Electronic Supplementary Material (ESI) for Dalton Transactions.
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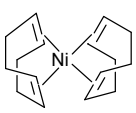
## I. General considerations

All manipulations were carried out using standard Schlenk techniques under inert atmosphere. Toluene, THF and pentane were dried by a solvent purification system (SPS-M-Braun). Commercial starting materials were purchased from Sigma-Aldrich, Strem and Alfa Aesar and used without further purification. NHC$^{IPr}$ [1], [Ni(DME)Cl$_2$][2], [Ni(dcpp)Cl$_2$][3] and **1**[4] were synthesized following published procedures. Deuterated solvents were purchased from Sigma-Aldrich or Eurisotop, freeze-pumped and stored over 4Å molecular sieves under argon. The $^1$H, $^{31}$P{$^1$H}, and $^{13}$C{$^1$H} NMR spectra were recorded on a Bruker AC 300 MHz instrument at 293 K unless otherwise stated. All chemical shifts are reported in ppm vs SiMe$_4$ and were determined with reference to residual solvent peaks. All coupling constants are given in Hertz. RPE spectra were recorded on a Bruker Elexsys E500. Elemental analyses were performed by Stephen Boyer (London Metropolitan University).

## II. Complex syntheses

### [Ni(COD)$_2$]

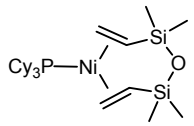


A solution containing COD (5mL, 40.77 mmol, 60eq) and reducing agent **1** (385 mg, 1.36 mmol, 2 eq) in 10 mL THF is cannulated into [Ni(DME)$Cl_2$] (150 mg, 0.68 mmol) in 5 mL THF at -20°C. The media is stirred until the temperature get to -10°C (3h). The suspension is then filtered and volatiles are evaporated. The orange oily solid is triturated 2 times with 2 mL of pentane and the yellow solid is dissolved in 2 mL of toluene and let overnight at -34°C to allow the formation of yellow crystals that were finally washed twice with cold pentane (101.7 mg, 54%).

$^1$H-NMR (300 MHz, $C_6D_6$) δ ppm 4.30 (s, 8H, CH=CH), 2.08 (s, 16H, $CH_2$).

$^{13}$C-NMR (75 MHz, $C_6D_6$) δ ppm 89.73 (CH=CH), 30.86 ($CH_2$).

## [Ni($PCy_3$)(($H_2C$=CHSi$Me_2$)$_2$O)] (2a)



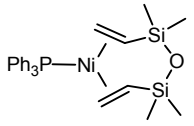

A solution containing $PCy_3$ (192 mg, 0.68 mmol, 1eq), reducing agent **1** (386 mg, 1.36 mmol, 2eq) and dvtms (254 mg, 1.36 mmol, 2eq) in 10 mL THF is cannulated into a solution of [Ni(DME)$Cl_2$] (150 mg, 0.68 mmol) in 5mL THF. The media is stirred 1h at 20°C. The clear yellow solution is the filtered and the volatiles are evaporated. The adding of 2mL of pentane led to the precipitation of the complex. The solid is finally washed with cold pentane (3x2mL). The complex **2a** is obtained as a yellow powder (278 mg, 77%). $^1$H, $^{31}$P, $^{13}$C NMR spectra are in accordance with those reported elsewhere.[5]

$^1$H-NMR (300 MHz, $C_6D_6$) δ ppm 2.97 (m, 2H, $CH_2$=CH), 2.63 (m, 4H, $CH_2$=CH), 2.07 (m, 3H, CH(Cy)), 1.47 (m, 30H, $CH_2$(Cy)), 0.61 (s, 6H, Me), 0.09 (s, 6H, Me).

$^{31}$P-NMR (121 MHz, $C_6D_6$) δ ppm 38.0.

$^{13}$C-NMR (75 MHz, $C_6D_6$) δ ppm 58.9 (CH, dvtms, $J_{C-P}$=7.1Hz), 55.7 ($CH_2$, dvtms, $J_{C-P}$= 4.9Hz), 36.6 (CH, PCy, $J_{C-P}$=15.6Hz), 30.9 (CH2, PCy), 28.2 ($CH_2$, PCy $J_{C-P}$=9.7Hz), 27.1 ($CH_2$, PCy), 2.4 (Me, dvtms $J_{C-P}$=1.8Hz), -0.1 (Me, dvtms).

## [Ni($PPh_3$)(($H_2C$=CHSi$Me_2$)$_2$O)] (2b)




A solution containing $PPh_3$ (179 mg, 0.68 mmol, 1eq), reducing agent **(1)** (386 mg, 1.36 mmol, 2eq) and dvtms (254 mg, 1.36 mmol, 2eq) in 10 mL THF is cannulated into a solution

of [Ni(DME)$Cl_2$] (150 mg, 0.68 mmol) in 5 mL de THF. The media is stirred 1h at 20°C. The clear yellow solution is the filtered and the volatiles are evaporated. The adding of 2mL of pentane led to the precipitation of the complex. The solid is finally washed with cold pentane (3x2mL). The complex **2b** is obtained as a yellow powder (161 mg, 43%). $^{1}$H, $^{31}$P, $^{13}$C NMR spectra are in accordance with those reported elsewhere.[5]

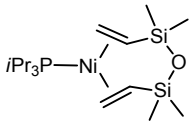
$^{1}$H-NMR (300 MHz, $C_6D_6$) δ ppm 7,4 (m, 6H, aromatics), 7.01 (m, 9H, aromatics), 3.11 (m, 2H, $CH_2$=CH), 2.94 (m, 2H, $CH_2$=CH), 2.77 (m, 2H, $CH_2$=CH), 0.50 (s, 6H, Me), 0.01 (s, 6H, Me).

$^{31}$P-NMR (121 MHz, $C_6D_6$) δ ppm 40.5.

$^{13}$C-NMR (75 MHz, $C_6D_6$) δ ppm 136.5 (C PPh, $J_{C-P}$=35.5Hz), 133.8 (CH PPh, $J_{C-P}$=11.7Hz), 129.5 (CH PPh, $J_{C-P}$=1.75Hz), 128.5 (C PPh, $J_{C-P}$=9.0Hz), 63.8 (CH, dvtms, $J_{C-P}$=2.40Hz), 62.6 ($CH_2$, dvtms, $J_{C-P}$=7.3Hz), 2.1($CH_3$, dvtms $J_{C-P}$=1.8Hz), -0.4 ($CH_3$, dvtms).

EA: Expected %C : 61.55 %H : 6.56 Obtained %C : 61.48 %H : 6.44

[Ni($PiPr_3$)(($H_2C$=CHSi$Me_2$)$_2$O)] (2c)



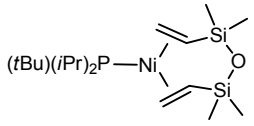

A solution containing $PiPr_3$ (109 mg, 0.68 mmol, 1eq), reducing agent **(1)** (386 mg, 1.36 mmol, 2 eq) and dvtms (254 mg, 0.68 mmol, 2 eq) in 10 mL THF is cannulated into a solution of [Ni(DME)$Cl_2$] (150 mg, 0.68 mmol) in 5mL THF. The media is stirred 1h at 20°C. The clear yellow solution is the filtered and the volatiles are evaporated. The adding of 2mL of pentane at -20°C led to the precipitation of the complex. The solid is finally washed with cold pentane (3x2mL). The complex **2c** is obtained as a yellow powder (65.6 mg, 24%).

$^{1}$H-NMR (300 MHz, $C_6D_6$) δ ppm 2.93 (m, 2H, CH=$CH_2$), 2.61 (m, 2H, CH=$CH_2$), 2.03 (sept, J=7.5Hz, 3H, CH(iPr)), 0.97 (dd, J=6.64, 11.77, 18H, $CH_3$(iPr)) 0.50 (s, 6H, Me), 0.01 (s, 6H, Me).

