths	2				3				4			
	Exp.	Cal.	Deviation		Exp.	Cal.	Deviation		Exp.	Cal.	Deviation	
La1-N1	2.455(4)	2.5048	0.05	avg. 0.02	2.5211(18)	2.5159	0.01	avg. 0.04	2.491(3)	2.5033	0.01	avg. 0.02
La1-N2	2.506(4)	2.5171	0.01		2.4775(18)	2.5134	0.04		2.539(3)	2.5498	0.01	
Ni1-P1	2.188(3)	2.1684	0.02		2.1703(6)	2.1542	0.02		2.1704(10)	2.1596	0.01	
Ni1-P2	2.166(2)	2.1547	0.01		2.1797(6)	2.1633	0.02		2.1812(10)	2.1727	0.01	
Ni1-I1/H1/N4	2.586(4)	2.6149	0.03		1.52(3)	1.6636	0.14		1.970(3)	2.0124	0.04	
La1-I1/H1/N3	3.672(5)	3.6385	0.03		2.57(3)	2.5946	0.02		2.484(3)	2.5279	0.04	
La1-Ni1	2.528(3)	2.5254	0.00		2.4778(3)	2.5191	0.04		2.5009(6)	2.5157	0.01	

Table S4. Bonding descriptors for La-Ni interactions in complexes **2–4**.

Complexes	Bond	MBO ^a	WBI ^b	LBO ^c	MOC ^d	MAC ^e	
						La	Ni
2	La-Ni	1.0786/ 1.0495	0.3260/ 0.3153	1.2711/ 1.2285	-0.9690/ -1.2226	0.5276/ 0.5331	-0.1684/ -0.1551
3		0.9200/ 0.9195	0.2892/ 0.2890	1.2051/ 1.2038	-3.1168/ -3.1139	0.4396/ 0.4455	-0.2250/ -0.2268
4		1.0557	0.6134	1.2300	-0.3723	0.6688	-0.0577
5		1.0557	0.6134	1.2300	-0.3723	0.6688	-0.0577
6		1.0557	0.6134	1.2300	-0.3723	0.6688	-0.0577

a: Mayer Bond Orders, b: Wiberg Bond Index, c: Löwdin Bond Orders, d: Mulliken Overlap Charges, e: Mulliken Atomic Charge

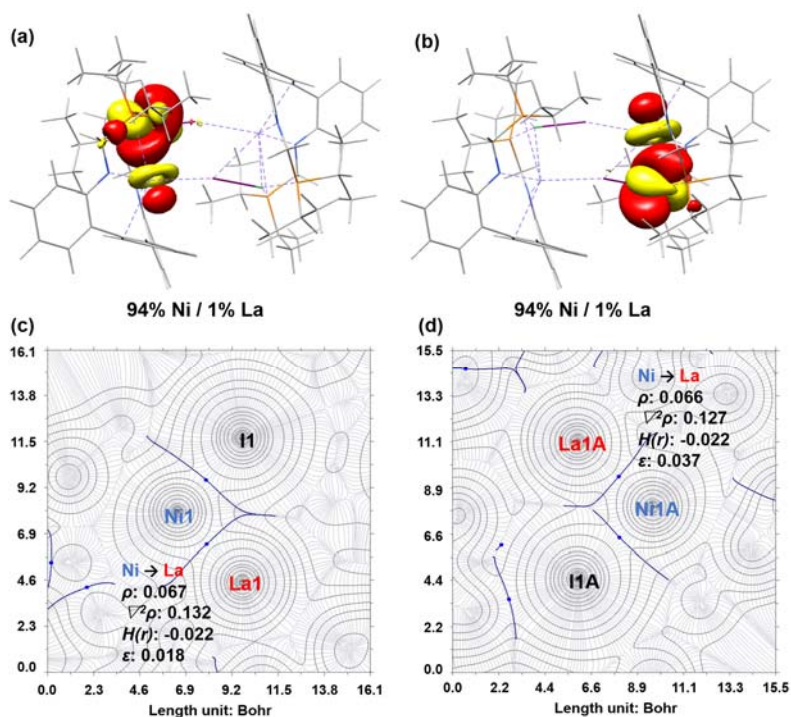


Figure S29. (a, b) NLMOs (isovalue = 0.015) and (c, d) the corresponding electron density contour plots for the dative Ni→La bond in **2**.

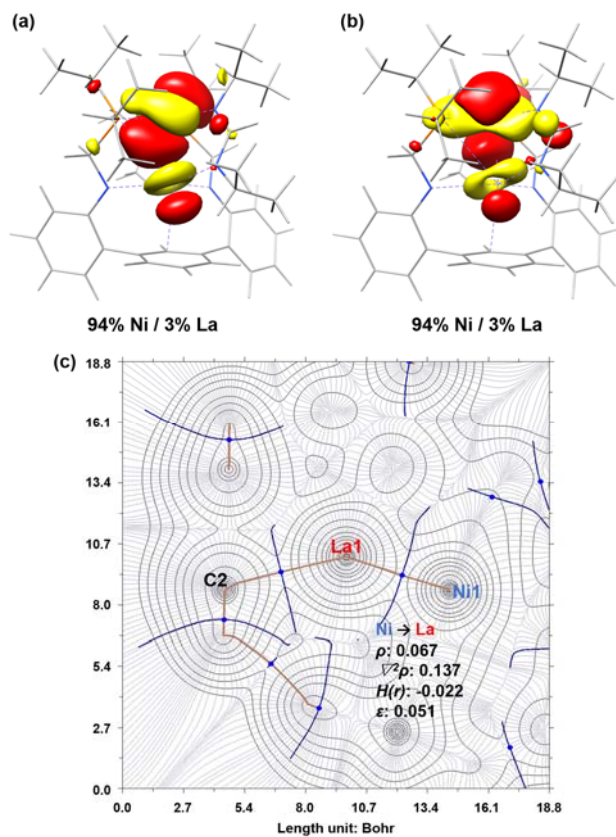


Figure S30. (a, b) NLMOs (isovalue = 0.015) and (c, d) the corresponding electron density contour plots for the dative Ni→La bond in **4**.

Table S5. Calculated QTAIM data (a.u.) for **2-4**.

Complexes	Bond	ρ^a	$\nabla^2\rho^b$	$H(r)^c$	ε^d
2	Ni→La	0.067/0.066	0.132/0.127	-0.022/-0.022	0.018/0.037
3		0.066/0.065	0.137/0.137	-0.021/-0.021	0.041/0.041
4		0.067	0.137	-0.022	0.051

a: Electron density, b: Laplacian of electron density, c: Energy density, d: Bond ellipticity.

DFT Optimized Cartesian Coordinates of All Structures

Coordinates of 2

La	11.32061598150332	8.28633007360238	8.54348984723250
Ni	9.10902995770466	7.71877515868687	9.60977057122549
P	10.05669386013162	7.27797291287216	11.50290475070440
C	7.62220064991578	6.09785278244000	12.39379794595267
H	7.29004591119002	6.17158125000123	11.33983972351014
H	7.26970745959265	7.00160149127447	12.93106261161807
H	7.11774103590459	5.22105858090221	12.85140991367697
H	10.74609974158566	5.63455041565700	13.96195173942673
P	8.24848931246610	9.50642282626727	8.75425220342045
C	7.33984618788231	10.99201740656953	6.44665285305206
H	7.97617988528892	11.85388138361317	6.73031332454791
H	6.32393158461598	11.16139130080657	6.86219492058796
H	7.24033983451993	10.99877295026920	5.34110402778623
H	7.06373200737065	11.18703905925079	11.16789214386956
N	12.54835401086334	7.00714472987171	10.31286319427479
N	10.72180002227396	10.69589980099013	8.86372198564405
C	14.37798249720593	8.13290035977204	8.41115766575875
C	13.97942433340971	9.37155428695464	8.98619960593938
H	14.02958115120808	9.49523840207136	10.07795619575032
C	13.48016779499383	10.42729039230239	8.19248755881517
C	13.42774499884694	10.25803485660822	6.78346646631933
H	13.01893798245089	11.07058524947407	6.16523545798900
C	13.87927513465043	9.06559235812741	6.19677793056754
H	13.82949485731326	8.93760631428973	5.10554205036385
C	14.33307953712232	8.00249682042752	7.00246589188684
H	14.61777054264825	7.04343510554334	6.54435111643853
C	14.77067661226085	6.99688357775262	9.27732339740237
C	16.02239929425738	6.38555649435793	9.10120460768280
H	16.69525363123485	6.78895172361082	8.32719113769967
C	16.43813259808023	5.31109912961128	9.90607131205076
H	17.42821250961292	4.85405031130393	9.76432886182661
C	15.56737799573778	4.85858515964513	10.90985610570395
H	15.87138529112443	4.02788820529087	11.56699774128628
C	14.30237395316138	5.43547999060661	11.08913874877534
H	13.64659664340985	5.02318968477871	11.86654745454213
C	13.83438661153333	6.50295741654394	10.25965231270995
C	11.73934656786544	6.46740053293529	11.38821314514023
H	12.23438884409504	6.56615299950285	12.38821567731818
H	11.53089846778081	5.37374298261438	11.25605649750216
C	12.96857307595348	11.67549828569351	8.82234760060855
C	13.84722005760347	12.73222442117524	9.09972661005615
H	14.91256726948225	12.60844705479066	8.84724286232453

C	13.39181643899719	13.92868613102243	9.68215172787380
H	14.09189481802275	14.74978032919052	9.89482877011648
C	12.02632564643487	14.04494379303716	9.98058166169423
H	11.64046188974250	14.97045321775081	10.43751419819896
C	11.13209147949437	12.99872069144456	9.71091833041971
H	10.07468476940021	13.13672925765300	9.96992759036091
C	11.56569115498398	11.77055401675652	9.12393648649408
C	9.32231983625577	10.97986064580671	9.14350054323240
H	8.95317867471801	11.87763700142943	8.58985081318416
H	9.14565724072223	11.19723801136796	10.22712925872121
La	8.97286388918437	4.59777777749831	5.38110269180842
Ni	11.25730029462625	5.23033293527221	4.49428108678103
P	10.55473990535178	5.48290047181266	2.45225631822331
C	11.69338030638584	6.54867659434105	1.38064427956170
H	12.42237890833327	5.80384036276621	0.99132663246965
C	12.46705570385985	7.56959500399267	2.22242767366975
H	12.98611262932239	7.08532144032265	3.07401192910493
H	13.22480278768022	8.09139673974775	1.60067155889272
H	11.79206295618603	8.33635919061552	2.65342670906116
C	10.98760657111542	7.21289284171666	0.19174169320235
H	10.27323551558510	7.98982940979694	0.53186898283420
H	11.73079262492742	7.71383000329375	-0.46393294032003
H	10.43043013225889	6.48784422036109	-0.43442275831085
C	10.15809188560735	4.08291477034128	1.25327318898818
H	9.94477711889657	4.58897683664740	0.28497203403680
C	11.35326764956026	3.14485707272248	1.06587876485233
H	11.59703780408995	2.63229306943471	2.01835472038936
H	11.11304688850206	2.36088645106344	0.31836346271784
H	12.26373653242893	3.67219527114499	0.71616570373207
C	8.90787387003870	3.31214764544555	1.68850142599657
H	8.01803606256840	3.96704090605651	1.74087860885743
H	8.69643522099613	2.48776050511740	0.97708387148835
H	9.05878871881800	2.85389222235349	2.68736078912463
P	12.09307290541716	3.47399831410275	5.40781754384939
C	12.40280103151614	3.11347840590012	7.23960045316885
H	13.29533336605050	2.44830791969884	7.24915482207413
C	11.25882376200630	2.36881593254985	7.93623946667180
H	11.05029873395698	1.38359196041044	7.47740309609875
H	11.51835679682495	2.20299722633457	9.00284727013815
H	10.31694081763011	2.95174428188441	7.93235670031705
C	12.76059727471298	4.42241430681265	7.94759211419246
H	11.87274747200573	5.08502076078936	8.00522624598043
H	13.10801896024566	4.23780193579406	8.98320655392810
H	13.56836128700584	4.97978452495667	7.43154900741055

C	13.85561500137046	3.22298770718864	4.77113376028516
H	14.45480304173095	3.70734601760844	5.57473392565177
C	14.26772386893335	1.75015477527221	4.67051055078682
H	13.71119602621759	1.22971626328455	3.86458582396902
H	15.34892095350059	1.66723626202153	4.43130837134149
H	14.09450757616743	1.19711609391730	5.61563860653283
C	14.10212681157417	3.98988953178264	3.46814854811519
H	13.78044393916604	5.04779088045363	3.56048924272475
H	15.17937949806663	3.97411972055443	3.19845430123062
H	13.53586476464361	3.54724417948128	2.62722113434972
N	8.03768040701739	5.91105630668672	3.46433642396273
N	9.69156205443660	2.22413733778606	4.94156598311464
C	5.96306646452476	4.71267746329197	5.07004472242193
C	6.45057023135224	3.52408536894643	4.45409599581593
H	6.56573930582702	3.49556309694413	3.36216110659810
C	6.85134569457368	2.40771392718073	5.21955219268390
C	6.68682346055965	2.45026388372399	6.63062060658625
H	7.01474786775417	1.58794394124514	7.22955950834006
C	6.12116196320893	3.57858922309916	7.24217357188121
H	5.99422152622753	3.60614263650127	8.33431537344070
C	5.78349952807623	4.71107567709308	6.47406195493212
H	5.42836333145703	5.62750751551022	6.96765039290383
C	5.71996728896084	5.94208191200432	4.27677471353151
C	4.48500308649401	6.60392596446086	4.38447313793675
H	3.71036199473146	6.15888186504965	5.02954902541529
C	4.21096458450169	7.78112254805776	3.66888708705741
H	3.23184110018507	8.27428176263180	3.75414367966625
C	5.21082310543719	8.29458538915387	2.82714256989618
H	5.02229280510310	9.21131929452567	2.24548441644941
C	6.45934749756739	7.66758180332462	2.71776340594383
H	7.22068971356691	8.12462694020371	2.07253536507396
C	6.78092122614067	6.48702692813764	3.45870218238297
C	8.94966516797129	6.43894548196781	2.46599812153836
H	8.51058894185982	6.42397630342255	1.43730298966481
H	9.24175963558605	7.50350976026926	2.66404108484062
C	7.48301699711066	1.21902080377825	4.58173692287704
C	6.67998796555814	0.17985619029253	4.09135517820676
H	5.58592193338103	0.27938204677453	4.17576787174661
C	7.24349997462020	-0.97004367934936	3.50963207422663
H	6.60082102809794	-1.77678893910340	3.12815731238958
C	8.64116076501818	-1.06072880488883	3.43735935190101
H	9.11188177060538	-1.95224462885372	2.99248203458063
C	9.46186322570558	-0.03139766345549	3.92064997599719
H	10.54949936309626	-0.14889441924239	3.83433051250828

