

Spin-state tuning at pseudotetrahedral  $d^7$  ions:  
Examining the structural and magnetic phenomena  
of 4-coordinate  $[\text{BP}_3]\text{Co}^{\text{II}}\text{-X}$  systems

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## **Supporting Information**

## Supporting Information:

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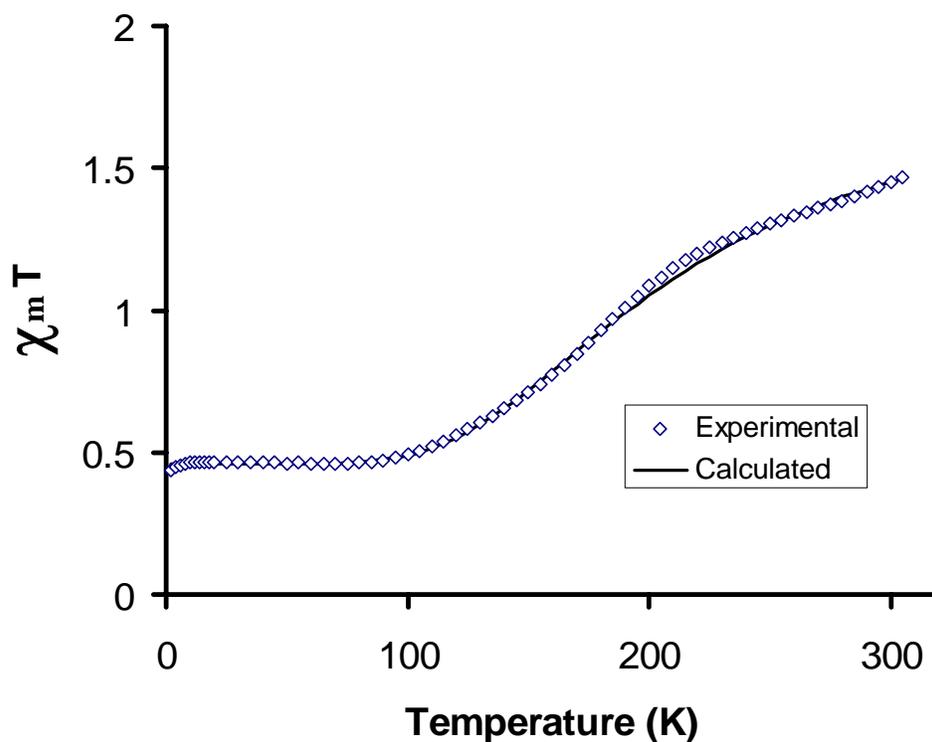
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I. SQUID data with calculated values for  $T_c$  and  $\Delta H$  for  $[\text{PhBP}_3]\text{CoOSiPh}_3$  (**2**).

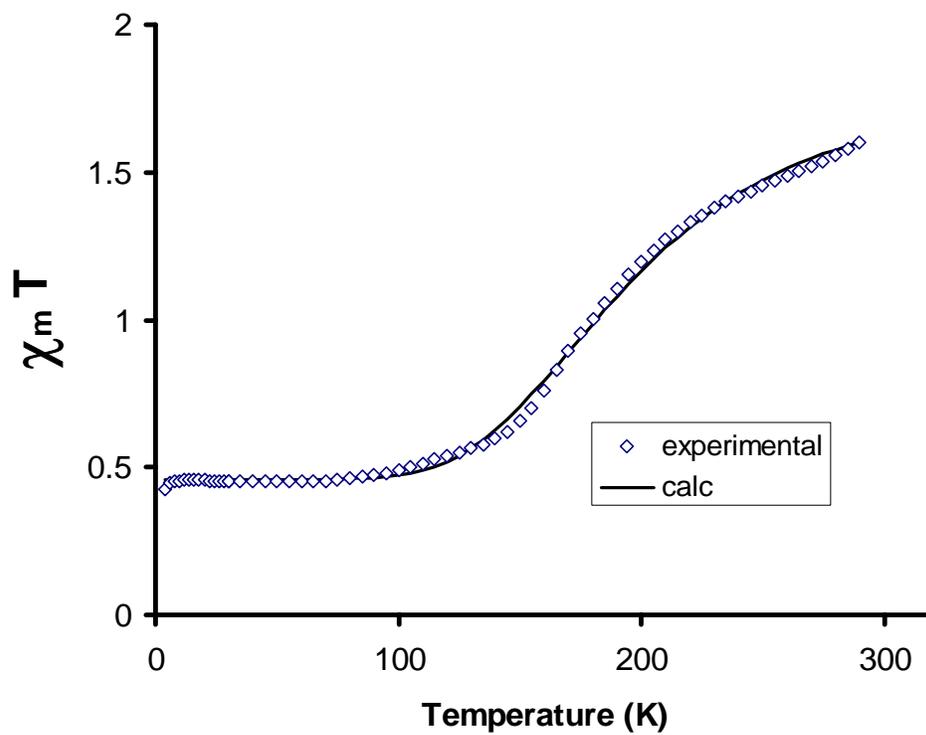
The thermodynamic variables for the spin crossover were taken from the following Boltzman equation for simple equilibria (Eq. 1). The data for the increasing path was fit according to this equation to determine  $T_c$  and  $\Delta H$ .

$$\frac{\chi T - (\chi T)_{LS}}{(\chi T)_{HS} - (\chi T)_{LS}} = \frac{1}{1 + e^{[(\Delta H/R)(1/T - 1/T_c)]}} \quad (\text{Eq. 1})$$

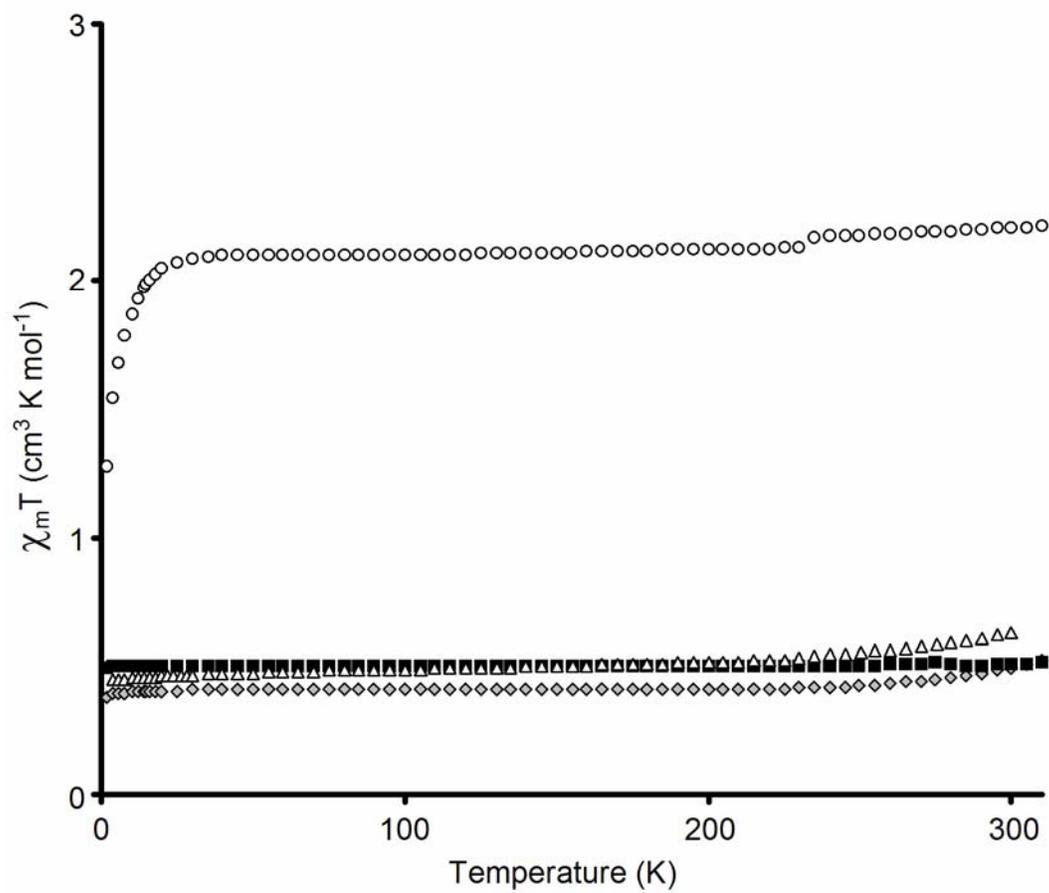
For the sample of  $[\text{PhBP}_3]\text{CoOSiPh}_3$  (**2**) with no solvent the value of  $T_c \approx 220$  K and  $\Delta H \approx 490$   $\text{cm}^{-1}$ .



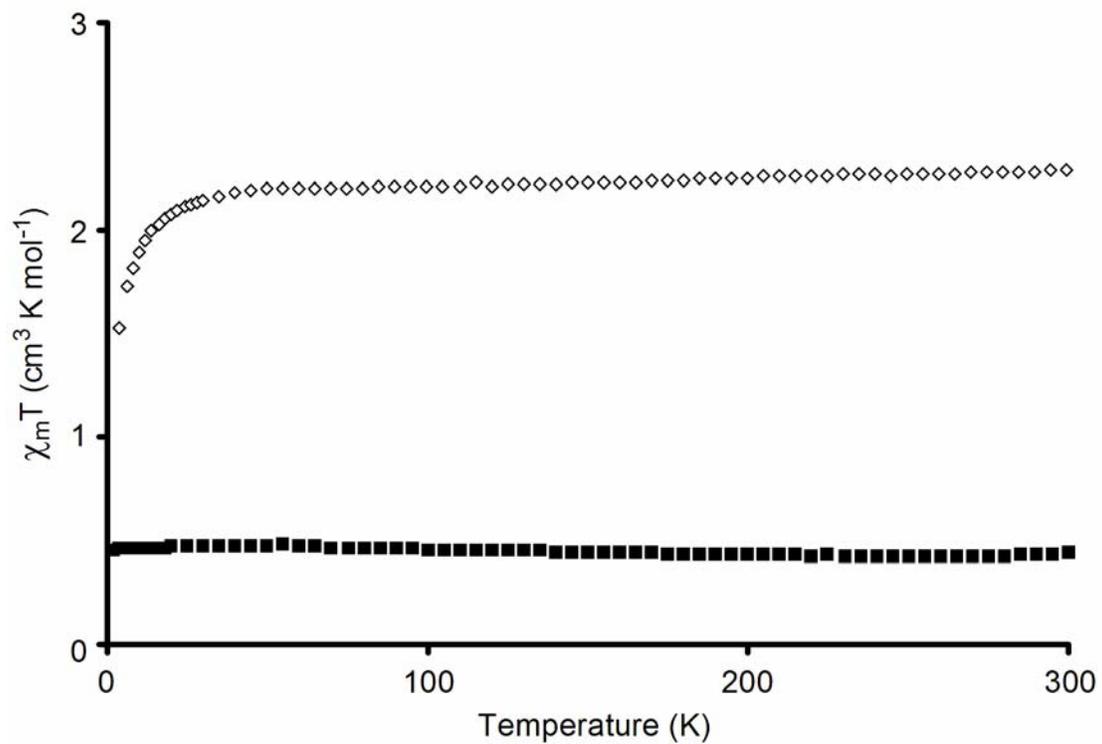
For the sample of  $[\text{PhBP}_3]\text{CoOSiPh}_3$  (**2**) with 3/2 equivalents of benzene solvent the value of  $T_c \approx 200$  K and  $\Delta H \approx 650$  cm<sup>-1</sup>.



SQUID data for [PhBP<sub>3</sub>]CoSPh (**5**), (◆), [PhBP<sub>3</sub>]CoS(2,6-Me<sub>2</sub>-Ph) (**6**) (■),  
[PhBP<sub>3</sub>]CoS(2,4,6-*i*-Pr<sub>3</sub>-Ph) (**7**) (Δ), [PhBP<sub>3</sub>]CoS2,4,6-*t*-Bu<sub>3</sub>-Ph) (**8**) (○).



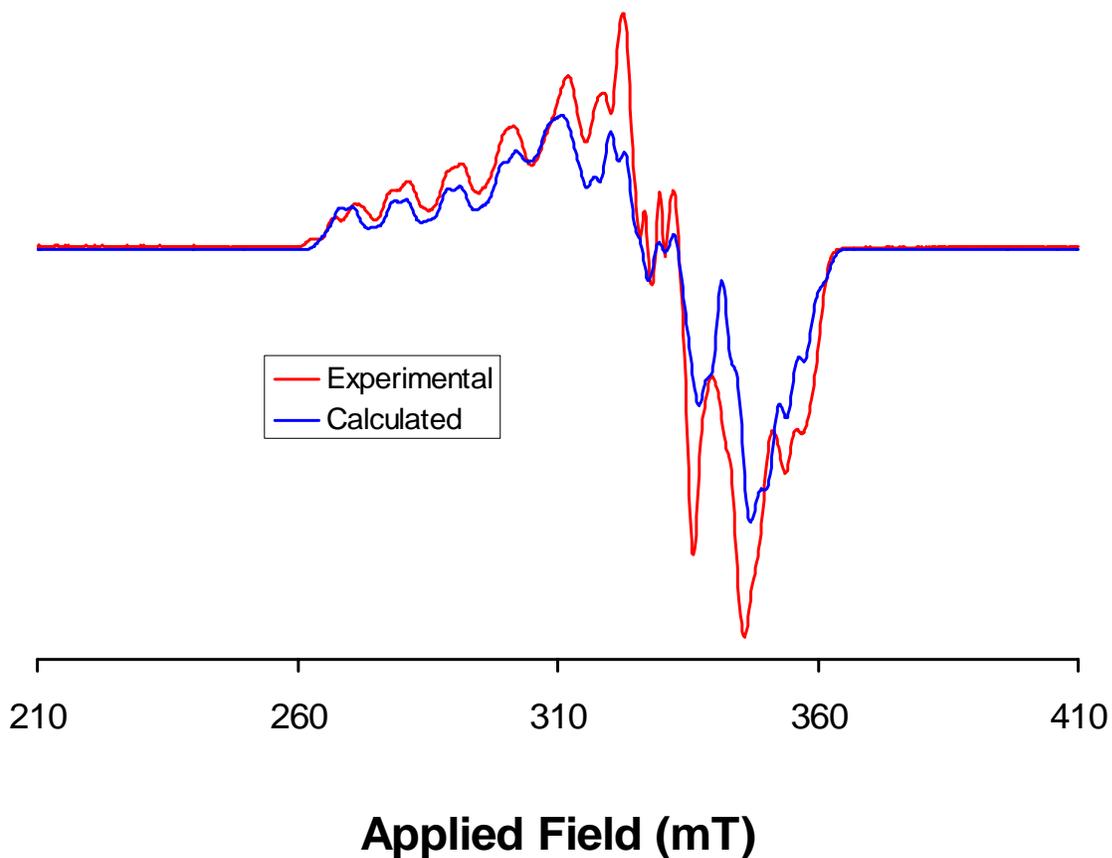
SQUID magnetization plot of  $\chi_m T$  versus T for  $[\text{PhBP}_3]\text{CoOCPh}_3$  (**12**) ( $\diamond$ ), and  $[\text{PhBP}_3]\text{CoSSiPh}_3$  (**9**) ( $\blacksquare$ ).



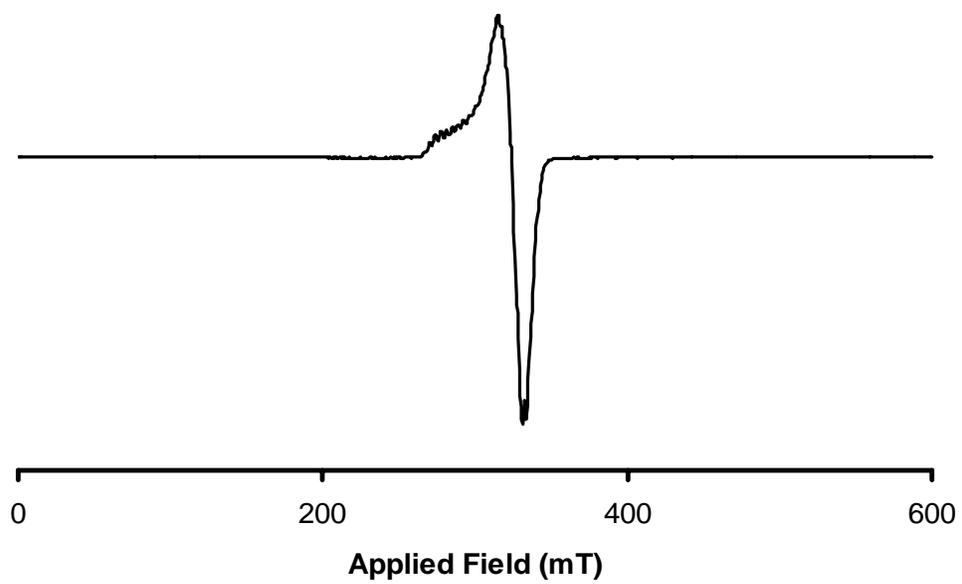
## II. Simulated EPR spectrum of [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub> (**2**).

The EPR simulation was performed with the program WINEPR *SimFonia* (Version 1.25, Bruker Analytische Messtechnik GmbH); this software is based on a second-order perturbation solution of the spin Hamiltonion:  $H = H \cdot g \cdot S + \Sigma S \cdot A \cdot I$ .

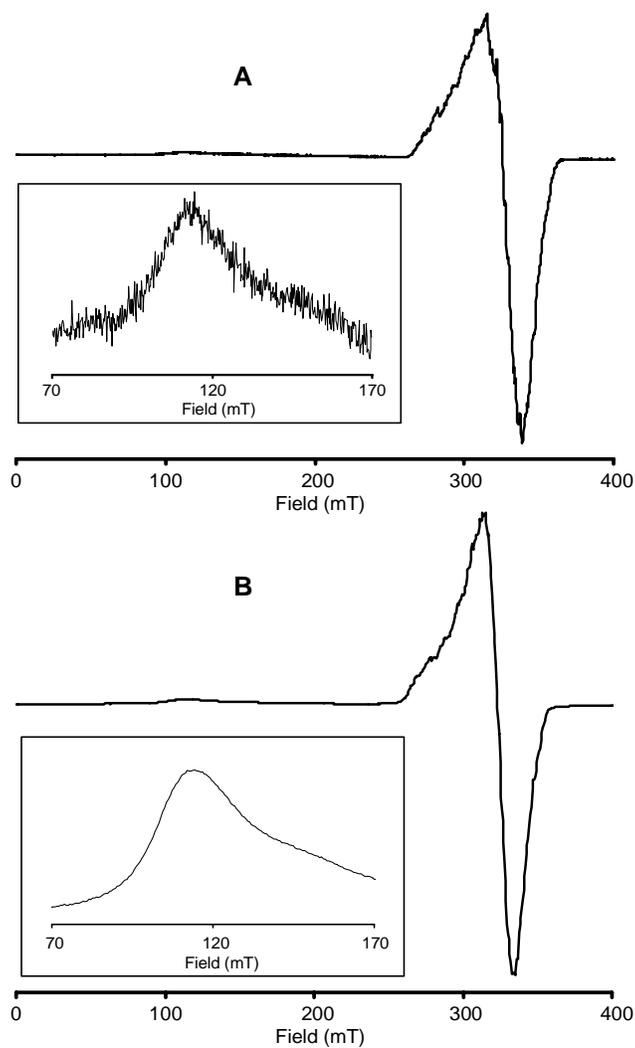
The solution of the Hamiltonion is:  $g_1 = 2.21$ ,  $g_2 = 2.05$ ,  $g_3 = 2.03$ ;  $a_{1(\text{Co})} = 105$  gauss,  $a_{2(\text{Co})} = 12$  gauss,  $a_{3(\text{Co})} = 65$  gauss;  $a_{1(\text{P})} = 28$  gauss,  $a_{2(\text{P})} = 27$  gauss,  $a_{3(\text{P})} = 34$  gauss.



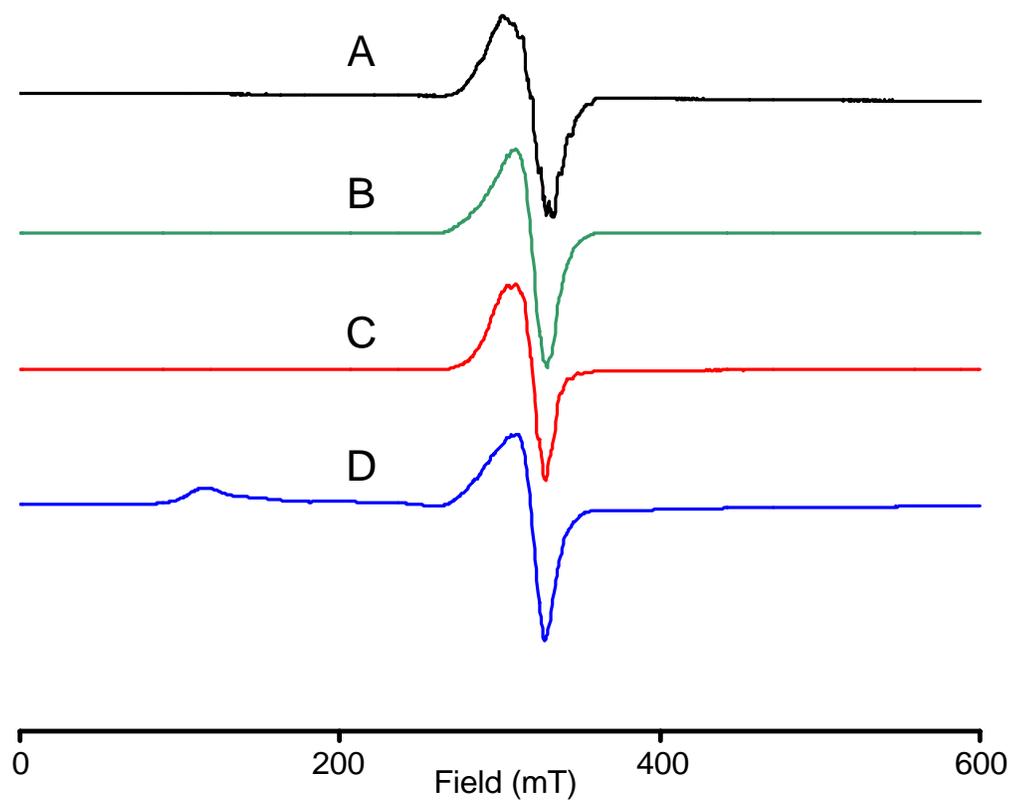
III. EPR spectrum of  $[\text{PhBP}_3]\text{CoSSiPh}_3$  (**9**) in toluene at 20 K.