$^{31}$P-NMR (121 MHz, $C_6D_6$) δ ppm 50.5.

$^{13}$C-NMR (75 MHz, $C_6D_6$) δ ppm 58.5 (CH, dvtms, $J_{C-P}$=6.9Hz), 55.1 ($CH_2$, dvtms, $J_{C-P}$=4.4Hz), 26.3 (CH, PiPr, $J_{C-P}$=16.2Hz), 20.1 ($CH_3$, PiPr, $J_{C-P}$=1.9Hz), 2.4 (Me, dvtms $J_{C-P}$=1.8Hz), 0.0 (Me, dvtms).

[Ni(P(tBu)(iPr)$_2$)(($H_2C$=CHSi$Me_2$)$_2$O)] (2d)



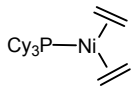
A solution containing P(tBu)(iPr)$_2$ (119 mg, 0.68mmol, 1eq), reducing agent **(1)** (386 mg, 1.36 mmol, 2 eq) and dvtms (254 mg, 0.68 mmol, 2 eq) in 10 mL THF is cannulated into a solution of [Ni(DME)Cl$_2$] (150 mg, 0.68 mmol) in 5mL THF. The media is stirred 1h at 20°C. The clear yellow solution is the filtered and the volatiles are evaporated. The adding of 2mL of pentane at -20°C led to the precipitation of the complex. The solid is finally washed with cold pentane (3x2mL). The complex **2d** is obtained as a yellow powder (124 mg, 43%). Crystals suitable for XRD analysis were obtained by slow diffusion of pentane into a solution of **2d** in THF at room temperature.

$^1$H-NMR (300 MHz, $C_6D_6$) δ ppm 2.68 (m, 6H, CH=CH$_2$), 2.20 (sept, 2H, CH(iPr)), 1.04 (m, 21H, CH$_3$(iPr+tBu)) 0.58 (s, 6H, Si-Me), 0.05 (s, 6H, Si-Me).

$^{31}$P-NMR (121 MHz, $C_6D_6$) δ ppm 50.5.

$^{13}$C-NMR (75 MHz, $C_6D_6$) δ ppm 58.2 (CH, dvtms), 53.9 (CH$_2$, dvtms), 33.6 (C, tBu, $J_{C-P}$=13.2Hz), 30.6 (CH3, tBu, $J_{C-P}$=4.9Hz), 25.5 (CH, iPr, $J_{C-P}$=12.7Hz), 22.4 (CH3, iPr, $J_{C-P}$=6.4Hz), 19.2 (CH3, iPr), 2.9(Me, dvtms $J_{C-P}$=1.8Hz), 0.4 (Me, dvtms).

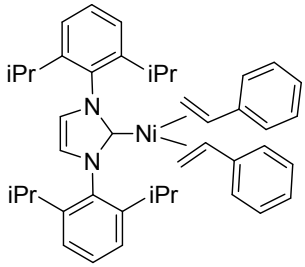
[Ni(PCy$_3$)(C$_2$H$_4$)$_2$] (3)




A solution containing PCy$_3$ (191 mg, 0.68 mmol, 1eq) and reducing agent **1** (386 mg, 1.34 mmol, 2eq) in 10 mL THF is cannulated into a suspension of [Ni(DME)Cl$_2$] (150 mg, 0.68 mmol) in 5 mL THF under 1 atm of C$_2$H$_4$ (bubling into the solution). The reaction mixture is stirred during 1h at RT. A clear yellow solution is obtained and analyzed by $^{31}$P NMR (no lock). The complex **3** was observed as unique product in the crude. THF was then evaporated and the oily residue was dissolved in 3mL of pentane. Placing the solution at -34°C led to the formation crystals suitable for XRD analysis.

$^{31}$P-NMR (121 MHz, no lock) δ ppm 39.1.

[Ni(NHCIPr)(CH$_2$=CHPh)$_2$] (4)



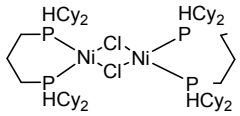

A solution of NHCIPr (319 mg, 0.82 mmol, 1.2eq) in 5mL THF is cannulated in a suspension of [Ni(DME)Cl$_2$] (150 mg, 0.68 mmol, 1eq), reducing agent **1** (386 mg, 1.36 mmol, 2eq) and

styrene (1 mL, 8.73 mmol, 12.8eq) in 10 mL THF à -20°C. The media is stirred 1h à -20°C and then 1h at 20°C. The solution is filtered and volatiles are evaporated. Adding of 2mL of pentane led to the precipitation of the complex. The suspension is placed 18h at -34°C and then filtered. Finally the complex is washed 3 times with 2 mL pentane at -20°C. The complex **4** is obtained as a yellow solid (198.1 mg, 44%). $^{1}$H, $^{13}$C NMR spectra are in accordance with those reported elsewhere.[6]

$^{1}$H-NMR (300 MHz, $C_6D_6$) δ ppm 0.98 (d(6.8Hz), 3H, $CH_3$, iPr), 1.00 (d(6.8Hz), 3H, $CH_3$, iPr), 1.11 (d(6.8Hz), 3H, $CH_3$, iPr), 1.37 (d(6.8Hz), 3H, $CH_3$, iPr), 2.67 (d(9.4 Hz), 2H, CHolef), 2.75 (d(12.7 Hz), 2H, CHolef), 2.88 (hept(6.8Hz), 2H, CH, iPr), 3.26 (dd(9.4Hz, 12.7 Hz), 2H, CHolef), 3.38 (hept(6.8Hz), 2H, CH, iPr), 6.12 (d(7.7Hz), 4H, CHarom), 6.69 (s, 2H, CHimid), 6.9-7.5 (m, 12H, CHarom).

$^{13}$C-NMR (75 MHz, $C_6D_6$) δ ppm 22.13, 22.80, 25.45, 27.06, 28.42, 29.05 ($CH_3$, iPr), 49.90, 72.99 (CH, iPr), 123.36, 124.09, 124.26, 124.46, 124.52, 126.58, 128.75, 129.83, 137.74, 146.05, 146.83, 146.89 (CHarom+imid), 204.1 (Ccarb).

### $[Ni(dcpp)Cl]_2$ (5)




A solution containing reducing agent **1** (150 mg, 0.53 mmol 2,4 eq) in 4mL THF is added to a suspension of $[Ni(dcpp)Cl_2]$ (126,0 mg, 0.22 mmol) in 4mL THF. The mixture is stirred 6h at 20°C. The clear yellow solution obtained is filtered and volatiles are evaporated. The pale red solid obtained is then washed 3 times with 4mL pentane (82.8 mg, 70%).

X-Band RPE at 20°C : g=2,14μB, $A_{iso}(^{31}P, n=2)$ = 74 G.

## III. Reduction mechanism investigations

A solution containing $PCy_3$ (19 mg, 0.068 mmol, 1eq), reducing agent **1** (37 mg, 0.136 mmol, 2eq) and dvtms (25 mg, 0.136 mmol, 2eq) in 0.4 mL toluene is added to $[Ni(DME)Cl_2]$ (15 mg, 0.068 mmol). The mixture is put in a closed and inert NMR tube and $^{31}$P NMR spectra are recorded after 5 and 30 minutes (Figure 1).

