Electronic Supplementary Information for Dalton Transactions

SUPPORTING INFORMATION

Syntheses, Structural studies, Photoelectron spectra and Density Functional Theory calculations on the "pseudo" tetraphospha-metallocenes [M(η-P2C3But3)2], (M= Ni, Pd, Pt).

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Table 1. Crystal data and structure refinement for [Pt(P2C3tBu3)2]

Identification code	aug499	
Empirical formula	C30 H54 P4 Pt	
Formula weight	733.70	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$ (No.14)	
Unit cell dimensions	a = 14.4887(4) Å	α= 90°.
	b = 15.3795(4) Å	β= 96.988(2)°.
	c = 15.2504(4) Å	γ = 90°.
Volume	3372.99(16) $Å_3$	
Z	4	
Density (calculated)	1.45 Mg/m_3	
Absorption coefficient	4.37 mm^{-1}	
F(000)	1488	
Crystal size	0.2 x 0.15 x 0.05 mm_3	
Theta range for data collection	4.14 to 27.87°.	
Index ranges	-19<=h<=18, -18<=k<=20, -18<=l<=20	
Reflections collected	22145	
Independent reflections	7982 [R(int) = 0.054]	
Reflections with I>2sigma(I)	5553	
Completeness to theta = 27.87°	99.4 %	
Tmax. and Tmin.	0.81, 0.58	
Refinement method	Full-matrix least-squares on F_2	
Data / restraints / parameters	7982 / 0 / 316	
Goodness-of-fit on F_2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.052, wR2 = 0.105	
R indices (all data)	R1 = 0.086, wR2 = 0.121	
Largest diff. peak and hole	3.18 and -3.38 $e.Å^{-3}$	(0.7 Å from Pt)
Data collection KappaCCD		
Absorption correction Multi-scan		
Program package WinGX		
Refinement using SHELXL-97		
Drawing using ORTEP-3 for Windows		

Table 3. Bond lengths [Å] and angles [°] for aug499.

Pt-C(3)	2.182(7)
Pt-C(18)	2.207(7)
Pt-P(1)	2.380(2)
Pt-P(2)	2.417(3)
Pt-P(3)	2.420(2)
Pt-P(4)	2.468(2)
P(1)-C(3)	1.777(7)
P(1)-C(1)	1.861(6)
P(2)-C(3)	1.765(6)
P(2)-C(2)	1.844(6)
P(3)-C(18)	1.760(7)
P(3)-C(16)	1.832(6)
P(4)-C(18)	1.757(7)
P(4)-C(17)	1.820(6)
C(1)-C(2)	1.368(9)
C(1)-C(4)	1.555(9)
C(2)-C(8)	1.560(9)
C(3)-C(12)	1.517(8)
C(4)-C(7)	1.514(11)
C(4)-C(6)	1.525(11)
C(4)-C(5)	1.539(11)
C(8)-C(10)	1.536(11)
C(8)-C(9)	1.538(11)
C(8)-C(11)	1.544(12)
C(12)-C(14)	1.522(9)
C(12)-C(13)	1.525(10)
C(12)-C(15)	1.527(10)
C(16)-C(17)	1.383(8)
C(16)-C(19)	1.558(8)
C(17)-C(23)	1.556(9)
C(18)-C(27)	1.519(9)
C(19)-C(21)	1.514(11)
C(19)-C(22)	1.524(12)
C(19)-C(20)	1.535(11)
C(23)-C(24)	1.538(10)
C(23)-C(26)	1.538(11)

C(23)-C(25)	1.543(11)
C(27)-C(29)	1.524(10)
C(27)-C(28)	1.527(10)
C(27)-C(30)	1.543(11)