C	8.91900877066924	1.15505043109911	4.50338941117251
C	11.12284258941032	1.99003680774330	4.82697140664518
H	11.46037940211878	1.08273082874685	5.38645534023340
H	11.43973989192672	1.82232761256353	3.76551304472942
I	10.69544384362515	7.61515374067274	5.45837137500760
I	8.91310221975440	5.34418691114450	8.57731556896485
C	9.14427939872159	5.94005817416089	12.47317745695629
H	9.41397392531574	5.03806538378595	11.87877999777997
C	9.64562619396226	5.75653618012745	13.90938508287773
H	9.18887340722471	4.85175512544958	14.36363761034713
H	9.36779146431704	6.61869376665664	14.55036342588359
C	10.36550854472022	8.69330435244762	12.69952758710761
H	10.70504464662582	8.24399218835296	13.65777495372354
C	9.06513783720860	9.47201094141675	12.92102312285632
H	8.66500541422531	9.80861631885761	11.94177820740808
H	9.24177936712869	10.36929057735736	13.54992849485249
H	8.28207916301264	8.86062605120833	13.41233415593644
C	11.47683310205545	9.59879554854391	12.14959103911048
H	12.43648275483018	9.05792504927850	12.03789392685657
H	11.64162969908288	10.46230006498627	12.82632943741760
H	11.20239213238870	10.00985345931865	11.15342829504629
C	7.93180358656443	9.65572948655646	6.90428956351172
H	8.94930023091165	9.56296114289691	6.46406524688953
C	7.10389643569557	8.45357586504321	6.43549941628518
H	6.06193464847489	8.50003225601553	6.81665234682074
H	7.54961965151393	7.50122870874378	6.78823841167257
H	7.04148538581406	8.42225481190650	5.32964220288677
C	6.53513071263232	9.89402684563942	9.46993072665228
H	5.89010465284980	9.98183280109609	8.56962052126309
C	6.44678707857858	11.21190985386404	10.24671699330706
H	5.39707525053221	11.39372118849929	10.56069667810348
H	6.77019739416993	12.08155129727749	9.64211441673285
C	6.04694180737804	8.70020375612883	10.29936715166892
H	6.67315233539315	8.57218033325401	11.20390861489212
H	6.10243372375129	7.75581410280445	9.72030673715448
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Coordinates of **3**

La	2.40383194426072	9.33563974331525	5.59700661215554
Ni	4.25683576769842	10.73875867060852	4.62678040343948
P	2.92178432001689	12.33874503525395	4.08016366884914
P	4.91593405343163	9.12807463648851	3.34162691097917
N	3.62230299303315	7.24765507493059	4.91008406998630
N	0.85214737533918	10.45949696913723	3.96633447556962

C	2.34030512474432	5.69753576084309	6.30334197460223
C	3.50703347718967	6.01113590443795	5.50819255480620
C	4.78519002450059	7.40313400167346	4.05896537660459
H	4.80867470198740	6.66134062716254	3.22010355190704
H	5.73682996521215	7.24377902498841	4.62120320064448
C	0.59325276415850	7.10923167139912	5.14891369784731
H	0.89006582141157	6.65813944741763	4.19116599405155
C	1.22505423751038	6.67130896342186	6.34698579528591
C	4.13643804067552	8.90833161002251	1.63884673861171
H	4.11616098798021	9.93980419526295	1.22894561372224
C	-0.87585452033861	10.45887185332361	2.17596091891988
H	-0.47840239918038	11.37895632825108	1.72895516107048
C	1.33015406845770	11.67875593542864	3.33955260511831
H	0.57192783497590	12.50232766289570	3.36373616741616
H	1.56115571418637	11.52170116811310	2.25572641106972
C	2.28623010391272	4.52743101447905	7.07772609006105
H	1.38411253580579	4.34406204105273	7.68336165710960
C	-0.34163246240765	8.16664271793866	5.15363364962239
C	-0.88060783568726	8.72886218261072	3.88589776878342
C	-0.27149921324568	9.92180497505648	3.35526073928754
C	6.76710667972133	9.25889951291616	3.02225019372311
H	7.06686027523730	8.40509431902022	2.37630665513692
C	-1.96991440404769	9.83684846816102	1.55723528819444
H	-2.39337327244406	10.28972116445243	0.64611389568474
C	4.52057564255766	5.00088517194861	5.46038449746080
H	5.41126359330232	5.15438851362960	4.83790500902265
C	3.50849247816962	13.47962919588667	2.69875503666268
H	2.64591545959094	14.13783613559619	2.45653848229866
C	1.42021808465170	12.78923814441795	6.38413349336427
H	0.51486420245550	12.35431623605852	5.91207445025785
H	1.09263100660362	13.47489100510983	7.19193764181748
H	1.98168002750541	11.97112984747435	6.88641736582189
C	-2.52625532410310	8.65775555100762	2.07479376886392
H	-3.38203535185982	8.17037504737180	1.58542642358350
C	0.82477597823482	7.25721413803261	7.57092750256715
H	1.31802557169702	6.94231017276011	8.49928927529759
C	3.32745390945878	3.58307858637832	7.05815280255473
H	3.26317391577734	2.66398502272252	7.65804042428550
C	-0.15778456280170	8.26777260077812	7.59543887941942
H	-0.46021328178887	8.70699476245062	8.55606160571243
C	-1.96953381603998	8.11866693427856	3.24867985983973
H	-2.39451788023770	7.20536376110659	3.69545429963602
C	7.52695367539522	9.18454953695564	4.35484147452221
H	8.59199337135668	9.46600366890434	4.21645197787542

H	7.50535248953808	8.17275290305113	4.80260376042677
H	7.06344488097924	9.87535526807046	5.08699293366272
C	2.28202585531939	13.55601283852354	5.37551827066807
H	3.19445370212400	13.90576947711583	5.90402257808102
C	-0.70977644449409	8.74835959501189	6.39874938679220
H	-1.43102195515737	9.57898289199646	6.40287845923045
C	4.67818780965743	14.34033369238674	3.19176762393351
H	4.44326124057353	14.90325175132865	4.11715763348437
H	4.97670981706987	15.07539765472001	2.41551264988149
H	5.56176401399077	13.69910354115183	3.39503899985415
C	2.68436090456191	8.44232417195630	1.82184886726385
H	2.63991923916205	7.40498095516354	2.21210038600998
H	2.14220429723027	8.46310286391103	0.85454520567301
H	2.12446694211324	9.09304505147708	2.52624062464095
C	1.53410184636559	14.77632928551580	4.82963603385369
H	2.17451147986798	15.42335302686859	4.19965202791556
H	1.18731324912714	15.40162539831719	5.67784618838282
H	0.64037335030464	14.48479677187292	4.23786227903333
C	3.90532253326840	12.69012110592564	1.44786296854770
H	4.72721755862372	11.98860641946321	1.68788818274448
H	4.25727511921988	13.37755674963444	0.65031300818444
H	3.06581696429408	12.09786225421436	1.03412819062371
C	4.43030991490901	3.82887825088805	6.22360231460660
H	5.24808515457843	3.09239817296915	6.16662083913905
C	7.05738452155339	10.57739866804363	2.29270964347583
H	6.72505144204636	11.43840029458617	2.91112221867304
H	6.53254827058287	10.64743700622576	1.31927793412764
H	8.14439493773212	10.69220153759311	2.09896003475062
C	4.91572260912293	8.00303841676635	0.67922377242108
H	5.92812192073715	8.39252224229486	0.45218617863763
H	4.37290381263438	7.91141263477989	-0.28520816365519
H	5.02755950852124	6.97633484014590	1.08650040994913
H	4.73331796972131	10.33071222907187	6.16726041973389
La	4.88043073629265	11.20185689537251	8.30367826648881
Ni	3.02650204394458	9.79775670938629	9.27288942255622
P	4.36037396558220	8.19736794786323	9.82050715240694
P	2.36651406079937	11.40709230179439	10.55902801034692
N	3.66124850613925	13.28909795407091	8.99327757283157
N	6.42966710756418	10.07730024169477	9.93611912994246
C	4.94426876188685	14.84256529218270	7.60431579488598
C	3.77658456824330	14.52657971449059	8.39715744745121
C	2.49686052793376	13.13214645242348	9.84225736024374
H	2.47074074085902	13.87387321047786	10.68107138033655
H	1.54645985592775	13.29042623110956	9.27770812951815

C	6.68983968547295	13.42739976047507	8.75764001513983
H	6.39148691953494	13.87493635157377	9.71655224262295
C	6.06028834391438	13.86977635747245	7.56005450582654
C	3.14591724348387	11.62594461972459	12.26203009161866
H	3.16783602407342	10.59397571059533	12.67064604326017
C	8.15757201718939	10.07553451737884	11.72666791080401
H	7.75876050476746	9.15609304275512	12.17374376701126
C	5.95055832844231	8.85851411424146	10.56309291717369
H	6.70897275681306	8.03511513275292	10.54080266513659
H	5.71773804460898	9.01657124723630	11.64637534720061
C	4.99837247169032	16.01389706840477	6.83170067575305
H	5.90120522151553	16.19898133439224	6.22764619819520
C	7.62548557448417	12.37067852644903	8.75061472578083
C	8.16422317827019	11.80606428196346	10.01742069748187
C	7.55379034765885	10.61370886303026	10.54757865046966
C	0.51527481729098	11.27567493697255	10.87834162210441
H	0.21615171987205	12.12594143009705	11.52913542433037
C	9.25281843585175	10.69563763420464	12.34520324172177
H	9.67578247208461	10.24189550739296	13.25608372378860
C	2.76209844587058	15.53597743491717	8.44483313144740
H	1.87054231005064	15.38092242282864	9.06568329769902
C	3.77428638874465	7.05482217019971	11.20081347348479
H	4.63784542106431	6.39784062940402	11.44281295304389
C	5.86385048770148	7.74927953607182	7.51744111323231
H	6.76792959746075	8.18574028394072	7.99057495496238
H	6.19400890227985	7.06396549391947	6.71039206154588
H	5.30132419157978	8.56606862991210	7.01429403213051
C	9.81096096851806	11.87392026192465	11.82769562600606
H	10.66771347669808	12.35976198979712	12.31683144736256
C	6.46438022540069	13.28962509546506	6.33466248072464
H	5.97626095687050	13.61200631779866	5.40620425251685
C	3.95632733182725	16.95728730821950	6.85101626032274
H	4.02069677831880	17.87731290496854	6.25257816016505
C	7.44626154816052	12.27862176218499	6.30822936743231
H	7.75107579373624	11.84429519124089	5.34612710339076
C	9.25448468566034	12.41429498725633	10.65429263112960
H	9.68042610626708	13.32729101727795	10.20784805783342
C	-0.24513366988109	11.35824936114225	9.54642405162222
H	-1.30793696311468	11.06701062287054	9.68180566822937
H	-0.23178225645450	12.37518795829935	9.11014690103739
H	0.22310163362626	10.67868826290973	8.80672831478839
C	5.00268800120729	6.98114496879198	8.52556106535725
H	4.09081816661708	6.63013972335741	7.99704441871331
C	7.99541684329434	11.79283537066454	7.50424284390778

H	8.71667486041288	10.96226286573885	7.49841840414873
C	2.60609636461629	6.19212098815795	10.70739119765440
H	2.84108724393450	5.63127114354510	9.78082877648440
H	2.31084271529215	5.45492957716395	11.48290863818906
H	1.72027843691372	6.83130541447490	10.50707268704995
C	4.59727470038653	12.09441801461496	12.07958433344815
H	4.64032472029437	13.13218115509431	11.69035661312036
H	5.13918825762570	12.07333805659214	13.04703867289465
H	5.15819364301766	11.44511361768570	11.37470868679136
C	5.75214191363740	5.76186781504671	9.07169309941155
H	5.11178766858191	5.11329594530509	9.70015416788080
H	6.10121993578695	5.13784755486007	8.22349616263862
H	6.64452695687688	6.05456631832890	9.66493001564192
C	3.37593664384467	7.84280858558045	12.45223916639264
H	2.55421019937008	8.54448998731215	12.21206507246315
H	3.02309597116129	7.15430198114655	13.24847117794842
H	4.21487022690951	8.43461082565052	12.86772831074372
C	2.85242351829971	16.70918863304073	7.68353150906525
H	2.03390474291133	17.44484586914199	7.74048904749045
C	0.22470179532036	9.95364065397908	11.60139290898378
H	0.55433741453720	9.09505277061040	10.97815485888579
H	0.75141359839104	9.87801819408161	12.57340417735306
H	-0.86207720266738	9.83947354630216	11.79684901175738
C	2.36519816313228	12.52869354717407	13.22283573222079
H	1.35386983646820	12.13669432655790	13.45028183562132
H	2.90842511232913	12.62083104420564	14.18699260586584
H	2.25077486370544	13.55546333865723	12.81638587857736
H	2.55458334231148	10.20960088263044	7.73149652488742