EPR spectrum of a glassy toluene solution of (A)  $[\text{PhBP}_3]\text{CoO}(4\text{-}^t\text{Bu-Ph})$  (**4**) at 20 K. Inset shows an expansion of the low field signal near 110 mT. EPR spectrum of a glassy toluene solution of (B)  $[\text{PhBP}_3]\text{CoO}(\text{C}_6\text{F}_5)$  (**5**) at 20 K. Inset shows an expansion of the low field signal near 110 mT.



Glassy toluene EPR spectra of (A)  $[\text{PhBP}_3]\text{CoSPh}$  (**5**) (—), (B)  $[\text{PhBP}_3]\text{CoS}(2,6\text{-Me}_2\text{-Ph})$  (**6**) (—), (C)  $[\text{PhBP}_3]\text{CoS}(2,4,6\text{-}^i\text{Pr}_3\text{-Ph})$  (**7**) (—), (D)  $[\text{PhBP}_3]\text{CoS}(2,4,6\text{-}^t\text{Bu}_3\text{-Ph})$  (**8**) (—).



IV. Table with experimental parameters for EPR spectra (2-12, 14-15).

	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>
Solvent	toluene						
Temperature (K)	20	20	20	77	77	10	20
$\nu$ (GHz)	9.475	9.474	9.380	9.380	9.379	9.378	9.379
Modulation frequency (kHz)	100	100	100	100	100	100	100
Modulation amplitude (gauss)	4	5	4	4	4	4	4
Microwave power (mW)	0.202	2.02	2.02	0.641	2.02	0.638	2.02
Conversion time (ms)	81.92	81.92	81.92	163.84	81.92	81.92	81.92
Time constant (ms)	20.48	20.48	20.48	40.96	20.48	20.48	20.48
Scans	2	4	3	1	2	1	3

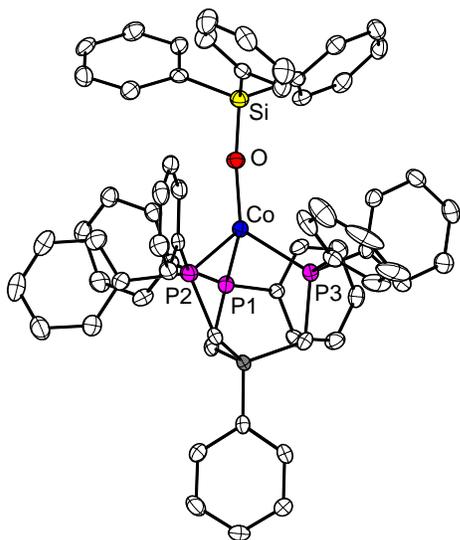
	<b>9</b>	<b>10</b>	<b>11</b>	<b>12</b>	<b>14</b>	<b>15</b>	<b>15</b>
Solvent	toluene	toluene	toluene	toluene	toluene	toluene	powder
Temperature (K)	20	20	20	20	20	20	20
$\nu$ (GHz)	9.380	9.378	9.378	9.379	9.377	9.378	9.382
Modulation frequency (kHz)	100	100	100	100	100	100	100
Modulation amplitude (gauss)	4	4	4	4	4	4	4
Microwave power (mW)	0.638	0.0639	0.00639	0.202	0.639	0.638	0.0638
Conversion time (ms)	81.92	81.92	81.92	81.92	81.92	81.92	81.92
Time constant (ms)	20.48	20.48	20.48	20.48	20.48	20.48	20.48
Scans	1	1	1	1	1	1	3

V. DFT reports for the geometry minimizations of **2**, **6**, and **{16}**.

[PhBP<sub>3</sub>]CoOSiPh<sub>3</sub>, **2**:

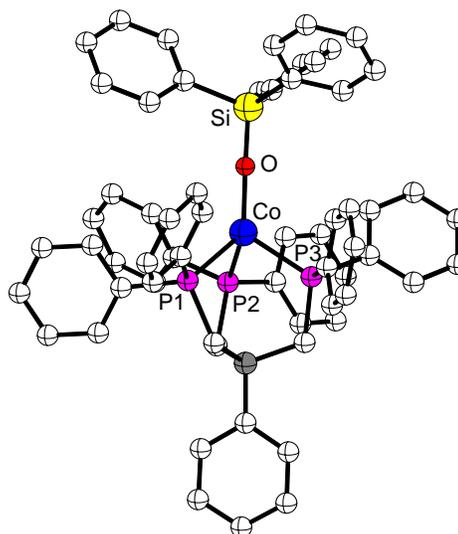
## [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub> – DFT

Experimental – dmj14



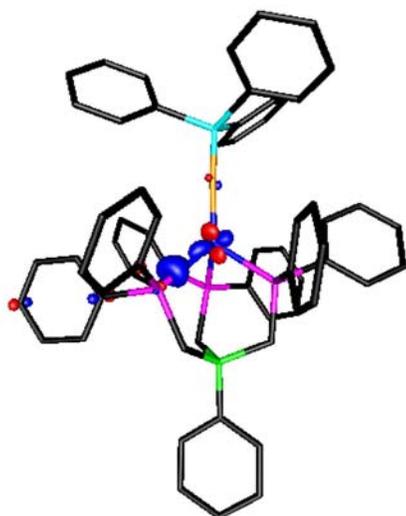
Co-O	1.80 Å	P1-Co-P2	91°
O-Si	1.61 Å	P1-Co-P3	86°
Co-P1	2.16 Å	P2-Co-P3	95°
Co-P2	2.28 Å	P1-Co-O	129°
Co-P3	2.17 Å	P2-Co-O	119°
		P3-Co-O	126°
		Co-O-Si	173°

Theoretical B3LYP - lacvp\*\*

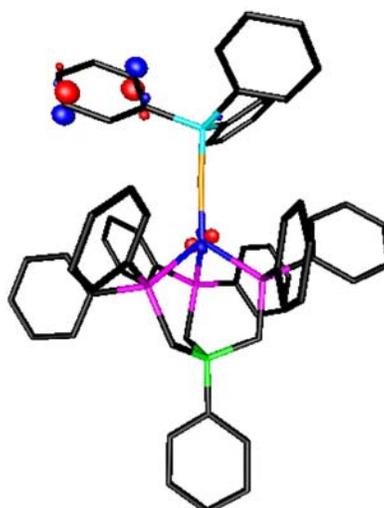


Co-O	1.85 Å	P1-Co-P2	89°
O-Si	1.64 Å	P1-Co-P3	95°
Co-P1	2.43 Å	P2-Co-P3	89°
Co-P2	2.22 Å	P1-Co-O	117°
Co-P3	2.25 Å	P2-Co-O	139°
		P3-Co-O	118°
		Co-O-Si	163°

# [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub> – DFT

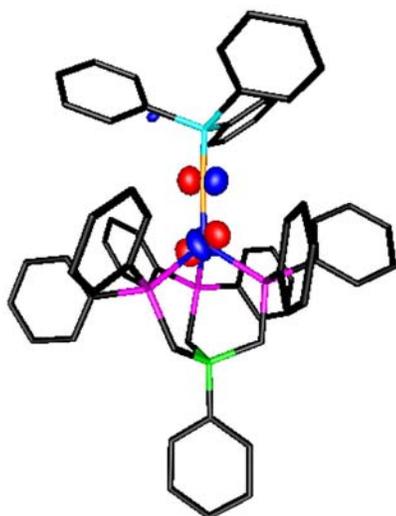


MO 255 – HOMO-6

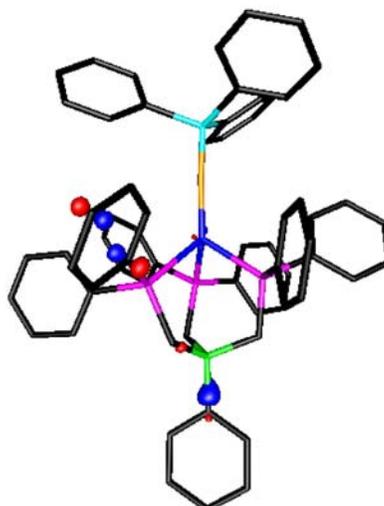


MO 256 – HOMO-5

# [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub> – DFT

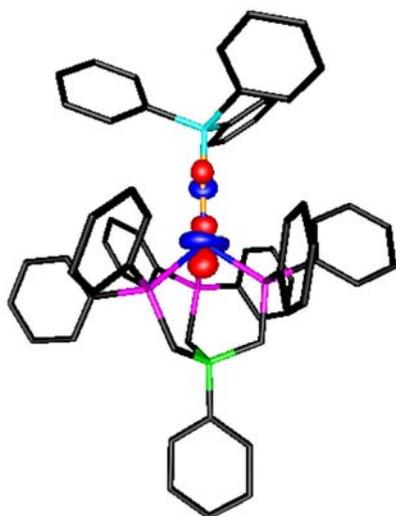


MO 257 – HOMO-4

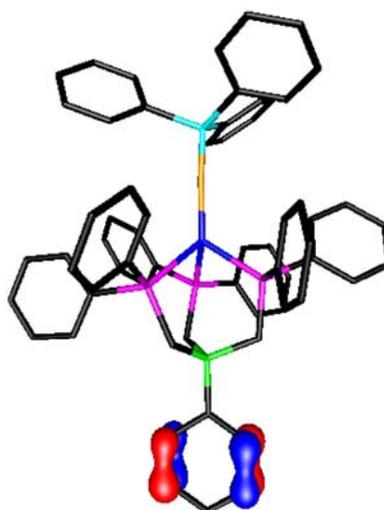


MO 258 – HOMO-3

# [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub> – DFT

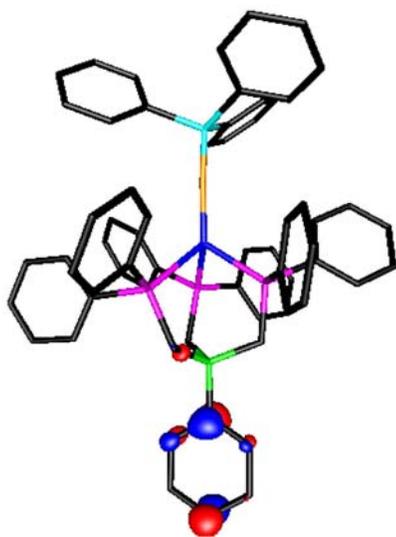


MO 259 – HOMO-2

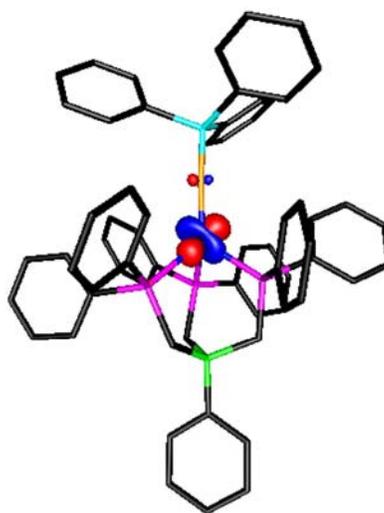


MO 260 – HOMO-1

# [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub> – DFT

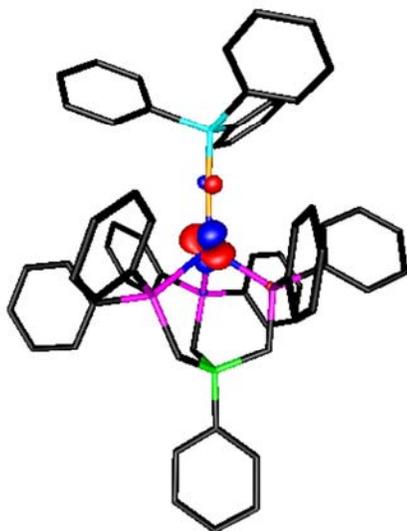


MO 261 – HOMO



MO 262 – SOMO

# [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub> – DFT



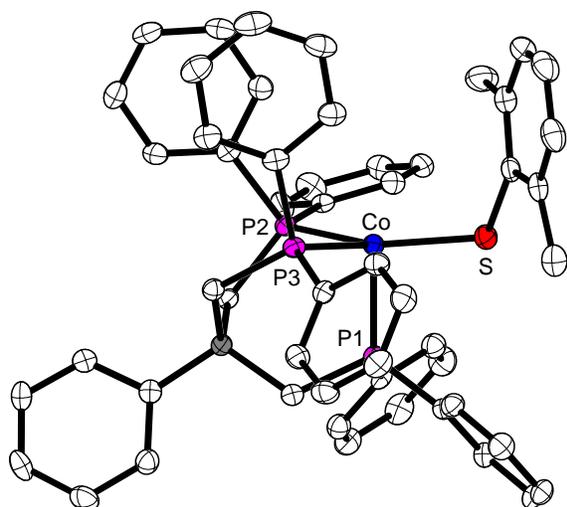
<u>Orbital Energies</u>	<u>(Hartrees)</u>	<u>(kcal/mol)</u>
255 – HOMO-6	-0.239893	-150.5
256 – HOMO-5	-0.239372	-150.2
257 – HOMO-4	-0.238171	-149.5
258 – HOMO-3	-0.236079	-148.1
259 – HOMO-2	-0.223829	-140.5
260 – HOMO-1	-0.218735	-137.3
261 – HOMO	-0.205300	-128.8
262 – SOMO	-0.236116	-148.2
263 – LUMO	-0.082007	-51.5

MO 263 – LUMO

[PhBP<sub>3</sub>]CoS(2,6-Me<sub>2</sub>-Ph), **6**:

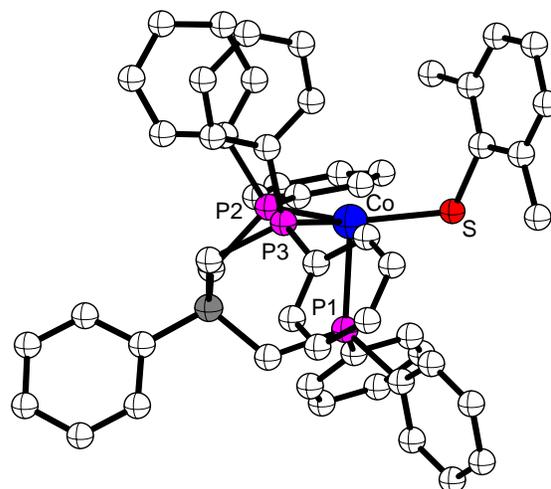
# [PhBP<sub>3</sub>]CoS(2,6-Me<sub>2</sub>-Ph) – DFT

Experimental – dmj39



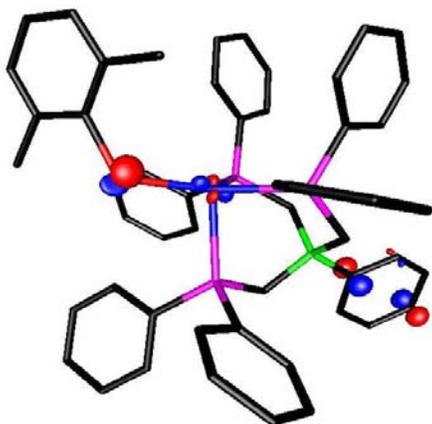
Co-S	2.17 Å	P1-Co-P2	89°
Co-P1	2.25 Å	P1-Co-P3	100°
Co-P2	2.20 Å	P2-Co-P3	87°
Co-P3	2.21 Å	P1-Co-S	96°
		P2-Co-S	147°
		P3-Co-S	123°

Theoretical B3LYP - lacvp\*\*

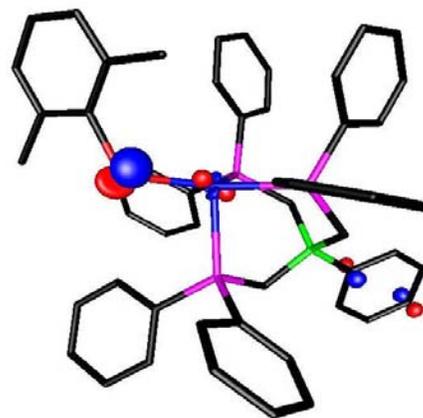


Co-S	2.22 Å	P1-Co-P2	89°
Co-P1	2.42 Å	P1-Co-P3	96°
Co-P2	2.27 Å	P2-Co-P3	89°
Co-P3	2.29 Å	P1-Co-S	100°
		P2-Co-S	145°
		P3-Co-S	122°

# [PhBP<sub>3</sub>]CoS(2,6-Me<sub>2</sub>-Ph) – DFT

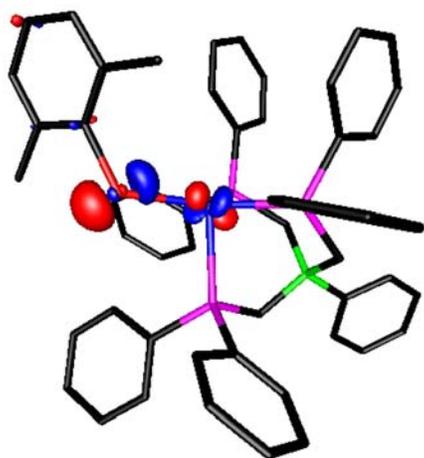


MO 223 – HOMO-2

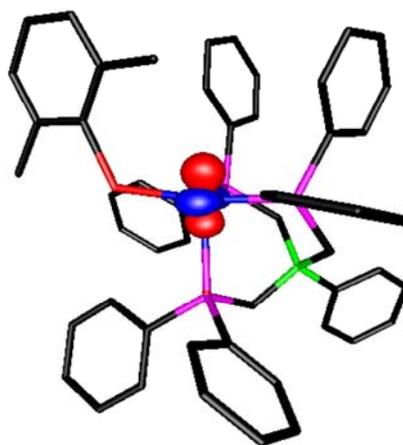


MO 224 – HOMO-1

# [PhBP<sub>3</sub>]CoS(2,6-Me<sub>2</sub>-Ph) – DFT

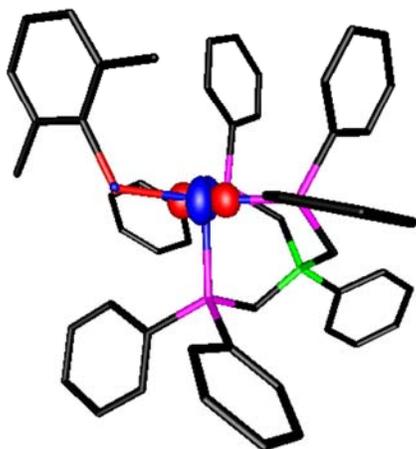


MO 225 – HOMO



MO 226 – SOMO

# [PhBP<sub>3</sub>]CoS(2,6-Me<sub>2</sub>-Ph) – DFT



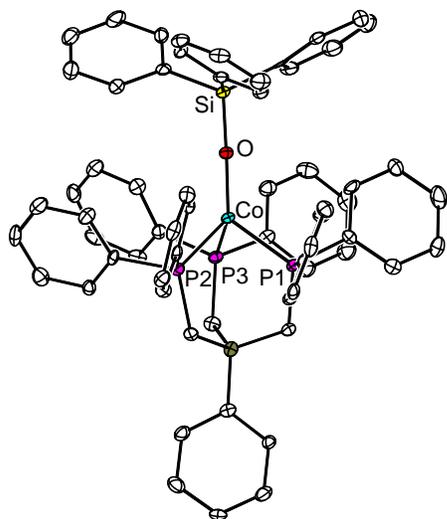
MO 227 – LUMO

<u>Orbital Energies</u>	<u>(Hartrees)</u>	<u>(kcal/mol)</u>
223 – HOMO-2	-0.208194	-130.6
224 – HOMO-1	-0.206318	-129.5
225 – HOMO	-0.202609	-127.1
226 – SOMO	-0.245234	-153.9
227 – LUMO	-0.089866	-56.4

{[PhBP<sub>3</sub>]CoOSiPh<sub>3</sub>}, {16}:

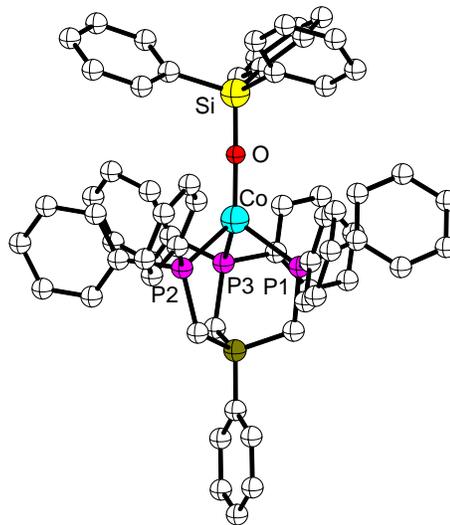
# {[PhBP<sub>3</sub>]CoOSiPh<sub>3</sub>}<sup>+</sup> – DFT

Experimental – dmj40



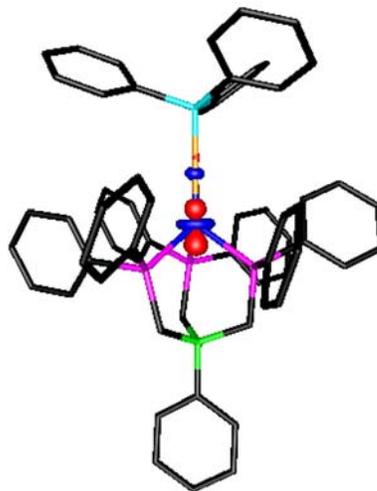
Co-O	1.77 Å	P1-Co-P2	91°
O-Si	1.65 Å	P1-Co-P3	90°
Co-P1	2.19 Å	P2-Co-P3	91°
Co-P2	2.18 Å	P1-Co-O	126°
Co-P3	2.18 Å	P2-Co-O	124°
		P3-Co-O	125°
		Co-O-Si	179°

Theoretical B3LYP - lacvp\*\*



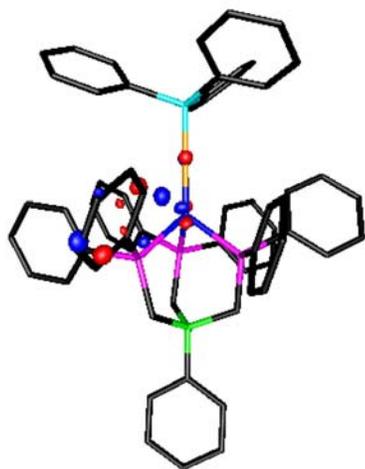
Co-O	1.78 Å	P1-Co-P2	91°
O-Si	1.68 Å	P1-Co-P3	91°
Co-P1	2.24 Å	P2-Co-P3	91°
Co-P2	2.24 Å	P1-Co-O	124°
Co-P3	2.23 Å	P2-Co-O	126°
		P3-Co-O	124°
		Co-O-Si	179°

$\{[\text{PhBP}_3]\text{CoOSiPh}_3\}^+$  – DFT

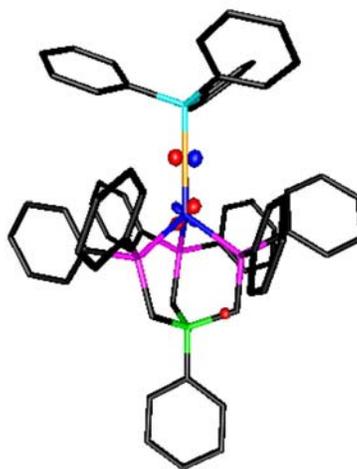


MO 241 – HOMO-20

$\{[\text{PhBP}_3]\text{CoOSiPh}_3\}^+ - \text{DFT}$

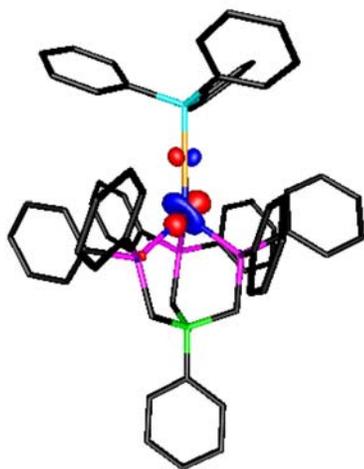


MO 245 – HOMO-16

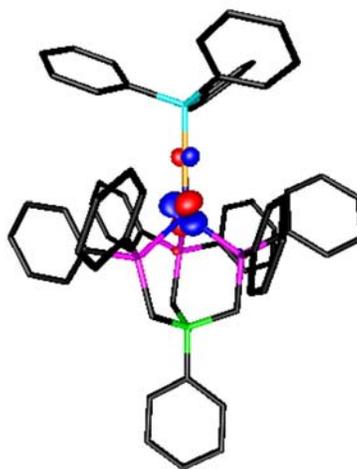


MO 246 – HOMO-15

$\{[\text{PhBP}_3]\text{CoOSiPh}_3\}^+ - \text{DFT}$



MO 262 – LUMO



MO 263 – LUMO+1

# $\{[\text{PhBP}_3]\text{CoOSiPh}_3\}^+$ – DFT

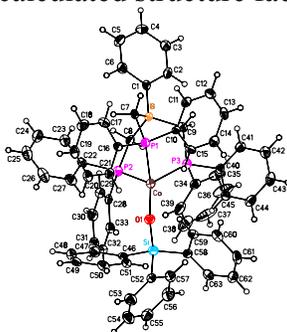
<u>Orbital Energies</u>	<u>(Hartrees)</u>	<u>(kcal/mol)</u>
241 – HOMO-20	-0.357658	-223.1
245 – HOMO-16	-0.344438	-216.6
246 – HOMO-15	-0.343270	-216.2
262 – LUMO	-0.195077	-126.7
263 – LUMO+1	-0.194074	-126.6

VI. X-ray reports for complexes **2** (low temperature), **2** (ambient temperature), **3**, **5**, **6**, **7**, **8**, **9**, **10**, **12**, **15**, {**16**} {BPh<sub>4</sub>}, and **17**.