C(3)-Pt-C(18)	164.1(2)
C(3)-Pt-P(1)	45.59(18)
C(18)-Pt-P(1)	145.57(18)
C(3)-Pt-P(2)	44.76(17)
C(18)-Pt-P(2)	120.42(18)
P(1)-Pt-P(2)	74.25(7)
C(3)-Pt-P(3)	151.43(17)
C(18)-Pt-P(3)	44.41(18)
P(1)-Pt-P(3)	108.91(7)
P(2)-Pt-P(3)	155.55(6)
C(3)-Pt-P(4)	128.07(18)
C(18)-Pt-P(4)	43.72(18)
P(1)-Pt-P(4)	167.83(6)
P(2)-Pt-P(4)	108.37(7)
P(3)-Pt-P(4)	73.85(7)
C(3)-P(1)-C(1)	97.7(3)
C(3)-P(1)-Pt	61.3(2)
C(1)-P(1)-Pt	90.2(2)
C(3)-P(2)-C(2)	98.2(3)
C(3)-P(2)-Pt	60.5(3)
C(2)-P(2)-Pt	93.9(2)
C(18)-P(3)-C(16)	97.0(3)
C(18)-P(3)-Pt	61.4(2)
C(16)-P(3)-Pt	82.6(2)
C(18)-P(4)-C(17)	97.9(3)
C(18)-P(4)-Pt	60.2(2)
C(17)-P(4)-Pt	83.7(2)
C(2)-C(1)-C(4)	135.0(6)
C(2)-C(1)-P(1)	114.9(4)
C(4)-C(1)-P(1)	110.0(4)
C(1)-C(2)-C(8)	131.9(6)
C(1)-C(2)-P(2)	113.2(4)
C(8)-C(2)-P(2)	114.9(5)

C(12)-C(3)-P(2)	125.0(5)
C(12)-C(3)-P(1)	125.0(5)
P(2)-C(3)-P(1)	109.7(3)
C(12)-C(3)-Pt	124.1(5)
P(2)-C(3)-Pt	74.7(3)
P(1)-C(3)-Pt	73.1(2)
C(7)-C(4)-C(6)	111.6(8)
C(7)-C(4)-C(5)	103.4(7)
C(6)-C(4)-C(5)	107.1(7)
C(7)-C(4)-C(1)	117.8(6)
C(6)-C(4)-C(1)	107.8(6)
C(5)-C(4)-C(1)	108.6(6)
C(10)-C(8)-C(9)	110.8(7)
C(10)-C(8)-C(11)	107.1(8)
C(9)-C(8)-C(11)	104.7(7)
C(10)-C(8)-C(2)	112.0(6)
C(9)-C(8)-C(2)	111.6(6)
C(11)-C(8)-C(2)	110.2(6)
C(3)-C(12)-C(14)	111.3(6)
C(3)-C(12)-C(13)	106.9(6)
C(14)-C(12)-C(13)	109.4(6)
C(3)-C(12)-C(15)	111.1(5)
C(14)-C(12)-C(15)	109.2(6)
C(13)-C(12)-C(15)	108.9(6)
C(17)-C(16)-C(19)	132.2(6)
C(17)-C(16)-P(3)	115.8(5)
C(19)-C(16)-P(3)	112.1(5)
C(16)-C(17)-C(23)	132.8(6)
C(16)-C(17)-P(4)	114.5(5)
C(23)-C(17)-P(4)	112.5(4)
C(27)-C(18)-P(4)	123.5(5)
C(27)-C(18)-P(3)	123.0(5)
P(4)-C(18)-P(3)	113.2(4)
C(27)-C(18)-Pt	122.5(5)
P(4)-C(18)-Pt	76.1(3)
P(3)-C(18)-Pt	74.2(3)
C(21)-C(19)-C(22)	112.0(8)
C(21)-C(19)-C(20)	106.0(8)

C(22)-C(19)-C(20)	103.7(8)
C(21)-C(19)-C(16)	111.4(6)
C(22)-C(19)-C(16)	112.0(7)
C(20)-C(19)-C(16)	111.4(6)
C(24)-C(23)-C(26)	104.1(7)
C(24)-C(23)-C(25)	110.5(8)
C(26)-C(23)-C(25)	106.5(7)
C(24)-C(23)-C(17)	115.8(6)
C(26)-C(23)-C(17)	111.5(6)
C(25)-C(23)-C(17)	108.1(6)
C(18)-C(27)-C(29)	111.7(6)
C(18)-C(27)-C(28)	111.4(6)
C(29)-C(27)-C(28)	109.8(6)
C(18)-C(27)-C(30)	106.6(6)
C(29)-C(27)-C(30)	109.1(6)
C(28)-C(27)-C(30)	108.0(7)