Coordinates of 4

La	1.85137776873639	1.98302449884173	12.52900730650471
Ni	2.07339239757919	-0.47256664115025	13.02861284494587
P	2.71944722178044	-0.79598507178667	10.97958004566941
P	0.05407730237564	-0.58603471737991	13.78582397346663
N	0.02625957536184	2.16230185963359	14.23296084487671
N	1.41645136195370	1.44674620698917	10.07447778519927
N	3.45745432255380	-0.10910057539429	14.44347358120952
N	4.05552052592678	2.04867213143366	13.76498328961268
C	-0.44263182892817	3.29884134674680	14.86739516536734
C	-1.20358435142118	3.27598720248325	16.07852038314958
H	-1.47052774419086	2.31325946746714	16.53309215423092
C	-0.45274553907319	0.91497007933079	14.79841847082916
H	-1.56816317199326	0.89834177540920	14.90500524907308
H	-0.04895944773183	0.72738857840383	15.82797026308424

C	0.64345022052586	2.14801140742603	9.16678698370986
C	0.82739997259332	4.15358394565535	10.66793967178566
C	1.74382732147738	0.09555570662741	9.65919249951312
H	2.31189491336070	0.05964618342010	8.69275704407181
H	0.82806747151889	-0.53190808864386	9.49401502273928
C	0.12989795418610	1.59680508139889	7.95144873110529
H	0.37690957236832	0.56346659361978	7.67499758038400
C	0.28058321099197	3.51481634401453	9.44053376436243
C	2.48712494737969	-2.59925202900681	10.47041794822734
H	1.39303847828586	-2.63194289643675	10.27152440274547
C	-0.13912249679052	4.60926119116031	14.34057494884285
C	-1.48939706386017	0.57629730664800	11.75355173233406
H	-0.56563570521867	0.73804079958964	11.15537766326755
H	-1.64098488596754	1.46883843478847	12.39084648376473
H	-2.33252171982155	0.51466950664959	11.03477573684661
C	0.07089284979405	4.21154581215247	11.85920104335746
H	-0.95428944140500	3.81297223056930	11.86218192611970
C	-1.39488985036723	-0.71043867798772	12.58380771273914
H	-2.31614839475652	-0.80732817091553	13.19776425251569
C	-1.59534193077878	4.45292936115229	16.73045037172476
H	-2.17339112047939	4.37566875778739	17.66558177298312
C	4.16608822030734	1.00206390182010	14.59551663967253
H	4.86852630649272	1.06673666364504	15.45947333259482
C	-0.69884926276711	2.33816375231115	7.09746404716010
H	-1.07338261669076	1.86377883647032	6.17582796883101
C	-0.26964760644086	-1.93452233368208	15.07576191380745
H	0.31201864916803	-1.54574454489852	15.94053022039504
C	1.93343514464294	5.24143943488489	13.04223676901347
H	2.36910943372664	5.63278796554142	13.97311172512633
C	0.62067299245370	4.71302391138904	13.07018275185222
C	2.76614869388017	-3.52208031796600	11.66298001828967
H	2.45692586656139	-4.56581589389014	11.44428707129430
H	2.20124790538453	-3.16718237011221	12.54827726197649
H	3.84159217360270	-3.53642885373238	11.93177836013312
C	4.49567311063541	-0.38694513032091	10.48604934349514
H	4.64906675416481	-0.78717303440823	9.46043716247273
C	-1.25629611459748	5.71644468236556	16.22084689690882
H	-1.56331658648715	6.63838942395089	16.73561505788040
C	-0.55483658407450	4.23720996272826	8.57771108223878
H	-0.80507065941015	5.27847626734511	8.83756184252571
C	-0.52231820805485	5.77406504638617	15.02396417203529
H	-0.25730528577570	6.74912831667600	14.58380941473700
C	-1.23595675940805	-1.94265980937717	11.68919019139044
H	-1.99812443845354	-1.94773186880209	10.88238414214839

H	-1.33201748535706	-2.89270425634806	12.25133443903200
H	-0.23224647775382	-1.93167307219961	11.21586277135995
C	2.15601685846898	4.65810003281764	10.68038366919441
H	2.75259275606389	4.59823049591902	9.75823801318682
C	-1.05879011786959	3.66108681669668	7.39743091026980
H	-1.71182675122219	4.23845818958297	6.72693339846794
C	4.70064924495117	1.13503490546183	10.45186458646125
H	3.98537384572003	1.64583656105425	9.77674968800129
H	5.73060512012132	1.37465179946045	10.11217299619041
H	4.59499122287027	1.55926225090305	11.47632148603482
C	2.68816699810069	5.22601856105496	11.84979581778428
H	3.70804432047913	5.64034807443991	11.84258472069982
C	3.22172908978077	-3.02061526891197	9.19438708724860
H	4.32079940192237	-3.04071242564495	9.34227102570367
H	3.00426826929910	-2.34495787689897	8.34254098434628
H	2.91402737302240	-4.04481342215772	8.89377391575961
C	3.52810436560535	-1.12522193565140	15.51180555525445
H	2.87868164050969	-1.95744687233309	15.16575561290491
C	2.93726483444558	-0.60361104996380	16.83049527513316
H	2.81879186739994	-1.41793586821391	17.57471312082886
H	1.94395577603817	-0.14624352786164	16.64588747297474
H	3.58472303888126	0.17739111368139	17.28032561901895
C	4.94390782932305	3.19921193429230	13.99358281966348
H	4.70981528323216	3.91997949183975	13.17966175922416
C	0.33446444273506	-3.28821733389225	14.68494396199061
H	-0.16213426794173	-3.72719533726962	13.79658679327418
H	0.22981063262370	-4.01484812569400	15.51813774467648
H	1.41327385111204	-3.19763295236217	14.45069241901451
C	4.94116974926614	-1.70366687861658	15.68119921356459
H	5.65641847186448	-0.93828350840307	16.04712372669407
H	5.31974576386039	-2.08790917444740	14.71299424936226
H	4.94270827793868	-2.53688533683247	16.41366561496597
C	-1.73887808920526	-2.06505906160674	15.49496861243614
H	-2.18588195158695	-1.09259463033536	15.78173337085278
H	-1.82958333703887	-2.74413718424827	16.36929456625654
H	-2.35645799953885	-2.49729968818090	14.68100884493437
C	5.46890829966228	-1.05221423746777	11.46722554914802
H	5.20636138377404	-0.76957518516845	12.50810856901511
H	6.51295192536991	-0.73017839226738	11.26841337678827
H	5.44350501765459	-2.15840534160981	11.40014966225582
C	4.64681188068804	3.90822472830985	15.32738497467470
H	4.91591399910473	3.26656314244255	16.19215671316244
H	3.56569711769562	4.14056261209472	15.41178857540468
H	5.21981023777256	4.85398726301550	15.42049039857010

C	6.43159676143941	2.83410381528818	13.85096043000873
H	7.07475739851745	3.73583265125683	13.91758552411116
H	6.61935739667337	2.34167851790388	12.87589818152828
H	6.75285290869994	2.13425703805042	14.65040714622618

The input files for all DFT calculations:

Input file for the geometry optimization of 2

! UKS BP RI def2-SVP Def2/J TightSCF SlowConv D3BJ UNO UCO

! Opt

%pal nprocs 24

end

%scf maxiter 2000

end

*xyz 0 1

La	11.313596770	8.507095159	8.656904640
Ni	9.079701770	7.887343159	9.664276640
P	9.976493770	7.405778159	11.600783640
C	7.966028356	5.755036129	12.449877250
H	7.374217657	6.327948379	11.952865339
H	7.544444797	5.508779669	13.278576145
H	8.152796081	4.967308355	11.939031206
H	10.640449302	5.615584588	13.981325895
P	8.208561770	9.666849159	8.789005640
C	8.843018165	10.648896070	6.309061913
H	9.230819036	11.326763119	6.866770437
H	8.469738567	11.055396089	5.523410630
H	9.520319839	10.018981320	6.052253649
H	6.589402357	12.106582026	8.368829504
N	12.420806770	7.134555159	10.364658640
N	10.655248770	10.877812159	9.132273640
C	14.364951770	8.455907159	8.791636640
C	13.888028770	9.613949159	9.429984640
H	13.876149770	9.655095159	10.358635640
C	13.429069770	10.702462159	8.685014640
C	13.509027770	10.656625159	7.305849640
H	13.206756770	11.374866159	6.798591640
C	14.032966770	9.555362159	6.686887640
H	14.111002770	9.544092159	5.760271640
C	14.449488770	8.461052159	7.419395640
H	14.790912770	7.716557159	6.978436640
C	14.698390770	7.231740159	9.551838640
C	15.969840770	6.678264159	9.439677640
H	16.644023163	7.120027889	8.847796817
C	16.324148770	5.525626159	10.130644640

H	17.241874297	5.137878824	10.044436399
C	15.385148770	4.937259159	10.929617640
H	15.625457078	4.110802730	11.438755820
C	14.116735770	5.456731159	11.048702640
H	13.460930552	4.996269134	11.646945266
C	13.709154770	6.619126159	10.356350640
C	11.569629770	6.505199159	11.387954640
H	12.044050770	6.490093159	12.233205640
H	11.386395770	5.587879159	11.131175640
C	12.833998770	11.920909159	9.359364640
C	13.634271770	12.960613159	9.731849640
H	14.623006292	12.894036618	9.597791412
C	13.091946770	14.118650159	10.299577640
H	13.681379433	14.879650931	10.570588637
C	11.744337770	14.184935159	10.472665640
H	11.347287114	14.997213149	10.899930481
C	10.910965770	13.156845159	10.072486640
H	9.922700834	13.259092733	10.185967257
C	11.418605770	11.964514159	9.507527640
C	9.204088770	11.121410159	9.269358640
H	8.955140770	11.876062159	8.712749640
H	9.006286770	11.353199159	10.190269640
La	9.019912770	4.489348159	5.279059640
Ni	11.253807770	5.109101159	4.271688640
P	10.357015770	5.590666159	2.335180640
C	11.433533770	6.540460159	1.118996640
H	12.160976770	5.936389159	0.860347640
C	12.071459770	7.698077159	1.857042640
H	12.714836770	7.360110159	2.487387640
H	12.518018770	8.272113159	1.227612640
H	11.398251770	8.194971159	2.322067640
C	10.794447770	7.018609159	-0.164623360
H	9.947034770	7.420981159	0.029899640
H	11.368738770	7.666541159	-0.583427360
H	10.670121770	6.273906159	-0.756847360
C	9.880998770	4.177062159	1.210386640
H	9.665407770	4.572993159	0.341471640
C	11.038367770	3.228032159	0.972217640
H	11.365746770	2.901640159	1.814297640
H	10.742200770	2.489578159	0.436309640
H	11.746495770	3.690786159	0.514379640
C	8.680288770	3.391954159	1.643798640
H	7.931791770	3.986050159	1.730204640
H	8.487056770	2.721465159	0.988515640

H	8.861104770	2.977164159	2.489242640
P	12.124947770	3.329594159	5.146959640
C	12.489321770	2.938596159	6.949981640
H	12.995133770	2.098485159	6.945273640
C	11.199947770	2.647622159	7.739261640
H	10.670101770	2.006108159	7.261082640
H	11.426264770	2.295699159	8.603413640
H	10.700342770	3.460363159	7.845690640
C	13.386514770	3.943180159	7.542633640
H	13.033930770	4.821253159	7.379668640
H	13.452423770	3.795104159	8.488455640
H	14.256830770	3.868828159	7.144919640
C	13.807263770	2.989745159	4.420128640
H	14.424619770	3.518473159	4.968484640
C	14.306780770	1.548480159	4.558598640
H	13.942461770	1.014012159	3.849949640
H	15.265730770	1.535812159	4.508970640
H	14.026049770	1.192616159	5.405123640
C	13.971874770	3.547967159	3.013270640
H	13.665173770	4.457275159	2.991350640
H	14.897284770	3.515635159	2.761295640
H	13.454484770	3.021623159	2.398004640
N	7.912702770	5.861889159	3.571305640
N	9.678260770	2.118631159	4.803691640
C	5.968558770	4.540537159	5.144328640
C	6.445480770	3.382494159	4.505979640
H	6.458259938	3.338234994	3.507041294
C	6.904440770	2.293981159	5.250950640
C	6.824482770	2.339819159	6.630114640
H	7.149571133	1.567359625	7.175663742
C	6.300542770	3.441081159	7.249076640
H	6.216629883	3.453199902	8.245476039
C	5.884021770	4.535391159	6.516568640
H	5.542597770	5.279887159	6.957527640
C	5.635118770	5.764704159	4.384126640
C	4.363668770	6.318179159	4.496287640
H	3.689485947	5.876415149	5.088167764
C	4.009360770	7.470817159	3.805320640
H	3.091635540	7.858565443	3.891527778
C	4.948361770	8.059184159	3.006346640
H	4.708052661	8.885640716	2.497209043
C	6.216774770	7.539712159	2.887262640
H	6.872579050	8.000175356	2.289019888
C	6.624355770	6.377318159	3.579613640

C	8.763880770	6.491244159	2.548009640
H	8.289459770	6.506350159	1.702759640
H	8.947113770	7.408565159	2.804789640
C	7.499511770	1.075534159	4.576599640
C	6.699238770	0.035830159	4.204114640
H	5.710504460	0.102407761	4.338173913
C	7.241563770	-1.122205841	3.636386640
H	6.652131106	-1.883206613	3.365375642
C	8.589172770	-1.188490841	3.463298640
H	8.986222519	-2.000769177	3.036033616
C	9.422543770	-0.160400841	3.863477640
H	10.410808597	-0.262649478	3.749997035
C	8.914904770	1.031929159	4.428436640
C	11.129420770	1.875033159	4.666605640
H	11.378369770	1.120381159	5.223214640
H	11.327222770	1.643245159	3.745694640
I	11.251870770	7.398824159	5.472502640
I	8.808742770	5.762171159	8.315298640
C	9.053043770	5.998097159	12.433405640
H	9.296162061	5.217985018	11.891944259
C	9.692473770	5.465825159	13.700408640
H	9.225436770	4.677938159	13.987000640
H	9.424540303	6.290890121	14.223079835
C	10.377691770	8.608806159	12.955438640
H	10.609190770	8.082613159	13.749801640
C	9.193234770	9.471991159	13.322384640
H	8.866105770	9.916318159	12.536551640
H	9.462786770	10.126218159	13.970924640
H	8.498481770	8.922183159	13.691574640
C	11.566892770	9.456401159	12.623109640
H	12.304261770	8.892209159	12.370055640
H	11.817216770	9.976604159	13.392035640
H	11.352472770	10.044336159	11.896417640
C	8.251540770	9.534855159	6.922286640
H	9.018654525	8.970430601	6.692330640
C	7.295705770	8.576933159	6.362866640
H	6.540907023	8.933753204	6.476524112
H	7.331732770	7.756638159	6.860321640
H	7.508338770	8.405269159	5.444144640
C	6.440649770	10.058019159	9.227817640
H	5.875485770	9.375539159	8.811022640
C	5.954821770	11.425158159	8.733478640
H	5.043692770	11.558460159	9.005669640
H	6.012793136	11.459099885	7.735737551