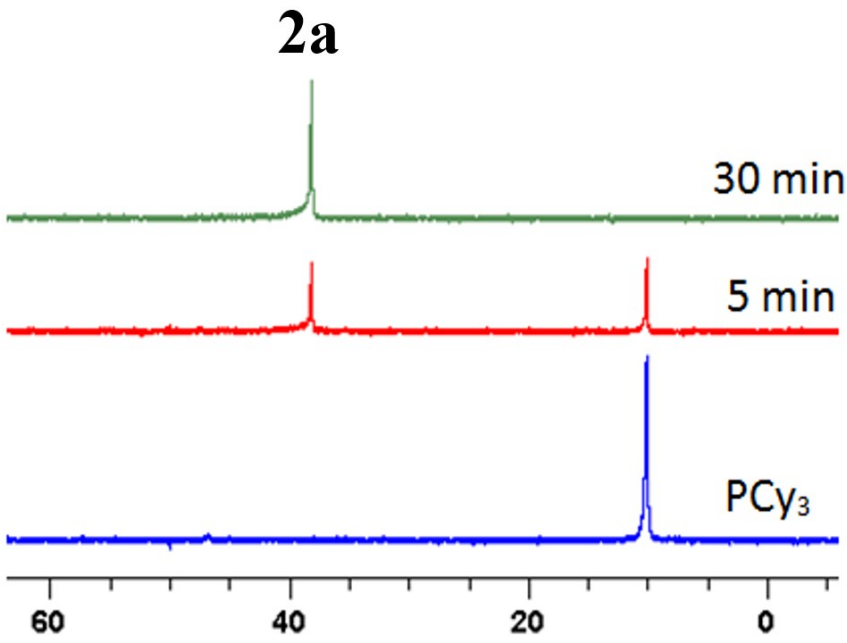



*Figure 1*

A solution containing $PCy_3$ (19 mg, 0.068 mmol, 1eq), reducing agent **1** (19 mg, 0.068 mmol, 1eq) and dvtms (25 mg, 0.136 mmol, 2eq) in 0.4 mL toluene is added to $[Ni(DME)Cl_2]$ (15 mg, 0.068 mmol). The mixture is put in a closed and inert NMR tube and $^{31}P$ NMR spectra are recorded after 5 and 30 minutes, 20h and after the adding of a second equivalent of **1**(Figure 2).

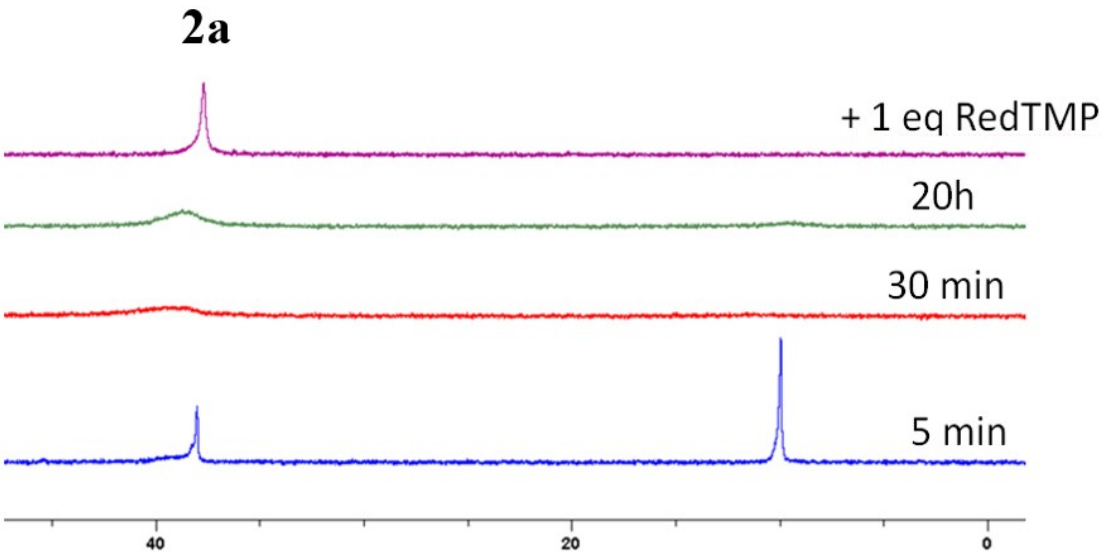



*Figure 2*

A solution containing $PCy_3$ (13 mg, 0.047mmol, 1eq), reducing agent **1** (13 mg, 0.047 mmol, 1eq) and dvtms (17 mg, 0.094 mmol, 2eq) in 10 mL toluene is added to $[Ni(DME)Cl_2]$ (15 mg, 0.068 mmol). The mixture is stirred at RT during 5h and then analyzed by EPR spectroscopy. EPR spectra at RT with two different simulations are presented in Figure 3.

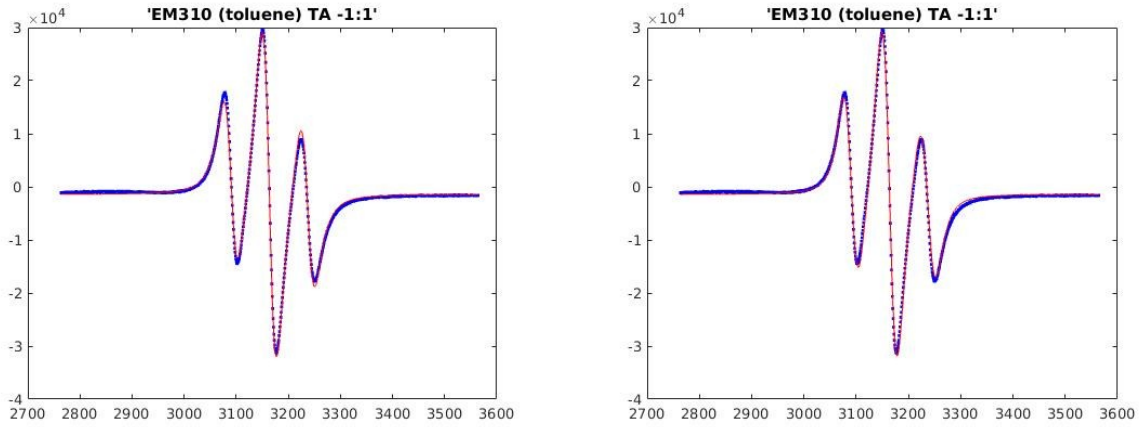



*Figure 3 EPR spectra at RT (Blue: experimental; red: simulated)*

# IV. Crystal data

## 1) Crystal data for complex 2d

CCDC Number : 1890834

| | |
|---|---|
| $C_{18}H_{41}NiOPSi_2$ | $Z = 2$ |
| $M_r = 419.38$ | $F(000) = 456$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.232$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 9.745$ (8) Å | Cell parameters from 8798 reflections |
| $b = 11.1357$ (11) Å | $\theta = 3.0$–$29.0°$ |
| $c = 11.7289$ (11) Å | $\mu = 1.04$ mm$^{-1}$ |
| $\alpha = 64.563$ (9)° | $T = 150$ K |
| $\beta = 81.647$ (7)° | Needle, brown |
| $\gamma = 80.817$ (7)° | 0.39 × 0.13 × 0.10 mm |
| $V = 1130.5$ (9) Å$^3$ | |

### *Data collection*

| | |
|---|---|
| Xcalibur, Atlas, Gemini ultra diffractometer | 5695 independent reflections |
| Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source | 4505 reflections with $I > 2.0\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.065$ |

| | |
|---|---|
| Detector resolution: 10.4685 pixels $mm^{-1}$ | $\theta_{max}$ = 29.3°, $\theta_{min}$ = 3.1° |
| Absorption correction: analytical *CrysAlis PRO* 1.171.38.46 (Rigaku Oxford Diffraction, 2015) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. | *h* = -13→13 |
| $T_{min}$ = 0.761, $T_{max}$ = 0.915 | *k* = -15→15 |
| 29745 measured reflections | *l* = -15→16 |

## *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: difference Fourier map |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.042 | Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = $1.0/[A_0*T_0(x) + A_1*T_1(x) \cdots + A_{n-1}]*T_{n-1}(x)]$ where $A_i$ are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta*F*/6*sigma*F*)$^2$]$^2$ $A_i$ are: 0.173E + 04 0.171E + 04 958. |
| $wR(F^2)$ = 0.075 | $(\Delta/\sigma)_{max}$ = 0.001 |
| *S* = 1.00 | $\Delta\rangle_{max}$ = 0.89 e Å$^{-3}$ |
| 5685 reflections | $\Delta\rangle_{min}$ = -1.00 e Å$^{-3}$ |
| 209 parameters | Extinction correction: Larson (1970), Equation 22 |
| 0 restraints | Extinction coefficient: 27 (5) |
| Primary atom site location: structure-invariant direct methods | |