A. X-ray report for [PhBP<sub>3</sub>]CoOSiPh<sub>3</sub>, **2** (low temperature).

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Table 6.	Observed and calculated structure factors (for deposit)



DMJ14

**Note:** The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 193897. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 193897."

**Table 1. Crystal data and structure refinement for DMJ14 (CCDC 193897).**

Empirical formula	C <sub>63</sub> H <sub>56</sub> BOP <sub>3</sub> SiCo 1½(C <sub>6</sub> H <sub>6</sub> )
Formula weight	1136.98
Crystallization Solvent	Benzene/petroleum ether
Crystal Habit	Block
Crystal size	0.37 x 0.28 x 0.22 mm <sup>3</sup>
Crystal color	Purple

### Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98 K	
θ range for 6856 reflections used in lattice determination	2.30 to 22.4°	
Unit cell dimensions	a = 13.1013(14) Å b = 14.4428(16) Å c = 16.9894(19) Å	α = 77.984(2)° β = 67.9620(10)° γ = 89.536(2)°
Volume	2905.8(6) Å <sup>3</sup>	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.299 Mg/m <sup>3</sup>	
F(000)	1192	
Data collection program	Bruker SMART v5.054	
θ range for data collection	1.70 to 22.63°	
Completeness to θ = 22.63°	74.8 %	
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -15 ≤ l ≤ 17	
Data collection scan type	ω scans at 3 φ settings	
Data reduction program	Bruker SAINT v6.022	
Reflections collected	11925	
Independent reflections	5788 [R <sub>int</sub> = 0.0383]	
Absorption coefficient	0.444 mm <sup>-1</sup>	
Absorption correction	None	
Max. and min. transmission	0.9085 and 0.8528	

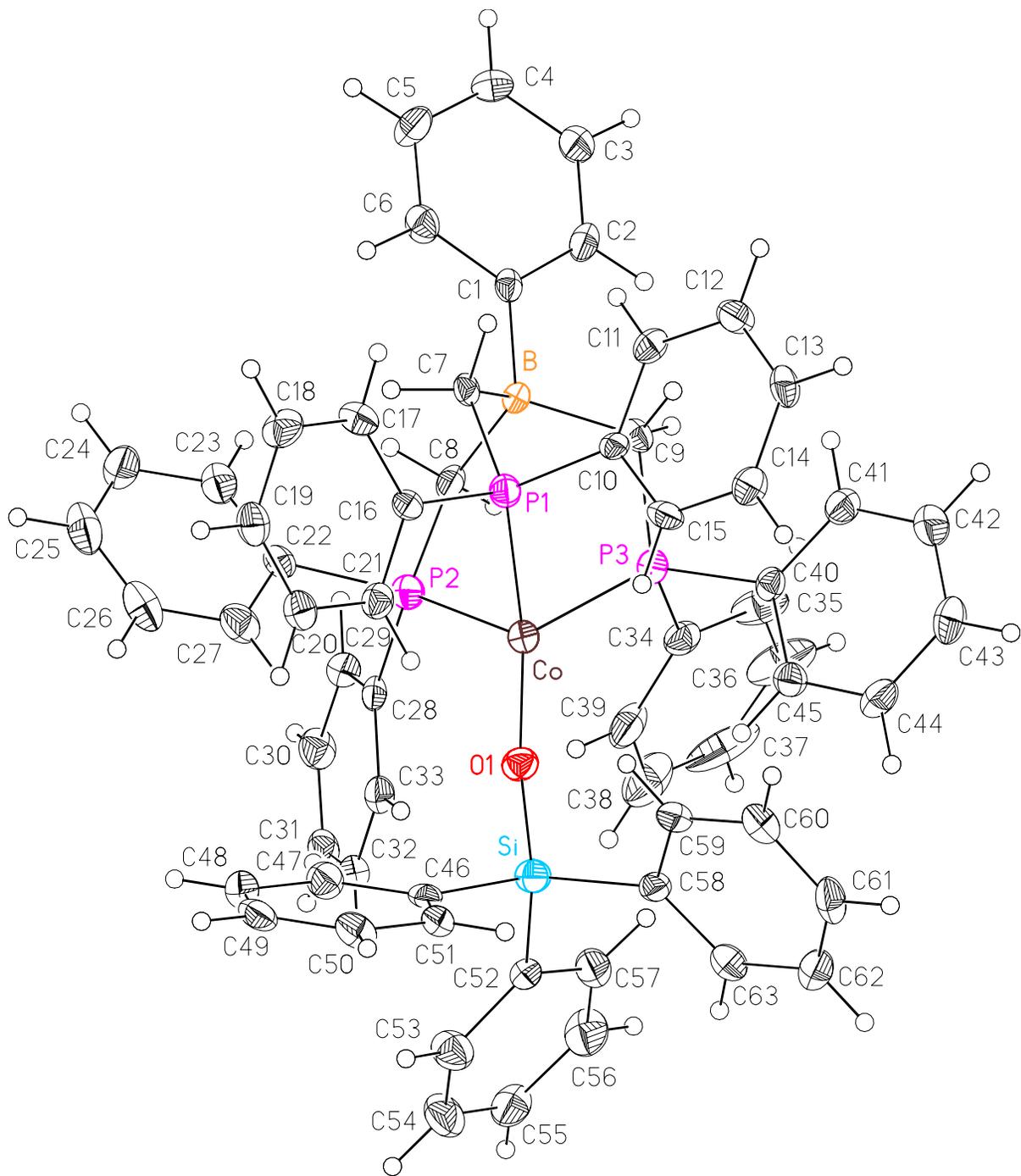
**Table 1 (cont.)****Structure solution and Refinement**

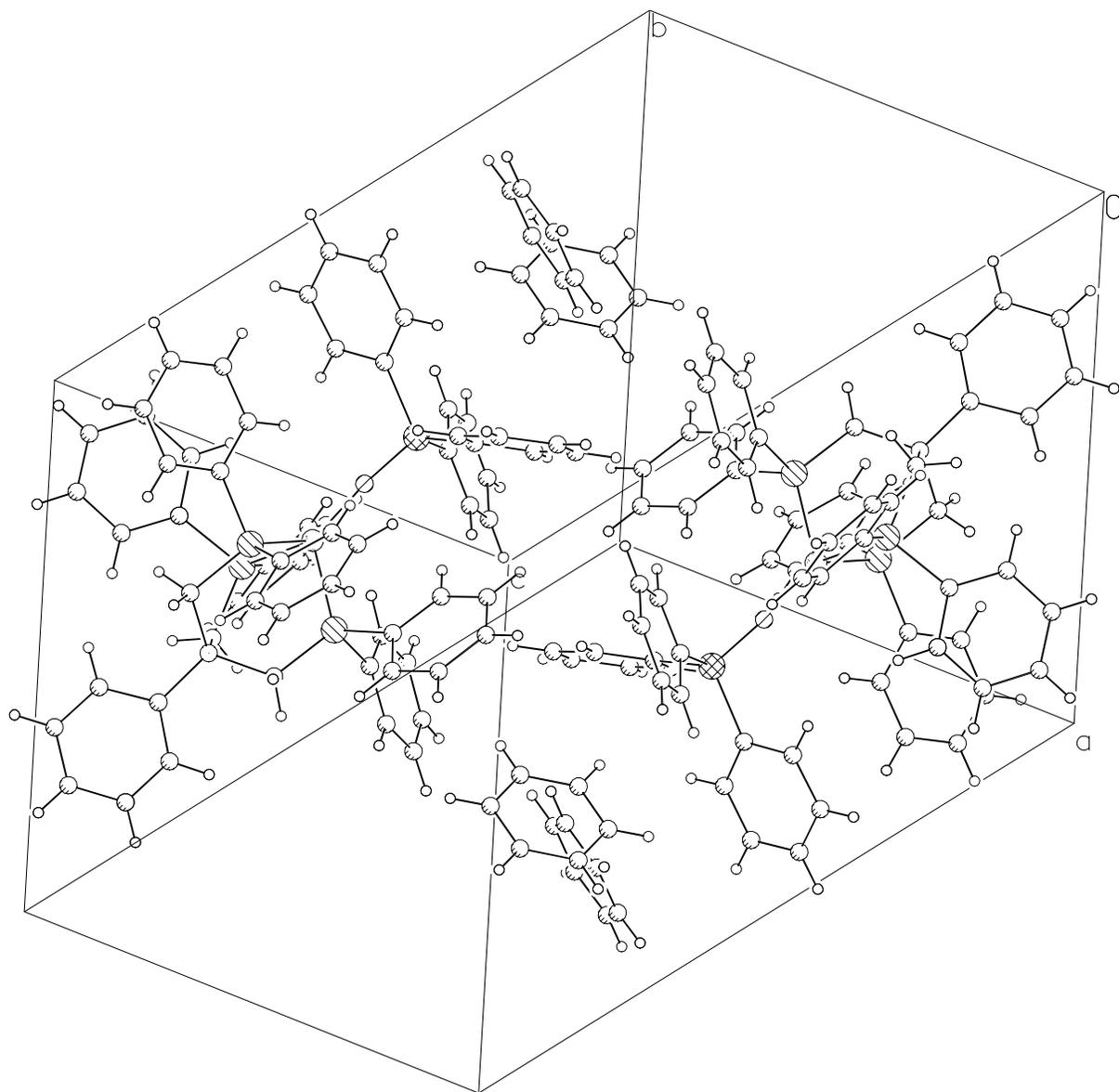
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	5788 / 0 / 712
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F <sup>2</sup>	1.486
Final R indices [I>2σ(I), 4721 reflections]	R1 = 0.0336, wR2 = 0.0673
R indices (all data)	R1 = 0.0456, wR2 = 0.0698
Type of weighting scheme used	Sigma
Weighting scheme used	w=1/σ <sup>2</sup> (F <sub>o</sub> <sup>2</sup> )
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.273 and -0.277 e.Å <sup>-3</sup>

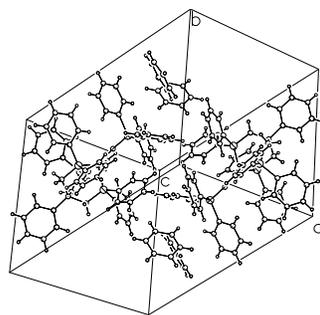
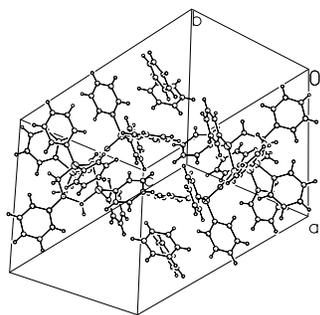
**Special Refinement Details**

Refinement of F<sup>2</sup> against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F<sup>2</sup>, conventional R-factors (R) are based on F, with F set to zero for negative F<sup>2</sup>. The threshold expression of F<sup>2</sup> > 2σ(F<sup>2</sup>) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F<sup>2</sup> are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.







**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for DMJ14 (CCDC 193897).  $U_{\text{eq}}$  is defined as the trace of the orthogonalized  $U_{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co	6253(1)	2771(1)	2410(1)	19(1)
P(1)	5662(1)	1360(1)	2469(1)	19(1)
P(2)	6920(1)	3118(1)	924(1)	22(1)
P(3)	4599(1)	3162(1)	2562(1)	20(1)
Si	7643(1)	3476(1)	3549(1)	22(1)
O(1)	7066(2)	3145(1)	2954(1)	22(1)
B	4819(3)	2221(2)	1157(2)	17(1)
C(1)	4190(3)	1913(2)	580(2)	17(1)
C(2)	3193(3)	2234(2)	573(2)	26(1)
C(3)	2658(3)	1934(2)	88(2)	31(1)
C(4)	3108(3)	1297(2)	-409(2)	30(1)
C(5)	4116(3)	981(2)	-450(2)	30(1)
C(6)	4637(3)	1286(2)	37(2)	24(1)
C(7)	5343(2)	1259(2)	1555(2)	17(1)
C(8)	5825(2)	3058(2)	529(2)	21(1)
C(9)	3941(2)	2628(2)	1989(2)	18(1)
C(10)	4486(2)	822(2)	3447(2)	15(1)
C(11)	3577(3)	343(2)	3434(2)	21(1)
C(12)	2697(3)	-39(2)	4201(2)	25(1)
C(13)	2713(3)	47(2)	4988(2)	24(1)
C(14)	3608(3)	520(2)	5013(2)	24(1)
C(15)	4481(3)	904(2)	4249(2)	21(1)
C(16)	6728(2)	565(2)	2518(2)	18(1)
C(17)	6719(3)	-314(2)	2304(2)	24(1)
C(18)	7540(3)	-918(2)	2319(2)	28(1)
C(19)	8391(3)	-653(2)	2536(2)	25(1)
C(20)	8418(3)	213(2)	2749(2)	24(1)
C(21)	7589(3)	814(2)	2748(2)	21(1)
C(22)	7961(2)	2340(2)	414(2)	20(1)
C(23)	8024(3)	2008(2)	-307(2)	29(1)
C(24)	8856(3)	1440(2)	-666(2)	35(1)
C(25)	9625(3)	1203(2)	-313(2)	36(1)
C(26)	9577(3)	1522(2)	398(2)	35(1)
C(27)	8753(3)	2089(2)	761(2)	28(1)
C(28)	7710(2)	4272(2)	384(2)	20(1)
C(29)	7752(3)	4749(2)	-425(2)	25(1)
C(30)	8372(3)	5617(2)	-822(2)	27(1)
C(31)	8924(3)	6002(2)	-403(2)	29(1)
C(32)	8880(3)	5529(2)	401(2)	26(1)
C(33)	8273(3)	4663(2)	795(2)	23(1)
C(34)	4618(3)	4438(2)	2183(2)	23(1)
C(35)	3665(3)	4855(2)	2188(2)	37(1)
C(36)	3693(4)	5836(3)	1894(3)	52(1)
C(37)	4694(5)	6375(3)	1576(2)	53(1)
C(38)	5625(4)	5973(3)	1585(2)	49(1)
C(39)	5582(3)	5009(3)	1892(2)	35(1)
C(40)	3699(3)	3019(2)	3697(2)	18(1)

C(41)	2612(3)	2621(2)	4044(2)	26(1)
C(42)	1970(3)	2544(2)	4915(2)	32(1)
C(43)	2389(3)	2855(2)	5450(2)	29(1)
C(44)	3464(3)	3253(2)	5118(2)	27(1)
C(45)	4108(3)	3327(2)	4249(2)	22(1)
C(46)	8830(2)	2730(2)	3518(2)	18(1)
C(47)	9617(3)	2659(2)	2714(2)	25(1)
C(48)	10493(3)	2092(2)	2640(2)	29(1)
C(49)	10598(3)	1569(2)	3388(2)	27(1)
C(50)	9833(3)	1625(2)	4192(2)	27(1)
C(51)	8966(3)	2192(2)	4255(2)	22(1)
C(52)	8161(3)	4752(2)	3079(2)	20(1)
C(53)	9260(3)	5083(2)	2772(2)	31(1)
C(54)	9618(3)	6025(3)	2353(2)	36(1)
C(55)	8871(3)	6655(2)	2247(2)	33(1)
C(56)	7773(3)	6358(2)	2559(2)	35(1)
C(57)	7426(3)	5422(2)	2971(2)	28(1)
C(58)	6668(2)	3293(2)	4708(2)	19(1)
C(59)	6175(3)	2378(2)	5158(2)	23(1)
C(60)	5490(3)	2181(2)	6028(2)	27(1)
C(61)	5275(3)	2896(3)	6476(2)	29(1)
C(62)	5729(3)	3806(2)	6062(2)	27(1)
C(63)	6414(3)	3999(2)	5187(2)	23(1)
C(71)	1206(3)	8051(3)	3409(2)	39(1)
C(72)	2275(3)	7852(3)	2974(3)	44(1)
C(73)	2954(3)	8511(3)	2253(3)	49(1)
C(74)	2584(3)	9359(3)	1967(3)	44(1)
C(75)	1518(4)	9556(3)	2415(3)	41(1)
C(76)	837(3)	8899(3)	3133(2)	40(1)
C(81)	8887(3)	5077(3)	5485(3)	56(1)
C(82)	9200(4)	4391(3)	5013(3)	56(1)
C(83)	10306(4)	4303(3)	4530(3)	58(1)

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**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for DMJ14 (CCDC 193897).**

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Co-B	3.526(4)	O(1)-Co-P(1)	129.45(7)
Co-P(1)	2.1564(9)	O(1)-Co-P(3)	125.82(7)
Co-P(2)	2.2838(10)	P(1)-Co-P(3)	85.88(3)
Co-P(3)	2.1694(9)	O(1)-Co-P(2)	119.42(7)
Co-O(1)	1.7989(19)	P(1)-Co-P(2)	91.38(3)
Si-O(1)	1.612(2)	P(3)-Co-P(2)	94.60(3)

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**Table 4. Bond lengths [Å] and angles [°] for DMJ14 (CCDC 193897).**

Co-O(1)	1.7989(19)	C(16)-C(21)	1.396(4)
Co-P(1)	2.1564(9)	C(17)-C(18)	1.383(4)
Co-P(3)	2.1694(9)	C(17)-H(17)	0.9500
Co-P(2)	2.2838(10)	C(18)-C(19)	1.378(4)
Co-B	3.526(4)	C(18)-H(18)	0.9500
P(1)-C(7)	1.785(3)	C(19)-C(20)	1.377(4)
P(1)-C(16)	1.816(3)	C(19)-H(19)	0.9500
P(1)-C(10)	1.816(3)	C(20)-C(21)	1.385(4)
P(2)-C(8)	1.807(3)	C(20)-H(20)	0.9500
P(2)-C(28)	1.835(3)	C(21)-H(21)	0.9500
P(2)-C(22)	1.835(3)	C(22)-C(23)	1.380(4)
P(3)-C(9)	1.799(3)	C(22)-C(27)	1.387(4)
P(3)-C(40)	1.812(3)	C(23)-C(24)	1.389(4)
P(3)-C(34)	1.819(3)	C(23)-H(23)	0.9500
Si-O(1)	1.612(2)	C(24)-C(25)	1.362(4)
Si-C(58)	1.867(3)	C(24)-H(24)	0.9500
Si-C(52)	1.868(3)	C(25)-C(26)	1.361(4)
Si-C(46)	1.875(3)	C(25)-H(25)	0.9500
B-C(1)	1.622(4)	C(26)-C(27)	1.383(4)
B-C(8)	1.665(4)	C(26)-H(26)	0.9500
B-C(9)	1.667(4)	C(27)-H(27)	0.9500
B-C(7)	1.673(4)	C(28)-C(33)	1.381(4)
C(1)-C(2)	1.386(4)	C(28)-C(29)	1.384(4)
C(1)-C(6)	1.395(4)	C(29)-C(30)	1.393(4)
C(2)-C(3)	1.394(4)	C(29)-H(29)	0.9500
C(2)-H(2)	0.9500	C(30)-C(31)	1.378(4)
C(3)-C(4)	1.360(4)	C(30)-H(30)	0.9500
C(3)-H(3)	0.9500	C(31)-C(32)	1.374(4)
C(4)-C(5)	1.376(4)	C(31)-H(31)	0.9500
C(4)-H(4)	0.9500	C(32)-C(33)	1.383(4)
C(5)-C(6)	1.388(4)	C(32)-H(32)	0.9500
C(5)-H(5)	0.9500	C(33)-H(33)	0.9500
C(6)-H(6)	0.9500	C(34)-C(39)	1.378(4)
C(7)-H(7A)	0.9900	C(34)-C(35)	1.380(4)
C(7)-H(7B)	0.9900	C(35)-C(36)	1.397(5)
C(8)-H(8A)	0.9900	C(35)-H(35)	0.9500
C(8)-H(8B)	0.9900	C(36)-C(37)	1.389(5)
C(9)-H(9A)	0.9900	C(36)-H(36)	0.9500
C(9)-H(9B)	0.9900	C(37)-C(38)	1.351(5)
C(10)-C(15)	1.389(4)	C(37)-H(37)	0.9500
C(10)-C(11)	1.391(4)	C(38)-C(39)	1.375(5)
C(11)-C(12)	1.384(4)	C(38)-H(38)	0.9500
C(11)-H(11)	0.9500	C(39)-H(39)	0.9500
C(12)-C(13)	1.377(4)	C(40)-C(45)	1.387(4)
C(12)-H(12)	0.9500	C(40)-C(41)	1.396(4)
C(13)-C(14)	1.381(4)	C(41)-C(42)	1.382(4)
C(13)-H(13)	0.9500	C(41)-H(41)	0.9500
C(14)-C(15)	1.377(4)	C(42)-C(43)	1.370(4)
C(14)-H(14)	0.9500	C(42)-H(42)	0.9500
C(15)-H(15)	0.9500	C(43)-C(44)	1.383(4)
C(16)-C(17)	1.393(4)	C(43)-H(43)	0.9500