C	6.256181770	9.947153159	10.744067640
H	6.908677770	10.495621159	11.186743640
H	6.370278770	9.033468159	11.014195640
H	5.374929770	10.244196159	10.981516640

*

Input file for the natural localized molecular orbital (NLMO) analysis of 2

! UKS BP RI def2-SVP Def2/J TightSCF SlowConv D3BJ UNO UCO

%pal nprocs 24
end

%NBO NBOKEYLIST = "\$NBO NBO NLMO AONLMO=C AONBO=P \$END"
end

%scf maxiter 2000
end

*xyz 0 1

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Ni	9.10902995770466	7.71877515868687	9.60977057122549
P	10.05669386013162	7.27797291287216	11.50290475070440
C	7.62220064991578	6.09785278244000	12.39379794595267
H	7.29004591119002	6.17158125000123	11.33983972351014
H	7.26970745959265	7.00160149127447	12.93106261161807
H	7.11774103590459	5.22105858090221	12.85140991367697
H	10.74609974158566	5.63455041565700	13.96195173942673
P	8.24848931246610	9.50642282626727	8.75425220342045
C	7.33984618788231	10.99201740656953	6.44665285305206
H	7.97617988528892	11.85388138361317	6.73031332454791
H	6.32393158461598	11.16139130080657	6.86219492058796
H	7.24033983451993	10.99877295026920	5.34110402778623
H	7.06373200737065	11.18703905925079	11.16789214386956
N	12.54835401086334	7.00714472987171	10.31286319427479
N	10.72180002227396	10.69589980099013	8.86372198564405
C	14.37798249720593	8.13290035977204	8.41115766575875
C	13.97942433340971	9.37155428695464	8.98619960593938
H	14.02958115120808	9.49523840207136	10.07795619575032
C	13.48016779499383	10.42729039230239	8.19248755881517
C	13.42774499884694	10.25803485660822	6.78346646631933
H	13.01893798245089	11.07058524947407	6.16523545798900
C	13.87927513465043	9.06559235812741	6.19677793056754
H	13.82949485731326	8.93760631428973	5.10554205036385

C	14.33307953712232	8.00249682042752	7.00246589188684
H	14.61777054264825	7.04343510554334	6.54435111643853
C	14.77067661226085	6.99688357775262	9.27732339740237
C	16.02239929425738	6.38555649435793	9.10120460768280
H	16.69525363123485	6.78895172361082	8.32719113769967
C	16.43813259808023	5.31109912961128	9.90607131205076
H	17.42821250961292	4.85405031130393	9.76432886182661
C	15.56737799573778	4.85858515964513	10.90985610570395
H	15.87138529112443	4.02788820529087	11.56699774128628
C	14.30237395316138	5.43547999060661	11.08913874877534
H	13.64659664340985	5.02318968477871	11.86654745454213
C	13.83438661153333	6.50295741654394	10.25965231270995
C	11.73934656786544	6.46740053293529	11.38821314514023
H	12.23438884409504	6.56615299950285	12.38821567731818
H	11.53089846778081	5.37374298261438	11.25605649750216
C	12.96857307595348	11.67549828569351	8.82234760060855
C	13.84722005760347	12.73222442117524	9.09972661005615
H	14.91256726948225	12.60844705479066	8.84724286232453
C	13.39181643899719	13.92868613102243	9.68215172787380
H	14.09189481802275	14.74978032919052	9.89482877011648
C	12.02632564643487	14.04494379303716	9.98058166169423
H	11.64046188974250	14.97045321775081	10.43751419819896
C	11.13209147949437	12.99872069144456	9.71091833041971
H	10.07468476940021	13.13672925765300	9.96992759036091
C	11.56569115498398	11.77055401675652	9.12393648649408
C	9.32231983625577	10.97986064580671	9.14350054323240
H	8.95317867471801	11.87763700142943	8.58985081318416
H	9.14565724072223	11.19723801136796	10.22712925872121
La	8.97286388918437	4.59777777749831	5.38110269180842
Ni	11.25730029462625	5.23033293527221	4.49428108678103
P	10.55473990535178	5.48290047181266	2.45225631822331
C	11.69338030638584	6.54867659434105	1.38064427956170
H	12.42237890833327	5.80384036276621	0.99132663246965
C	12.46705570385985	7.56959500399267	2.22242767366975
H	12.98611262932239	7.08532144032265	3.07401192910493
H	13.22480278768022	8.09139673974775	1.60067155889272
H	11.79206295618603	8.33635919061552	2.65342670906116
C	10.98760657111542	7.21289284171666	0.19174169320235
H	10.27323551558510	7.98982940979694	0.53186898283420
H	11.73079262492742	7.71383000329375	-0.46393294032003
H	10.43043013225889	6.48784422036109	-0.43442275831085
C	10.15809188560735	4.08291477034128	1.25327318898818
H	9.94477711889657	4.58897683664740	0.28497203403680
C	11.35326764956026	3.14485707272248	1.06587876485233

H	11.59703780408995	2.63229306943471	2.01835472038936
H	11.11304688850206	2.36088645106344	0.31836346271784
H	12.26373653242893	3.67219527114499	0.71616570373207
C	8.90787387003870	3.31214764544555	1.68850142599657
H	8.01803606256840	3.96704090605651	1.74087860885743
H	8.69643522099613	2.48776050511740	0.97708387148835
H	9.05878871881800	2.85389222235349	2.68736078912463
P	12.09307290541716	3.47399831410275	5.40781754384939
C	12.40280103151614	3.11347840590012	7.23960045316885
H	13.29533336605050	2.44830791969884	7.24915482207413
C	11.25882376200630	2.36881593254985	7.93623946667180
H	11.05029873395698	1.38359196041044	7.47740309609875
H	11.51835679682495	2.20299722633457	9.00284727013815
H	10.31694081763011	2.95174428188441	7.93235670031705
C	12.76059727471298	4.42241430681265	7.94759211419246
H	11.87274747200573	5.08502076078936	8.00522624598043
H	13.10801896024566	4.23780193579406	8.98320655392810
H	13.56836128700584	4.97978452495667	7.43154900741055
C	13.85561500137046	3.22298770718864	4.77113376028516
H	14.45480304173095	3.70734601760844	5.57473392565177
C	14.26772386893335	1.75015477527221	4.67051055078682
H	13.71119602621759	1.22971626328455	3.86458582396902
H	15.34892095350059	1.66723626202153	4.43130837134149
H	14.09450757616743	1.19711609391730	5.61563860653283
C	14.10212681157417	3.98988953178264	3.46814854811519
H	13.78044393916604	5.04779088045363	3.56048924272475
H	15.17937949806663	3.97411972055443	3.19845430123062
H	13.53586476464361	3.54724417948128	2.62722113434972
N	8.03768040701739	5.91105630668672	3.46433642396273
N	9.69156205443660	2.22413733778606	4.94156598311464
C	5.96306646452476	4.71267746329197	5.07004472242193
C	6.45057023135224	3.52408536894643	4.45409599581593
H	6.56573930582702	3.49556309694413	3.36216110659810
C	6.85134569457368	2.40771392718073	5.21955219268390
C	6.68682346055965	2.45026388372399	6.63062060658625
H	7.01474786775417	1.58794394124514	7.22955950834006
C	6.12116196320893	3.57858922309916	7.24217357188121
H	5.99422152622753	3.60614263650127	8.33431537344070
C	5.78349952807623	4.71107567709308	6.47406195493212
H	5.42836333145703	5.62750751551022	6.96765039290383
C	5.71996728896084	5.94208191200432	4.27677471353151
C	4.48500308649401	6.60392596446086	4.38447313793675
H	3.71036199473146	6.15888186504965	5.02954902541529
C	4.21096458450169	7.78112254805776	3.66888708705741

H	3.23184110018507	8.27428176263180	3.75414367966625
C	5.21082310543719	8.29458538915387	2.82714256989618
H	5.02229280510310	9.21131929452567	2.24548441644941
C	6.45934749756739	7.66758180332462	2.71776340594383
H	7.22068971356691	8.12462694020371	2.07253536507396
C	6.78092122614067	6.48702692813764	3.45870218238297
C	8.94966516797129	6.43894548196781	2.46599812153836
H	8.51058894185982	6.42397630342255	1.43730298966481
H	9.24175963558605	7.50350976026926	2.66404108484062
C	7.48301699711066	1.21902080377825	4.58173692287704
C	6.67998796555814	0.17985619029253	4.09135517820676
H	5.58592193338103	0.27938204677453	4.17576787174661
C	7.24349997462020	-0.97004367934936	3.50963207422663
H	6.60082102809794	-1.77678893910340	3.12815731238958
C	8.64116076501818	-1.06072880488883	3.43735935190101
H	9.11188177060538	-1.95224462885372	2.99248203458063
C	9.46186322570558	-0.03139766345549	3.92064997599719
H	10.54949936309626	-0.14889441924239	3.83433051250828
C	8.91900877066924	1.15505043109911	4.50338941117251
C	11.12284258941032	1.99003680774330	4.82697140664518
H	11.46037940211878	1.08273082874685	5.38645534023340
H	11.43973989192672	1.82232761256353	3.76551304472942
I	10.69544384362515	7.61515374067274	5.45837137500760
I	8.91310221975440	5.34418691114450	8.57731556896485
C	9.14427939872159	5.94005817416089	12.47317745695629
H	9.41397392531574	5.03806538378595	11.87877999779997
C	9.64562619396226	5.75653618012745	13.90938508287773
H	9.18887340722471	4.85175512544958	14.36363761034713
H	9.36779146431704	6.61869376665664	14.55036342588359
C	10.36550854472022	8.69330435244762	12.69952758710761
H	10.70504464662582	8.24399218835296	13.65777495372354
C	9.06513783720860	9.47201094141675	12.92102312285632
H	8.66500541422531	9.80861631885761	11.94177820740808
H	9.24177936712869	10.36929057735736	13.54992849485249
H	8.28207916301264	8.86062605120833	13.41233415593644
C	11.47683310205545	9.59879554854391	12.14959103911048
H	12.43648275483018	9.05792504927850	12.03789392685657
H	11.64162969908288	10.46230006498627	12.82632943741760
H	11.20239213238870	10.00985345931865	11.15342829504629
C	7.93180358656443	9.65572948655646	6.90428956351172
H	8.94930023091165	9.56296114289691	6.46406524688953
C	7.10389643569557	8.45357586504321	6.43549941628518
H	6.06193464847489	8.50003225601553	6.81665234682074
H	7.54961965151393	7.50122870874378	6.78823841167257

H	7.04148538581406	8.42225481190650	5.32964220288677
C	6.53513071263232	9.89402684563942	9.46993072665228
H	5.89010465284980	9.98183280109609	8.56962052126309
C	6.44678707857858	11.21190985386404	10.24671699330706
H	5.39707525053221	11.39372118849929	10.56069667810348
H	6.77019739416993	12.08155129727749	9.64211441673285
C	6.04694180737804	8.70020375612883	10.29936715166892
H	6.67315233539315	8.57218033325401	11.20390861489212
H	6.10243372375129	7.75581410280445	9.72030673715448
H	4.99546626340457	8.84522896919983	10.62660675744664

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Input file for the AIM analysis (single-point) of 2

! UKS BP RI ZORA-def2-SVP SARC/J TightSCF SlowConv D3BJ UNO UCO ZORA

%pal nprocs 24
end

%scf maxiter 2000
end

%basis newgto La "SARC-ZORA-TZVP" end
newgto I "SARC-ZORA-TZVP" end
end

*xyz 0 1

La	11.32061598150332	8.28633007360238	8.54348984723250
Ni	9.10902995770466	7.71877515868687	9.60977057122549
P	10.05669386013162	7.27797291287216	11.50290475070440
C	7.62220064991578	6.09785278244000	12.39379794595267
H	7.29004591119002	6.17158125000123	11.33983972351014
H	7.26970745959265	7.00160149127447	12.93106261161807
H	7.11774103590459	5.22105858090221	12.85140991367697
H	10.74609974158566	5.63455041565700	13.96195173942673
P	8.24848931246610	9.50642282626727	8.75425220342045
C	7.33984618788231	10.99201740656953	6.44665285305206
H	7.97617988528892	11.85388138361317	6.73031332454791
H	6.32393158461598	11.16139130080657	6.86219492058796
H	7.24033983451993	10.99877295026920	5.34110402778623
H	7.06373200737065	11.18703905925079	11.16789214386956
N	12.54835401086334	7.00714472987171	10.31286319427479
N	10.72180002227396	10.69589980099013	8.86372198564405
C	14.37798249720593	8.13290035977204	8.41115766575875