Symmetry transformations used to generate equivalent atoms:

```
 Least-squares planes (x,y,z in crystal coordinates) and deviations from
them
 (* indicates atom used to define plane)

  8.0173 (0.0333) x - 6.2467 (0.0302) y + 9.9812 (0.0230) z = 1.7917
(0.0133)

 *   -0.0283 (0.0018)  P1
 *    0.0282 (0.0018)  P2
 *    0.0601 (0.0038)  C1
 *   -0.0599 (0.0038)  C2
     -0.4170 (0.0083)  C3

 Rms deviation of fitted atoms =   0.0469


  12.0323 (0.0559) x - 2.4379 (0.0819) y + 6.5431 (0.0748) z = 3.4413
(0.0275)

 Angle to previous plane (with approximate esd) = 24.18 ( 0.54 )

 *    0.0000 (0.0000)  P1
 *    0.0000 (0.0000)  P2
 *    0.0000 (0.0000)  C3
      1.9120 (0.0019)  Pt

 Rms deviation of fitted atoms =   0.0000


  11.0667 (0.0743) x - 3.6622 (0.0297) y + 7.6637 (0.0993) z = 6.8553
```

(0.0162)

Angle to previous plane (with approximate esd) = 7.05 (0.96)

```
*    0.0000 (0.0000)  P3
*    0.0000 (0.0000)  P4
*    0.0000 (0.0000)  C18
    -1.9525 (0.0019)  Pt
```

Rms deviation of fitted atoms = 0.0000

8.7505 (0.0337) x - 4.3044 (0.0232) y + 10.1756 (0.0317) z = 6.2360
(0.0126)

Angle to previous plane (with approximate esd) = 12.67 (0.79)

```
*    0.0087 (0.0018)  P3
*   -0.0087 (0.0018)  P4
*   -0.0185 (0.0038)  C16
*    0.0185 (0.0038)  C17
     0.2122 (0.0083)  C18
```

Rms deviation of fitted atoms = 0.0144

Table 1. Crystal data and structure refinement for [Pd(P2C3tBu3)2]

Identification code	MAR499
Empirical formula	C30 H54 P4 Pd
Formula weight	645.0
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$ (No.14)
Unit cell dimensions(Å and deg.)	a=11.046(3) alpha=90 b=28.537(9) beta=105.12(2) c=16.175(5) gamma=90
Volume	4922(3) $Å^3$
Z, Calculated density	6, 1.31 $Mg.m^{-3}$
Absorption coefficient	0.78 mm^{-1}
F(000)	2040
Crystal size	0.30 x 0.20 x 0.05 mm
Theta range for data collection	2 to 23 deg.
Limiting indices	0<=h<=12 0<=k<=31 -17<=l<=17
Reflections collected / unique	7228 / 6830 [R(int) = 0.0975]
Reflections with I>2sigma(I)	3571
Completeness to theta = 23.00	99.8 %
Abs. correction from psi-scans	Tmax.=1.00 ,Tmin.=0.81
Refinement method	Full-matrix on all F^2
Data / restraints / parameters	6830 / 186 / 475

Goodness-of-fit on F^2 0.987

Final R indices [I>2sigma(I)] R1 = 0.075, wR2 = 0.140

R indices (all data) R1 = 0.169, wR2 = 0.178

Largest diff. peak and hole 0.84 and -0.98 e.$Å^{-3}$

Maximum shift/e.s.d. 0.001

There are two independent molecules; one in a general position and the other on an inversion centre.
All non-H atoms were anisotropic. In order to prevent some C atoms becoming non-positive-definite, constraints (DELU) were applied to Uij's.

Programs used were :
Data collection - Enraf-Nonius CAD4 software
Structure solution - SHELXS-97
Structure refinement - SHELXL-97
Interactive graphics and final drawings - ORTEP

References :

Enraf-Nonius(1989) CAD4 Software. Version 5.0. Enraf-Nonius,The Netherlands.
Sheldrick,G.M.(1997) SHELXS-97. Program for Crystal Structure Solution. Univ. of Gottingen, Germany.
Sheldrick,G.M.(1997) SHELXL-97. Program for Crystal Structure Refinement. Univ. of Gottingen, Germany.