C(44)-C(45)	1.380(4)	C(83)-H(83)	0.9500
C(44)-H(44)	0.9500		
C(45)-H(45)	0.9500	O(1)-Co-P(1)	129.45(7)
C(46)-C(47)	1.392(4)	O(1)-Co-P(3)	125.82(7)
C(46)-C(51)	1.401(4)	P(1)-Co-P(3)	85.88(3)
C(47)-C(48)	1.387(4)	O(1)-Co-P(2)	119.42(7)
C(47)-H(47)	0.9500	P(1)-Co-P(2)	91.38(3)
C(48)-C(49)	1.391(4)	P(3)-Co-P(2)	94.60(3)
C(48)-H(48)	0.9500	C(7)-P(1)-C(16)	108.00(14)
C(49)-C(50)	1.376(4)	C(7)-P(1)-C(10)	107.61(14)
C(49)-H(49)	0.9500	C(16)-P(1)-C(10)	102.34(13)
C(50)-C(51)	1.380(4)	C(7)-P(1)-Co	113.97(10)
C(50)-H(50)	0.9500	C(16)-P(1)-Co	108.16(11)
C(51)-H(51)	0.9500	C(10)-P(1)-Co	115.90(10)
C(52)-C(53)	1.385(4)	C(8)-P(2)-C(28)	107.85(15)
C(52)-C(57)	1.393(4)	C(8)-P(2)-C(22)	106.96(15)
C(53)-C(54)	1.392(4)	C(28)-P(2)-C(22)	99.41(14)
C(53)-H(53)	0.9500	C(8)-P(2)-Co	111.39(10)
C(54)-C(55)	1.366(4)	C(28)-P(2)-Co	115.72(11)
C(54)-H(54)	0.9500	C(22)-P(2)-Co	114.54(11)
C(55)-C(56)	1.370(4)	C(9)-P(3)-C(40)	110.74(14)
C(55)-H(55)	0.9500	C(9)-P(3)-C(34)	105.99(14)
C(56)-C(57)	1.380(4)	C(40)-P(3)-C(34)	100.43(14)
C(56)-H(56)	0.9500	C(9)-P(3)-Co	116.57(10)
C(57)-H(57)	0.9500	C(40)-P(3)-Co	111.92(10)
C(58)-C(63)	1.395(4)	C(34)-P(3)-Co	109.78(12)
C(58)-C(59)	1.404(4)	O(1)-Si-C(58)	111.55(12)
C(59)-C(60)	1.381(4)	O(1)-Si-C(52)	108.21(12)
C(59)-H(59)	0.9500	C(58)-Si-C(52)	111.21(14)
C(60)-C(61)	1.373(4)	O(1)-Si-C(46)	108.28(12)
C(60)-H(60)	0.9500	C(58)-Si-C(46)	107.66(14)
C(61)-C(62)	1.375(4)	C(52)-Si-C(46)	109.89(14)
C(61)-H(61)	0.9500	Si-O(1)-Co	172.47(13)
C(62)-C(63)	1.387(4)	C(1)-B-C(8)	109.3(2)
C(62)-H(62)	0.9500	C(1)-B-C(9)	110.9(2)
C(63)-H(63)	0.9500	C(8)-B-C(9)	109.6(2)
C(71)-C(76)	1.368(4)	C(1)-B-C(7)	108.2(2)
C(71)-C(72)	1.377(5)	C(8)-B-C(7)	110.3(2)
C(71)-H(71)	0.9500	C(9)-B-C(7)	108.5(2)
C(72)-C(73)	1.382(5)	C(2)-C(1)-C(6)	114.4(3)
C(72)-H(72)	0.9500	C(2)-C(1)-B	124.5(3)
C(73)-C(74)	1.375(5)	C(6)-C(1)-B	121.0(3)
C(73)-H(73)	0.9500	C(1)-C(2)-C(3)	123.1(3)
C(74)-C(75)	1.377(5)	C(1)-C(2)-H(2)	118.4
C(74)-H(74)	0.9500	C(3)-C(2)-H(2)	118.4
C(75)-C(76)	1.379(5)	C(4)-C(3)-C(2)	120.3(3)
C(75)-H(75)	0.9500	C(4)-C(3)-H(3)	119.8
C(76)-H(76)	0.9500	C(2)-C(3)-H(3)	119.8
C(81)-C(82)	1.367(5)	C(3)-C(4)-C(5)	119.0(3)
C(81)-C(83)#1	1.381(5)	C(3)-C(4)-H(4)	120.5
C(81)-H(81)	0.9500	C(5)-C(4)-H(4)	120.5
C(82)-C(83)	1.392(5)	C(4)-C(5)-C(6)	119.9(3)
C(82)-H(82)	0.9500	C(4)-C(5)-H(5)	120.1
C(83)-C(81)#1	1.381(5)	C(6)-C(5)-H(5)	120.1

C(5)-C(6)-C(1)	123.2(3)	C(20)-C(21)-C(16)	121.1(3)
C(5)-C(6)-H(6)	118.4	C(20)-C(21)-H(21)	119.5
C(1)-C(6)-H(6)	118.4	C(16)-C(21)-H(21)	119.5
B-C(7)-P(1)	113.9(2)	C(23)-C(22)-C(27)	117.8(3)
B-C(7)-H(7A)	108.8	C(23)-C(22)-P(2)	124.3(3)
P(1)-C(7)-H(7A)	108.8	C(27)-C(22)-P(2)	117.8(3)
B-C(7)-H(7B)	108.8	C(22)-C(23)-C(24)	120.6(3)
P(1)-C(7)-H(7B)	108.8	C(22)-C(23)-H(23)	119.7
H(7A)-C(7)-H(7B)	107.7	C(24)-C(23)-H(23)	119.7
B-C(8)-P(2)	113.6(2)	C(25)-C(24)-C(23)	120.5(3)
B-C(8)-H(8A)	108.9	C(25)-C(24)-H(24)	119.7
P(2)-C(8)-H(8A)	108.9	C(23)-C(24)-H(24)	119.7
B-C(8)-H(8B)	108.9	C(26)-C(25)-C(24)	119.8(3)
P(2)-C(8)-H(8B)	108.9	C(26)-C(25)-H(25)	120.1
H(8A)-C(8)-H(8B)	107.7	C(24)-C(25)-H(25)	120.1
B-C(9)-P(3)	113.9(2)	C(25)-C(26)-C(27)	120.3(3)
B-C(9)-H(9A)	108.8	C(25)-C(26)-H(26)	119.9
P(3)-C(9)-H(9A)	108.8	C(27)-C(26)-H(26)	119.9
B-C(9)-H(9B)	108.8	C(26)-C(27)-C(22)	121.0(3)
P(3)-C(9)-H(9B)	108.8	C(26)-C(27)-H(27)	119.5
H(9A)-C(9)-H(9B)	107.7	C(22)-C(27)-H(27)	119.5
C(15)-C(10)-C(11)	118.1(3)	C(33)-C(28)-C(29)	119.8(3)
C(15)-C(10)-P(1)	118.6(2)	C(33)-C(28)-P(2)	119.1(2)
C(11)-C(10)-P(1)	123.3(2)	C(29)-C(28)-P(2)	121.1(3)
C(12)-C(11)-C(10)	120.6(3)	C(28)-C(29)-C(30)	119.7(3)
C(12)-C(11)-H(11)	119.7	C(28)-C(29)-H(29)	120.2
C(10)-C(11)-H(11)	119.7	C(30)-C(29)-H(29)	120.2
C(13)-C(12)-C(11)	120.3(3)	C(31)-C(30)-C(29)	119.9(3)
C(13)-C(12)-H(12)	119.9	C(31)-C(30)-H(30)	120.1
C(11)-C(12)-H(12)	119.9	C(29)-C(30)-H(30)	120.1
C(12)-C(13)-C(14)	119.9(3)	C(32)-C(31)-C(30)	120.5(3)
C(12)-C(13)-H(13)	120.1	C(32)-C(31)-H(31)	119.8
C(14)-C(13)-H(13)	120.1	C(30)-C(31)-H(31)	119.8
C(15)-C(14)-C(13)	119.7(3)	C(31)-C(32)-C(33)	119.8(3)
C(15)-C(14)-H(14)	120.1	C(31)-C(32)-H(32)	120.1
C(13)-C(14)-H(14)	120.1	C(33)-C(32)-H(32)	120.1
C(14)-C(15)-C(10)	121.4(3)	C(28)-C(33)-C(32)	120.3(3)
C(14)-C(15)-H(15)	119.3	C(28)-C(33)-H(33)	119.8
C(10)-C(15)-H(15)	119.3	C(32)-C(33)-H(33)	119.8
C(17)-C(16)-C(21)	117.9(3)	C(39)-C(34)-C(35)	118.7(3)
C(17)-C(16)-P(1)	120.2(2)	C(39)-C(34)-P(3)	120.7(3)
C(21)-C(16)-P(1)	121.9(2)	C(35)-C(34)-P(3)	120.6(3)
C(18)-C(17)-C(16)	120.8(3)	C(34)-C(35)-C(36)	119.9(4)
C(18)-C(17)-H(17)	119.6	C(34)-C(35)-H(35)	120.0
C(16)-C(17)-H(17)	119.6	C(36)-C(35)-H(35)	120.0
C(19)-C(18)-C(17)	120.4(3)	C(37)-C(36)-C(35)	119.1(4)
C(19)-C(18)-H(18)	119.8	C(37)-C(36)-H(36)	120.4
C(17)-C(18)-H(18)	119.8	C(35)-C(36)-H(36)	120.4
C(20)-C(19)-C(18)	119.9(3)	C(38)-C(37)-C(36)	121.1(4)
C(20)-C(19)-H(19)	120.1	C(38)-C(37)-H(37)	119.5
C(18)-C(19)-H(19)	120.1	C(36)-C(37)-H(37)	119.5
C(19)-C(20)-C(21)	120.0(3)	C(37)-C(38)-C(39)	119.2(4)
C(19)-C(20)-H(20)	120.0	C(37)-C(38)-H(38)	120.4
C(21)-C(20)-H(20)	120.0	C(39)-C(38)-H(38)	120.4

C(38)-C(39)-C(34)	121.9(4)	C(56)-C(57)-C(52)	122.1(3)
C(38)-C(39)-H(39)	119.1	C(56)-C(57)-H(57)	118.9
C(34)-C(39)-H(39)	119.1	C(52)-C(57)-H(57)	118.9
C(45)-C(40)-C(41)	118.2(3)	C(63)-C(58)-C(59)	116.3(3)
C(45)-C(40)-P(3)	118.3(3)	C(63)-C(58)-Si	124.8(2)
C(41)-C(40)-P(3)	123.5(3)	C(59)-C(58)-Si	118.9(2)
C(42)-C(41)-C(40)	120.2(3)	C(60)-C(59)-C(58)	122.1(3)
C(42)-C(41)-H(41)	119.9	C(60)-C(59)-H(59)	119.0
C(40)-C(41)-H(41)	119.9	C(58)-C(59)-H(59)	119.0
C(43)-C(42)-C(41)	120.7(3)	C(61)-C(60)-C(59)	119.6(3)
C(43)-C(42)-H(42)	119.7	C(61)-C(60)-H(60)	120.2
C(41)-C(42)-H(42)	119.7	C(59)-C(60)-H(60)	120.2
C(42)-C(43)-C(44)	120.0(3)	C(60)-C(61)-C(62)	120.5(3)
C(42)-C(43)-H(43)	120.0	C(60)-C(61)-H(61)	119.8
C(44)-C(43)-H(43)	120.0	C(62)-C(61)-H(61)	119.8
C(45)-C(44)-C(43)	119.5(3)	C(61)-C(62)-C(63)	119.6(3)
C(45)-C(44)-H(44)	120.2	C(61)-C(62)-H(62)	120.2
C(43)-C(44)-H(44)	120.2	C(63)-C(62)-H(62)	120.2
C(44)-C(45)-C(40)	121.4(3)	C(62)-C(63)-C(58)	122.0(3)
C(44)-C(45)-H(45)	119.3	C(62)-C(63)-H(63)	119.0
C(40)-C(45)-H(45)	119.3	C(58)-C(63)-H(63)	119.0
C(47)-C(46)-C(51)	116.3(3)	C(76)-C(71)-C(72)	120.0(4)
C(47)-C(46)-Si	119.0(2)	C(76)-C(71)-H(71)	120.0
C(51)-C(46)-Si	124.6(3)	C(72)-C(71)-H(71)	120.0
C(48)-C(47)-C(46)	122.3(3)	C(71)-C(72)-C(73)	119.0(4)
C(48)-C(47)-H(47)	118.8	C(71)-C(72)-H(72)	120.5
C(46)-C(47)-H(47)	118.8	C(73)-C(72)-H(72)	120.5
C(47)-C(48)-C(49)	119.5(3)	C(74)-C(73)-C(72)	121.3(4)
C(47)-C(48)-H(48)	120.2	C(74)-C(73)-H(73)	119.4
C(49)-C(48)-H(48)	120.2	C(72)-C(73)-H(73)	119.4
C(50)-C(49)-C(48)	119.5(3)	C(73)-C(74)-C(75)	119.2(4)
C(50)-C(49)-H(49)	120.2	C(73)-C(74)-H(74)	120.4
C(48)-C(49)-H(49)	120.2	C(75)-C(74)-H(74)	120.4
C(49)-C(50)-C(51)	120.2(3)	C(74)-C(75)-C(76)	119.7(4)
C(49)-C(50)-H(50)	119.9	C(74)-C(75)-H(75)	120.1
C(51)-C(50)-H(50)	119.9	C(76)-C(75)-H(75)	120.1
C(50)-C(51)-C(46)	122.1(3)	C(71)-C(76)-C(75)	120.9(3)
C(50)-C(51)-H(51)	118.9	C(71)-C(76)-H(76)	119.6
C(46)-C(51)-H(51)	118.9	C(75)-C(76)-H(76)	119.6
C(53)-C(52)-C(57)	116.3(3)	C(82)-C(81)-C(83)#1	118.6(4)
C(53)-C(52)-Si	124.2(3)	C(82)-C(81)-H(81)	120.7
C(57)-C(52)-Si	119.4(2)	C(83)#1-C(81)-H(81)	120.7
C(52)-C(53)-C(54)	121.9(3)	C(81)-C(82)-C(83)	121.5(4)
C(52)-C(53)-H(53)	119.0	C(81)-C(82)-H(82)	119.2
C(54)-C(53)-H(53)	119.0	C(83)-C(82)-H(82)	119.2
C(55)-C(54)-C(53)	119.8(3)	C(81)#1-C(83)-C(82)	119.8(4)
C(55)-C(54)-H(54)	120.1	C(81)#1-C(83)-H(83)	120.1
C(53)-C(54)-H(54)	120.1	C(82)-C(83)-H(83)	120.1
C(54)-C(55)-C(56)	120.0(3)		
C(54)-C(55)-H(55)	120.0		
C(56)-C(55)-H(55)	120.0		
C(55)-C(56)-C(57)	119.9(3)		
C(55)-C(56)-H(56)	120.1		
C(57)-C(56)-H(56)	120.1		

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Symmetry transformations used to generate equivalent atoms:

#1  $-x+2, -y+1, -z+1$

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for DMJ14 (CCDC 193897).  
The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

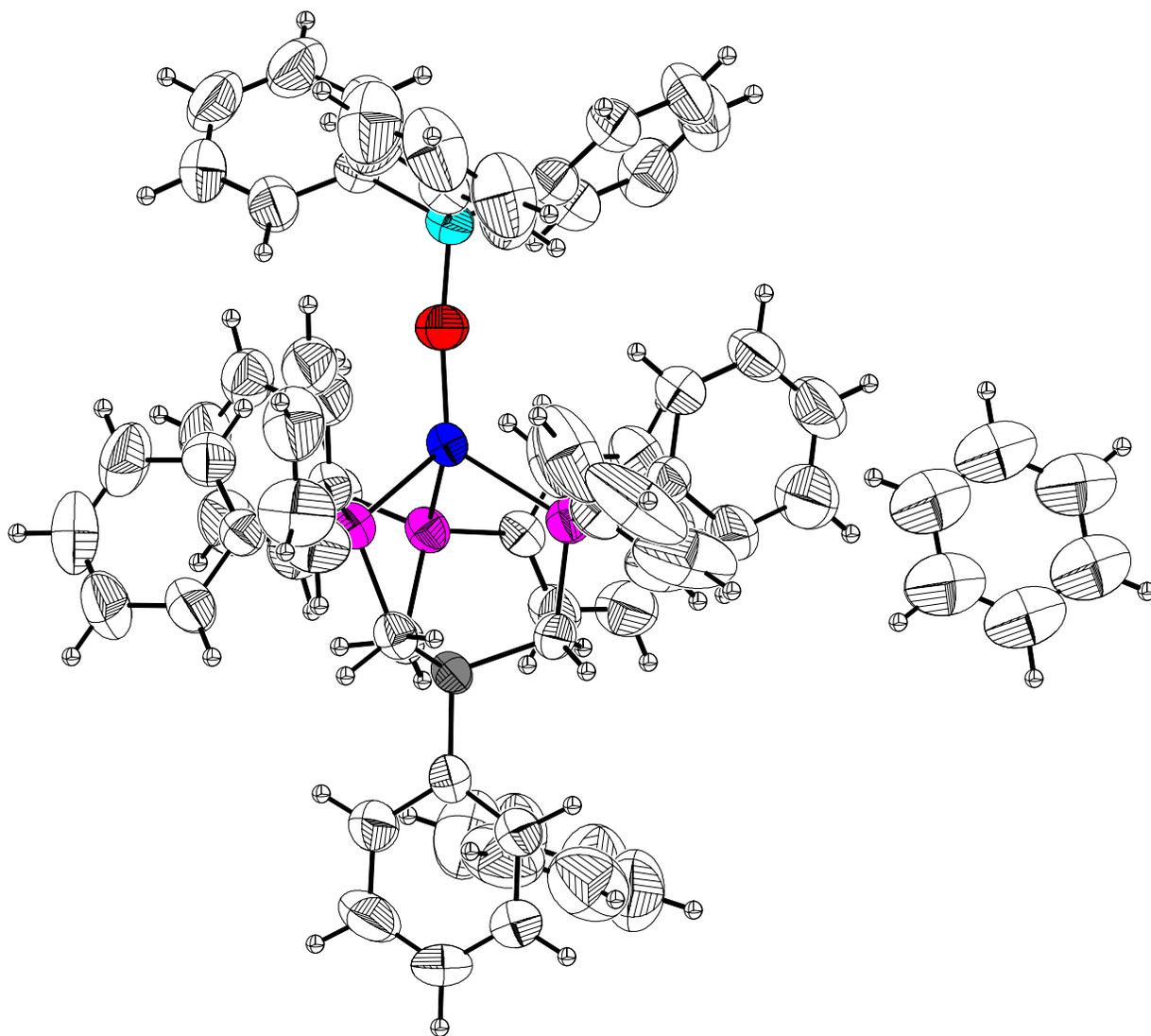
	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Co	169(3)	205(3)	191(3)	-57(2)	-54(2)	10(2)
P(1)	173(5)	181(5)	198(6)	-44(4)	-55(4)	17(4)
P(2)	199(6)	251(6)	191(6)	-61(4)	-52(4)	-7(4)
P(3)	186(6)	213(5)	193(5)	-67(4)	-54(4)	27(4)
Si	220(6)	217(6)	225(6)	-56(5)	-86(5)	-1(5)
O(1)	229(13)	225(13)	232(13)	-74(10)	-120(11)	37(10)
B	160(20)	180(20)	170(20)	-77(18)	-45(19)	23(19)
C(1)	150(20)	130(20)	170(20)	-15(16)	-13(17)	4(16)
C(2)	230(20)	320(20)	240(20)	-154(17)	-63(18)	71(19)
C(3)	200(20)	430(30)	360(20)	-190(20)	-120(20)	55(19)
C(4)	290(30)	360(20)	310(20)	-150(20)	-157(19)	0(20)
C(5)	360(30)	300(20)	290(20)	-164(18)	-120(20)	80(20)
C(6)	190(20)	290(20)	280(20)	-80(18)	-114(18)	73(18)
C(7)	135(19)	174(19)	150(20)	-26(15)	8(16)	-21(15)
C(8)	210(20)	240(20)	200(20)	-117(16)	-72(17)	64(16)
C(9)	139(19)	169(19)	220(20)	-20(15)	-62(16)	19(15)
C(10)	160(20)	106(19)	200(20)	-54(15)	-80(17)	26(16)
C(11)	270(20)	230(20)	140(20)	-55(17)	-80(19)	23(18)
C(12)	200(20)	280(20)	250(20)	-44(18)	-90(20)	-34(18)
C(13)	180(20)	250(20)	180(20)	3(17)	17(17)	-6(18)
C(14)	270(20)	240(20)	180(20)	-41(17)	-80(20)	32(18)
C(15)	160(20)	190(20)	290(20)	-52(18)	-110(20)	-8(17)
C(16)	170(20)	150(20)	170(20)	-16(16)	-18(17)	-42(16)
C(17)	210(20)	250(20)	290(20)	-40(18)	-129(18)	-7(18)
C(18)	340(20)	180(20)	360(20)	-104(17)	-160(20)	79(19)
C(19)	210(20)	290(20)	240(20)	-34(18)	-74(18)	78(18)
C(20)	210(20)	260(20)	200(20)	-25(17)	-55(17)	23(18)
C(21)	220(20)	210(20)	180(20)	-42(16)	-42(17)	11(18)
C(22)	160(20)	200(20)	180(20)	-2(17)	-18(17)	-53(16)
C(23)	230(20)	350(20)	270(20)	-84(19)	-62(19)	12(19)
C(24)	320(30)	360(20)	320(20)	-155(19)	-30(20)	10(20)
C(25)	220(30)	300(20)	420(30)	-20(20)	-10(20)	53(19)
C(26)	200(20)	390(30)	370(30)	10(20)	-80(20)	30(20)
C(27)	230(20)	320(20)	250(20)	-5(18)	-70(20)	-47(19)
C(28)	150(20)	280(20)	180(20)	-110(18)	-25(17)	43(16)
C(29)	220(20)	280(20)	260(20)	-107(19)	-56(18)	-6(19)
C(30)	260(20)	260(20)	220(20)	-15(19)	-38(19)	-14(19)
C(31)	210(20)	220(20)	340(30)	-80(20)	35(19)	-38(17)
C(32)	170(20)	310(20)	300(30)	-150(20)	-44(18)	13(19)
C(33)	190(20)	260(20)	210(20)	-72(18)	-18(18)	9(19)
C(34)	280(20)	240(20)	170(20)	-65(17)	-83(18)	0(20)
C(35)	570(30)	260(30)	480(30)	-130(20)	-400(20)	100(20)
C(36)	940(40)	400(30)	620(30)	-240(20)	-670(30)	280(30)
C(37)	1260(50)	170(30)	310(30)	-30(20)	-470(30)	20(30)
C(38)	720(40)	350(30)	240(30)	-60(20)	-20(20)	-60(30)
C(39)	440(30)	240(30)	280(20)	-121(19)	20(20)	-10(20)
C(40)	180(20)	180(20)	190(20)	-63(16)	-76(18)	61(17)