C	13.97942433340971	9.37155428695464	8.98619960593938
H	14.02958115120808	9.49523840207136	10.07795619575032
C	13.48016779499383	10.42729039230239	8.19248755881517
C	13.42774499884694	10.25803485660822	6.78346646631933
H	13.01893798245089	11.07058524947407	6.16523545798900
C	13.87927513465043	9.06559235812741	6.19677793056754
H	13.82949485731326	8.93760631428973	5.10554205036385
C	14.33307953712232	8.00249682042752	7.00246589188684
H	14.61777054264825	7.04343510554334	6.54435111643853
C	14.77067661226085	6.99688357775262	9.27732339740237
C	16.02239929425738	6.38555649435793	9.10120460768280
H	16.69525363123485	6.78895172361082	8.32719113769967
C	16.43813259808023	5.31109912961128	9.90607131205076
H	17.42821250961292	4.85405031130393	9.76432886182661
C	15.56737799573778	4.85858515964513	10.90985610570395
H	15.87138529112443	4.02788820529087	11.56699774128628
C	14.30237395316138	5.43547999060661	11.08913874877534
H	13.64659664340985	5.02318968477871	11.86654745454213
C	13.83438661153333	6.50295741654394	10.25965231270995
C	11.73934656786544	6.46740053293529	11.38821314514023
H	12.23438884409504	6.56615299950285	12.38821567731818
H	11.53089846778081	5.37374298261438	11.25605649750216
C	12.96857307595348	11.67549828569351	8.82234760060855
C	13.84722005760347	12.73222442117524	9.09972661005615
H	14.91256726948225	12.60844705479066	8.84724286232453
C	13.39181643899719	13.92868613102243	9.68215172787380
H	14.09189481802275	14.74978032919052	9.89482877011648
C	12.02632564643487	14.04494379303716	9.98058166169423
H	11.64046188974250	14.97045321775081	10.43751419819896
C	11.13209147949437	12.99872069144456	9.71091833041971
H	10.07468476940021	13.13672925765300	9.96992759036091
C	11.56569115498398	11.77055401675652	9.12393648649408
C	9.32231983625577	10.97986064580671	9.14350054323240
H	8.95317867471801	11.87763700142943	8.58985081318416
H	9.14565724072223	11.19723801136796	10.22712925872121
La	8.97286388918437	4.59777777749831	5.38110269180842
Ni	11.25730029462625	5.23033293527221	4.49428108678103
P	10.55473990535178	5.48290047181266	2.45225631822331
C	11.69338030638584	6.54867659434105	1.38064427956170
H	12.42237890833327	5.80384036276621	0.99132663246965
C	12.46705570385985	7.56959500399267	2.22242767366975
H	12.98611262932239	7.08532144032265	3.07401192910493
H	13.22480278768022	8.09139673974775	1.60067155889272
H	11.79206295618603	8.33635919061552	2.65342670906116

C	10.98760657111542	7.21289284171666	0.19174169320235
H	10.27323551558510	7.98982940979694	0.53186898283420
H	11.73079262492742	7.71383000329375	-0.46393294032003
H	10.43043013225889	6.48784422036109	-0.43442275831085
C	10.15809188560735	4.08291477034128	1.25327318898818
H	9.94477711889657	4.58897683664740	0.28497203403680
C	11.35326764956026	3.14485707272248	1.06587876485233
H	11.59703780408995	2.63229306943471	2.01835472038936
H	11.11304688850206	2.36088645106344	0.31836346271784
H	12.26373653242893	3.67219527114499	0.71616570373207
C	8.90787387003870	3.31214764544555	1.68850142599657
H	8.01803606256840	3.96704090605651	1.74087860885743
H	8.69643522099613	2.48776050511740	0.97708387148835
H	9.05878871881800	2.85389222235349	2.68736078912463
P	12.09307290541716	3.47399831410275	5.40781754384939
C	12.40280103151614	3.11347840590012	7.23960045316885
H	13.29533336605050	2.44830791969884	7.24915482207413
C	11.25882376200630	2.36881593254985	7.93623946667180
H	11.05029873395698	1.38359196041044	7.47740309609875
H	11.51835679682495	2.20299722633457	9.00284727013815
H	10.31694081763011	2.95174428188441	7.93235670031705
C	12.76059727471298	4.42241430681265	7.94759211419246
H	11.87274747200573	5.08502076078936	8.00522624598043
H	13.10801896024566	4.23780193579406	8.98320655392810
H	13.56836128700584	4.97978452495667	7.43154900741055
C	13.85561500137046	3.22298770718864	4.77113376028516
H	14.45480304173095	3.70734601760844	5.57473392565177
C	14.26772386893335	1.75015477527221	4.67051055078682
H	13.71119602621759	1.22971626328455	3.86458582396902
H	15.34892095350059	1.66723626202153	4.43130837134149
H	14.09450757616743	1.19711609391730	5.61563860653283
C	14.10212681157417	3.98988953178264	3.46814854811519
H	13.78044393916604	5.04779088045363	3.56048924272475
H	15.17937949806663	3.97411972055443	3.19845430123062
H	13.53586476464361	3.54724417948128	2.62722113434972
N	8.03768040701739	5.91105630668672	3.46433642396273
N	9.69156205443660	2.22413733778606	4.94156598311464
C	5.96306646452476	4.71267746329197	5.07004472242193
C	6.45057023135224	3.52408536894643	4.45409599581593
H	6.56573930582702	3.49556309694413	3.36216110659810
C	6.85134569457368	2.40771392718073	5.21955219268390
C	6.68682346055965	2.45026388372399	6.63062060658625
H	7.01474786775417	1.58794394124514	7.22955950834006
C	6.12116196320893	3.57858922309916	7.24217357188121

H	5.99422152622753	3.60614263650127	8.33431537344070
C	5.78349952807623	4.71107567709308	6.47406195493212
H	5.42836333145703	5.62750751551022	6.96765039290383
C	5.71996728896084	5.94208191200432	4.27677471353151
C	4.48500308649401	6.60392596446086	4.38447313793675
H	3.71036199473146	6.15888186504965	5.02954902541529
C	4.21096458450169	7.78112254805776	3.66888708705741
H	3.23184110018507	8.27428176263180	3.75414367966625
C	5.21082310543719	8.29458538915387	2.82714256989618
H	5.02229280510310	9.21131929452567	2.24548441644941
C	6.45934749756739	7.66758180332462	2.71776340594383
H	7.22068971356691	8.12462694020371	2.07253536507396
C	6.78092122614067	6.48702692813764	3.45870218238297
C	8.94966516797129	6.43894548196781	2.46599812153836
H	8.51058894185982	6.42397630342255	1.43730298966481
H	9.24175963558605	7.50350976026926	2.66404108484062
C	7.48301699711066	1.21902080377825	4.58173692287704
C	6.67998796555814	0.17985619029253	4.09135517820676
H	5.58592193338103	0.27938204677453	4.17576787174661
C	7.24349997462020	-0.97004367934936	3.50963207422663
H	6.60082102809794	-1.77678893910340	3.12815731238958
C	8.64116076501818	-1.06072880488883	3.43735935190101
H	9.11188177060538	-1.95224462885372	2.99248203458063
C	9.46186322570558	-0.03139766345549	3.92064997599719
H	10.54949936309626	-0.14889441924239	3.83433051250828
C	8.91900877066924	1.15505043109911	4.50338941117251
C	11.12284258941032	1.99003680774330	4.82697140664518
H	11.46037940211878	1.08273082874685	5.38645534023340
H	11.43973989192672	1.82232761256353	3.76551304472942
I	10.69544384362515	7.61515374067274	5.45837137500760
I	8.91310221975440	5.34418691114450	8.57731556896485
C	9.14427939872159	5.94005817416089	12.47317745695629
H	9.41397392531574	5.03806538378595	11.87877999779997
C	9.64562619396226	5.75653618012745	13.90938508287773
H	9.18887340722471	4.85175512544958	14.36363761034713
H	9.36779146431704	6.61869376665664	14.55036342588359
C	10.36550854472022	8.69330435244762	12.69952758710761
H	10.70504464662582	8.24399218835296	13.65777495372354
C	9.06513783720860	9.47201094141675	12.92102312285632
H	8.66500541422531	9.80861631885761	11.94177820740808
H	9.24177936712869	10.36929057735736	13.54992849485249
H	8.28207916301264	8.86062605120833	13.41233415593644
C	11.47683310205545	9.59879554854391	12.14959103911048
H	12.43648275483018	9.05792504927850	12.03789392685657

H	11.64162969908288	10.46230006498627	12.82632943741760
H	11.20239213238870	10.00985345931865	11.15342829504629
C	7.93180358656443	9.65572948655646	6.90428956351172
H	8.94930023091165	9.56296114289691	6.46406524688953
C	7.10389643569557	8.45357586504321	6.43549941628518
H	6.06193464847489	8.50003225601553	6.81665234682074
H	7.54961965151393	7.50122870874378	6.78823841167257
H	7.04148538581406	8.42225481190650	5.32964220288677
C	6.53513071263232	9.89402684563942	9.46993072665228
H	5.89010465284980	9.98183280109609	8.56962052126309
C	6.44678707857858	11.21190985386404	10.24671699330706
H	5.39707525053221	11.39372118849929	10.56069667810348
H	6.77019739416993	12.08155129727749	9.64211441673285
C	6.04694180737804	8.70020375612883	10.29936715166892
H	6.67315233539315	8.57218033325401	11.20390861489212
H	6.10243372375129	7.75581410280445	9.72030673715448
H	4.99546626340457	8.84522896919983	10.62660675744664

*

Input file for the geometry optimization of 3

! UKS BP RI def2-SVP Def2/J TightSCF SlowConv D3BJ UNO UCO

! Opt

%pal nprocs 24

end

%scf maxiter 2000

end

*xyz 0 1

La	2.340636801	9.360542283	5.569533482
Ni	4.160945801	10.741735283	4.611056482
P	2.820100801	12.340450283	4.013954482
P	4.898114801	9.137075283	3.333040482
N	3.524074801	7.300336283	4.867632482
N	0.783203801	10.457788283	3.918467482
C	2.282596801	5.739960283	6.245304482
C	3.424726801	6.045228283	5.452225482
C	4.712866801	7.430727283	4.028826482
H	4.657087801	6.780846283	3.284074482
H	5.514518801	7.210068283	4.565523482
C	0.529031801	7.142884283	5.119622482
H	0.725772684	6.671556072	4.259888371

C	1.175663801	6.717066283	6.300066482
C	4.205673801	8.926728283	1.614564482
H	4.244252801	9.823632283	1.174173482
C	-0.899656199	10.380702283	2.092412482
H	-0.521960425	11.198586998	1.658349703
C	1.261577801	11.675583283	3.256456482
H	0.556702801	12.368824283	3.307202482
H	1.425453801	11.479875283	2.299925482
C	2.241717801	4.578134283	7.011280482
H	1.456595891	4.414387733	7.608583298
C	-0.375541199	8.201177283	5.120456482
C	-0.930899199	8.742009283	3.849806482
C	-0.317983199	9.906295283	3.291760482
C	6.733742801	9.211496283	3.064928482
H	6.995395801	8.446171283	2.477138482
C	-1.977166199	9.741257283	1.504622482
H	-2.357934719	10.111675194	0.657388213
C	4.414981801	5.042290283	5.366746482
H	5.194863097	5.174408237	4.754921336
C	3.423211801	13.492435283	2.686596482
H	2.666344801	14.093377283	2.428588482
C	1.395188801	12.773443283	6.354412482
H	0.628404801	12.329256283	5.936648482
H	1.077825801	13.401059283	7.036812482
H	1.974175801	12.101955283	6.772300482
C	-2.540763199	8.610184283	2.052244482
H	-3.317092457	8.156816889	1.614327950
C	0.809750801	7.325963283	7.495105482
H	1.230460520	7.023257574	8.350308724
C	3.265116801	3.641621283	6.965135482
H	3.234800458	2.818427151	7.532085514
C	-0.133535199	8.350018283	7.521096482
H	-0.403019925	8.756520933	8.394099104
C	-1.996055199	8.118760283	3.233106482
H	-2.385233685	7.294822986	3.645013554
C	7.501777801	9.087666283	4.388116482
H	8.426584801	9.384673283	4.257381482
H	7.497327801	8.152936283	4.682094482
H	7.072295801	9.646560283	5.068793482
C	2.183119801	13.533028283	5.292665482
H	2.981835801	13.926453283	5.747997482
C	-0.697590199	8.806999283	6.344543482
H	-1.338703138	9.574146742	6.365967223
C	4.566112801	14.363753283	3.211284482

H	4.284806801	14.809027283	4.037721482
H	4.797586801	15.038481283	2.539225482
H	5.348271801	13.801927283	3.392875482
C	2.733176801	8.540683283	1.706853482
H	2.652500801	7.653845283	2.116305482
H	2.343110801	8.521781283	0.807864482
H	2.256530801	9.198149283	2.255657482
C	1.342607801	14.705719283	4.771590482
H	1.874089801	15.232754283	4.138864482
H	1.072356801	15.273429283	5.523291482
H	0.544685801	14.360349283	4.319593482
C	3.884756801	12.748432283	1.439436482
H	4.635832801	12.162004283	1.668228482
H	4.170097801	13.394826283	0.760315482
H	3.145312801	12.210019283	1.087610482
C	4.326674801	3.878619283	6.114375482
H	5.050791554	3.193428357	6.035836821
C	7.088517801	10.507812283	2.347738482
H	6.828836801	11.271045283	2.905575482
H	6.611690801	10.550106283	1.493434482
H	8.054699801	10.536575283	2.185244482
C	4.956439801	7.954132283	0.706401482
H	5.880401801	8.258889283	0.593958482
H	4.515097801	7.918009283	-0.168167518
H	4.953013801	7.061390283	1.110696482
H	4.567769801	10.553530283	6.061559482
La	4.943579801	11.176574283	8.332661482
Ni	3.123271801	9.795381283	9.291138482
P	4.464116801	8.196666283	9.888241482
P	2.386101801	11.400041283	10.569154482
N	3.760141801	13.236780283	9.034562482
N	6.501012801	10.079328283	9.983727482
C	5.001620801	14.797156283	7.656890482
C	3.859489801	14.491888283	8.449969482
C	2.571349801	13.106389283	9.873369482
H	2.627128801	13.756270283	10.618120482
H	1.769697801	13.327048283	9.336671482
C	6.755184801	13.394232283	8.782573482
H	6.568284801	13.841987283	9.599307482
C	6.108552801	13.820050283	7.602128482
C	3.078543801	11.610388283	12.287630482
H	3.039963801	10.713484283	12.728021482
C	8.183873801	10.156414283	11.809782482
H	7.825052801	9.379404283	12.222152482