## *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²) for (I)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.69978 (4) | 0.54637 (4) | 0.31137 (4) | 0.0167 |
| P2 | 0.82021 (8) | 0.72306 (7) | 0.21557 (7) | 0.0163 |
| C3 | 1.0117 (3) | 0.6754 (3) | 0.2335 (3) | 0.0217 |
| C4 | 1.0682 (3) | 0.5535 (3) | 0.2056 (3) | 0.0298 |
| H42 | 1.1477 | 0.5065 | 0.2522 | 0.0453* |
| H43 | 0.9992 | 0.4921 | 0.2296 | 0.0445* |
| H41 | 1.0963 | 0.5794 | 0.1183 | 0.0450* |

| | | | | |
|---|---|---|---|---|
| C5 | 1.1086 (3) | 0.7855 (3) | 0.1648 (3) | 0.0328 |
| H51 | 1.2017 | 0.7495 | 0.1883 | 0.0485* |
| H52 | 1.0799 | 0.8604 | 0.1873 | 0.0485* |
| H53 | 1.1092 | 0.8172 | 0.0737 | 0.0486* |
| H31 | 1.0186 | 0.6468 | 0.3234 | 0.0259* |
| C6 | 0.7684 (3) | 0.8487 (3) | 0.2892 (3) | 0.0200 |
| C7 | 0.7972 (4) | 0.9930 (3) | 0.2022 (3) | 0.0319 |
| H72 | 0.7419 | 1.0265 | 0.1306 | 0.0482* |
| H73 | 0.7699 | 1.0496 | 0.2472 | 0.0479* |
| H71 | 0.8939 | 0.9983 | 0.1735 | 0.0477* |
| C8 | 0.8467 (3) | 0.8056 (3) | 0.4082 (3) | 0.0276 |
| H81 | 0.8316 | 0.7132 | 0.4677 | 0.0406* |
| H83 | 0.8125 | 0.8639 | 0.4499 | 0.0409* |
| H82 | 0.9455 | 0.8101 | 0.3856 | 0.0407* |
| C9 | 0.6123 (3) | 0.8453 (3) | 0.3316 (3) | 0.0328 |
| H92 | 0.5923 | 0.7565 | 0.3922 | 0.0485* |
| H91 | 0.5817 | 0.9053 | 0.3722 | 0.0485* |
| H93 | 0.5564 | 0.8699 | 0.2609 | 0.0487* |
| C10 | 0.8158 (3) | 0.8299 (3) | 0.0411 (3) | 0.0234 |
| C11 | 0.6723 (3) | 0.9016 (3) | -0.0016 (3) | 0.0298 |
| H112 | 0.6848 | 0.9723 | -0.0846 | 0.0450* |
| H113 | 0.6247 | 0.9404 | 0.0536 | 0.0445* |
| H111 | 0.6155 | 0.8424 | -0.0068 | 0.0446* |
| C12 | 0.8749 (4) | 0.7499 (4) | -0.0365 (3) | 0.0338 |
| H121 | 0.8575 | 0.8046 | -0.1248 | 0.0504* |
| H122 | 0.9744 | 0.7253 | -0.0305 | 0.0509* |
| H123 | 0.8289 | 0.6694 | -0.0066 | 0.0507* |
| H101 | 0.8763 | 0.8977 | 0.0230 | 0.0274* |
| C13 | 0.7177 (3) | 0.3772 (3) | 0.4720 (3) | 0.0188 |
| C14 | 0.8148 (3) | 0.4627 (3) | 0.4610 (3) | 0.0218 |
| H141 | 0.9132 | 0.4393 | 0.4425 | 0.0260* |
| H142 | 0.8026 | 0.5098 | 0.5153 | 0.0264* |
| Si15 | 0.75969 (9) | 0.22171 (8) | 0.44688 (8) | 0.0185 |
| O16 | 0.6372 (2) | 0.2119 (2) | 0.36887 (19) | 0.0210 |
| Si17 | 0.55800 (9) | 0.33529 (8) | 0.25199 (8) | 0.0191 |
| C18 | 0.5259 (3) | 0.4866 (3) | 0.2840 (3) | 0.0218 |
| C19 | 0.5499 (3) | 0.6145 (3) | 0.1909 (3) | 0.0249 |
| H192 | 0.4898 | 0.6941 | 0.1933 | 0.0310* |
| H191 | 0.5808 | 0.6271 | 0.1045 | 0.0305* |
| H181 | 0.4529 | 0.4817 | 0.3525 | 0.0263* |

| | | | | |
|---|---|---|---|---|
| C20 | 0.3922 (3) | 0.2764 (3) | 0.2447 (3) | 0.0299 |
| H201 | 0.3413 | 0.3443 | 0.1768 | 0.0454* |
| H202 | 0.3343 | 0.2574 | 0.3226 | 0.0456* |
| H203 | 0.4112 | 0.1966 | 0.2301 | 0.0452* |
| C21 | 0.6687 (3) | 0.3699 (3) | 0.0996 (3) | 0.0291 |
| H213 | 0.6176 | 0.4316 | 0.0288 | 0.0443* |
| H212 | 0.7525 | 0.4055 | 0.0984 | 0.0443* |
| H211 | 0.6956 | 0.2881 | 0.0878 | 0.0439* |
| C22 | 0.9303 (3) | 0.2155 (3) | 0.3536 (3) | 0.0262 |
| H221 | 0.9527 | 0.1286 | 0.3530 | 0.0395* |
| H222 | 1.0038 | 0.2307 | 0.3890 | 0.0390* |
| H223 | 0.9276 | 0.2795 | 0.2683 | 0.0386* |
| C23 | 0.7607 (3) | 0.0723 (3) | 0.6020 (3) | 0.0254 |
| H233 | 0.7651 | -0.0079 | 0.5909 | 0.0387* |
| H232 | 0.8376 | 0.0671 | 0.6459 | 0.0381* |
| H231 | 0.6772 | 0.0793 | 0.6543 | 0.0384* |
| H131 | 0.6343 | 0.3764 | 0.5306 | 0.0227* |