Table 3. Bond lengths [Å] and angles [deg]

Pd(1)-P(1)	2.428(4)	Pd(1)-P(2)	2.473(3)
Pd(1)-P(3)	2.419(3)	Pd(1)-P(4)	2.459(4)
Pd(1)-C(1)	2.201(11)	Pd(1)-C(16)	2.219(11)
P(1)-C(1)	1.738(11)	P(1)-C(3)	1.848(12)
P(2)-C(1)	1.731(12)	P(2)-C(2)	1.853(11)
P(3)-C(16)	1.715(12)	P(3)-C(17)	1.864(11)
P(4)-C(16)	1.770(11)	P(4)-C(18)	1.823(12)
C(1)-C(4)	1.553(15)	C(2)-C(3)	1.349(16)
C(2)-C(8)	1.535(16)	C(3)-C(12)	1.584(15)
C(4)-C(6)	1.506(16)	C(4)-C(7)	1.531(15)
C(4)-C(5)	1.539(15)	C(8)-C(9)	1.523(16)
C(8)-C(11)	1.530(15)	C(8)-C(10)	1.555(16)
C(12)-C(13)	1.519(17)	C(12)-C(15)	1.523(17)
C(12)-C(14)	1.542(16)	C(16)-C(19)	1.537(15)
C(17)-C(18)	1.364(16)	C(17)-C(23)	1.552(16)
C(18)-C(27)	1.576(15)	C(19)-C(21)	1.515(16)
C(19)-C(22)	1.523(17)	C(19)-C(20)	1.540(16)
C(23)-C(25)	1.494(16)	C(23)-C(24)	1.521(15)
C(23)-C(26)	1.551(16)	C(27)-C(28)	1.521(17)
C(27)-C(29)	1.538(16)	C(27)-C(30)	1.542(17)
Pd(2)-C(31)	2.211(11)	Pd(2)-P(5)	2.445(3)
Pd(2)-P(6)	2.456(3)	P(5)-C(31)	1.753(12)
P(5)-C(32)	1.831(11)	P(6)-C(31)	1.752(11)
P(6)-C(33)	1.847(12)	C(31)-C(34)	1.525(15)
C(32)-C(33)	1.383(15)	C(32)-C(38)	1.539(16)
C(33)-C(42)	1.559(15)	C(34)-C(36)	1.493(16)
C(34)-C(37)	1.495(17)	C(34)-C(35)	1.519(16)
C(38)-C(39)	1.532(16)	C(38)-C(41)	1.540(17)
C(38)-C(40)	1.562(17)	C(42)-C(43)	1.519(16)
C(42)-C(44)	1.549(17)	C(42)-C(45)	1.560(16)

C(1)-Pd(1)-C(16)	176.3(4)	C(1)-Pd(1)-P(3)	138.1(3)
C(16)-Pd(1)-P(3)	43.1(3)	C(1)-Pd(1)-P(1)	43.7(3)
C(16)-Pd(1)-P(1)	139.8(3)	P(3)-Pd(1)-P(1)	106.12(12
C(1)-Pd(1)-P(4)	132.2(3)	C(16)-Pd(1)-P(4)	44.1(3)
P(3)-Pd(1)-P(4)	73.25(12	P(1)-Pd(1)-P(4)	172.51(11
C(1)-Pd(1)-P(2)	43.0(3)	C(16)-Pd(1)-P(2)	136.0(3)
P(3)-Pd(1)-P(2)	176.90(11	P(1)-Pd(1)-P(2)	72.97(12
P(4)-Pd(1)-P(2)	108.05(12	C(1)-P(1)-C(3)	96.0(5)
C(1)-P(1)-Pd(1)	61.2(4)	C(3)-P(1)-Pd(1)	85.9(4)
C(1)-P(2)-C(2)	96.9(5)	C(1)-P(2)-Pd(1)	60.1(4)
C(2)-P(2)-Pd(1)	88.2(4)	C(16)-P(3)-C(17)	97.8(5)
C(16)-P(3)-Pd(1)	62.2(4)	C(17)-P(3)-Pd(1)	87.3(4)
C(16)-P(4)-C(18)	96.3(5)	C(16)-P(4)-Pd(1)	60.7(4)
C(18)-P(4)-Pd(1)	87.3(4)	C(4)-C(1)-P(2)	123.1(8)
C(4)-C(1)-P(1)	122.5(9)	P(2)-C(1)-P(1)	114.3(6)