C	6.022638801	8.861533283	10.645738482
H	6.727513801	8.168292283	10.594992482
H	5.858762801	9.057241283	11.602269482
C	5.042498801	15.958982283	6.890914482
H	5.827620710	16.122728833	6.293611666
C	7.659757801	12.335939283	8.781739482
C	8.215116801	11.795107283	10.052388482
C	7.602199801	10.630821283	10.610434482
C	0.550473801	11.325620283	10.837266482
H	0.288820801	12.090945283	11.425056482
C	9.261382801	10.795859283	12.397572482
H	9.623146801	10.443929283	13.202520482
C	2.869234801	15.494826283	8.535448482
H	2.089353504	15.362708330	9.147273628
C	3.861004801	7.044681283	11.215598482
H	4.617872801	6.443739283	11.473606482
C	5.889027801	7.763673283	7.547782482
H	6.655811801	8.207860283	7.965546482
H	6.206390801	7.136057283	6.865382482
H	5.310040801	8.435161283	7.129894482
C	9.824979801	11.926932283	11.849950482
H	10.562526801	12.357651283	12.265990482
C	6.474465801	13.211153283	6.407089482
H	6.074840801	13.498688283	5.594746482
C	4.019099801	16.895495283	6.937059482
H	4.049416143	17.718689416	6.370109449
C	7.417751801	12.187098283	6.381098482
H	7.673728801	11.800971283	5.551854482
C	9.280271801	12.418356283	10.669088482
H	9.650006801	13.201127283	10.277761482
C	-0.217561199	11.449450283	9.514079482
H	-1.142367199	11.152443283	9.644813482
H	-0.213111199	12.384180283	9.220100482
H	0.211920801	10.890556283	8.833401482
C	5.101096801	7.004088283	8.609530482
H	4.302380801	6.610663283	8.154197482
C	7.981807801	11.730117283	7.557651482
H	8.590728801	11.001490283	7.537303482
C	2.718103801	6.173363283	10.690910482
H	3.005150722	5.719002086	9.847607471
H	2.481918473	5.484902144	11.376649318
H	1.935944801	6.735189283	10.509319482
C	4.551040801	11.996433283	12.195341482
H	4.631715801	12.883271283	11.785889482

H	4.941106801	12.015335283	13.094330482
H	5.027686801	11.338967283	11.646538482
C	5.941608801	5.831397283	9.130604482
H	5.399331383	5.293657192	9.776182360
H	6.217377332	5.252096733	8.363556512
H	6.755873747	6.183841112	9.591859232
C	3.399459801	7.788684283	12.462758482
H	2.648383801	8.375112283	12.233966482
H	3.108303097	7.129115746	13.155721048
H	4.138903801	8.327097283	12.814584482
C	2.957541801	16.658497283	7.787819482
H	2.233425047	17.343688210	7.866358143
C	0.195698801	10.029304283	11.554456482
H	0.455380801	9.266071283	10.996619482
H	0.672525801	9.987010283	12.408760482
H	-0.770483199	10.000541283	11.716950482
C	2.327776801	12.582984283	13.195793482
H	1.403814801	12.278227283	13.308236482
H	2.769118801	12.619107283	14.070362482
H	2.331202801	13.475726283	12.791498482
H	2.716446801	9.983586283	7.840635482

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Input file for the natural localized molecular orbital (NLMO) analysis of 3