*Atomic displacement parameters (Å²) for (I)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.01672 (19) | 0.01584 (19) | 0.0176 (2) | -0.00234 (14) | -0.00095 (15) | -0.00703 (15) |
| P2 | 0.0167 (4) | 0.0167 (4) | 0.0147 (4) | -0.0022 (3) | -0.0008 (3) | -0.0058 (3) |
| C3 | 0.0196 (15) | 0.0230 (15) | 0.0185 (14) | -0.0016 (12) | -0.0018 (11) | -0.0050 (12) |
| C4 | 0.0282 (17) | 0.0281 (17) | 0.0257 (17) | 0.0034 (14) | 0.0040 (13) | -0.0084 (14) |
| C5 | 0.0201 (16) | 0.0360 (19) | 0.0357 (19) | -0.0088 (14) | 0.0022 (14) | -0.0082 (16) |
| C6 | 0.0236 (15) | 0.0188 (14) | 0.0211 (15) | -0.0027 (12) | -0.0006 (12) | -0.0119 (12) |
| C7 | 0.049 (2) | 0.0186 (16) | 0.0284 (17) | -0.0047 (15) | -0.0031 (16) | -0.0101 (14) |
| C8 | 0.0338 (18) | 0.0302 (17) | 0.0229 (16) | -0.0043 (14) | -0.0035 (13) | -0.0143 (14) |
| C9 | 0.0278 (18) | 0.0365 (19) | 0.040 (2) | -0.0021 (14) | 0.0048 (15) | -0.0248 (17) |
| C10 | 0.0272 (16) | 0.0224 (15) | 0.0175 (14) | -0.0061 (12) | -0.0003 (12) | -0.0048 (12) |
| C11 | 0.0364 (19) | 0.0252 (17) | 0.0226 (16) | -0.0009 (14) | -0.0098 (14) | -0.0037 (13) |
| C12 | 0.0367 (19) | 0.046 (2) | 0.0197 (16) | -0.0031 (16) | 0.0001 (14) | -0.0156 (15) |
| C13 | 0.0250 (15) | 0.0148 (13) | 0.0119 (13) | -0.0025 (11) | -0.0014 (11) | -0.0012 (11) |
| C14 | 0.0257 (16) | 0.0216 (15) | 0.0181 (14) | -0.0016 (12) | -0.0089 (12) | -0.0065 (12) |
| Si15 | 0.0205 (4) | 0.0167 (4) | 0.0177 (4) | -0.0016 (3) | -0.0005 (3) | -0.0070 (3) |
| O16 | 0.0248 (11) | 0.0179 (10) | 0.0212 (11) | -0.0035 (8) | -0.0026 (9) | -0.0083 (9) |
| Si17 | 0.0199 (4) | 0.0181 (4) | 0.0200 (4) | -0.0031 (3) | -0.0010 (3) | -0.0082 (3) |
| C18 | 0.0160 (14) | 0.0227 (15) | 0.0286 (16) | -0.0018 (11) | -0.0041 (12) | -0.0119 (13) |
| C19 | 0.0233 (15) | 0.0207 (15) | 0.0318 (17) | 0.0021 (12) | -0.0161 (13) | -0.0094 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20 | 0.0308 (18) | 0.0265 (17) | 0.0346 (19) | -0.0079 (14) | -0.0080 (15) | -0.0115 (15) |
| C21 | 0.0347 (18) | 0.0250 (16) | 0.0235 (16) | -0.0004 (14) | 0.0023 (14) | -0.0087 (13) |
| C22 | 0.0250 (16) | 0.0280 (17) | 0.0270 (16) | -0.0001 (13) | -0.0015 (13) | -0.0140 (14) |
| C23 | 0.0267 (16) | 0.0222 (16) | 0.0251 (16) | -0.0018 (13) | -0.0043 (13) | -0.0073 (13) |

*Geometric parameters (Å, º) for (I)*

| | | | |
|---|---|---|---|
| Ni1—P2 | 2.2284 (10) | C11—H113 | 0.953 |
| Ni1—C13 | 2.018 (3) | C11—H111 | 0.952 |
| Ni1—C14 | 2.010 (3) | C12—H121 | 0.974 |
| Ni1—C18 | 2.030 (3) | C12—H122 | 0.969 |
| Ni1—C19 | 2.008 (3) | C12—H123 | 0.969 |
| P2—C3 | 1.874 (3) | C13—C14 | 1.402 (4) |
| P2—C6 | 1.908 (3) | C13—Si15 | 1.852 (3) |
| P2—C10 | 1.877 (3) | C13—H131 | 0.983 |
| C3—C4 | 1.530 (4) | C14—H141 | 0.971 |
| C3—C5 | 1.531 (4) | C14—H142 | 0.969 |
| C3—H31 | 0.971 | Si15—O16 | 1.649 (2) |
| C4—H42 | 0.960 | Si15—C22 | 1.862 (3) |
| C4—H43 | 0.962 | Si15—C23 | 1.865 (3) |
| C4—H41 | 0.947 | O16—Si17 | 1.647 (2) |
| C5—H51 | 0.960 | Si17—C18 | 1.849 (3) |
| C5—H52 | 0.968 | Si17—C20 | 1.864 (3) |
| C5—H53 | 0.970 | Si17—C21 | 1.867 (3) |
| C6—C7 | 1.535 (4) | C18—C19 | 1.404 (4) |
| C6—C8 | 1.541 (4) | C18—H181 | 0.981 |
| C6—C9 | 1.532 (4) | C19—H192 | 0.990 |
| C7—H72 | 0.966 | C19—H191 | 0.970 |
| C7—H73 | 0.969 | C20—H201 | 0.964 |
| C7—H71 | 0.955 | C20—H202 | 0.959 |
| C8—H81 | 0.984 | C20—H203 | 0.960 |
| C8—H83 | 0.964 | C21—H213 | 0.965 |
| C8—H82 | 0.965 | C21—H212 | 0.958 |
| C9—H92 | 0.969 | C21—H211 | 0.969 |
| C9—H91 | 0.965 | C22—H221 | 0.960 |
| C9—H93 | 0.974 | C22—H222 | 0.949 |
| C10—C11 | 1.532 (4) | C22—H223 | 0.948 |
| C10—C12 | 1.528 (4) | C23—H233 | 0.950 |
| C10—H101 | 0.965 | C23—H232 | 0.950 |
| C11—H112 | 0.959 | C23—H231 | 0.959 |
| | | | |

| | | | |
|---|---|---|---|
| P2—Ni1—C13 | 133.98 (9) | H113—C11—H111 | 109.3 |
| P2—Ni1—C14 | 93.36 (9) | C10—C12—H121 | 108.6 |
| C13—Ni1—C14 | 40.75 (11) | C10—C12—H122 | 111.2 |
| P2—Ni1—C18 | 137.27 (9) | H121—C12—H122 | 109.1 |
| C13—Ni1—C18 | 88.71 (12) | C10—C12—H123 | 110.1 |
| C14—Ni1—C18 | 129.03 (13) | H121—C12—H123 | 108.7 |
| P2—Ni1—C19 | 96.57 (10) | H122—C12—H123 | 109.1 |
| C13—Ni1—C19 | 129.30 (12) | Ni1—C13—C14 | 69.31 (16) |
| C14—Ni1—C19 | 167.35 (13) | Ni1—C13—Si15 | 114.46 (14) |
| C18—Ni1—C19 | 40.71 (12) | C14—C13—Si15 | 125.2 (2) |
| Ni1—P2—C3 | 111.96 (11) | Ni1—C13—H131 | 109.0 |
| Ni1—P2—C6 | 111.77 (10) | C14—C13—H131 | 115.8 |
| C3—P2—C6 | 104.49 (14) | Si15—C13—H131 | 113.6 |
| Ni1—P2—C10 | 120.98 (10) | C13—C14—Ni1 | 69.94 (16) |
| C3—P2—C10 | 102.59 (14) | C13—C14—H141 | 119.5 |
| C6—P2—C10 | 103.40 (13) | Ni1—C14—H141 | 115.8 |
| P2—C3—C4 | 112.7 (2) | C13—C14—H142 | 120.4 |
| P2—C3—C5 | 117.7 (2) | Ni1—C14—H142 | 115.0 |
| C4—C3—C5 | 109.7 (3) | H141—C14—H142 | 110.6 |
| P2—C3—H31 | 103.8 | C13—Si15—O16 | 108.82 (12) |
| C4—C3—H31 | 105.9 | C13—Si15—C22 | 112.98 (14) |
| C5—C3—H31 | 106.0 | O16—Si15—C22 | 107.91 (14) |
| C3—C4—H42 | 110.2 | C13—Si15—C23 | 110.37 (13) |
| C3—C4—H43 | 111.5 | O16—Si15—C23 | 107.51 (13) |
| H42—C4—H43 | 107.9 | C22—Si15—C23 | 109.09 (15) |
| C3—C4—H41 | 111.1 | Si15—O16—Si17 | 127.17 (13) |
| H42—C4—H41 | 108.0 | O16—Si17—C18 | 109.49 (12) |
| H43—C4—H41 | 108.1 | O16—Si17—C20 | 106.19 (14) |
| C3—C5—H51 | 108.9 | C18—Si17—C20 | 111.89 (14) |
| C3—C5—H52 | 111.2 | O16—Si17—C21 | 109.75 (13) |
| H51—C5—H52 | 108.9 | C18—Si17—C21 | 109.96 (15) |
| C3—C5—H53 | 110.5 | C20—Si17—C21 | 109.48 (16) |
| H51—C5—H53 | 108.4 | Si17—C18—Ni1 | 114.41 (15) |
| H52—C5—H53 | 108.8 | Si17—C18—C19 | 122.9 (2) |
| P2—C6—C7 | 115.3 (2) | Ni1—C18—C19 | 68.80 (16) |
| P2—C6—C8 | 110.1 (2) | Si17—C18—H181 | 114.1 |
| C7—C6—C8 | 107.0 (3) | Ni1—C18—H181 | 110.2 |
| P2—C6—C9 | 107.2 (2) | C19—C18—H181 | 117.2 |
| C7—C6—C9 | 109.4 (3) | C18—C19—Ni1 | 70.49 (17) |
| C8—C6—C9 | 107.6 (3) | C18—C19—H192 | 119.7 |