C(4)-C(1)-Pd(1) 117.6(7) P(2)-C(1)-Pd(1) 76.9(4)
P(1)-C(1)-Pd(1) 75.1(4) C(3)-C(2)-C(8) 132.9(10)
C(3)-C(2)-P(2) 113.3(9) C(8)-C(2)-P(2) 113.7(8)
C(2)-C(3)-C(12) 133.4(11) C(2)-C(3)-P(1) 116.5(8)
C(12)-C(3)-P(1) 109.8(8) C(6)-C(4)-C(7) 108.9(10)
C(6)-C(4)-C(5) 108.3(9) C(7)-C(4)-C(5) 109.5(10)
C(6)-C(4)-C(1) 108.2(9) C(7)-C(4)-C(1) 112.6(9)
C(5)-C(4)-C(1) 109.2(9) C(9)-C(8)-C(11) 111.1(10)
C(9)-C(8)-C(2) 109.5(10) C(11)-C(8)-C(2) 115.1(10)
C(9)-C(8)-C(10) 106.7(11) C(11)-C(8)-C(10) 102.9(11)
C(2)-C(8)-C(10) 111.1(9) C(13)-C(12)-C(15) 107.7(11)
C(13)-C(12)-C(14) 110.0(11) C(15)-C(12)-C(14) 103.8(9)
C(13)-C(12)-C(3) 108.0(9) C(15)-C(12)-C(3) 110.4(9)
C(14)-C(12)-C(3) 116.6(10) C(19)-C(16)-P(3) 125.2(8)
C(19)-C(16)-P(4) 121.6(8) P(3)-C(16)-P(4) 113.2(6)
C(19)-C(16)-Pd(1) 117.9(8) P(3)-C(16)-Pd(1) 74.6(4)
P(4)-C(16)-Pd(1) 75.1(4) C(18)-C(17)-C(23) 138.3(10)
C(18)-C(17)-P(3) 113.0(9) C(23)-C(17)-P(3) 108.4(8)
C(17)-C(18)-C(27) 129.9(11) C(17)-C(18)-P(4) 116.6(8)
C(27)-C(18)-P(4) 113.3(9) C(21)-C(19)-C(22) 108.6(11)
C(21)-C(19)-C(16) 113.3(9) C(22)-C(19)-C(16) 105.6(10)
C(21)-C(19)-C(20) 109.4(10) C(22)-C(19)-C(20) 108.7(10)
C(16)-C(19)-C(20) 111.1(10) C(25)-C(23)-C(24) 105.8(10)
C(25)-C(23)-C(26) 108.6(11) C(24)-C(23)-C(26) 107.2(10)
C(25)-C(23)-C(17) 111.2(10) C(24)-C(23)-C(17) 118.1(10)
C(26)-C(23)-C(17) 105.6(10) C(28)-C(27)-C(29) 106.5(10)
C(28)-C(27)-C(30) 105.0(11) C(29)-C(27)-C(30) 111.2(11)
C(28)-C(27)-C(18) 111.3(10) C(29)-C(27)-C(18) 112.5(10)
C(30)-C(27)-C(18) 109.9(9) C(31)-Pd(2)-C(31)' 180
C(31)-Pd(2)-P(5) 43.9(3) C(31)'-Pd(2)-P(5) 136.1(3)
C(31)-Pd(2)-P(5)' 136.1(3) C(31)'-Pd(2)-P(5)' 43.9(3)
P(5)-Pd(2)-P(5)' 180 C(31)-Pd(2)-P(6) 43.7(3)
C(31)'-Pd(2)-P(6) 136.3(3) P(5)-Pd(2)-P(6) 72.77(10
P(5)'-Pd(2)-P(6) 107.23(10 C(31)-Pd(2)-P(6)' 136.3(3)
C(31)'-Pd(2)-P(6)' 43.7(3) P(5)-Pd(2)-P(6)' 107.23(10
P(5)'-Pd(2)-P(6)' 72.77(10 P(6)-Pd(2)-P(6)' 180
C(31)-P(5)-C(32) 98.0(5) C(31)-P(5)-Pd(2) 60.9(4)
C(32)-P(5)-Pd(2) 89.0(4) C(31)-P(6)-C(33) 98.1(5)
C(31)-P(6)-Pd(2) 60.7(4) C(33)-P(6)-Pd(2) 88.0(4)
C(34)-C(31)-P(6) 123.8(9) C(34)-C(31)-P(5) 124.1(9)
P(6)-C(31)-P(5) 112.0(6) C(34)-C(31)-Pd(2) 118.6(7)
P(6)-C(31)-Pd(2) 75.6(4) P(5)-C(31)-Pd(2) 75.2(4)
C(33)-C(32)-C(38) 130.1(10) C(33)-C(32)-P(5) 114.9(8)
C(38)-C(32)-P(5) 114.9(8) C(32)-C(33)-C(42) 134.0(11)
C(32)-C(33)-P(6) 114.0(8) C(42)-C(33)-P(6) 111.6(8)
C(36)-C(34)-C(37) 110.1(11) C(36)-C(34)-C(35) 108.1(11)
C(37)-C(34)-C(35) 110.3(11) C(36)-C(34)-C(31) 107.3(10)
C(37)-C(34)-C(31) 110.3(10) C(35)-C(34)-C(31) 110.8(9)
C(39)-C(38)-C(32) 113.1(10) C(39)-C(38)-C(41) 111.0(11)
C(32)-C(38)-C(41) 113.5(10) C(39)-C(38)-C(40) 103.4(11)