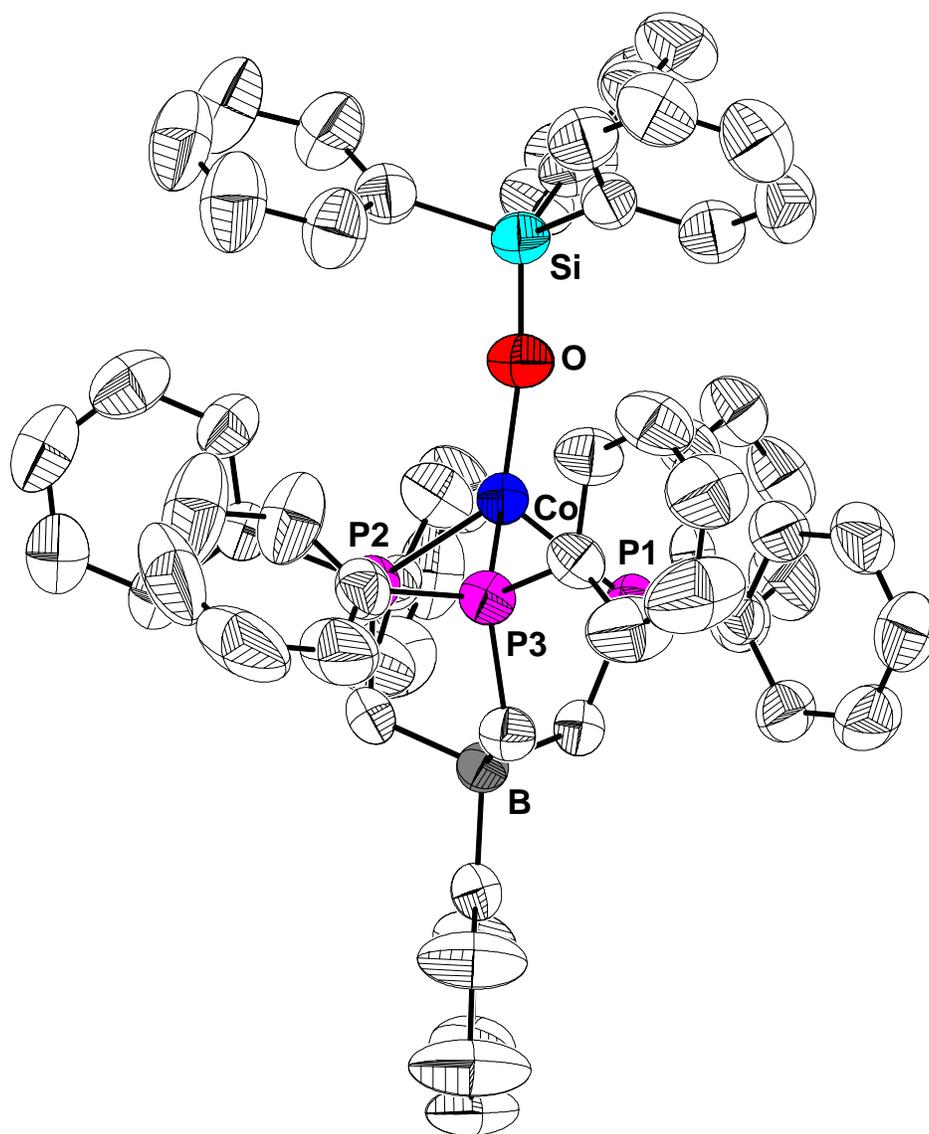
C(41)	250(20)	310(20)	250(20)	-133(18)	-110(20)	54(19)
C(42)	240(20)	430(30)	270(30)	-120(20)	-40(20)	-17(19)
C(43)	310(30)	330(20)	160(20)	-48(18)	-10(20)	50(20)
C(44)	330(30)	290(20)	240(20)	-127(18)	-140(20)	89(19)
C(45)	190(20)	200(20)	270(20)	-69(17)	-100(20)	39(16)
C(46)	180(20)	170(20)	200(20)	-48(17)	-61(18)	-58(16)
C(47)	230(20)	270(20)	250(20)	-56(17)	-94(19)	15(19)
C(48)	230(20)	330(20)	300(20)	-129(19)	-32(19)	-10(20)
C(49)	160(20)	240(20)	450(30)	-110(20)	-140(20)	12(17)
C(50)	230(20)	290(20)	270(20)	-4(18)	-100(20)	-47(19)
C(51)	170(20)	220(20)	250(20)	-72(17)	-55(17)	-16(18)
C(52)	200(20)	230(20)	190(20)	-86(16)	-63(17)	3(19)
C(53)	270(30)	230(20)	400(20)	-48(19)	-120(20)	0(19)
C(54)	250(20)	300(30)	430(30)	-50(20)	-40(20)	-50(20)
C(55)	390(30)	210(20)	270(20)	-52(17)	0(20)	-60(20)
C(56)	380(30)	210(30)	410(30)	-50(20)	-120(20)	70(20)
C(57)	220(20)	270(20)	330(20)	-86(19)	-56(18)	10(20)
C(58)	170(20)	190(20)	260(20)	-92(19)	-108(17)	41(17)
C(59)	190(20)	250(20)	280(20)	-85(18)	-109(19)	-4(18)
C(60)	190(20)	310(20)	280(30)	-20(20)	-76(19)	-13(18)
C(61)	190(20)	460(30)	180(20)	-60(20)	-36(17)	70(20)
C(62)	280(20)	300(30)	240(20)	-104(19)	-90(19)	69(19)
C(63)	200(20)	230(20)	240(20)	-5(19)	-74(18)	-19(17)
C(71)	310(30)	510(30)	340(30)	-80(20)	-130(20)	70(20)
C(72)	360(30)	430(30)	510(30)	-120(20)	-160(20)	100(20)
C(73)	240(30)	590(30)	660(30)	-280(30)	-150(30)	100(30)
C(74)	380(30)	480(30)	480(30)	-140(20)	-190(20)	-60(20)
C(75)	520(30)	410(30)	440(30)	-170(20)	-290(30)	150(20)
C(76)	330(30)	640(30)	330(30)	-220(20)	-180(20)	200(20)
C(81)	470(30)	560(30)	770(30)	-340(30)	-280(30)	100(30)
C(82)	430(40)	490(30)	840(40)	-180(30)	-330(30)	70(20)
C(83)	520(30)	570(30)	850(40)	-330(30)	-390(30)	130(30)

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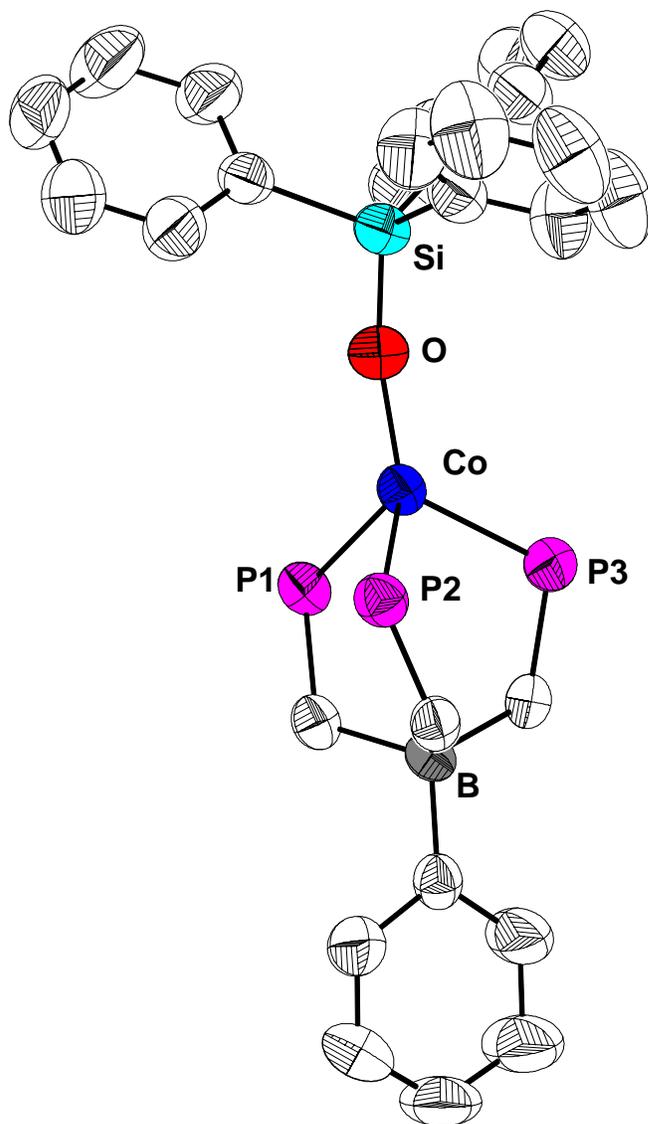
B. X-ray report for  $[\text{PhBP}_3]\text{CoOSiPh}_3$ , **2** (ambient temperature).

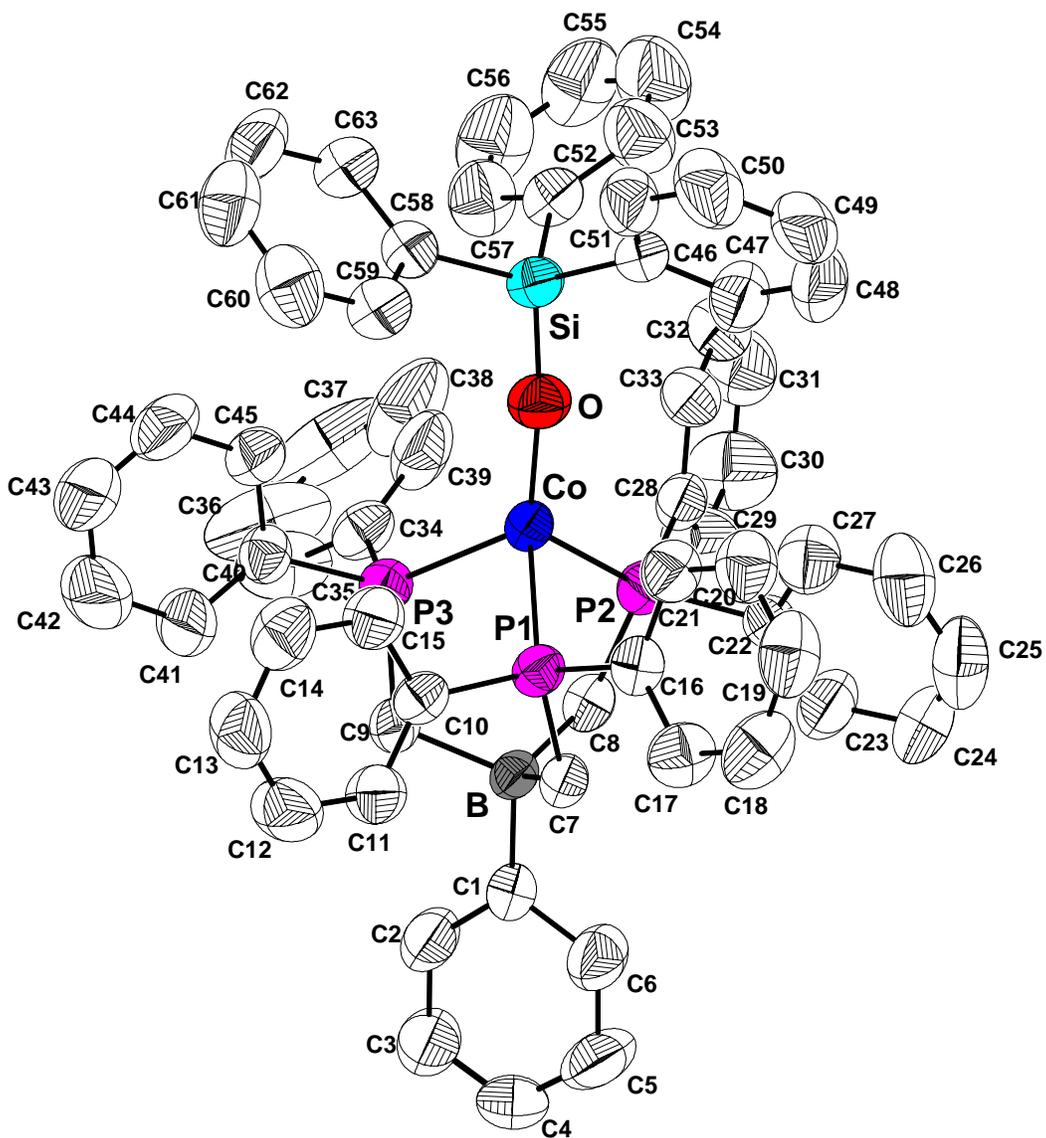
## Crystal Structure Report for DMJ 44, $[\text{PhBP}_3]\text{CoOSiPh}_3$ , 295 K





Phosphine aryl rings omitted for clarity.





**Table 1. Crystal Data and Structure Analysis Details for dmj44.**

Empirical formula	C <sub>63</sub> H <sub>56</sub> BOP <sub>3</sub> SiCo • 1/2(C <sub>6</sub> H <sub>6</sub> )
Formula weight	1136.98
Crystallization solvent	Benzene/Petroleum Ether
Crystal shape	Irregular block
Crystal color	blue/purple
Crystal size	0.35 x 0.40 x 0.45 mm

### Data Collection

Preliminary photograph(s)	Rotation
Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoK $\alpha$
Data collection temperature	295 K
Theta range for 3445 reflections used in lattice determination	2.30 to 22.27°
Unit cell dimensions	a = 13.4295(15) Å $\alpha$ = 78.183(2)° b = 14.5619(17) Å $\beta$ = 68.286(2)° c = 17.357(2) Å $\gamma$ = 88.981(2)°
Volume	3080.3(6) Å <sup>3</sup>
Z	2
Crystal system	Triclinic
Space group	P $\bar{1}$ (# 2)
Density (calculated)	1.226 g/cm <sup>3</sup>
F(000)	1192
Theta range for data collection	1.7 to 28.4°
Completeness to theta = 28.37°	76.4%
Index ranges	-17 ≤ h ≤ 14, -19 ≤ k ≤ 19, -22 ≤ l ≤ 16
Reflections collected	17923
Independent reflections	11774 [R <sub>int</sub> = 0.0597]
Reflections > 2 $\sigma$ (I)	5552
Average $\sigma$ (I)/(net I)	0.1177
Absorption coefficient	0.42 mm <sup>-1</sup>

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	Direct methods
Secondary solution method	Difference map
Hydrogen placement	Calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	11774 / 0 / 712
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	1.06
Final R indices [I>2σ(I), 5552 reflections]	R1 = 0.0534, wR2 = 0.0738
R indices (all data)	R1 = 0.1288, wR2 = 0.0854
Type of weighting scheme used	Sigma
Weighting scheme used	w=1/σ <sup>2</sup> (Fo <sup>2</sup> )
Max shift/error	0.015
Average shift/error	0.001
Largest diff. peak and hole	0.46 and -0.31 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

**Special Refinement Details**

Refinement of F<sup>2</sup> against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F<sup>2</sup>, conventional R-factors (R) are based on F, with F set to zero for negative F<sup>2</sup>. The threshold expression of F<sup>2</sup> > 2σ(F<sup>2</sup>) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F<sup>2</sup> are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

A crystal fragment was mounted on a fiber with epoxy and then coated with two coats of epoxy to protect it from air and solvent loss. There was a decrease in intensity during collection as the crystal decomposed. A significant portion of the data had to be discarded. This was based on a decrease in total intensity and an increase in R for data merging. Although the data is only 76% complete to 28.4° the data to parameter ratio is still above 16:1 for all data and better than 7:1 for data with I>2σ. Most of the missing data is at high angles, whereas most of the low angle data is above 90% completion.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj44.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co	8634(1)	2245(1)	2627(1)	45(1)
P(1)	8149(1)	3763(1)	2521(1)	49(1)
P(2)	7830(1)	1871(1)	4090(1)	51(1)
P(3)	7164(1)	1776(1)	2416(1)	52(1)
Si	11103(1)	1611(1)	1515(1)	55(1)
O	9993(2)	2018(2)	2034(1)	65(1)
B	6051(3)	2850(3)	3742(2)	45(1)
C(1)	4881(3)	3176(2)	4263(2)	49(1)
C(2)	3950(4)	2989(3)	4170(3)	106(2)
C(3)	2953(4)	3301(4)	4613(3)	130(2)
C(4)	2865(4)	3837(3)	5177(3)	98(2)
C(5)	3752(4)	4022(3)	5326(3)	95(2)
C(6)	4727(3)	3705(3)	4882(2)	81(1)
C(7)	6907(2)	3817(2)	3388(2)	47(1)
C(8)	6416(2)	2026(2)	4383(2)	49(1)
C(9)	6018(2)	2428(2)	2921(2)	50(1)
C(10)	7949(3)	4253(2)	1541(2)	48(1)
C(11)	7082(3)	4756(2)	1505(2)	69(1)
C(12)	6981(4)	5106(3)	745(3)	90(1)
C(13)	7730(4)	4969(3)	1(3)	89(1)
C(14)	8595(4)	4476(3)	18(2)	83(1)
C(15)	8701(3)	4121(3)	788(2)	69(1)
C(16)	9148(3)	4603(2)	2522(2)	50(1)
C(17)	8853(3)	5429(3)	2793(2)	72(1)
C(18)	9617(4)	6052(3)	2805(3)	90(1)
C(19)	10679(4)	5833(3)	2541(3)	86(1)
C(20)	10967(4)	5014(3)	2279(2)	79(1)
C(21)	10214(3)	4395(3)	2273(2)	64(1)
C(22)	8354(3)	2643(2)	4589(2)	51(1)
C(23)	7740(3)	2955(3)	5296(3)	86(1)
C(24)	8200(5)	3530(4)	5647(3)	107(2)
C(25)	9257(5)	3780(3)	5293(3)	100(2)
C(26)	9883(4)	3471(3)	4589(3)	101(2)
C(27)	9432(4)	2904(3)	4239(2)	79(1)
C(28)	8010(3)	716(2)	4641(2)	55(1)
C(29)	7205(4)	244(3)	5376(3)	85(1)
C(30)	7370(4)	-636(3)	5793(3)	112(2)
C(31)	8324(5)	-1044(3)	5462(4)	104(2)
C(32)	9117(4)	-585(4)	4721(3)	92(2)
C(33)	8957(3)	294(3)	4321(2)	70(1)
C(34)	6753(4)	535(3)	2823(2)	61(1)
C(35)	5822(4)	166(3)	2804(3)	106(2)
C(36)	5519(5)	-786(5)	3121(4)	155(3)
C(37)	6149(7)	-1354(5)	3457(4)	160(4)
C(38)	7071(7)	-1008(4)	3461(4)	143(3)
C(39)	7372(4)	-62(3)	3131(3)	98(2)

C(40)	7380(3)	1913(2)	1294(2)	54(1)
C(41)	6643(4)	2254(3)	961(3)	103(2)
C(42)	6861(5)	2321(4)	104(3)	142(2)
C(43)	7818(5)	2057(3)	-416(3)	105(2)
C(44)	8544(4)	1724(3)	-94(3)	85(1)
C(45)	8342(3)	1651(3)	765(2)	68(1)
C(46)	12254(3)	2311(2)	1534(2)	54(1)
C(47)	12203(4)	2562(3)	2268(2)	79(1)
C(48)	13003(5)	3088(4)	2320(3)	102(2)
C(49)	13902(4)	3398(3)	1614(4)	96(2)
C(50)	13976(4)	3181(3)	874(3)	101(2)
C(51)	13169(4)	2638(3)	838(3)	79(1)
C(52)	11124(3)	344(3)	2019(2)	64(1)
C(53)	11816(4)	36(3)	2424(3)	95(2)
C(54)	11759(5)	-901(4)	2841(3)	121(2)
C(55)	11026(6)	-1526(3)	2842(3)	116(2)
C(56)	10337(5)	-1250(3)	2448(3)	117(2)
C(57)	10388(4)	-319(3)	2045(3)	88(1)
C(58)	11293(3)	1718(3)	370(2)	56(1)
C(59)	11243(3)	2597(3)	-105(3)	73(1)
C(60)	11436(4)	2757(3)	-975(3)	94(2)
C(61)	11696(4)	2031(4)	-1387(3)	97(2)
C(62)	11747(3)	1171(4)	-945(3)	92(2)
C(63)	11552(3)	1004(3)	-72(3)	76(1)
C(64)	4615(9)	5790(7)	2947(5)	142(3)
C(65)	5243(7)	6591(8)	2656(7)	159(3)
C(66)	5247(7)	7223(6)	1998(7)	157(3)
C(67)	4581(9)	7091(6)	1617(4)	151(3)
C(68)	3934(6)	6301(9)	1865(6)	149(3)
C(69)	3954(6)	5660(6)	2527(7)	143(2)
C(70)	5644(8)	-48(6)	439(7)	187(3)
C(71)	4635(11)	88(7)	788(5)	235(4)
C(72)	3996(6)	143(8)	343(9)	248(5)

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**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj44.**