| | | | |
|---|---|---|---|
| C6—C7—H72 | 109.2 | Ni1—C19—H192 | 113.6 |
| C6—C7—H73 | 110.0 | C18—C19—H191 | 120.1 |
| H72—C7—H73 | 107.8 | Ni1—C19—H191 | 115.6 |
| C6—C7—H71 | 111.4 | H192—C19—H191 | 111.3 |
| H72—C7—H71 | 110.1 | Si17—C20—H201 | 110.2 |
| H73—C7—H71 | 108.3 | Si17—C20—H202 | 110.7 |
| C6—C8—H81 | 110.4 | H201—C20—H202 | 108.2 |
| C6—C8—H83 | 109.6 | Si17—C20—H203 | 110.5 |
| H81—C8—H83 | 108.7 | H201—C20—H203 | 108.6 |
| C6—C8—H82 | 110.6 | H202—C20—H203 | 108.6 |
| H81—C8—H82 | 108.6 | Si17—C21—H213 | 110.6 |
| H83—C8—H82 | 108.9 | Si17—C21—H212 | 111.5 |
| C6—C9—H92 | 111.1 | H213—C21—H212 | 109.4 |
| C6—C9—H91 | 110.3 | Si17—C21—H211 | 110.2 |
| H92—C9—H91 | 107.5 | H213—C21—H211 | 107.2 |
| C6—C9—H93 | 112.0 | H212—C21—H211 | 107.7 |
| H92—C9—H93 | 106.8 | Si15—C22—H221 | 109.5 |
| H91—C9—H93 | 109.0 | Si15—C22—H222 | 111.8 |
| P2—C10—C11 | 115.2 (2) | H221—C22—H222 | 107.6 |
| P2—C10—C12 | 111.4 (2) | Si15—C22—H223 | 111.6 |
| C11—C10—C12 | 109.1 (3) | H221—C22—H223 | 107.7 |
| P2—C10—H101 | 105.0 | H222—C22—H223 | 108.4 |
| C11—C10—H101 | 107.4 | Si15—C23—H233 | 111.3 |
| C12—C10—H101 | 108.3 | Si15—C23—H232 | 110.7 |
| C10—C11—H112 | 108.7 | H233—C23—H232 | 109.1 |
| C10—C11—H113 | 111.9 | Si15—C23—H231 | 109.7 |
| H112—C11—H113 | 107.9 | H233—C23—H231 | 108.4 |
| C10—C11—H111 | 111.2 | H232—C23—H231 | 107.4 |
| H112—C11—H111 | 107.6 | | |

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## 2) Crystal data for complex 3

CCDC Number : 1880112

*Crystal data*

$C_{22}H_{36}NiP$
$M_r = 390.21$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.5546\ (10)$ Å
$b = 17.1029\ (15)$ Å
$c = 13.3750\ (15)$ Å
$\beta = 100.00\ (1)°$
$V = 2152.4\ (4)$ Å$^3$
$Z = 4$

$F(000) = 844$
$D_x = 1.204$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8714 reflections
$\theta = 3.7–29.4°$
$\mu = 0.98$ mm$^{-1}$
$T = 150$ K
Needle, yellow
0.37 × 0.14 × 0.09 mm

*Data collection*

Xcalibur, Atlas, Gemini ultra diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.4685 pixels mm$^{-1}$
$\omega$ scans

Absorption correction: analytical *CrysAlis PRO* 1.171.38.46 (Rigaku Oxford Diffraction, 2015) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
$T_{min} = 0.799$, $T_{max} = 0.925$
26929 measured reflections
5472 independent reflections
4351 reflections with $I > 2.0\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 29.8°$, $\theta_{min} = 2.8°$
$h = -13 \rightarrow 13$
$k = -23 \rightarrow 23$
$l = -17 \rightarrow 18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.138$
$S = 1.01$
5461 reflections
217 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
H-atom parameters constrained

Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [weight] = $1.0/[A_0*T_0(x) + A_1*T_1(x) \cdots + A_{n-1}]*T_{n-1}(x)]$ where $A_i$ are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 1982) W = [weight] * $[1-(\text{delta}F/6*\text{sigma}F)^2]^2$ $A_i$ are: 672. 998. 511. 118.
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.00$ e Å$^{-3}$
$\Delta\rho_{min} = -0.98$ e Å$^{-3}$

*Special details*

*Experimental*. The crystal was placed in the cold stream of an Oxford Cryosystems open-flow nitrogen cryostat (Cosier & Glazer, 1986) with a nominal stability of 0.1 K.