C(32)-C(38)-C(40)	109.5(10)	C(41)-C(38)-C(40)	105.5(11)
C(43)-C(42)-C(44)	110.6(10)	C(43)-C(42)-C(33)	108.2(10)
C(44)-C(42)-C(33)	115.6(10)	C(43)-C(42)-C(45)	105.9(10)
C(44)-C(42)-C(45)	106.5(10)	C(33)-C(42)-C(45)	109.6(9)

Symmetry transformations used to generate equivalent atoms:
' -x,1-y,-z

Table 1. Crystal data and structure refinement for [Ni(P2C3tBu3)2]

Identification code	MAR999
Empirical formula	C30 H54 Ni P4
Formula weight	597.3
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$ (No.14)
Unit cell dimensions(Å and deg.)	a=17.396(4) alpha=90 b= 9.479(2) beta=103.84(3) c=20.102(8) gamma=90
Volume	3219(2) $Å^3$
Z, Calculated density	4, 1.23 $Mg.m^{-3}$
Absorption coefficient	0.82 mm^{-1}
F(000)	1288
Crystal size	0.4 x 0.2 x 0.1 mm
Theta range for data collection	2 to 25 deg.
Limiting indices	0<=h<=20 0<=k<=11 -23<=l<=23
Reflections collected / unique	5840 / 5652 [R(int) = 0.0380]
Reflections with I>2sigma(I)	4140
Completeness to theta = 24.98	99.9 %
Abs. correction from psi-scans	not applied
Refinement method	Full-matrix on all F^2
Data / restraints / parameters	5652 / 0 / 316
Goodness-of-fit on F^2	1.014

Final R indices [I>2sigma(I)] R1 = 0.046, wR2 = 0.094

R indices (all data) R1 = 0.075, wR2 = 0.106

Largest diff. peak and hole 0.41 and -0.32 e.Å^{-3}

Maximum shift/e.s.d. 0.001

Programs used were :
Data collection - Enraf-Nonius CAD4 software
Structure solution - SHELXS-97
Structure refinement - SHELXL-97
Interactive graphics and final drawings - ORTEP

References :

Enraf-Nonius(1989) CAD4 Software. Version 5.0. Enraf-Nonius,The Netherlands.
Sheldrick,G.M.(1997) SHELXS-97. Program for Crystal Structure Solution. Univ. of Gottingen, Germany.
Sheldrick,G.M.(1997) SHELXL-97. Program for Crystal

Table 3. Bond lengths [Å] and angles [deg]

Ni-P(1)	2.294(1)	Ni-P(2)	2.260(1)
Ni-C(1)	2.014(3)	Ni-P(3)	2.320(1)
Ni-P(4)	2.397(1)	Ni-C(16)	2.235(4)
Ni-C(17)	2.193(3)	Ni-C(18)	2.149(3)
Ni-M(1)	1.736(4)	P(1)-C(1)	1.758(4)
P(1)-C(3)	1.869(4)	P(2)-C(1)	1.767(4)
P(2)-C(2)	1.884(4)	P(3)-C(16)	1.764(4)
P(3)-C(18)	1.789(3)	P(4)-C(16)	1.740(4)
P(4)-C(17)	1.800(4)	C(1)-C(4)	1.536(5)
C(2)-C(3)	1.348(5)	C(2)-C(8)	1.548(5)
C(3)-C(12)	1.556(5)	C(4)-C(7)	1.518(5)
C(4)-C(6)	1.523(5)	C(4)-C(5)	1.531(5)
C(8)-C(11)	1.524(5)	C(8)-C(9)	1.537(5)
C(8)-C(10)	1.544(5)	C(12)-C(15)	1.537(5)
C(12)-C(13)	1.540(5)	C(12)-C(14)	1.542(5)
C(16)-C(19)	1.537(5)	C(17)-C(18)	1.433(5)
C(17)-C(23)	1.570(5)	C(18)-C(27)	1.568(5)
C(19)-C(21)	1.520(5)	C(19)-C(22)	1.535(5)
C(19)-C(20)	1.538(5)	C(23)-C(26)	1.535(5)
C(23)-C(24)	1.539(5)	C(23)-C(25)	1.540(5)
C(27)-C(29)	1.531(5)	C(27)-C(30)	1.534(5)
C(27)-C(28)	1.542(5)		