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Co-O	1.796(2)
Co-P(3)	2.277(1)
Co-P(1)	2.284(1)
Co-P(2)	2.310(1)
Si-O	1.606(2)
O-Co-P(3)	124.88(8)
O-Co-P(1)	118.93(8)
P(3)-Co-P(1)	91.54(4)
O-Co-P(2)	124.45(8)
P(3)-Co-P(2)	94.53(4)
P(1)-Co-P(2)	94.05(4)
Si-O-Co	168.3(2)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj44.**

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Co-O	1.796(2)
Co-P(3)	2.2774(10)
Co-P(1)	2.2841(10)
Co-P(2)	2.3103(10)
P(1)-C(7)	1.799(3)
P(1)-C(10)	1.819(3)
P(1)-C(16)	1.832(3)
P(2)-C(8)	1.798(3)
P(2)-C(28)	1.817(4)
P(2)-C(22)	1.840(3)
P(3)-C(34)	1.816(4)
P(3)-C(9)	1.824(3)
P(3)-C(40)	1.829(3)
Si-O	1.606(2)
Si-C(52)	1.877(4)
Si-C(46)	1.881(4)
Si-C(58)	1.881(3)
B-C(1)	1.616(5)
B-C(8)	1.660(4)
B-C(9)	1.677(4)
B-C(7)	1.691(5)
C(1)-C(2)	1.357(4)
C(1)-C(6)	1.399(4)
C(2)-C(3)	1.396(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.344(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.351(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.379(5)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(15)	1.372(4)
C(10)-C(11)	1.378(4)
C(11)-C(12)	1.370(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.361(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.362(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.389(4)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(17)	1.380(4)
C(16)-C(21)	1.381(4)

C(17)-C(18)	1.391(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.381(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.362(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.371(4)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.364(4)
C(22)-C(27)	1.372(4)
C(23)-C(24)	1.400(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.343(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.361(6)
C(25)-H(25)	0.9500
C(26)-C(27)	1.384(5)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(33)	1.375(5)
C(28)-C(29)	1.384(5)
C(29)-C(30)	1.395(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.375(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.377(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.380(5)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.358(5)
C(34)-C(35)	1.384(5)
C(35)-C(36)	1.389(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.373(8)
C(36)-H(36)	0.9500
C(37)-C(38)	1.348(8)
C(37)-H(37)	0.9500
C(38)-C(39)	1.383(6)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(41)	1.359(4)
C(40)-C(45)	1.381(5)
C(41)-C(42)	1.388(5)
C(41)-H(41)	0.9500
C(42)-C(43)	1.370(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.332(5)
C(43)-H(43)	0.9500
C(44)-C(45)	1.394(5)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(51)	1.372(5)

C(46)-C(47)	1.375(4)
C(47)-C(48)	1.370(5)
C(47)-H(47)	0.9500
C(48)-C(49)	1.364(5)
C(48)-H(48)	0.9500
C(49)-C(50)	1.353(5)
C(49)-H(49)	0.9500
C(50)-C(51)	1.381(5)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-C(57)	1.377(5)
C(52)-C(53)	1.379(5)
C(53)-C(54)	1.396(5)
C(53)-H(53)	0.9500
C(54)-C(55)	1.352(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.353(6)
C(55)-H(55)	0.9500
C(56)-C(57)	1.382(5)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(63)	1.379(4)
C(58)-C(59)	1.389(4)
C(59)-C(60)	1.405(5)
C(59)-H(59)	0.9500
C(60)-C(61)	1.365(5)
C(60)-H(60)	0.9500
C(61)-C(62)	1.343(5)
C(61)-H(61)	0.9500
C(62)-C(63)	1.408(5)
C(62)-H(62)	0.9500
C(63)-H(63)	0.9500
C(64)-C(65)	1.345(8)
C(64)-C(69)	1.377(8)
C(64)-H(64)	0.9500
C(65)-C(66)	1.311(7)
C(65)-H(65)	0.9500
C(66)-C(67)	1.329(7)
C(66)-H(66)	0.9500
C(67)-C(68)	1.350(7)
C(67)-H(67)	0.9500
C(68)-C(69)	1.331(7)
C(68)-H(68)	0.9500
C(69)-H(69)	0.9500
C(70)-C(71)	1.294(9)
C(70)-C(72)#1	1.298(9)
C(70)-H(70)	0.9500
C(71)-C(72)	1.342(9)
C(71)-H(71)	0.9500
C(72)-C(70)#1	1.298(9)
C(72)-H(72)	0.9500
O-Co-P(3)	124.88(8)
O-Co-P(1)	118.93(8)

P(3)-Co-P(1)	91.54(4)
O-Co-P(2)	124.45(8)
P(3)-Co-P(2)	94.53(4)
P(1)-Co-P(2)	94.05(4)
C(7)-P(1)-C(10)	107.53(15)
C(7)-P(1)-C(16)	108.62(15)
C(10)-P(1)-C(16)	103.02(15)
C(7)-P(1)-Co	109.09(10)
C(10)-P(1)-Co	113.83(11)
C(16)-P(1)-Co	114.37(12)
C(8)-P(2)-C(28)	108.74(17)
C(8)-P(2)-C(22)	107.59(16)
C(28)-P(2)-C(22)	101.43(14)
C(8)-P(2)-Co	108.34(10)
C(28)-P(2)-Co	118.06(13)
C(22)-P(2)-Co	112.13(12)
C(34)-P(3)-C(9)	107.15(17)
C(34)-P(3)-C(40)	101.85(16)
C(9)-P(3)-C(40)	109.37(16)
C(34)-P(3)-Co	114.76(15)
C(9)-P(3)-Co	110.12(10)
C(40)-P(3)-Co	113.14(12)
O-Si-C(52)	109.51(15)
O-Si-C(46)	109.14(14)
C(52)-Si-C(46)	109.63(18)
O-Si-C(58)	111.63(14)
C(52)-Si-C(58)	109.63(17)
C(46)-Si-C(58)	107.25(17)
Si-O-Co	168.33(15)
C(1)-B-C(8)	109.4(3)
C(1)-B-C(9)	110.1(3)
C(8)-B-C(9)	109.7(3)
C(1)-B-C(7)	106.6(3)
C(8)-B-C(7)	110.6(3)
C(9)-B-C(7)	110.3(3)
C(2)-C(1)-C(6)	112.0(3)
C(2)-C(1)-B	126.2(3)
C(6)-C(1)-B	121.8(3)
C(1)-C(2)-C(3)	125.0(4)
C(1)-C(2)-H(2)	117.5
C(3)-C(2)-H(2)	117.5
C(4)-C(3)-C(2)	120.1(4)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	118.0(4)
C(3)-C(4)-H(4)	121.0
C(5)-C(4)-H(4)	121.0
C(4)-C(5)-C(6)	120.7(4)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(5)-C(6)-C(1)	124.0(4)
C(5)-C(6)-H(6)	118.0
C(1)-C(6)-H(6)	118.0
B-C(7)-P(1)	115.9(2)

B-C(7)-H(7A)	108.3
P(1)-C(7)-H(7A)	108.3
B-C(7)-H(7B)	108.3
P(1)-C(7)-H(7B)	108.3
H(7A)-C(7)-H(7B)	107.4
B-C(8)-P(2)	117.0(2)
B-C(8)-H(8A)	108.1
P(2)-C(8)-H(8A)	108.1
B-C(8)-H(8B)	108.1
P(2)-C(8)-H(8B)	108.1
H(8A)-C(8)-H(8B)	107.3
B-C(9)-P(3)	116.0(2)
B-C(9)-H(9A)	108.3
P(3)-C(9)-H(9A)	108.3
B-C(9)-H(9B)	108.3
P(3)-C(9)-H(9B)	108.3
H(9A)-C(9)-H(9B)	107.4
C(15)-C(10)-C(11)	117.5(3)
C(15)-C(10)-P(1)	118.7(3)
C(11)-C(10)-P(1)	123.8(3)
C(12)-C(11)-C(10)	120.8(4)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(13)-C(12)-C(11)	121.3(4)
C(13)-C(12)-H(12)	119.4
C(11)-C(12)-H(12)	119.4
C(12)-C(13)-C(14)	119.1(4)
C(12)-C(13)-H(13)	120.4
C(14)-C(13)-H(13)	120.4
C(13)-C(14)-C(15)	119.7(4)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(10)-C(15)-C(14)	121.5(4)
C(10)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(17)-C(16)-C(21)	119.1(3)
C(17)-C(16)-P(1)	121.2(3)
C(21)-C(16)-P(1)	119.7(3)
C(16)-C(17)-C(18)	120.7(4)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	119.0(4)
C(19)-C(18)-H(18)	120.5
C(17)-C(18)-H(18)	120.5
C(20)-C(19)-C(18)	120.2(4)
C(20)-C(19)-H(19)	119.9
C(18)-C(19)-H(19)	119.9
C(19)-C(20)-C(21)	120.9(4)
C(19)-C(20)-H(20)	119.5
C(21)-C(20)-H(20)	119.5
C(20)-C(21)-C(16)	120.1(4)
C(20)-C(21)-H(21)	119.9
C(16)-C(21)-H(21)	119.9
C(23)-C(22)-C(27)	118.0(4)

C(23)-C(22)-P(2)	123.9(3)
C(27)-C(22)-P(2)	118.0(3)
C(22)-C(23)-C(24)	120.6(4)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	120.4(5)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	119.8(5)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1
C(25)-C(26)-C(27)	120.1(5)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(22)-C(27)-C(26)	121.1(4)
C(22)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.5
C(33)-C(28)-C(29)	119.1(4)
C(33)-C(28)-P(2)	119.7(3)
C(29)-C(28)-P(2)	121.2(3)
C(28)-C(29)-C(30)	120.0(4)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	120.0(5)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(32)	120.2(5)
C(30)-C(31)-H(31)	119.9
C(32)-C(31)-H(31)	119.9
C(31)-C(32)-C(33)	119.6(5)
C(31)-C(32)-H(32)	120.2
C(33)-C(32)-H(32)	120.2
C(28)-C(33)-C(32)	121.2(4)
C(28)-C(33)-H(33)	119.4
C(32)-C(33)-H(33)	119.4
C(39)-C(34)-C(35)	118.2(4)
C(39)-C(34)-P(3)	120.6(4)
C(35)-C(34)-P(3)	121.1(4)
C(34)-C(35)-C(36)	120.3(5)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9
C(37)-C(36)-C(35)	119.3(7)
C(37)-C(36)-H(36)	120.3
C(35)-C(36)-H(36)	120.3
C(38)-C(37)-C(36)	120.9(8)
C(38)-C(37)-H(37)	119.5
C(36)-C(37)-H(37)	119.5
C(37)-C(38)-C(39)	119.1(7)
C(37)-C(38)-H(38)	120.5
C(39)-C(38)-H(38)	120.5
C(34)-C(39)-C(38)	122.0(5)
C(34)-C(39)-H(39)	119.0
C(38)-C(39)-H(39)	119.0
C(41)-C(40)-C(45)	119.0(3)

C(41)-C(40)-P(3)	123.3(3)
C(45)-C(40)-P(3)	117.7(3)
C(40)-C(41)-C(42)	119.8(4)
C(40)-C(41)-H(41)	120.1
C(42)-C(41)-H(41)	120.1
C(43)-C(42)-C(41)	120.9(4)
C(43)-C(42)-H(42)	119.6
C(41)-C(42)-H(42)	119.6
C(44)-C(43)-C(42)	119.6(4)
C(44)-C(43)-H(43)	120.2
C(42)-C(43)-H(43)	120.2
C(43)-C(44)-C(45)	120.5(4)
C(43)-C(44)-H(44)	119.8
C(45)-C(44)-H(44)	119.8
C(40)-C(45)-C(44)	120.3(4)
C(40)-C(45)-H(45)	119.9
C(44)-C(45)-H(45)	119.9
C(51)-C(46)-C(47)	115.0(4)
C(51)-C(46)-Si	124.3(3)
C(47)-C(46)-Si	120.6(3)
C(48)-C(47)-C(46)	123.5(4)
C(48)-C(47)-H(47)	118.3
C(46)-C(47)-H(47)	118.3
C(49)-C(48)-C(47)	119.7(4)
C(49)-C(48)-H(48)	120.1
C(47)-C(48)-H(48)	120.1
C(50)-C(49)-C(48)	118.7(5)
C(50)-C(49)-H(49)	120.6
C(48)-C(49)-H(49)	120.6
C(49)-C(50)-C(51)	120.7(5)
C(49)-C(50)-H(50)	119.7
C(51)-C(50)-H(50)	119.7
C(46)-C(51)-C(50)	122.3(4)
C(46)-C(51)-H(51)	118.8
C(50)-C(51)-H(51)	118.8
C(57)-C(52)-C(53)	116.5(4)
C(57)-C(52)-Si	120.6(3)
C(53)-C(52)-Si	122.8(4)
C(52)-C(53)-C(54)	121.1(4)
C(52)-C(53)-H(53)	119.5
C(54)-C(53)-H(53)	119.5
C(55)-C(54)-C(53)	120.1(5)
C(55)-C(54)-H(54)	120.0
C(53)-C(54)-H(54)	120.0
C(54)-C(55)-C(56)	120.5(5)
C(54)-C(55)-H(55)	119.8
C(56)-C(55)-H(55)	119.8
C(55)-C(56)-C(57)	119.3(5)
C(55)-C(56)-H(56)	120.4
C(57)-C(56)-H(56)	120.4
C(52)-C(57)-C(56)	122.6(4)
C(52)-C(57)-H(57)	118.7
C(56)-C(57)-H(57)	118.7
C(63)-C(58)-C(59)	115.5(3)

C(63)-C(58)-Si	125.8(3)
C(59)-C(58)-Si	118.6(3)
C(58)-C(59)-C(60)	122.7(4)
C(58)-C(59)-H(59)	118.6
C(60)-C(59)-H(59)	118.6
C(61)-C(60)-C(59)	119.7(4)
C(61)-C(60)-H(60)	120.2
C(59)-C(60)-H(60)	120.2
C(62)-C(61)-C(60)	119.0(4)
C(62)-C(61)-H(61)	120.5
C(60)-C(61)-H(61)	120.5
C(61)-C(62)-C(63)	121.6(4)
C(61)-C(62)-H(62)	119.2
C(63)-C(62)-H(62)	119.2
C(58)-C(63)-C(62)	121.4(4)
C(58)-C(63)-H(63)	119.3
C(62)-C(63)-H(63)	119.3
C(65)-C(64)-C(69)	116.9(8)
C(65)-C(64)-H(64)	121.5
C(69)-C(64)-H(64)	121.5
C(66)-C(65)-C(64)	122.4(9)
C(66)-C(65)-H(65)	118.8
C(64)-C(65)-H(65)	118.8
C(65)-C(66)-C(67)	119.5(8)
C(65)-C(66)-H(66)	120.3
C(67)-C(66)-H(66)	120.3
C(66)-C(67)-C(68)	121.7(8)
C(66)-C(67)-H(67)	119.2
C(68)-C(67)-H(67)	119.2
C(69)-C(68)-C(67)	118.0(8)
C(69)-C(68)-H(68)	121.0
C(67)-C(68)-H(68)	121.0
C(68)-C(69)-C(64)	121.6(8)
C(68)-C(69)-H(69)	119.2
C(64)-C(69)-H(69)	119.2
C(71)-C(70)-C(72)#1	117.7(9)
C(71)-C(70)-H(70)	121.2
C(72)#1-C(70)-H(70)	121.2
C(70)-C(71)-C(72)	120.5(8)
C(70)-C(71)-H(71)	119.8
C(72)-C(71)-H(71)	119.8
C(70)#1-C(72)-C(71)	121.9(8)
C(70)#1-C(72)-H(72)	119.1
C(71)-C(72)-H(72)	119.1

---

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj44. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co	486(3)	443(3)	431(3)	-126(2)	-175(3)	30(2)
P(1)	565(7)	437(6)	457(6)	-111(5)	-184(5)	54(5)
P(2)	553(7)	527(6)	446(6)	-117(5)	-171(5)	29(5)
P(3)	513(7)	545(6)	522(6)	-142(5)	-183(6)	20(5)
Si	524(7)	562(7)	565(7)	-185(6)	-177(6)	92(6)
O	526(17)	697(16)	734(17)	-255(14)	-186(14)	84(13)
B	490(30)	460(30)	390(20)	-140(20)	-150(20)	70(20)
C(1)	550(30)	480(20)	430(20)	-90(18)	-180(20)	-30(20)
C(2)	650(30)	1720(50)	1210(40)	-1060(40)	-410(30)	300(30)
C(3)	660(40)	2310(60)	1420(50)	-1270(50)	-500(30)	470(40)
C(4)	600(30)	1430(40)	1020(40)	-620(30)	-270(30)	430(30)
C(5)	880(40)	1030(40)	930(40)	-590(30)	-150(30)	200(30)
C(6)	600(30)	1060(30)	850(30)	-490(30)	-220(30)	-10(30)
C(7)	560(20)	440(20)	430(20)	-112(17)	-210(19)	24(19)
C(8)	530(30)	470(20)	390(20)	-72(17)	-116(19)	-74(19)
C(9)	460(20)	500(20)	570(20)	-164(18)	-210(20)	-30(18)
C(10)	550(30)	400(20)	450(20)	-85(18)	-140(20)	3(19)
C(11)	820(30)	780(30)	450(30)	-110(20)	-240(20)	230(20)
C(12)	930(40)	1040(40)	700(30)	-110(30)	-330(30)	330(30)
C(13)	1140(40)	910(40)	720(30)	-60(30)	-530(30)	110(30)
C(14)	970(40)	940(30)	480(30)	-110(20)	-200(30)	30(30)
C(15)	730(30)	800(30)	500(30)	-110(20)	-190(20)	110(20)
C(16)	590(30)	400(20)	460(20)	-10(18)	-190(20)	-80(20)
C(17)	750(30)	530(30)	830(30)	-150(20)	-250(30)	-60(20)
C(18)	1010(40)	670(30)	960(40)	-260(30)	-230(30)	-240(30)
C(19)	790(40)	1020(40)	680(30)	-80(30)	-210(30)	-410(30)
C(20)	750(40)	880(30)	730(30)	-150(30)	-290(30)	-100(30)
C(21)	570(30)	660(30)	650(30)	-160(20)	-180(20)	-70(20)
C(22)	580(30)	500(20)	470(20)	-87(19)	-220(20)	90(20)
C(23)	770(30)	1140(40)	770(30)	-500(30)	-230(30)	20(30)
C(24)	1310(50)	1190(40)	1010(40)	-640(30)	-570(40)	180(40)
C(25)	1530(60)	780(40)	950(40)	-80(30)	-810(50)	-160(40)
C(26)	920(40)	1180(40)	1020(40)	-110(30)	-500(40)	-400(30)
C(27)	660(30)	990(30)	680(30)	-220(30)	-190(30)	-50(30)
C(28)	650(30)	550(20)	520(30)	-180(20)	-250(20)	40(20)
C(29)	920(40)	650(30)	810(30)	20(30)	-220(30)	150(30)
C(30)	1210(50)	880(40)	1010(40)	90(30)	-290(40)	70(40)
C(31)	1480(60)	740(40)	1110(50)	-130(40)	-770(40)	250(40)
C(32)	990(40)	1010(40)	1030(40)	-400(30)	-600(40)	360(30)
C(33)	850(30)	670(30)	690(30)	-160(20)	-400(30)	210(30)
C(34)	720(30)	560(30)	460(20)	-120(20)	-100(20)	20(30)
C(35)	740(40)	680(40)	1510(50)	-280(30)	-90(40)	-130(30)
C(36)	1020(50)	870(50)	1990(70)	-480(50)	450(50)	-370(40)
C(37)	2330(110)	610(50)	930(50)	-170(40)	470(60)	-200(60)
C(38)	2880(110)	610(50)	990(50)	-240(40)	-920(60)	260(50)
C(39)	1710(50)	600(30)	900(40)	-300(30)	-740(40)	180(30)

C(40)	510(30)	610(20)	510(20)	-140(20)	-180(20)	-50(20)
C(41)	980(40)	1680(50)	600(30)	-450(30)	-410(30)	500(30)
C(42)	1480(60)	2200(60)	910(40)	-560(40)	-750(40)	920(50)
C(43)	1210(50)	1390(40)	630(30)	-410(30)	-360(30)	350(40)
C(44)	790(40)	1010(40)	680(30)	-400(30)	-90(30)	40(30)
C(45)	630(30)	810(30)	640(30)	-280(20)	-200(20)	100(20)
C(46)	520(30)	590(20)	560(30)	-210(20)	-220(20)	110(20)
C(47)	710(30)	1020(30)	670(30)	-290(30)	-220(30)	-50(30)
C(48)	910(40)	1390(50)	1050(40)	-620(40)	-520(40)	50(40)
C(49)	720(40)	1040(40)	1380(50)	-430(40)	-600(40)	50(30)
C(50)	630(40)	1390(50)	990(40)	-200(40)	-320(30)	-90(30)
C(51)	590(30)	1140(40)	670(30)	-310(30)	-220(30)	0(30)
C(52)	690(30)	640(30)	600(30)	-190(20)	-200(20)	70(20)
C(53)	1060(40)	780(40)	1140(40)	-110(30)	-610(30)	100(30)
C(54)	1690(60)	840(40)	1370(50)	-100(40)	-960(50)	200(40)
C(55)	1970(70)	620(40)	980(40)	-120(30)	-690(40)	100(40)
C(56)	1810(60)	610(40)	1150(50)	-120(30)	-660(40)	-130(40)
C(57)	1100(40)	640(30)	1000(40)	-130(30)	-510(30)	-50(30)
C(58)	550(30)	580(30)	550(20)	-90(20)	-200(20)	20(20)
C(59)	740(30)	730(30)	730(30)	-220(30)	-260(30)	80(20)
C(60)	1060(40)	1030(40)	690(30)	90(30)	-410(30)	-30(30)
C(61)	1110(40)	1180(40)	640(30)	-190(30)	-340(30)	-130(40)
C(62)	1040(40)	1110(40)	680(30)	-450(30)	-270(30)	80(30)
C(63)	800(30)	750(30)	780(30)	-310(30)	-290(30)	140(20)
C(64)	1560(80)	1440(70)	1190(60)	-300(60)	-450(60)	790(60)
C(65)	1780(80)	1600(80)	1800(90)	-430(70)	-1090(70)	100(70)
C(66)	1720(80)	1470(70)	1640(80)	-250(60)	-800(60)	-330(50)
C(67)	1730(80)	1650(80)	1150(50)	-30(50)	-660(60)	-200(60)
C(68)	1270(60)	2160(90)	1100(60)	-430(60)	-440(50)	-400(70)
C(69)	1380(70)	1320(60)	1330(70)	-370(60)	-160(60)	-160(50)
C(70)	1030(80)	2910(90)	1860(90)	-920(70)	-540(60)	440(60)
C(71)	1200(80)	4330(130)	1990(80)	-1610(90)	-670(80)	980(80)
C(72)	1040(70)	4560(140)	2460(120)	-1910(110)	-780(90)	950(80)

---

**Table 6. Hydrogen coordinates (  $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj44.**

	x	y	z	$U_{\text{iso}}$
H(2)	398	262	377	128
H(3)	234	313	452	156
H(4)	220	408	546	117
H(5)	370	437	574	114
H(6)	533	385	500	97
H(7A)	708	394	387	56
H(7B)	653	436	321	56
H(8A)	606	142	443	58
H(8B)	614	217	496	58
H(9A)	596	296	249	59
H(9B)	536	201	312	59
H(11)	655	486	201	83
H(12)	638	545	74	108
H(13)	765	522	-52	106
H(14)	912	437	-50	99
H(15)	931	378	79	83
H(17)	812	557	297	86
H(18)	941	662	299	108
H(19)	1121	626	254	103
H(20)	1170	487	210	94
H(21)	1043	382	210	77
H(23)	699	278	555	104
H(24)	776	374	614	128
H(25)	956	417	553	120
H(26)	1063	364	434	122
H(27)	988	269	375	94
H(29)	654	52	560	102
H(30)	682	-95	630	134
H(31)	844	-164	575	124
H(32)	977	-87	449	111
H(33)	951	61	382	85
H(35)	539	56	257	128
H(36)	488	-104	310	187
H(37)	593	-200	369	192
H(38)	751	-141	369	171
H(39)	803	18	312	117
H(41)	598	245	131	123
H(42)	634	255	-12	170
H(43)	796	211	-100	126
H(44)	920	153	-45	102
H(45)	887	142	99	82
H(47)	1158	236	277	95
H(48)	1293	324	285	122
H(49)	1446	376	164	115
H(50)	1459	340	37	121
H(51)	1325	249	31	94
H(53)	1234	47	242	114

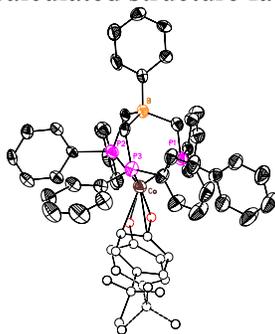
H(54)	1224	-110	312	145
H(55)	1099	-216	312	139
H(56)	982	-169	245	140
H(57)	990	-13	178	106
H(59)	1107	311	17	88
H(60)	1139	337	-128	113
H(61)	1184	213	-198	117
H(62)	1192	66	-123	110
H(63)	1160	39	22	91
H(64)	463	533	342	170
H(65)	570	670	294	191
H(66)	572	777	179	188
H(67)	456	757	116	182
H(68)	348	620	158	179
H(69)	350	510	271	172
H(70)	611	-8	75	224
H(71)	435	15	136	282
H(72)	326	25	61	298

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C. X-ray report for [PhBP<sub>3</sub>]CoO(4-*t*Bu-Ph), **3**.