Cosier, J. & Glazer, A·*M*., 1986. J. Appl. Cryst. 105–107.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ni1 | 0.59275 (5) | 0.38524 (3) | 0.59028 (3) | 0.0238 |
| P2 | 0.64091 (9) | 0.37330 (5) | 0.75551 (6) | 0.0188 |
| C3 | 0.5646 (4) | 0.4548 (2) | 0.8218 (3) | 0.0221 |
| C4 | 0.4029 (4) | 0.4590 (2) | 0.7891 (3) | 0.0255 |
| C5 | 0.3388 (4) | 0.5253 (2) | 0.8429 (3) | 0.0311 |
| C6 | 0.4059 (4) | 0.6040 (2) | 0.8259 (3) | 0.0327 |
| C7 | 0.5670 (4) | 0.6003 (2) | 0.8585 (3) | 0.0299 |
| C8 | 0.6315 (4) | 0.5344 (2) | 0.8034 (3) | 0.0269 |
| H82 | 0.7339 | 0.5324 | 0.8281 | 0.0318* |
| H81 | 0.6137 | 0.5451 | 0.7310 | 0.0317* |
| H72 | 0.6068 | 0.6496 | 0.8417 | 0.0360* |
| H71 | 0.5893 | 0.5920 | 0.9316 | 0.0358* |
| H62 | 0.3677 | 0.6447 | 0.8637 | 0.0388* |
| H61 | 0.3850 | 0.6169 | 0.7539 | 0.0388* |
| H52 | 0.3533 | 0.5141 | 0.9153 | 0.0380* |
| H51 | 0.2374 | 0.5278 | 0.8165 | 0.0383* |
| H41 | 0.3530 | 0.4260 | 0.7441 | 0.0332* |
| H31 | 0.5855 | 0.4436 | 0.8948 | 0.0268* |
| C9 | 0.8339 (3) | 0.3781 (2) | 0.8113 (3) | 0.0211 |
| C10 | 0.8764 (4) | 0.3834 (2) | 0.9267 (3) | 0.0266 |
| C11 | 1.0354 (4) | 0.4017 (2) | 0.9549 (3) | 0.0320 |
| C12 | 1.1261 (4) | 0.3414 (2) | 0.9112 (3) | 0.0331 |
| C13 | 1.0796 (4) | 0.3322 (2) | 0.7962 (3) | 0.0305 |
| C14 | 0.9207 (4) | 0.3142 (2) | 0.7699 (3) | 0.0236 |
| H141 | 0.8931 | 0.3115 | 0.6963 | 0.0290* |
| H142 | 0.9022 | 0.2639 | 0.8001 | 0.0290* |
| H132 | 1.0973 | 0.3810 | 0.7641 | 0.0369* |
| H131 | 1.1331 | 0.2910 | 0.7709 | 0.0369* |
| H122 | 1.2258 | 0.3578 | 0.9263 | 0.0401* |
| H121 | 1.1159 | 0.2916 | 0.9441 | 0.0398* |
| H112 | 1.0626 | 0.4029 | 1.0285 | 0.0387* |
| H111 | 1.0524 | 0.4530 | 0.9276 | 0.0388* |
| H101 | 0.8227 | 0.4243 | 0.9529 | 0.0319* |
| H102 | 0.8571 | 0.3337 | 0.9574 | 0.0321* |
| H91 | 0.8653 | 0.4269 | 0.7852 | 0.0256* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.5610 (4) | 0.2850 (2) | 0.8046 (3) | 0.0241 |
| C16 | 0.6141 (4) | 0.2078 (2) | 0.7642 (3) | 0.0278 |
| C17 | 0.5191 (4) | 0.1396 (2) | 0.7838 (4) | 0.0384 |
| C18 | 0.5129 (5) | 0.1321 (2) | 0.8962 (4) | 0.0417 |
| C19 | 0.4658 (5) | 0.2085 (2) | 0.9392 (4) | 0.0422 |
| C20 | 0.5606 (4) | 0.2771 (2) | 0.9183 (3) | 0.0311 |
| H201 | 0.5268 | 0.3251 | 0.9447 | 0.0378* |
| H202 | 0.6569 | 0.2673 | 0.9528 | 0.0383* |
| H192 | 0.4688 | 0.2031 | 1.0120 | 0.0512* |
| H191 | 0.3689 | 0.2193 | 0.9064 | 0.0512* |
| H182 | 0.4466 | 0.0910 | 0.9058 | 0.0500* |
| H181 | 0.6065 | 0.1185 | 0.9331 | 0.0498* |
| H172 | 0.5551 | 0.0914 | 0.7590 | 0.0461* |
| H171 | 0.4234 | 0.1485 | 0.7469 | 0.0457* |
| H162 | 0.7100 | 0.1971 | 0.8001 | 0.0339* |
| H161 | 0.6162 | 0.2122 | 0.6921 | 0.0335* |
| H151 | 0.4605 | 0.2881 | 0.7737 | 0.0293* |
| C21 | 0.6789 (5) | 0.4384 (3) | 0.4836 (3) | 0.0369 |
| C22 | 0.7659 (4) | 0.4476 (2) | 0.5777 (3) | 0.0319 |
| H221 | 0.8470 | 0.4679 | 0.6117 | 0.0402* |
| H211 | 0.6673 | 0.4494 | 0.4168 | 0.0473* |
| C23 | 0.4363 (5) | 0.3554 (3) | 0.4789 (3) | 0.0381 |
| C24 | 0.4102 (5) | 0.3268 (3) | 0.5711 (3) | 0.0384 |
| H241 | 0.3520 | 0.2995 | 0.6029 | 0.0476* |
| H231 | 0.4047 | 0.3586 | 0.4116 | 0.0481* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.0268 (2) | 0.0225 (2) | 0.0202 (2) | 0.00357 (17) | −0.00116 (17) | −0.00260 (16) |
| P2 | 0.0175 (4) | 0.0186 (4) | 0.0194 (4) | −0.0006 (3) | 0.0007 (3) | −0.0005 (3) |
| C3 | 0.0226 (15) | 0.0207 (15) | 0.0220 (15) | −0.0013 (12) | 0.0010 (12) | 0.0007 (12) |
| C4 | 0.0189 (15) | 0.0264 (17) | 0.0307 (18) | 0.0035 (13) | 0.0029 (13) | −0.0047 (14) |
| C5 | 0.0259 (18) | 0.034 (2) | 0.034 (2) | 0.0077 (15) | 0.0055 (15) | −0.0012 (16) |
| C6 | 0.039 (2) | 0.0251 (17) | 0.0328 (19) | 0.0085 (16) | 0.0019 (16) | −0.0007 (15) |
| C7 | 0.036 (2) | 0.0195 (16) | 0.0335 (19) | 0.0018 (15) | 0.0048 (15) | −0.0046 (14) |
| C8 | 0.0298 (18) | 0.0176 (15) | 0.0336 (19) | −0.0027 (13) | 0.0064 (14) | 0.0002 (13) |
| C9 | 0.0172 (14) | 0.0228 (15) | 0.0231 (16) | −0.0002 (12) | 0.0030 (12) | −0.0010 (12) |
| C10 | 0.0186 (15) | 0.0351 (19) | 0.0240 (16) | −0.0002 (14) | −0.0023 (13) | −0.0001 (14) |
| C11 | 0.0225 (17) | 0.039 (2) | 0.0315 (19) | −0.0024 (15) | −0.0049 (14) | −0.0073 (16) |
| C12 | 0.0188 (16) | 0.034 (2) | 0.044 (2) | 0.0002 (15) | −0.0032 (15) | −0.0038 (17) |
| C13 | 0.0188 (16) | 0.0297 (18) | 0.043 (2) | 0.0016 (14) | 0.0048 (15) | −0.0045 (16) |
| C14 | 0.0202 (15) | 0.0222 (16) | 0.0279 (17) | 0.0026 (13) | 0.0027 (13) | −0.0023 (13) |
| C15 | 0.0188 (15) | 0.0209 (16) | 0.0316 (18) | −0.0007 (12) | 0.0021 (13) | −0.0007 (13) |
| C16 | 0.0257 (17) | 0.0194 (16) | 0.038 (2) | −0.0018 (13) | 0.0055 (15) | −0.0016 (14) |
| C17 | 0.0288 (19) | 0.0228 (18) | 0.065 (3) | −0.0027 (15) | 0.0105 (19) | −0.0036 (18) |
| C18 | 0.033 (2) | 0.0245 (19) | 0.073 (3) | 0.0017 (16) | 0.022 (2) | 0.013 (2) |
| C19 | 0.047 (3) | 0.029 (2) | 0.058 (3) | −0.0001 (19) | 0.028 (2) | 0.0090 (19) |
| C20 | 0.037 (2) | 0.0237 (17) | 0.035 (2) | −0.0022 (15) | 0.0129 (16) | 0.0038 (15) |
| C21 | 0.046 (2) | 0.041 (2) | 0.0246 (18) | 0.0082 (19) | 0.0092 (17) | 0.0069 (16) |
| C22 | 0.0310 (19) | 0.037 (2) | 0.0281 (18) | −0.0033 (16) | 0.0075 (15) | 0.0073 (16) |
| C23 | 0.041 (2) | 0.038 (2) | 0.0277 (19) | −0.0017 (18) | −0.0164 (16) | −0.0107 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.034 (2) | 0.034 (2) | 0.042 (2) | −0.0109 (17) | −0.0075 (17) | −0.0052 (18) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—P2 | 2.1873 (10) | C11—H111 | 0.976 |
| Ni1—C21 | 1.987 (4) | C12—C13 | 1.534 (6) |
| Ni1—C22 | 2.000 (4) | C12—H122 | 0.979 |
| Ni1—C23 | 1.985 (4) | C12—H121 | 0.971 |
| Ni1—C24 | 1.988 (4) | C13—C14 | 1.529 (5) |
| P2—C3 | 1.867 (4) | C13—H132 | 0.968 |
| P2—C9 | 1.867 (3) | C13—H131 | 0.966 |
| P2—C15 | 1.863 (4) | C14—H141 | 0.975 |
| C3—C4 | 1.533 (5) | C14—H142 | 0.980 |
| C3—C8 | 1.541 (5) | C15—C16 | 1.545 (5) |
| C3—H31 | 0.981 | C15—C20 | 1.527 (5) |
| C4—C5 | 1.526 (5) | C15—H151 | 0.979 |
| C4—H41 | 0.899 | C16—C17 | 1.530 (5) |
| C5—C6 | 1.526 (6) | C16—H162 | 0.975 |
| C5—H52 | 0.974 | C16—H161 | 0.971 |
| C5—H51 | 0.972 | C17—C18 | 1.519 (7) |
| C6—C7 | 1.526 (5) | C17—H172 | 0.973 |
| C6—H62 | 0.968 | C17—H171 | 0.973 |
| C6—H61 | 0.974 | C18—C19 | 1.527 (6) |
| C7—C8 | 1.533 (5) | C18—H182 | 0.969 |
| C7—H72 | 0.968 | C18—H181 | 0.971 |
| C7—H71 | 0.974 | C19—C20 | 1.538 (5) |
| C8—H82 | 0.977 | C19—H192 | 0.973 |
| C8—H81 | 0.971 | C19—H191 | 0.971 |
| C9—C10 | 1.529 (5) | C20—H201 | 0.970 |
| C9—C14 | 1.533 (5) | C20—H202 | 0.969 |
| C9—H91 | 0.972 | C21—C22 | 1.392 (6) |
| C10—C11 | 1.533 (5) | C21—H211 | 0.901 |
| C10—H101 | 0.969 | C22—H221 | 0.897 |
| C10—H102 | 0.975 | C23—C24 | 1.389 (6) |
| C11—C12 | 1.527 (5) | C23—H231 | 0.900 |
| C11—H112 | 0.973 | C24—H241 | 0.889 |
| | | | |
| P2—Ni1—C21 | 136.69 (13) | C11—C12—C13 | 111.6 (3) |
| P2—Ni1—C22 | 95.89 (12) | C11—C12—H122 | 108.9 |
| C21—Ni1—C22 | 40.88 (17) | C13—C12—H122 | 109.8 |
| P2—Ni1—C23 | 137.14 (15) | C11—C12—H121 | 108.1 |
| C21—Ni1—C23 | 86.01 (19) | C13—C12—H121 | 109.2 |
| C22—Ni1—C23 | 126.90 (18) | H122—C12—H121 | 109.2 |
| P2—Ni1—C24 | 96.26 (13) | C12—C13—C14 | 110.8 (3) |
| C21—Ni1—C24 | 126.95 (19) | C12—C13—H132 | 108.3 |
| C22—Ni1—C24 | 167.83 (17) | C14—C13—H132 | 108.4 |
| C23—Ni1—C24 | 40.94 (19) | C12—C13—H131 | 110.4 |
| Ni1—P2—C3 | 112.29 (11) | C14—C13—H131 | 109.7 |
| Ni1—P2—C9 | 114.80 (11) | H132—C13—H131 | 109.3 |
| C3—P2—C9 | 102.55 (15) | C9—C14—C13 | 110.6 (3) |
| Ni1—P2—C15 | 113.88 (12) | C9—C14—H141 | 109.3 |
| C3—P2—C15 | 102.72 (15) | C13—C14—H141 | 109.0 |