! UKS BP RI def2-SVP Def2/J TightSCF SlowConv D3BJ UNO UCO

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%pal nprocs 24
end
```

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%NBO NBOKEYLIST = "$NBO NBO NLMO AONLMO=C AONBO=P $END"
end
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%scf maxiter 2000
end
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*xyz 0 1
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La	2.40383194426072	9.33563974331525	5.59700661215554
Ni	4.25683576769842	10.73875867060852	4.62678040343948
P	2.92178432001689	12.33874503525395	4.08016366884914
P	4.91593405343163	9.12807463648851	3.34162691097917
N	3.62230299303315	7.24765507493059	4.91008406998630
N	0.85214737533918	10.45949696913723	3.96633447556962
C	2.34030512474432	5.69753576084309	6.30334197460223
C	3.50703347718967	6.01113590443795	5.50819255480620

C	4.78519002450059	7.40313400167346	4.05896537660459
H	4.80867470198740	6.66134062716254	3.22010355190704
H	5.73682996521215	7.24377902498841	4.62120320064448
C	0.59325276415850	7.10923167139912	5.14891369784731
H	0.89006582141157	6.65813944741763	4.19116599405155
C	1.22505423751038	6.67130896342186	6.34698579528591
C	4.13643804067552	8.90833161002251	1.63884673861171
H	4.11616098798021	9.93980419526295	1.22894561372224
C	-0.87585452033861	10.45887185332361	2.17596091891988
H	-0.47840239918038	11.37895632825108	1.72895516107048
C	1.33015406845770	11.67875593542864	3.33955260511831
H	0.57192783497590	12.50232766289570	3.36373616741616
H	1.56115571418637	11.52170116811310	2.25572641106972
C	2.28623010391272	4.52743101447905	7.07772609006105
H	1.38411253580579	4.34406204105273	7.68336165710960
C	-0.34163246240765	8.16664271793866	5.15363364962239
C	-0.88060783568726	8.72886218261072	3.88589776878342
C	-0.27149921324568	9.92180497505648	3.35526073928754
C	6.76710667972133	9.25889951291616	3.02225019372311
H	7.06686027523730	8.40509431902022	2.37630665513692
C	-1.96991440404769	9.83684846816102	1.55723528819444
H	-2.39337327244406	10.28972116445243	0.64611389568474
C	4.52057564255766	5.00088517194861	5.46038449746080
H	5.41126359330232	5.15438851362960	4.83790500902265
C	3.50849247816962	13.47962919588667	2.69875503666268
H	2.64591545959094	14.13783613559619	2.45653848229866
C	1.42021808465170	12.78923814441795	6.38413349336427
H	0.51486420245550	12.35431623605852	5.91207445025785
H	1.09263100660362	13.47489100510983	7.19193764181748
H	1.98168002750541	11.97112984747435	6.88641736582189
C	-2.52625532410310	8.65775555100762	2.07479376886392
H	-3.38203535185982	8.17037504737180	1.58542642358350
C	0.82477597823482	7.25721413803261	7.57092750256715
H	1.31802557169702	6.94231017276011	8.49928927529759
C	3.32745390945878	3.58307858637832	7.05815280255473
H	3.26317391577734	2.66398502272252	7.65804042428550
C	-0.15778456280170	8.26777260077812	7.59543887941942
H	-0.46021328178887	8.70699476245062	8.55606160571243
C	-1.96953381603998	8.11866693427856	3.24867985983973
H	-2.39451788023770	7.20536376110659	3.69545429963602
C	7.52695367539522	9.18454953695564	4.35484147452221
H	8.59199337135668	9.46600366890434	4.21645197787542
H	7.50535248953808	8.17275290305113	4.80260376042677
H	7.06344488097924	9.87535526807046	5.08699293366272

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H	3.19445370212400	13.90576947711583	5.90402257808102
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H	-1.43102195515737	9.57898289199646	6.40287845923045
C	4.67818780965743	14.34033369238674	3.19176762393351
H	4.44326124057353	14.90325175132865	4.11715763348437
H	4.97670981706987	15.07539765472001	2.41551264988149
H	5.56176401399077	13.69910354115183	3.39503899985415
C	2.68436090456191	8.44232417195630	1.82184886726385
H	2.63991923916205	7.40498095516354	2.21210038600998
H	2.14220429723027	8.46310286391103	0.85454520567301
H	2.12446694211324	9.09304505147708	2.52624062464095
C	1.53410184636559	14.77632928551580	4.82963603385369
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H	1.18731324912714	15.40162539831719	5.67784618838282
H	0.64037335030464	14.48479677187292	4.23786227903333
C	3.90532253326840	12.69012110592564	1.44786296854770
H	4.72721755862372	11.98860641946321	1.68788818274448
H	4.25727511921988	13.37755674963444	0.65031300818444
H	3.06581696429408	12.09786225421436	1.03412819062371
C	4.43030991490901	3.82887825088805	6.22360231460660
H	5.24808515457843	3.09239817296915	6.16662083913905
C	7.05738452155339	10.57739866804363	2.29270964347583
H	6.72505144204636	11.43840029458617	2.91112221867304
H	6.53254827058287	10.64743700622576	1.31927793412764
H	8.14439493773212	10.69220153759311	2.09896003475062
C	4.91572260912293	8.00303841676635	0.67922377242108
H	5.92812192073715	8.39252224229486	0.45218617863763
H	4.37290381263438	7.91141263477989	-0.28520816365519
H	5.02755950852124	6.97633484014590	1.08650040994913
H	4.73331796972131	10.33071222907187	6.16726041973389
La	4.88043073629265	11.20185689537251	8.30367826648881
Ni	3.02650204394458	9.79775670938629	9.27288942255622
P	4.36037396558220	8.19736794786323	9.82050715240694
P	2.36651406079937	11.40709230179439	10.55902801034692
N	3.66124850613925	13.28909795407091	8.99327757283157
N	6.42966710756418	10.07730024169477	9.93611912994246
C	4.94426876188685	14.84256529218270	7.60431579488598
C	3.77658456824330	14.52657971449059	8.39715744745121
C	2.49686052793376	13.13214645242348	9.84225736024374
H	2.47074074085902	13.87387321047786	10.68107138033655
H	1.54645985592775	13.29042623110956	9.27770812951815
C	6.68983968547295	13.42739976047507	8.75764001513983
H	6.39148691953494	13.87493635157377	9.71655224262295

C	6.06028834391438	13.86977635747245	7.56005450582654
C	3.14591724348387	11.62594461972459	12.26203009161866
H	3.16783602407342	10.59397571059533	12.67064604326017
C	8.15757201718939	10.07553451737884	11.72666791080401
H	7.75876050476746	9.15609304275512	12.17374376701126
C	5.95055832844231	8.85851411424146	10.56309291717369
H	6.70897275681306	8.03511513275292	10.54080266513659
H	5.71773804460898	9.01657124723630	11.64637534720061
C	4.99837247169032	16.01389706840477	6.83170067575305
H	5.90120522151553	16.19898133439224	6.22764619819520
C	7.62548557448417	12.37067852644903	8.75061472578083
C	8.16422317827019	11.80606428196346	10.01742069748187
C	7.55379034765885	10.61370886303026	10.54757865046966
C	0.51527481729098	11.27567493697255	10.87834162210441
H	0.21615171987205	12.12594143009705	11.52913542433037
C	9.25281843585175	10.69563763420464	12.34520324172177
H	9.67578247208461	10.24189550739296	13.25608372378860
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H	1.87054231005064	15.38092242282864	9.06568329769902
C	3.77428638874465	7.05482217019971	11.20081347348479
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C	5.86385048770148	7.74927953607182	7.51744111323231
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H	6.19400890227985	7.06396549391947	6.71039206154588
H	5.30132419157978	8.56606862991210	7.01429403213051
C	9.81096096851806	11.87392026192465	11.82769562600606
H	10.66771347669808	12.35976198979712	12.31683144736256
C	6.46438022540069	13.28962509546506	6.33466248072464
H	5.97626095687050	13.61200631779866	5.40620425251685
C	3.95632733182725	16.95728730821950	6.85101626032274
H	4.02069677831880	17.87731290496854	6.25257816016505
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H	9.68042610626708	13.32729101727795	10.20784805783342
C	-0.24513366988109	11.35824936114225	9.54642405162222
H	-1.30793696311468	11.06701062287054	9.68180566822937
H	-0.23178225645450	12.37518795829935	9.11014690103739
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C	5.00268800120729	6.98114496879198	8.52556106535725
H	4.09081816661708	6.63013972335741	7.99704441871331
C	7.99541684329434	11.79283537066454	7.50424284390778
H	8.71667486041288	10.96226286573885	7.49841840414873
C	2.60609636461629	6.19212098815795	10.70739119765440

H	2.84108724393450	5.63127114354510	9.78082877648440
H	2.31084271529215	5.45492957716395	11.48290863818906
H	1.72027843691372	6.83130541447490	10.50707268704995
C	4.59727470038653	12.09441801461496	12.07958433344815
H	4.64032472029437	13.13218115509431	11.69035661312036
H	5.13918825762570	12.07333805659214	13.04703867289465
H	5.15819364301766	11.44511361768570	11.37470868679136
C	5.75214191363740	5.76186781504671	9.07169309941155
H	5.11178766858191	5.11329594530509	9.70015416788080
H	6.10121993578695	5.13784755486007	8.22349616263862
H	6.64452695687688	6.05456631832890	9.66493001564192
C	3.37593664384467	7.84280858558045	12.45223916639264
H	2.55421019937008	8.54448998731215	12.21206507246315
H	3.02309597116129	7.15430198114655	13.24847117794842
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C	2.85242351829971	16.70918863304073	7.68353150906525
H	2.03390474291133	17.44484586914199	7.74048904749045
C	0.22470179532036	9.95364065397908	11.60139290898378
H	0.55433741453720	9.09505277061040	10.97815485888579
H	0.75141359839104	9.87801819408161	12.57340417735306
H	-0.86207720266738	9.83947354630216	11.79684901175738
C	2.36519816313228	12.52869354717407	13.22283573222079
H	1.35386983646820	12.13669432655790	13.45028183562132
H	2.90842511232913	12.62083104420564	14.18699260586584
H	2.25077486370544	13.55546333865723	12.81638587857736
H	2.55458334231148	10.20960088263044	7.73149652488742

*

Input file for the AIM analysis (single-point) of 3

! UKS BP RI ZORA-def2-SVP SARC/J TightSCF SlowConv D3BJ UNO UCO ZORA

%pal nprocs 24

end

%scf maxiter 2000

end

%basis newgto La "SARC-ZORA-TZVP" end

end

*xyz 0 1

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N	3.62230299303315	7.24765507493059	4.91008406998630
N	0.85214737533918	10.45949696913723	3.96633447556962
C	2.34030512474432	5.69753576084309	6.30334197460223
C	3.50703347718967	6.01113590443795	5.50819255480620
C	4.78519002450059	7.40313400167346	4.05896537660459
H	4.80867470198740	6.66134062716254	3.22010355190704
H	5.73682996521215	7.24377902498841	4.62120320064448
C	0.59325276415850	7.10923167139912	5.14891369784731
H	0.89006582141157	6.65813944741763	4.19116599405155
C	1.22505423751038	6.67130896342186	6.34698579528591
C	4.13643804067552	8.90833161002251	1.63884673861171
H	4.11616098798021	9.93980419526295	1.22894561372224
C	-0.87585452033861	10.45887185332361	2.17596091891988
H	-0.47840239918038	11.37895632825108	1.72895516107048
C	1.33015406845770	11.67875593542864	3.33955260511831
H	0.57192783497590	12.50232766289570	3.36373616741616
H	1.56115571418637	11.52170116811310	2.25572641106972
C	2.28623010391272	4.52743101447905	7.07772609006105
H	1.38411253580579	4.34406204105273	7.68336165710960
C	-0.34163246240765	8.16664271793866	5.15363364962239
C	-0.88060783568726	8.72886218261072	3.88589776878342
C	-0.27149921324568	9.92180497505648	3.35526073928754
C	6.76710667972133	9.25889951291616	3.02225019372311
H	7.06686027523730	8.40509431902022	2.37630665513692
C	-1.96991440404769	9.83684846816102	1.55723528819444
H	-2.39337327244406	10.28972116445243	0.64611389568474
C	4.52057564255766	5.00088517194861	5.46038449746080
H	5.41126359330232	5.15438851362960	4.83790500902265
C	3.50849247816962	13.47962919588667	2.69875503666268
H	2.64591545959094	14.13783613559619	2.45653848229866
C	1.42021808465170	12.78923814441795	6.38413349336427
H	0.51486420245550	12.35431623605852	5.91207445025785
H	1.09263100660362	13.47489100510983	7.19193764181748
H	1.98168002750541	11.97112984747435	6.88641736582189
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H	-3.38203535185982	8.17037504737180	1.58542642358350
C	0.82477597823482	7.25721413803261	7.57092750256715
H	1.31802557169702	6.94231017276011	8.49928927529759
C	3.32745390945878	3.58307858637832	7.05815280255473
H	3.26317391577734	2.66398502272252	7.65804042428550
C	-0.15778456280170	8.26777260077812	7.59543887941942

H	-0.46021328178887	8.70699476245062	8.55606160571243
C	-1.96953381603998	8.11866693427856	3.24867985983973
H	-2.39451788023770	7.20536376110659	3.69545429963602
C	7.52695367539522	9.18454953695564	4.35484147452221
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H	-1.43102195515737	9.57898289199646	6.40287845923045
C	4.67818780965743	14.34033369238674	3.19176762393351
H	4.44326124057353	14.90325175132865	4.11715763348437
H	4.97670981706987	15.07539765472001	2.41551264988149
H	5.56176401399077	13.69910354115183	3.39503899985415
C	2.68436090456191	8.44232417195630	1.82184886726385
H	2.63991923916205	7.40498095516354	2.21210038600998
H	2.14220429723027	8.46310286391103	0.85454520567301
H	2.12446694211324	9.09304505147708	2.52624062464095
C	1.53410184636559	14.77632928551580	4.82963603385369
H	2.17451147986798	15.42335302686859	4.19965202791556
H	1.18731324912714	15.40162539831719	5.67784618838282
H	0.64037335030464	14.48479677187292	4.23786227903333
C	3.90532253326840	12.69012110592564	1.44786296854770
H	4.72721755862372	11.98860641946321	1.68788818274448
H	4.25727511921988	13.37755674963444	0.65031300818444
H	3.06581696429408	12.09786225421436	1.03412819062371
C	4.43030991490901	3.82887825088805	6.22360231460660
H	5.24808515457843	3.09239817296915	6.16662083913905
C	7.05738452155339	10.57739866804363	2.29270964347583
H	6.72505144204636	11.43840029458617	2.91112221867304
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H	8.14439493773212	10.69220153759311	2.09896003475062
C	4.91572260912293	8.00303841676635	0.67922377242108
H	5.92812192073715	8.39252224229486	0.45218617863763
H	4.37290381263438	7.91141263477989	-0.28520816365519
H	5.02755950852124	6.97633484014590	1.08650040994913
H	4.73331796972131	10.33071222907187	6.16726041973389
La	4.88043073629265	11.20185689537251	8.30367826648881
Ni	3.02650204394458	9.79775670938629	9.27288942255622
P	4.36037396558220	8.19736794786323	9.82050715240694
P	2.36651406079937	11.40709230179439	10.55902801034692
N	3.66124850613925	13.28909795407091	8.99327757283157
N	6.42966710756418	10.07730024169477	9.93611912994246

C	4.94426876188685	14.84256529218270	7.60431579488598
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H	1.54645985592775	13.29042623110956	9.27770812951815
C	6.68983968547295	13.42739976047507	8.75764001513983
H	6.39148691953494	13.87493635157377	9.71655224262295
C	6.06028834391438	13.86977635747245	7.56005450582654
C	3.14591724348387	11.62594461972459	12.26203009161866
H	3.16783602407342	10.59397571059533	12.67064604326017
C	8.15757201718939	10.07553451737884	11.72666791080401
H	7.75876050476746	9.15609304275512	12.17374376701126
C	5.95055832844231	8.85851411424146	10.56309291717369
H	6.70897275681306	8.03511513275292	10.54080266513659
H	5.71773804460898	9.01657124723630	11.64637534720061
C	4.99837247169032	16.01389706840477	6.83170067575305
H	5.90120522151553	16.19898133439224	6.22764619819520
C	7.62548557448417	12.37067852644903	8.75061472578083
C	8.16422317827019	11.80606428196346	10.01742069748187
C	7.55379034765885	10.61370886303026	10.54757865046966
C	0.51527481729098	11.27567493697255	10.87834162210441
H	0.21615171987205	12.12594143009705	11.52913542433037
C	9.25281843585175	10.69563763420464	12.34520324172177
H	9.67578247208461	10.24189550739296	13.25608372378860
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C	3.77428638874465	7.05482217019971	11.20081347348479
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C	5.86385048770148	7.74927953607182	7.51744111323231
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H	5.30132419157978	8.56606862991210	7.01429403213051
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H	10.66771347669808	12.35976198979712	12.31683144736256
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C	7.44626154816052	12.27862176218499	6.30822936743231
H	7.75107579373624	11.84429519124089	5.34612710339076
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H	9.68042610626708	13.32729101727795	10.20784805783342
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H	-1.30793696311468	11.06701062287054	9.68180566822937

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C	5.00268800120729	6.98114496879198	8.52556106535725
H	4.09081816661708	6.63013972335741	7.99704441871331
C	7.99541684329434	11.79283537066454	7.50424284390778
H	8.71667486041288	10.96226286573885	7.49841840414873
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H	2.84108724393450	5.63127114354510	9.78082877648440
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H	1.72027843691372	6.83130541447490	10.50707268704995
C	4.59727470038653	12.09441801461496	12.07958433344815
H	4.64032472029437	13.13218115509431	11.69035661312036
H	5.13918825762570	12.07333805659214	13.04703867289465
H	5.15819364301766	11.44511361768570	11.37470868679136
C	5.75214191363740	5.76186781504671	9.07169309941155