Contents

Table 1.	Crystal data
Figures	Figures for publication
Table 2.	Atomic Coordinates
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Table 5.	Anisotropic displacement parameters
Table 6.	Hydrogen atomic coordinates
Table 7.	Observed and calculated structure factors (for deposit)



DMJ19

**Note:** The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 194087. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 194087."

**Table 1. Crystal data and structure refinement for DMJ19 (CCDC 194087).**

Empirical formula	C <sub>55</sub> H <sub>54</sub> BOP <sub>3</sub> Co
Formula weight	893.63
Crystallization Solvent	Petroleum ether
Crystal Habit	Fragment
Crystal size	0.33 x 0.25 x 0.22 mm <sup>3</sup>
Crystal color	Red

### Data Collection

Preliminary Photos	Rotation
Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoK $\alpha$
Data Collection Temperature	98(2) K
$\theta$ range for 27451 reflections used in lattice determination	2.29 to 22.91°
Unit cell dimensions	a = 38.2238(8) Å c = 12.4091(5) Å
Volume	18130.4(9) Å <sup>3</sup>
Z	16
Crystal system	Tetragonal
Space group	I4 <sub>1</sub> /a
Density (calculated)	1.310 Mg/m <sup>3</sup>
F(000)	7504
$\theta$ range for data collection	1.51 to 23.70°
Completeness to $\theta = 23.70^\circ$	88.3 %
Index ranges	-41 $\leq$ h $\leq$ 41, -42 $\leq$ k $\leq$ 42, -12 $\leq$ l $\leq$ 13
Data collection scan type	$\omega$ scans at 7 $\phi$ settings
Reflections collected	99401
Independent reflections	6071 [R <sub>int</sub> = 0.0769]
Absorption coefficient	0.525 mm <sup>-1</sup>
Absorption correction	None
Max. and min. transmission	0.8933 and 0.8459

**Table 1 (cont.)****Structure solution and Refinement**

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on $F^2$
Data / restraints / parameters	6071 / 32 / 519
Treatment of hydrogen atoms	Riding
Goodness-of-fit on $F^2$	3.011
Final R indices [ $I > 2\sigma(I)$ , 4119 reflections]	$R_1 = 0.0560$ , $wR_2 = 0.0808$
R indices (all data)	$R_1 = 0.0970$ , $wR_2 = 0.0837$
Type of weighting scheme used	Sigma
Weighting scheme used	$w = 1/\sigma^2(F_o^2)$
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	0.824 and -0.555 e.Å <sup>-3</sup>

**Special Refinement Details**

The aryl oxide ligand is disordered over two sites (O1A-C55A and O1B-C55B), each with a distinctly different bonding mode. Both orientations were refined isotropically with restraints on distances and angles within the ligand itself, as follows. The aryl ring was restrained with AFIX 66, FLAT was applied to atoms O1 to C52, carbon-carbon distances in the t-Butyl group were restrained with DFIX and angles within the t-Butyl group as well as angles between the aryl ring and atoms bonded to it were restrained to be equal using DFIX with a free variable. The actual list of restraints follows;

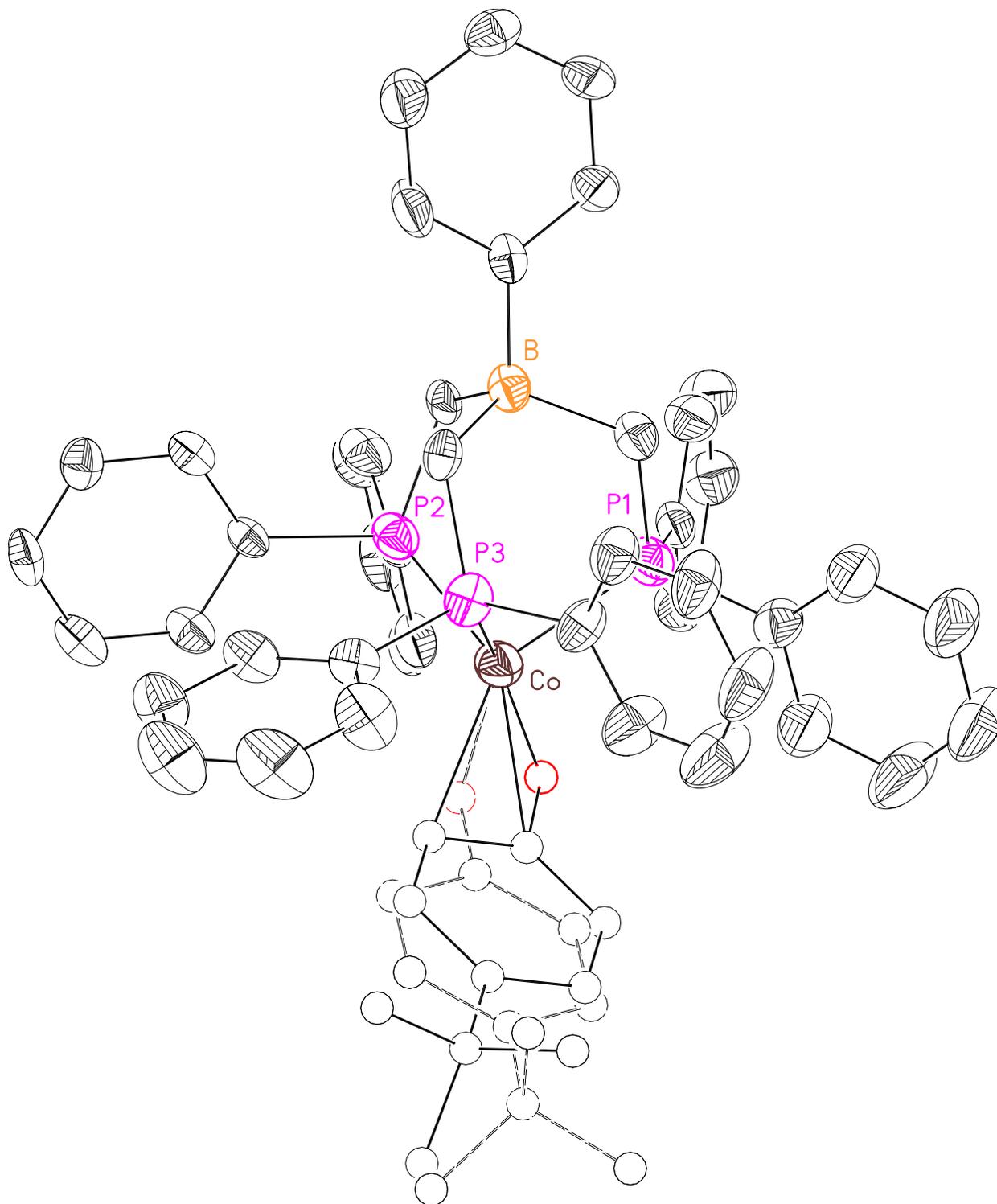
```
DFIX 1.55 0.01 C49B C52B
DFIX 1.54 0.001 C52B C53B C52B C54B C52B C55B
DFIX 41 0.1 C53B C54B C53B C55B C54B C55B
DFIX 31 0.1 C48B C52B C50B C52B
DFIX 21 0.1 O1B C47B O1B C51B
FLAT 0.1 O1B > C52B

WGHT 0.000000
FVAR 0.03716 2.35268 2.54338 2.47245 0.49054
```