M(1)-Ni-C(1)	160.6(1)	M(1)-Ni-P(2)	137.7(1)
M(1)-Ni-P(1)	142.1(1)	C(1)-P(1)-C(3)	98.37(16
C(1)-P(1)-Ni	57.82(11	C(3)-P(1)-Ni	99.10(11
C(1)-P(2)-C(2)	99.00(16	C(1)-P(2)-Ni	58.50(11
C(2)-P(2)-Ni	96.90(11	C(16)-P(3)-C(18)	95.93(16
C(16)-P(4)-C(17)	95.76(16	C(4)-C(1)-P(1)	125.4(3)
C(4)-C(1)-P(2)	126.5(3)	P(1)-C(1)-P(2)	107.29(19
C(4)-C(1)-Ni	126.0(2)	P(1)-C(1)-Ni	74.57(13
P(2)-C(1)-Ni	73.08(13	C(3)-C(2)-C(8)	135.9(3)
C(3)-C(2)-P(2)	113.0(3)	C(8)-C(2)-P(2)	111.0(2)
C(2)-C(3)-C(12)	131.7(3)	C(2)-C(3)-P(1)	113.4(3)
C(12)-C(3)-P(1)	114.6(2)	C(7)-C(4)-C(6)	108.6(3)
C(7)-C(4)-C(5)	109.3(3)	C(6)-C(4)-C(5)	109.4(3)
C(7)-C(4)-C(1)	112.2(3)	C(6)-C(4)-C(1)	111.6(3)
C(5)-C(4)-C(1)	105.6(3)	C(11)-C(8)-C(9)	109.2(3)
C(11)-C(8)-C(10)	104.9(3)	C(9)-C(8)-C(10)	107.9(3)
C(11)-C(8)-C(2)	116.5(3)	C(9)-C(8)-C(2)	108.6(3)
C(10)-C(8)-C(2)	109.3(3)	C(15)-C(12)-C(13)	112.2(3)
C(15)-C(12)-C(14)	105.0(3)	C(13)-C(12)-C(14)	105.0(3)
C(15)-C(12)-C(3)	115.0(3)	C(13)-C(12)-C(3)	108.2(3)
C(14)-C(12)-C(3)	110.9(3)	C(19)-C(16)-P(4)	122.6(3)
C(19)-C(16)-P(3)	120.0(3)	P(4)-C(16)-P(3)	116.9(2)
C(18)-C(17)-C(23)	130.4(3)	C(18)-C(17)-P(4)	116.0(2)

C(23)-C(17)-P(4)	113.3(2)	C(17)-C(18)-C(27)	132.6(3)
C(17)-C(18)-P(3)	115.3(2)	C(27)-C(18)-P(3)	111.8(2)
C(21)-C(19)-C(22)	108.0(3)	C(21)-C(19)-C(16)	113.0(3)
C(22)-C(19)-C(16)	112.2(3)	C(21)-C(19)-C(20)	109.1(3)
C(22)-C(19)-C(20)	108.8(3)	C(16)-C(19)-C(20)	105.6(3)
C(26)-C(23)-C(24)	110.5(3)	C(26)-C(23)-C(25)	104.8(3)
C(24)-C(23)-C(25)	105.2(3)	C(26)-C(23)-C(17)	110.2(3)
C(24)-C(23)-C(17)	114.4(3)	C(25)-C(23)-C(17)	111.1(3)
C(29)-C(27)-C(30)	105.2(3)	C(29)-C(27)-C(28)	110.3(3)
C(30)-C(27)-C(28)	106.4(3)	C(29)-C(27)-C(18)	115.4(3)
C(30)-C(27)-C(18)	110.9(3)	C(28)-C(27)-C(18)	108.4(3)

M(1) is the centroid of the P(3),P(4),C(16),C(17),C(18) ring

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 11.6032 (0.0154) x - 2.6763 (0.0086) y + 16.6650 (0.0176) z = 1.5922 (0.0074)