H	5.11178766858191	5.11329594530509	9.70015416788080
H	6.10121993578695	5.13784755486007	8.22349616263862
H	6.64452695687688	6.05456631832890	9.66493001564192
C	3.37593664384467	7.84280858558045	12.45223916639264
H	2.55421019937008	8.54448998731215	12.21206507246315
H	3.02309597116129	7.15430198114655	13.24847117794842
H	4.21487022690951	8.43461082565052	12.86772831074372
C	2.85242351829971	16.70918863304073	7.68353150906525
H	2.03390474291133	17.44484586914199	7.74048904749045
C	0.22470179532036	9.95364065397908	11.60139290898378
H	0.55433741453720	9.09505277061040	10.97815485888579
H	0.75141359839104	9.87801819408161	12.57340417735306
H	-0.86207720266738	9.83947354630216	11.79684901175738
C	2.36519816313228	12.52869354717407	13.22283573222079
H	1.35386983646820	12.13669432655790	13.45028183562132
H	2.90842511232913	12.62083104420564	14.18699260586584
H	2.25077486370544	13.55546333865723	12.81638587857736
H	2.55458334231148	10.20960088263044	7.73149652488742

*

Input file for the geometry optimization of 4

! UKS BP RI def2-SVP Def2/J TightSCF SlowConv D3BJ UNO UCO

! Opt

%pal nprocs 24

end

%scf maxiter 2000

end

*xyz 0 1

La	1.853835	2.033032	12.612467
Ni	2.071227	-0.408643	13.107723
P	2.730832	-0.825550	11.070829
P	0.029764	-0.531907	13.833880
N	0.005587	2.187459	14.275506
N	1.480641	1.465478	10.165504
N	3.421413	-0.031268	14.492094
N	4.021242	2.119324	13.823016
C	-0.561593	3.308079	14.871468
C	-1.336904	3.292976	16.068221
H	-1.485841	2.482243	16.498897
C	-0.452516	0.926163	14.873193
H	-1.418101	0.947488	14.968605
H	-0.067134	0.831418	15.758549
C	0.793314	2.159819	9.186029
C	0.845697	4.150178	10.706974
C	1.813838	0.101235	9.758539
H	2.357037	0.133497	8.955197
H	0.996757	-0.375641	9.545658
C	0.419788	1.640828	7.918574
H	0.673892	0.774958	7.692001
C	0.399478	3.507281	9.439520
C	2.397478	-2.582007	10.562122
H	1.424383	-2.690944	10.612959
C	-0.374370	4.591863	14.283438
C	-1.578248	0.628707	11.850270
H	-0.797640	0.721152	11.298522
H	-1.657343	1.394839	12.423091
H	-2.357330	0.563157	11.293521
C	0.009890	4.192001	11.833026
H	-0.863593	3.880729	11.764601
C	-1.452337	-0.641408	12.707311
H	-2.254688	-0.713839	13.264491
C	-1.873924	4.447528	16.606243
H	-2.370027	4.394749	17.391134
C	4.137539	1.061989	14.621426
H	4.761711	1.098436	15.309990
C	-0.306103	2.383144	7.018423
H	-0.513022	2.012876	6.190214
C	-0.236707	-1.904755	15.085297
H	0.326225	-1.674738	15.853375

C	1.758830	5.209549	13.134969
H	2.079626	5.546479	13.940018
C	0.464793	4.693875	13.059094
C	2.977108	-3.588775	11.560566
H	2.645292	-4.466686	11.357705
H	2.713853	-3.344622	12.450337
H	3.934725	-3.586025	11.497038
C	4.492458	-0.521155	10.539705
H	4.613108	-0.885832	9.638898
C	-1.691424	5.682112	16.004418
H	-2.071077	6.451226	16.363375
C	-0.371563	4.209169	8.525573
H	-0.650826	5.070343	8.736419
C	-0.922320	5.736846	14.845602
H	-0.771004	6.558816	14.437740
C	-1.393730	-1.872892	11.788191
H	-2.126953	-1.844039	11.168138
H	-1.454296	-2.670694	12.317814
H	-0.565367	-1.871739	11.303385
C	2.146501	4.659428	10.820787
H	2.723030	4.619376	10.091474
C	-0.737229	3.662558	7.304678
H	-1.255561	4.142423	6.700335
C	4.776518	0.975720	10.500043
H	4.177299	1.398285	9.880646
H	5.683037	1.121033	10.217564
H	4.650104	1.349252	11.374518
C	2.575522	5.217723	11.998571
H	3.419105	5.607092	12.041078
C	2.776761	-2.945555	9.134296
H	3.732750	-2.960008	9.050816
H	2.412088	-2.294741	8.530384
H	2.423955	-3.813040	8.920501
C	3.641009	-1.115817	15.483640
H	3.040401	-1.851455	15.240944
C	3.248137	-0.667553	16.883876
H	3.218696	-1.429138	17.468043
H	2.382673	-0.252287	16.856768
H	3.894446	-0.037947	17.212000
C	4.984656	3.214795	14.029947
H	4.791365	3.880528	13.337590
C	0.282056	-3.252942	14.583489
H	-0.334216	-3.615775	13.942778
H	0.368767	-3.858892	15.322734

H	1.139762	-3.131589	14.167660
C	5.055982	-1.662991	15.431908
H	5.670932	-0.988778	15.730165
H	5.268972	-1.913472	14.529773
H	5.123190	-2.432295	16.001883
C	-1.653321	-2.035749	15.638839
H	-1.939913	-1.189307	15.988587
H	-1.664172	-2.692311	16.338681
H	-2.247681	-2.308727	14.935134
C	5.487567	-1.202715	11.476069
H	5.312034	-0.934835	12.381394
H	6.381283	-0.947013	11.235029
H	5.397061	-2.155778	11.401764
C	4.785217	3.921453	15.361206
H	4.986339	3.315520	16.077809
H	3.874318	4.213647	15.434098
H	5.370535	4.680936	15.410266
C	6.414236	2.792946	13.814394
H	6.978041	3.570421	13.795649
H	6.487657	2.325839	12.978253
H	6.689653	2.215144	14.528893

*

Input file for the natural localized molecular orbital (NLMO) analysis of 4

! UKS BP RI def2-SVP Def2/J TightSCF SlowConv D3BJ UNO UCO

%pal nprocs 24
end

%NBO NBOKEYLIST = "\$NBO NBO NLMO AONLMO=C AONBO=P \$END"
end

%scf maxiter 2000
end

*xyz 0 1

La	1.85137776873639	1.98302449884173	12.52900730650471
Ni	2.07339239757919	-0.47256664115025	13.02861284494587
P	2.71944722178044	-0.79598507178667	10.97958004566941
P	0.05407730237564	-0.58603471737991	13.78582397346663
N	0.02625957536184	2.16230185963359	14.23296084487671
N	1.41645136195370	1.44674620698917	10.07447778519927
N	3.45745432255380	-0.10910057539429	14.44347358120952

N	4.05552052592678	2.04867213143366	13.76498328961268
C	-0.44263182892817	3.29884134674680	14.86739516536734
C	-1.20358435142118	3.27598720248325	16.07852038314958
H	-1.47052774419086	2.31325946746714	16.53309215423092
C	-0.45274553907319	0.91497007933079	14.79841847082916
H	-1.56816317199326	0.89834177540920	14.90500524907308
H	-0.04895944773183	0.72738857840383	15.82797026308424
C	0.64345022052586	2.14801140742603	9.16678698370986
C	0.82739997259332	4.15358394565535	10.66793967178566
C	1.74382732147738	0.09555570662741	9.65919249951312
H	2.31189491336070	0.05964618342010	8.69275704407181
H	0.82806747151889	-0.53190808864386	9.49401502273928
C	0.12989795418610	1.59680508139889	7.95144873110529
H	0.37690957236832	0.56346659361978	7.67499758038400
C	0.28058321099197	3.51481634401453	9.44053376436243
C	2.48712494737969	-2.59925202900681	10.47041794822734
H	1.39303847828586	-2.63194289643675	10.27152440274547
C	-0.13912249679052	4.60926119116031	14.34057494884285
C	-1.48939706386017	0.57629730664800	11.75355173233406
H	-0.56563570521867	0.73804079958964	11.15537766326755
H	-1.64098488596754	1.46883843478847	12.39084648376473
H	-2.33252171982155	0.51466950664959	11.03477573684661
C	0.07089284979405	4.21154581215247	11.85920104335746
H	-0.95428944140500	3.81297223056930	11.86218192611970
C	-1.39488985036723	-0.71043867798772	12.58380771273914
H	-2.31614839475652	-0.80732817091553	13.19776425251569
C	-1.59534193077878	4.45292936115229	16.73045037172476
H	-2.17339112047939	4.37566875778739	17.66558177298312
C	4.16608822030734	1.00206390182010	14.59551663967253
H	4.86852630649272	1.06673666364504	15.45947333259482
C	-0.69884926276711	2.33816375231115	7.09746404716010
H	-1.07338261669076	1.86377883647032	6.17582796883101
C	-0.26964760644086	-1.93452233368208	15.07576191380745
H	0.31201864916803	-1.54574454489852	15.94053022039504
C	1.93343514464294	5.24143943488489	13.04223676901347
H	2.36910943372664	5.63278796554142	13.97311172512633
C	0.62067299245370	4.71302391138904	13.07018275185222
C	2.76614869388017	-3.52208031796600	11.66298001828967
H	2.45692586656139	-4.56581589389014	11.44428707129430
H	2.20124790538453	-3.16718237011221	12.54827726197649
H	3.84159217360270	-3.53642885373238	11.93177836013312
C	4.49567311063541	-0.38694513032091	10.48604934349514
H	4.64906675416481	-0.78717303440823	9.46043716247273
C	-1.25629611459748	5.71644468236556	16.22084689690882

H	-1.56331658648715	6.63838942395089	16.73561505788040
C	-0.55483658407450	4.23720996272826	8.57771108223878
H	-0.80507065941015	5.27847626734511	8.83756184252571
C	-0.52231820805485	5.77406504638617	15.02396417203529
H	-0.25730528577570	6.74912831667600	14.58380941473700
C	-1.23595675940805	-1.94265980937717	11.68919019139044
H	-1.99812443845354	-1.94773186880209	10.88238414214839
H	-1.33201748535706	-2.89270425634806	12.25133443903200
H	-0.23224647775382	-1.93167307219961	11.21586277135995
C	2.15601685846898	4.65810003281764	10.68038366919441
H	2.75259275606389	4.59823049591902	9.75823801318682
C	-1.05879011786959	3.66108681669668	7.39743091026980
H	-1.71182675122219	4.23845818958297	6.72693339846794
C	4.70064924495117	1.13503490546183	10.45186458646125
H	3.98537384572003	1.64583656105425	9.77674968800129
H	5.73060512012132	1.37465179946045	10.11217299619041
H	4.59499122287027	1.55926225090305	11.47632148603482
C	2.68816699810069	5.22601856105496	11.84979581778428
H	3.70804432047913	5.64034807443991	11.84258472069982
C	3.22172908978077	-3.02061526891197	9.19438708724860
H	4.32079940192237	-3.04071242564495	9.34227102570367
H	3.00426826929910	-2.34495787689897	8.34254098434628
H	2.91402737302240	-4.04481342215772	8.89377391575961
C	3.52810436560535	-1.12522193565140	15.51180555525445
H	2.87868164050969	-1.95744687233309	15.16575561290491
C	2.93726483444558	-0.60361104996380	16.83049527513316
H	2.81879186739994	-1.41793586821391	17.57471312082886
H	1.94395577603817	-0.14624352786164	16.64588747297474
H	3.58472303888126	0.17739111368139	17.28032561901895
C	4.94390782932305	3.19921193429230	13.99358281966348
H	4.70981528323216	3.91997949183975	13.17966175922416
C	0.33446444273506	-3.28821733389225	14.68494396199061
H	-0.16213426794173	-3.72719533726962	13.79658679327418
H	0.22981063262370	-4.01484812569400	15.51813774467648
H	1.41327385111204	-3.19763295236217	14.45069241901451
C	4.94116974926614	-1.70366687861658	15.68119921356459
H	5.65641847186448	-0.93828350840307	16.04712372669407
H	5.31974576386039	-2.08790917444740	14.71299424936226
H	4.94270827793868	-2.53688533683247	16.41366561496597
C	-1.73887808920526	-2.06505906160674	15.49496861243614
H	-2.18588195158695	-1.09259463033536	15.78173337085278
H	-1.82958333703887	-2.74413718424827	16.36929456625654
H	-2.35645799953885	-2.49729968818090	14.68100884493437
C	5.46890829966228	-1.05221423746777	11.46722554914802

H	5.20636138377404	-0.76957518516845	12.50810856901511
H	6.51295192536991	-0.73017839226738	11.26841337678827
H	5.44350501765459	-2.15840534160981	11.40014966225582
C	4.64681188068804	3.90822472830985	15.32738497467470
H	4.91591399910473	3.26656314244255	16.19215671316244
H	3.56569711769562	4.14056261209472	15.41178857540468
H	5.21981023777256	4.85398726301550	15.42049039857010
C	6.43159676143941	2.83410381528818	13.85096043000873
H	7.07475739851745	3.73583265125683	13.91758552411116
H	6.61935739667337	2.34167851790388	12.87589818152828
H	6.75285290869994	2.13425703805042	14.65040714622618

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Input file for the AIM analysis (single-point) of 4

! UKS BP RI ZORA-def2-SVP SARC/J TightSCF SlowConv D3BJ UNO UCO ZORA

%pal nprocs 24

end

%scf maxiter 2000

end

%basis newgto La "SARC-ZORA-TZVP" end

end

*xyz 0 1

La	1.85137776873639	1.98302449884173	12.52900730650471
Ni	2.07339239757919	-0.47256664115025	13.02861284494587
P	2.71944722178044	-0.79598507178667	10.97958004566941
P	0.05407730237564	-0.58603471737991	13.78582397346663
N	0.02625957536184	2.16230185963359	14.23296084487671
N	1.41645136195370	1.44674620698917	10.07447778519927
N	3.45745432255380	-0.10910057539429	14.44347358120952
N	4.05552052592678	2.04867213143366	13.76498328961268
C	-0.44263182892817	3.29884134674680	14.86739516536734
C	-1.20358435142118	3.27598720248325	16.07852038314958
H	-1.47052774419086	2.31325946746714	16.53309215423092
C	-0.45274553907319	0.91497007933079	14.79841847082916
H	-1.56816317199326	0.89834177540920	14.90500524907308
H	-0.04895944773183	0.72738857840383	15.82797026308424
C	0.64345022052586	2.14801140742603	9.16678698370986
C	0.82739997259332	4.15358394565535	10.66793967178566
C	1.74382732147738	0.09555570662741	9.65919249951312

H	2.31189491336070	0.05964618342010	8.69275704407181
H	0.82806747151889	-0.53190808864386	9.49401502273928
C	0.12989795418610	1.59680508139889	7.95144873110529
H	0.37690957236832	0.56346659361978	7.67499758038400
C	0.28058321099197	3.51481634401453	9.44053376436243
C	2.48712494737969	-2.59925202900681	10.47041794822734
H	1.39303847828586	-2.63194289643675	10.27152440274547
C	-0.13912249679052	4.60926119116031	14.34057494884285
C	-1.48939706386017	0.57629730664800	11.75355173233406
H	-0.56563570521867	0.73804079958964	11.15537766326755
H	-1.64098488596754	1.46883843478847	12.39084648376473
H	-2.33252171982155	0.51466950664959	11.03477573684661
C	0.07089284979405	4.21154581215247	11.85920104335746
H	-0.95428944140500	3.81297223056930	11.86218192611970
C	-1.39488985036723	-0.71043867798772	12.58380771273914
H	-2.31614839475652	-0.80732817091553	13.19776425251569
C	-1.59534193077878	4.45292936115229	16.73045037172476
H	-2.17339112047939	4.37566875778739	17.66558177298312
C	4.16608822030734	1.00206390182010	14.59551663967253
H	4.86852630649272	1.06673666364504	15.45947333259482
C	-0.69884926276711	2.33816375231115	7.09746404716010
H	-1.07338261669076	1.86377883647032	6.17582796883101
C	-0.26964760644086	-1.93452233368208	15.07576191380745
H	0.31201864916803	-1.54574454489852	15.94053022039504
C	1.93343514464294	5.24143943488489	13.04223676901347
H	2.36910943372664	5.63278796554142	13.97311172512633
C	0.62067299245370	4.71302391138904	13.07018275185222
C	2.76614869388017	-3.52208031796600	11.66298001828967
H	2.45692586656139	-4.56581589389014	11.44428707129430
H	2.20124790538453	-3.16718237011221	12.54827726197649
H	3.84159217360270	-3.53642885373238	11.93177836013312
C	4.49567311063541	-0.38694513032091	10.48604934349514
H	4.64906675416481	-0.78717303440823	9.46043716247273
C	-1.25629611459748	5.71644468236556	16.22084689690882
H	-1.56331658648715	6.63838942395089	16.73561505788040
C	-0.55483658407450	4.23720996272826	8.57771108223878
H	-0.80507065941015	5.27847626734511	8.83756184252571
C	-0.52231820805485	5.77406504638617	15.02396417203529
H	-0.25730528577570	6.74912831667600	14.58380941473700
C	-1.23595675940805	-1.94265980937717	11.68919019139044
H	-1.99812443845354	-1.94773186880209	10.88238414214839
H	-1.33201748535706	-2.89270425634806	12.25133443903200
H	-0.23224647775382	-1.93167307219961	11.21586277135995
C	2.15601685846898	4.65810003281764	10.68038366919441

H	2.75259275606389	4.59823049591902	9.75823801318682
C	-1.05879011786959	3.66108681669668	7.39743091026980
H	-1.71182675122219	4.23845818958297	6.72693339846794
C	4.70064924495117	1.13503490546183	10.45186458646125
H	3.98537384572003	1.64583656105425	9.77674968800129
H	5.73060512012132	1.37465179946045	10.11217299619041
H	4.59499122287027	1.55926225090305	11.47632148603482
C	2.68816699810069	5.22601856105496	11.84979581778428
H	3.70804432047913	5.64034807443991	11.84258472069982
C	3.22172908978077	-3.02061526891197	9.19438708724860
H	4.32079940192237	-3.04071242564495	9.34227102570367
H	3.00426826929910	-2.34495787689897	8.34254098434628
H	2.91402737302240	-4.04481342215772	8.89377391575961
C	3.52810436560535	-1.12522193565140	15.51180555525445
H	2.87868164050969	-1.95744687233309	15.16575561290491
C	2.93726483444558	-0.60361104996380	16.83049527513316
H	2.81879186739994	-1.41793586821391	17.57471312082886
H	1.94395577603817	-0.14624352786164	16.64588747297474
H	3.58472303888126	0.17739111368139	17.28032561901895
C	4.94390782932305	3.19921193429230	13.99358281966348
H	4.70981528323216	3.91997949183975	13.17966175922416
C	0.33446444273506	-3.28821733389225	14.68494396199061
H	-0.16213426794173	-3.72719533726962	13.79658679327418
H	0.22981063262370	-4.01484812569400	15.51813774467648
H	1.41327385111204	-3.19763295236217	14.45069241901451
C	4.94116974926614	-1.70366687861658	15.68119921356459
H	5.65641847186448	-0.93828350840307	16.04712372669407
H	5.31974576386039	-2.08790917444740	14.71299424936226
H	4.94270827793868	-2.53688533683247	16.41366561496597
C	-1.73887808920526	-2.06505906160674	15.49496861243614
H	-2.18588195158695	-1.09259463033536	15.78173337085278
H	-1.82958333703887	-2.74413718424827	16.36929456625654
H	-2.35645799953885	-2.49729968818090	14.68100884493437
C	5.46890829966228	-1.05221423746777	11.46722554914802
H	5.20636138377404	-0.76957518516845	12.50810856901511
H	6.51295192536991	-0.73017839226738	11.26841337678827
H	5.44350501765459	-2.15840534160981	11.40014966225582
C	4.64681188068804	3.90822472830985	15.32738497467470
H	4.91591399910473	3.26656314244255	16.19215671316244
H	3.56569711769562	4.14056261209472	15.41178857540468
H	5.21981023777256	4.85398726301550	15.42049039857010
C	6.43159676143941	2.83410381528818	13.85096043000873
H	7.07475739851745	3.73583265125683	13.91758552411116
H	6.61935739667337	2.34167851790388	12.87589818152828

H	6.75285290869994	2.13425703805042	14.65040714622618
*			

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