| | | | |
|---|---|---|---|
| C9—P2—C15 | 109.38 (16) | C9—C14—H142 | 109.2 |
| P2—C3—C4 | 110.9 (2) | C13—C14—H142 | 108.9 |
| P2—C3—C8 | 112.1 (2) | H141—C14—H142 | 109.8 |
| C4—C3—C8 | 109.8 (3) | P2—C15—C16 | 112.9 (2) |
| P2—C3—H31 | 107.3 | P2—C15—C20 | 119.6 (3) |
| C4—C3—H31 | 108.3 | C16—C15—C20 | 109.3 (3) |
| C8—C3—H31 | 108.3 | P2—C15—H151 | 103.8 |
| C3—C4—C5 | 111.6 (3) | C16—C15—H151 | 104.9 |
| C3—C4—H41 | 123.5 | C20—C15—H151 | 104.7 |
| C5—C4—H41 | 124.9 | C15—C16—C17 | 110.5 (3) |
| C4—C5—C6 | 111.8 (3) | C15—C16—H162 | 109.0 |
| C4—C5—H52 | 108.8 | C17—C16—H162 | 107.8 |
| C6—C5—H52 | 109.3 | C15—C16—H161 | 110.4 |
| C4—C5—H51 | 108.5 | C17—C16—H161 | 110.1 |
| C6—C5—H51 | 109.1 | H162—C16—H161 | 108.9 |
| H52—C5—H51 | 109.3 | C16—C17—C18 | 111.1 (4) |
| C5—C6—C7 | 110.5 (3) | C16—C17—H172 | 109.3 |
| C5—C6—H62 | 110.5 | C18—C17—H172 | 110.1 |
| C7—C6—H62 | 109.5 | C16—C17—H171 | 109.0 |
| C5—C6—H61 | 109.1 | C18—C17—H171 | 108.7 |
| C7—C6—H61 | 108.4 | H172—C17—H171 | 108.5 |
| H62—C6—H61 | 108.8 | C17—C18—C19 | 111.4 (4) |
| C6—C7—C8 | 111.3 (3) | C17—C18—H182 | 109.3 |
| C6—C7—H72 | 108.3 | C19—C18—H182 | 109.2 |
| C8—C7—H72 | 108.8 | C17—C18—H181 | 109.4 |
| C6—C7—H71 | 109.1 | C19—C18—H181 | 108.6 |
| C8—C7—H71 | 109.9 | H182—C18—H181 | 109.0 |
| H72—C7—H71 | 109.4 | C18—C19—C20 | 111.3 (3) |
| C3—C8—C7 | 111.0 (3) | C18—C19—H192 | 109.7 |
| C3—C8—H82 | 109.5 | C20—C19—H192 | 109.8 |
| C7—C8—H82 | 108.9 | C18—C19—H191 | 108.2 |
| C3—C8—H81 | 108.7 | C20—C19—H191 | 108.5 |
| C7—C8—H81 | 109.0 | H192—C19—H191 | 109.3 |
| H82—C8—H81 | 109.7 | C19—C20—C15 | 110.6 (3) |
| P2—C9—C10 | 118.5 (2) | C19—C20—H201 | 109.6 |
| P2—C9—C14 | 112.5 (2) | C15—C20—H201 | 110.2 |
| C10—C9—C14 | 110.0 (3) | C19—C20—H202 | 108.8 |
| P2—C9—H91 | 103.9 | C15—C20—H202 | 108.8 |
| C10—C9—H91 | 105.5 | H201—C20—H202 | 108.8 |
| C14—C9—H91 | 105.2 | Ni1—C21—C22 | 70.0 (2) |
| C9—C10—C11 | 109.8 (3) | Ni1—C21—H211 | 144.4 |
| C9—C10—H101 | 110.1 | C22—C21—H211 | 145.5 |
| C11—C10—H101 | 109.1 | C21—C22—Ni1 | 69.1 (2) |
| C9—C10—H102 | 109.8 | C21—C22—H221 | 146.0 |
| C11—C10—H102 | 109.0 | Ni1—C22—H221 | 144.9 |
| H101—C10—H102 | 109.0 | Ni1—C23—C24 | 69.7 (2) |
| C10—C11—C12 | 111.9 (3) | Ni1—C23—H231 | 144.4 |
| C10—C11—H112 | 109.5 | C24—C23—H231 | 146.0 |
| C12—C11—H112 | 109.4 | C23—C24—Ni1 | 69.4 (2) |
| C10—C11—H111 | 108.3 | C23—C24—H241 | 146.4 |
| C12—C11—H111 | 108.8 | Ni1—C24—H241 | 144.2 |
| H112—C11—H111 | 109.0 | | |

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