* -0.0250 (0.0009) P1
* 0.0247 (0.0009) P2
* -0.0524 (0.0019) C2
* 0.0526 (0.0019) C3
0.5157 (0.0037) C1
-0.1680 (0.0054) C8
0.3543 (0.0054) C12

Rms deviation of fitted atoms = 0.0411

- 5.3372 (0.0458) x - 0.2982 (0.0180) y + 20.0422 (0.0116) z = 3.9791 (0.0124)

Angle to previous plane (with approximate esd) = 29.61 (0.19)

* 0.0000 (0.0000) P1
* 0.0000 (0.0000) P2
* 0.0000 (0.0000) C1
-1.7778 (0.0012) Ni
0.2129 (0.0092) C4
0.7958 (0.0062) C2
0.9034 (0.0060) C3

Rms deviation of fitted atoms = 0.0000

7.6315 (0.0195) x + 1.5392 (0.0100) y - 19.3608 (0.0109) z = 0.2392 (0.0042)

Angle to previous plane (with approximate esd) = 11.34 (0.17)

* 0.0184 (0.0016) P3
* 0.0132 (0.0016) P4
* -0.0201 (0.0016) C16
* -0.0002 (0.0020) C17
* -0.0112 (0.0020) C18
   -1.7341 (0.0016) Ni
    0.1015 (0.0056) C19
    0.1515 (0.0053) C23
    0.0936 (0.0051) C27

Rms deviation of fitted atoms = 0.0144

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 9.3639 (0.0278) x - 3.1825 (0.0925) y + 11.6745 (0.0476) z = 1.9056 (0.0324)

* 0.0175 (0.0031) P1
* -0.0170 (0.0030) P2
* 0.0370 (0.0066) C2
* -0.0375 (0.0068) C3
    0.2791 (0.0126) C1
   -1.8924 (0.0043) Pd1
    0.1974 (0.0188) C8
   -0.0208 (0.0186) C12

Rms deviation of fitted atoms = 0.0290

- 10.5771 (0.0322) x + 1.1993 (0.1746) y + 8.4932 (0.1522) z = 1.3415 (0.0381)

Angle to previous plane (with approximate esd) = 17.27 (0.73)

* 0.0000 (0.0001) P1
* 0.0000 (0.0001) P2
* 0.0000 (0.0000) C1
   -1.9696 (0.0029) Pd1
    0.0304 (0.0327) C4

Rms deviation of fitted atoms = 0.0000

10.6232 (0.0180) x - 3.4276 (0.2109) y - 7.9035 (0.1445) z = 2.1352 (0.0218)

Angle to previous plane (with approximate esd) = 5.01 (0.67)

* 0.0000 (0.0001) P3
* 0.0000 (0.0001) P4
* 0.0000 (0.0000) C16
   -1.9549 (0.0032) Pd1
   -0.0083 (0.0326) C19

Rms deviation of fitted atoms = 0.0000

9.5868 (0.0252) x + 2.1522 (0.1011) y - 11.3286 (0.0481) z = 1.7928 (0.0331)

Angle to previous plane (with approximate esd) = 18.82 (0.61)

* 0.0057 (0.0030) P3
* -0.0060 (0.0032) P4
* -0.0122 (0.0065) C17
* 0.0125 (0.0067) C18
   0.3094 (0.0128) C16
   -1.8798 (0.0043) Pd1
   0.0664 (0.0182) C23
   0.1587 (0.0187) C27

Rms deviation of fitted atoms = 0.0097

- 0.8449 (0.1198) x + 18.7740 (0.0512) y + 12.0219 (0.0200) z = 7.4145 (0.0261)

Angle to previous plane (with approximate esd) = 67.38 (0.62)

* 0.0000 (0.0000) P5
* 0.0000 (0.0000) P6
* 0.0000 (0.0000) C31
   1.9725 (0.0024) Pd2
   -0.0460 (0.0303) C34

Rms deviation of fitted atoms = 0.0000

2.5149 (0.0500) x + 16.8736 (0.0655) y + 11.1201 (0.0351) z = 6.5547 (0.0307)

Angle to previous plane (with approximate esd) = 17.97 (0.43)

* 0.0060 (0.0031) P5
* -0.0059 (0.0030) P6
* -0.0125 (0.0064) C32
* 0.0124 (0.0064) C33
   -0.3021 (0.0120) C31
   1.8821 (0.0041) Pd2
   -0.1377 (0.0184) C38
   -0.0811 (0.0179) C42

Rms deviation of fitted atoms = 0.0097