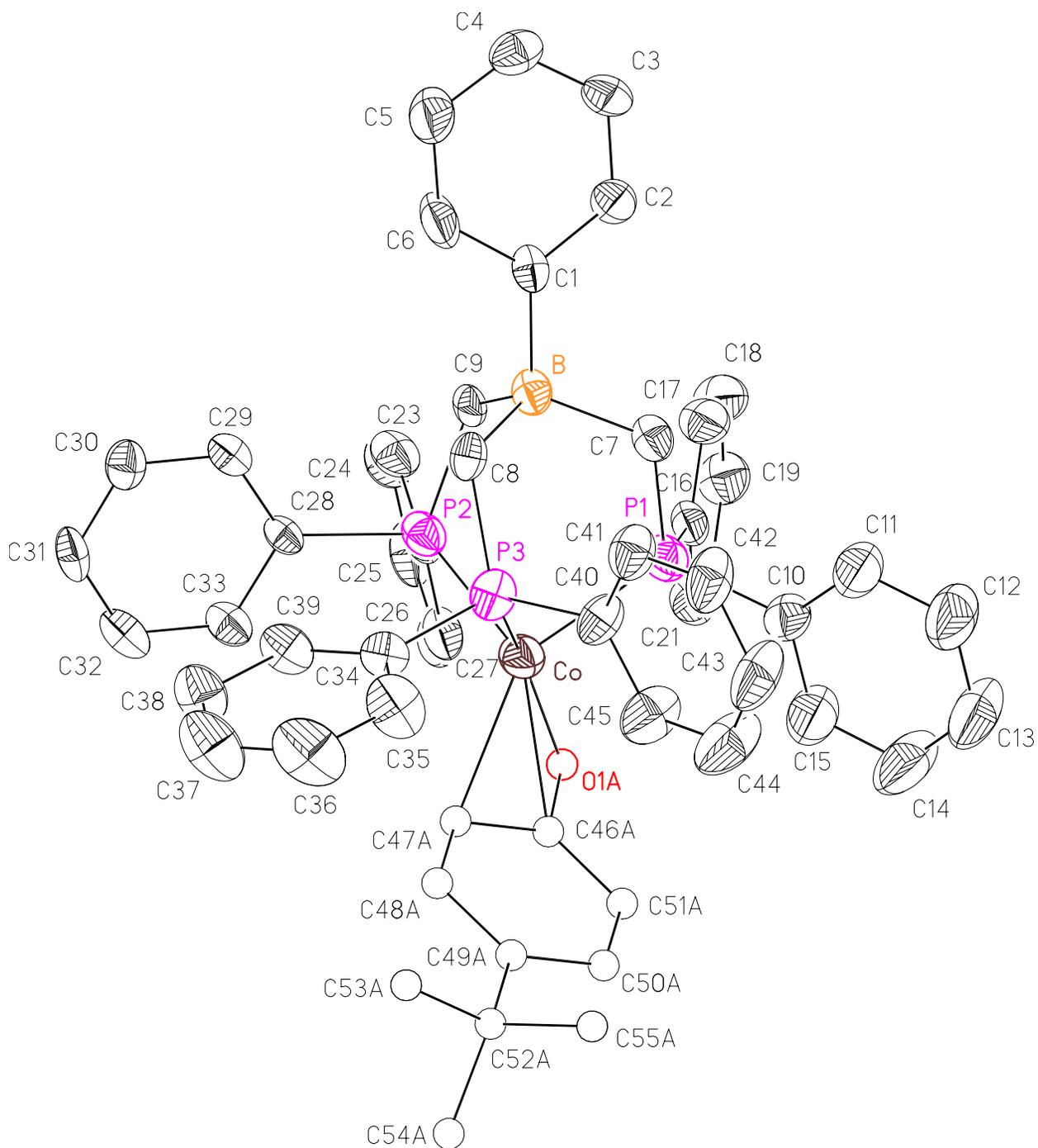
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DFIX 1.55 0.01 C49A C52A
DFIX 1.54 0.001 C52A C53A C52A C54A C52A C55A
DFIX 41 0.1 C53A C54A C53A C55A C54A C55A
DFIX 31 0.1 C48A C52A C50A C52A
DFIX 21 0.1 O1A C47A O1A C51A
FLAT 0.1 O1A > C52
```

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

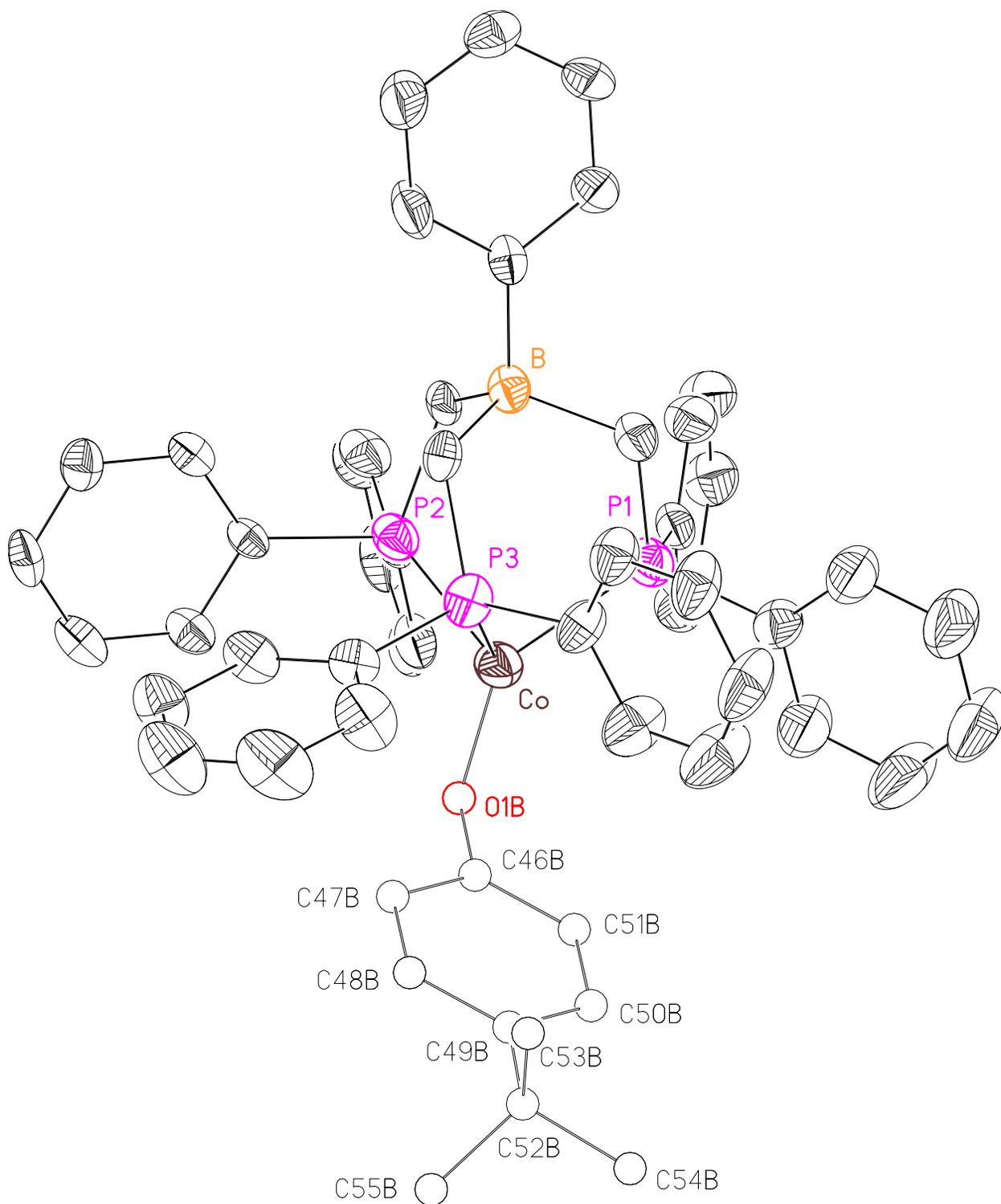
All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.



**Figure 1.** DMJ19 showing both orientations of the aryl-oxide ligand. The  $\eta^3$  orientation is shown with solid lines and the  $\eta^1$  orientation with dotted lines. Hydrogen atoms and labels on carbon and oxygen are omitted for clarity. Orientation of view is identical to Figures 2 and 3.



**Figure 2.** DMJ19 showing the  $\eta^3$  orientation of the aryl-oxide ligand only. All atoms are labeled except for C20 and C22 which are obscured by atoms C42 and P2, respectively. Hydrogen atoms are omitted for clarity.



**Figure 3.** Partially labeled view of DMJ19 showing only the  $\eta^1$  orientation of the aryl-oxide. Hydrogen labels are omitted for clarity. Orientation of view is identical to Figures 1 and 2.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for DMJ19 (CCDC 194087).  $U_{eq}$  is defined as the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{eq}$	Occ
Co	3998(1)	870(1)	980(1)	38(1)	1
P(1)	4261(1)	941(1)	2585(1)	37(1)	1
P(2)	3626(1)	455(1)	1678(1)	34(1)	1
P(3)	4414(1)	498(1)	458(1)	36(1)	1
B	4294(1)	180(1)	2573(4)	31(1)	1
C(1)	4419(1)	-154(1)	3287(3)	27(1)	1
C(2)	4573(1)	-138(1)	4292(3)	36(1)	1
C(3)	4656(1)	-430(1)	4898(3)	42(1)	1
C(4)	4590(1)	-755(1)	4510(4)	42(1)	1
C(5)	4443(1)	-786(1)	3515(4)	62(2)	1
C(6)	4361(1)	-493(1)	2928(4)	59(2)	1
C(7)	4483(1)	548(1)	2996(3)	33(1)	1
C(8)	4413(1)	111(1)	1295(3)	29(1)	1
C(9)	3859(1)	200(1)	2672(3)	28(1)	1
C(10)	4567(1)	1300(1)	2711(3)	40(1)	1
C(11)	4897(1)	1264(1)	3136(4)	64(2)	1
C(12)	5121(1)	1547(2)	3242(4)	81(2)	1
C(13)	5019(1)	1872(1)	2900(4)	77(2)	1
C(14)	4693(2)	1912(1)	2457(4)	82(2)	1
C(15)	4471(1)	1630(1)	2362(4)	61(2)	1
C(16)	3943(1)	1044(1)	3637(3)	33(1)	1
C(17)	3918(1)	858(1)	4596(4)	43(1)	1
C(18)	3666(1)	943(1)	5360(3)	47(1)	1
C(19)	3439(1)	1217(1)	5183(4)	45(1)	1
C(20)	3459(1)	1406(1)	4232(4)	45(1)	1
C(21)	3709(1)	1316(1)	3467(3)	38(1)	1
C(22)	3228(1)	611(1)	2316(3)	33(1)	1
C(23)	3048(1)	403(1)	3048(3)	39(1)	1
C(24)	2736(1)	515(1)	3491(3)	44(1)	1
C(25)	2602(1)	838(1)	3210(4)	45(1)	1
C(26)	2778(1)	1046(1)	2490(4)	44(1)	1
C(27)	3088(1)	934(1)	2040(3)	38(1)	1
C(28)	3435(1)	144(1)	723(3)	26(1)	1
C(29)	3504(1)	-214(1)	725(3)	32(1)	1
C(30)	3372(1)	-428(1)	-73(3)	36(1)	1
C(31)	3166(1)	-292(1)	-881(3)	39(1)	1
C(32)	3090(1)	63(1)	-878(3)	41(1)	1
C(33)	3222(1)	277(1)	-83(3)	34(1)	1
C(34)	4382(1)	350(1)	-939(3)	33(1)	1
C(35)	4643(1)	405(1)	-1693(4)	56(1)	1
C(36)	4596(1)	289(1)	-2752(4)	70(2)	1
C(37)	4292(1)	120(1)	-3057(4)	68(2)	1
C(38)	4034(1)	65(1)	-2306(4)	49(1)	1
C(39)	4080(1)	180(1)	-1258(3)	40(1)	1
C(40)	4846(1)	691(1)	489(3)	38(1)	1
C(41)	5148(1)	512(1)	760(3)	44(1)	1
C(42)	5474(1)	670(1)	684(4)	54(1)	1

C(43)	5504(1)	1009(1)	333(4)	64(2)	1
C(44)	5208(1)	1192(1)	70(4)	70(2)	1
C(45)	4882(1)	1035(1)	152(4)	57(1)	1
O(1A)	3778(1)	1310(1)	912(4)	21(2)	0.491(4)
C(46A)	3942(1)	1366(2)	-17(4)	27(2)	0.491(4)
C(47A)	3927(1)	1095(1)	-761(5)	21(2)	0.491(4)
C(48A)	4110(2)	1120(1)	-1726(4)	42(3)	0.491(4)
C(49A)	4308(2)	1417(2)	-1948(4)	53(3)	0.491(4)
C(50A)	4322(2)	1688(2)	-1204(6)	48(5)	0.491(4)
C(51A)	4139(2)	1663(1)	-239(5)	72(5)	0.491(4)
C(52A)	4521(2)	1440(3)	-3039(6)	88(4)	0.491(4)
C(53A)	4591(3)	1094(3)	-3640(9)	114(5)	0.491(4)
C(54A)	4335(3)	1647(3)	-3936(8)	81(5)	0.491(4)
C(55A)	4884(3)	1592(4)	-2767(13)	173(8)	0.491(4)
O(1B)	3734(2)	1158(2)	126(6)	99(3)	0.509(4)
C(46B)	3930(2)	1297(2)	-645(5)	55(3)	0.509(4)
C(47B)	3977(2)	1113(1)	-1601(6)	97(5)	0.509(4)
C(48B)	4196(2)	1245(2)	-2396(5)	54(3)	0.509(4)
C(49B)	4369(2)	1561(2)	-2236(5)	63(3)	0.509(4)
C(50B)	4322(2)	1745(2)	-1280(6)	91(7)	0.509(4)
C(51B)	4103(2)	1613(2)	-484(5)	55(4)	0.509(4)
C(52B)	4616(2)	1676(2)	-3117(7)	68(3)	0.509(4)
C(53B)	4927(2)	1420(3)	-3100(9)	83(4)	0.509(4)
C(54B)	4760(2)	2046(2)	-2907(7)	68(3)	0.509(4)
C(55B)	4454(4)	1686(5)	-4253(9)	162(8)	0.509(4)

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**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for DMJ19 (CCDC 194087).**

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Co-P(1)	2.2467(12)		
Co-P(2)	2.2999(13)		
Co-P(3)	2.2268(12)		
Co-O(1B)	1.832(7)	Co-O(1A)	1.885(4)
		Co-C(46A)	2.277(5)
		Co-C(47A)	2.341(5)
P(1)-Co-P(2)	91.48(4)		
P(1)-Co-P(3)	90.96(4)		
P(2)-Co-P(3)	96.35(4)		
O(1B)-Co-P(1)	133.4(3)	O(1A)-Co-P(1)	97.58(15)
O(1B)-Co-P(2)	106.9(2)	O(1A)-Co-P(2)	110.83(14)
O(1B)-Co-P(3)	127.5(3)	O(1A)-Co-P(3)	151.16(14)
P(1)-Co-C(46A)	115.05(15)		
P(2)-Co-C(46A)	136.13(14)		
P(3)-Co-C(46A)	116.21(12)		
P(1)-Co-C(47A)	145.63(12)		
P(2)-Co-C(47A)	121.94(12)		
P(3)-Co-C(47A)	92.81(14)		
C(46B)-O(1B)-Co	110.3(4)	C(46A)-O(1A)-Co	88.4(3)
O(1B)-Co-O(1A)	35.9(2)		

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**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for DMJ19 (CCDC 194087).**

Co-O(1B)	1.832(7)	C(17)-H(17)	0.9500
Co-O(1A)	1.885(4)	C(18)-C(19)	1.379(5)
Co-P(3)	2.2268(12)	C(18)-H(18)	0.9500
Co-P(1)	2.2467(12)	C(19)-C(20)	1.386(5)
Co-C(46A)	2.277(5)	C(19)-H(19)	0.9500
Co-P(2)	2.2999(13)	C(20)-C(21)	1.390(5)
Co-C(47A)	2.341(5)	C(20)-H(20)	0.9500
P(1)-C(7)	1.798(4)	C(21)-H(21)	0.9500
P(1)-C(10)	1.810(4)	C(22)-C(27)	1.389(5)
P(1)-C(16)	1.827(4)	C(22)-C(23)	1.391(5)
P(2)-C(9)	1.806(3)	C(23)-C(24)	1.382(5)
P(2)-C(22)	1.815(4)	C(23)-H(23)	0.9500
P(2)-C(28)	1.829(4)	C(24)-C(25)	1.383(5)
P(3)-C(8)	1.807(4)	C(24)-H(24)	0.9500
P(3)-C(40)	1.810(4)	C(25)-C(26)	1.372(5)
P(3)-C(34)	1.827(4)	C(25)-H(25)	0.9500
B-C(1)	1.624(6)	C(26)-C(27)	1.378(5)
B-C(7)	1.667(5)	C(26)-H(26)	0.9500
B-C(8)	1.669(5)	C(27)-H(27)	0.9500
B-C(9)	1.671(5)	C(28)-C(33)	1.386(5)
C(1)-C(2)	1.380(5)	C(28)-C(29)	1.395(5)
C(1)-C(6)	1.386(5)	C(29)-C(30)	1.379(5)
C(2)-C(3)	1.383(5)	C(29)-H(29)	0.9500
C(2)-H(2)	0.9500	C(30)-C(31)	1.378(5)
C(3)-C(4)	1.357(5)	C(30)-H(30)	0.9500
C(3)-H(3)	0.9500	C(31)-C(32)	1.385(5)
C(4)-C(5)	1.361(5)	C(31)-H(31)	0.9500
C(4)-H(4)	0.9500	C(32)-C(33)	1.379(5)
C(5)-C(6)	1.373(5)	C(32)-H(32)	0.9500
C(5)-H(5)	0.9500	C(33)-H(33)	0.9500
C(6)-H(6)	0.9500	C(34)-C(39)	1.382(5)
C(7)-H(7A)	0.9900	C(34)-C(35)	1.384(5)
C(7)-H(7B)	0.9900	C(35)-C(36)	1.398(6)
C(8)-H(8A)	0.9900	C(35)-H(35)	0.9500
C(8)-H(8B)	0.9900	C(36)-C(37)	1.382(6)
C(9)-H(9A)	0.9900	C(36)-H(36)	0.9500
C(9)-H(9B)	0.9900	C(37)-C(38)	1.374(5)
C(10)-C(11)	1.376(5)	C(37)-H(37)	0.9500
C(10)-C(15)	1.383(5)	C(38)-C(39)	1.384(5)
C(11)-C(12)	1.387(6)	C(38)-H(38)	0.9500
C(11)-H(11)	0.9500	C(39)-H(39)	0.9500
C(12)-C(13)	1.371(6)	C(40)-C(41)	1.381(5)
C(12)-H(12)	0.9500	C(40)-C(45)	1.387(5)
C(13)-C(14)	1.371(6)	C(41)-C(42)	1.387(5)
C(13)-H(13)	0.9500	C(41)-H(41)	0.9500
C(14)-C(15)	1.378(6)	C(42)-C(43)	1.372(5)
C(14)-H(14)	0.9500	C(42)-H(42)	0.9500
C(15)-H(15)	0.9500	C(43)-C(44)	1.369(6)
C(16)-C(21)	1.387(5)	C(43)-H(43)	0.9500
C(16)-C(17)	1.390(5)	C(44)-C(45)	1.386(5)
C(17)-C(18)	1.390(5)	C(44)-H(44)	0.9500

C(45)-H(45)	0.9500	O(1A)-Co-P(1)	97.58(15)
O(1A)-C(46A)	1.330(6)	P(3)-Co-P(1)	90.96(4)
C(46A)-C(47A)	1.3900	O(1B)-Co-C(46A)	29.8(3)
C(46A)-C(51A)	1.3900	O(1A)-Co-C(46A)	35.74(17)
C(47A)-C(48A)	1.3900	P(3)-Co-C(46A)	116.21(12)
C(47A)-H(47A)	0.9500	P(1)-Co-C(46A)	115.05(15)
C(48A)-C(49A)	1.3900	O(1B)-Co-P(2)	106.9(2)
C(48A)-H(48A)	0.9500	O(1A)-Co-P(2)	110.83(14)
C(49A)-C(50A)	1.3900	P(3)-Co-P(2)	96.35(4)
C(49A)-C(52A)	1.584(7)	P(1)-Co-P(2)	91.48(4)
C(50A)-C(51A)	1.3900	C(46A)-Co-P(2)	136.13(14)
C(50A)-H(50A)	0.9500	O(1B)-Co-C(47A)	35.0(3)
C(51A)-H(51A)	0.9500	O(1A)-Co-C(47A)	65.05(19)
C(52A)-C(54A)	1.5398(11)	P(3)-Co-C(47A)	92.81(14)
C(52A)-C(55A)	1.5401(11)	P(1)-Co-C(47A)	145.63(12)
C(52A)-C(53A)	1.5403(11)	C(46A)-Co-C(47A)	35.00(7)
C(53A)-H(53A)	0.9800	P(2)-Co-C(47A)	121.94(12)
C(53A)-H(53B)	0.9800	C(7)-P(1)-C(10)	107.68(19)
C(53A)-H(53C)	0.9800	C(7)-P(1)-C(16)	106.97(19)
C(54A)-H(54A)	0.9800	C(10)-P(1)-C(16)	101.75(18)
C(54A)-H(54B)	0.9800	C(7)-P(1)-Co	111.22(12)
C(54A)-H(54C)	0.9800	C(10)-P(1)-Co	117.18(15)
C(55A)-H(55A)	0.9800	C(16)-P(1)-Co	111.24(13)
C(55A)-H(55B)	0.9800	C(9)-P(2)-C(22)	106.96(18)
C(55A)-H(55C)	0.9800	C(9)-P(2)-C(28)	106.85(18)
O(1B)-C(46B)	1.327(8)	C(22)-P(2)-C(28)	99.27(17)
C(46B)-C(47B)	1.3900	C(9)-P(2)-Co	108.90(13)
C(46B)-C(51B)	1.3900	C(22)-P(2)-Co	117.11(15)
C(47B)-C(48B)	1.3900	C(28)-P(2)-Co	116.81(13)
C(47B)-H(47B)	0.9500	C(8)-P(3)-C(40)	108.9(2)
C(48B)-C(49B)	1.3900	C(8)-P(3)-C(34)	107.04(17)
C(48B)-H(48B)	0.9500	C(40)-P(3)-C(34)	101.93(19)
C(49B)-C(50B)	1.3900	C(8)-P(3)-Co	110.65(12)
C(49B)-C(52B)	1.510(7)	C(40)-P(3)-Co	112.62(15)
C(50B)-C(51B)	1.3900	C(34)-P(3)-Co	115.22(13)
C(50B)-H(50B)	0.9500	C(1)-B-C(7)	111.4(3)
C(51B)-H(51B)	0.9500	C(1)-B-C(8)	108.4(3)
C(52B)-C(54B)	1.5386(11)	C(7)-B-C(8)	108.3(3)
C(52B)-C(55B)	1.5398(11)	C(1)-B-C(9)	106.8(3)
C(52B)-C(53B)	1.5401(11)	C(7)-B-C(9)	111.6(3)
C(53B)-H(53D)	0.9800	C(8)-B-C(9)	110.2(3)
C(53B)-H(53E)	0.9800	C(2)-C(1)-C(6)	113.7(4)
C(53B)-H(53F)	0.9800	C(2)-C(1)-B	125.5(4)
C(54B)-H(54D)	0.9800	C(6)-C(1)-B	120.8(4)
C(54B)-H(54E)	0.9800	C(1)-C(2)-C(3)	123.5(4)
C(54B)-H(54F)	0.9800	C(1)-C(2)-H(2)	118.3
C(55B)-H(55D)	0.9800	C(3)-C(2)-H(2)	118.3
C(55B)-H(55E)	0.9800	C(4)-C(3)-C(2)	120.3(4)
C(55B)-H(55F)	0.9800	C(4)-C(3)-H(3)	119.8
		C(2)-C(3)-H(3)	119.8
O(1B)-Co-O(1A)	35.9(2)	C(3)-C(4)-C(5)	118.6(4)
O(1B)-Co-P(3)	127.5(3)	C(3)-C(4)-H(4)	120.7
O(1A)-Co-P(3)	151.16(14)	C(5)-C(4)-H(4)	120.7
O(1B)-Co-P(1)	133.4(3)	C(4)-C(5)-C(6)	120.2(4)

C(4)-C(5)-H(5)	119.9	C(19)-C(20)-H(20)	120.3
C(6)-C(5)-H(5)	119.9	C(21)-C(20)-H(20)	120.3
C(5)-C(6)-C(1)	123.7(4)	C(16)-C(21)-C(20)	121.6(4)
C(5)-C(6)-H(6)	118.1	C(16)-C(21)-H(21)	119.2
C(1)-C(6)-H(6)	118.1	C(20)-C(21)-H(21)	119.2
B-C(7)-P(1)	114.3(3)	C(27)-C(22)-C(23)	118.5(4)
B-C(7)-H(7A)	108.7	C(27)-C(22)-P(2)	120.6(4)
P(1)-C(7)-H(7A)	108.7	C(23)-C(22)-P(2)	120.8(3)
B-C(7)-H(7B)	108.7	C(24)-C(23)-C(22)	120.7(4)
P(1)-C(7)-H(7B)	108.7	C(24)-C(23)-H(23)	119.7
H(7A)-C(7)-H(7B)	107.6	C(22)-C(23)-H(23)	119.7
B-C(8)-P(3)	114.8(3)	C(23)-C(24)-C(25)	119.8(4)
B-C(8)-H(8A)	108.6	C(23)-C(24)-H(24)	120.1
P(3)-C(8)-H(8A)	108.6	C(25)-C(24)-H(24)	120.1
B-C(8)-H(8B)	108.6	C(26)-C(25)-C(24)	120.1(4)
P(3)-C(8)-H(8B)	108.6	C(26)-C(25)-H(25)	120.0
H(8A)-C(8)-H(8B)	107.5	C(24)-C(25)-H(25)	120.0
B-C(9)-P(2)	117.8(3)	C(25)-C(26)-C(27)	120.2(4)
B-C(9)-H(9A)	107.9	C(25)-C(26)-H(26)	119.9
P(2)-C(9)-H(9A)	107.9	C(27)-C(26)-H(26)	119.9
B-C(9)-H(9B)	107.9	C(26)-C(27)-C(22)	120.7(4)
P(2)-C(9)-H(9B)	107.9	C(26)-C(27)-H(27)	119.6
H(9A)-C(9)-H(9B)	107.2	C(22)-C(27)-H(27)	119.6
C(11)-C(10)-C(15)	117.1(4)	C(33)-C(28)-C(29)	118.2(4)
C(11)-C(10)-P(1)	123.3(4)	C(33)-C(28)-P(2)	117.7(3)
C(15)-C(10)-P(1)	119.5(4)	C(29)-C(28)-P(2)	124.1(3)
C(10)-C(11)-C(12)	121.6(5)	C(30)-C(29)-C(28)	120.8(4)
C(10)-C(11)-H(11)	119.2	C(30)-C(29)-H(29)	119.6
C(12)-C(11)-H(11)	119.2	C(28)-C(29)-H(29)	119.6
C(13)-C(12)-C(11)	120.2(5)	C(31)-C(30)-C(29)	120.5(4)
C(13)-C(12)-H(12)	119.9	C(31)-C(30)-H(30)	119.8
C(11)-C(12)-H(12)	119.9	C(29)-C(30)-H(30)	119.8
C(14)-C(13)-C(12)	119.0(5)	C(30)-C(31)-C(32)	119.1(4)
C(14)-C(13)-H(13)	120.5	C(30)-C(31)-H(31)	120.4
C(12)-C(13)-H(13)	120.5	C(32)-C(31)-H(31)	120.4
C(13)-C(14)-C(15)	120.4(5)	C(33)-C(32)-C(31)	120.5(4)
C(13)-C(14)-H(14)	119.8	C(33)-C(32)-H(32)	119.7
C(15)-C(14)-H(14)	119.8	C(31)-C(32)-H(32)	119.7
C(14)-C(15)-C(10)	121.6(5)	C(32)-C(33)-C(28)	120.8(4)
C(14)-C(15)-H(15)	119.2	C(32)-C(33)-H(33)	119.6
C(10)-C(15)-H(15)	119.2	C(28)-C(33)-H(33)	119.6
C(21)-C(16)-C(17)	118.1(4)	C(39)-C(34)-C(35)	118.6(4)
C(21)-C(16)-P(1)	118.8(3)	C(39)-C(34)-P(3)	118.2(3)
C(17)-C(16)-P(1)	123.1(3)	C(35)-C(34)-P(3)	123.2(4)
C(16)-C(17)-C(18)	120.8(4)	C(34)-C(35)-C(36)	119.7(4)
C(16)-C(17)-H(17)	119.6	C(34)-C(35)-H(35)	120.1
C(18)-C(17)-H(17)	119.6	C(36)-C(35)-H(35)	120.1
C(19)-C(18)-C(17)	120.3(4)	C(37)-C(36)-C(35)	120.8(4)
C(19)-C(18)-H(18)	119.8	C(37)-C(36)-H(36)	119.6
C(17)-C(18)-H(18)	119.8	C(35)-C(36)-H(36)	119.6
C(18)-C(19)-C(20)	119.8(4)	C(38)-C(37)-C(36)	119.4(5)
C(18)-C(19)-H(19)	120.1	C(38)-C(37)-H(37)	120.3
C(20)-C(19)-H(19)	120.1	C(36)-C(37)-H(37)	120.3
C(19)-C(20)-C(21)	119.4(4)	C(37)-C(38)-C(39)	119.8(4)

C(37)-C(38)-H(38)	120.1	C(52A)-C(53A)-H(53A)	109.5
C(39)-C(38)-H(38)	120.1	C(52A)-C(53A)-H(53B)	109.5
C(34)-C(39)-C(38)	121.7(4)	H(53A)-C(53A)-H(53B)	109.5
C(34)-C(39)-H(39)	119.1	C(52A)-C(53A)-H(53C)	109.5
C(38)-C(39)-H(39)	119.1	H(53A)-C(53A)-H(53C)	109.5
C(41)-C(40)-C(45)	117.3(4)	H(53B)-C(53A)-H(53C)	109.5
C(41)-C(40)-P(3)	124.5(3)	C(52A)-C(54A)-H(54A)	109.5
C(45)-C(40)-P(3)	118.0(4)	C(52A)-C(54A)-H(54B)	109.5
C(40)-C(41)-C(42)	121.3(4)	H(54A)-C(54A)-H(54B)	109.5
C(40)-C(41)-H(41)	119.3	C(52A)-C(54A)-H(54C)	109.5
C(42)-C(41)-H(41)	119.3	H(54A)-C(54A)-H(54C)	109.5
C(43)-C(42)-C(41)	120.4(4)	H(54B)-C(54A)-H(54C)	109.5
C(43)-C(42)-H(42)	119.8	C(52A)-C(55A)-H(55A)	109.5
C(41)-C(42)-H(42)	119.8	C(52A)-C(55A)-H(55B)	109.5
C(44)-C(43)-C(42)	119.3(4)	H(55A)-C(55A)-H(55B)	109.5
C(44)-C(43)-H(43)	120.4	C(52A)-C(55A)-H(55C)	109.5
C(42)-C(43)-H(43)	120.4	H(55A)-C(55A)-H(55C)	109.5
C(43)-C(44)-C(45)	120.3(5)	H(55B)-C(55A)-H(55C)	109.5
C(43)-C(44)-H(44)	119.9	C(46B)-O(1B)-Co	110.3(4)
C(45)-C(44)-H(44)	119.9	O(1B)-C(46B)-C(47B)	119.0(6)
C(44)-C(45)-C(40)	121.4(4)	O(1B)-C(46B)-C(51B)	120.9(6)
C(44)-C(45)-H(45)	119.3	C(47B)-C(46B)-C(51B)	120.0
C(40)-C(45)-H(45)	119.3	C(48B)-C(47B)-C(46B)	120.0
C(46A)-O(1A)-Co	88.4(3)	C(48B)-C(47B)-H(47B)	120.0
O(1A)-C(46A)-C(47A)	115.8(4)	C(46B)-C(47B)-H(47B)	120.0
O(1A)-C(46A)-C(51A)	124.1(4)	C(47B)-C(48B)-C(49B)	120.0
C(47A)-C(46A)-C(51A)	120.0	C(47B)-C(48B)-H(48B)	120.0
O(1A)-C(46A)-Co	55.9(3)	C(49B)-C(48B)-H(48B)	120.0
C(47A)-C(46A)-Co	75.0(3)	C(50B)-C(49B)-C(48B)	120.0
C(51A)-C(46A)-Co	137.4(3)	C(50B)-C(49B)-C(52B)	123.4(5)
C(46A)-C(47A)-C(48A)	120.0	C(48B)-C(49B)-C(52B)	116.5(5)
C(46A)-C(47A)-Co	70.0(3)	C(49B)-C(50B)-C(51B)	120.0
C(48A)-C(47A)-Co	139.6(3)	C(49B)-C(50B)-H(50B)	120.0
C(46A)-C(47A)-H(47A)	120.0	C(51B)-C(50B)-H(50B)	120.0
C(48A)-C(47A)-H(47A)	120.0	C(50B)-C(51B)-C(46B)	120.0
Co-C(47A)-H(47A)	65.2	C(50B)-C(51B)-H(51B)	120.0
C(49A)-C(48A)-C(47A)	120.0	C(46B)-C(51B)-H(51B)	120.0
C(49A)-C(48A)-H(48A)	120.0	C(49B)-C(52B)-C(54B)	111.6(6)
C(47A)-C(48A)-H(48A)	120.0	C(49B)-C(52B)-C(55B)	114.8(9)
C(50A)-C(49A)-C(48A)	120.0	C(54B)-C(52B)-C(55B)	106.0(9)
C(50A)-C(49A)-C(52A)	120.3(5)	C(49B)-C(52B)-C(53B)	106.8(7)
C(48A)-C(49A)-C(52A)	119.7(5)	C(54B)-C(52B)-C(53B)	107.8(7)
C(49A)-C(50A)-C(51A)	120.0	C(55B)-C(52B)-C(53B)	109.7(9)
C(49A)-C(50A)-H(50A)	120.0	C(52B)-C(53B)-H(53D)	109.5
C(51A)-C(50A)-H(50A)	120.0	C(52B)-C(53B)-H(53E)	109.5
C(50A)-C(51A)-C(46A)	120.0	H(53D)-C(53B)-H(53E)	109.5
C(50A)-C(51A)-H(51A)	120.0	C(52B)-C(53B)-H(53F)	109.5
C(46A)-C(51A)-H(51A)	120.0	H(53D)-C(53B)-H(53F)	109.5
C(54A)-C(52A)-C(55A)	112.3(10)	H(53E)-C(53B)-H(53F)	109.5
C(54A)-C(52A)-C(53A)	99.9(8)	C(52B)-C(54B)-H(54D)	109.5
C(55A)-C(52A)-C(53A)	105.8(9)	C(52B)-C(54B)-H(54E)	109.5
C(54A)-C(52A)-C(49A)	114.1(8)	H(54D)-C(54B)-H(54E)	109.5
C(55A)-C(52A)-C(49A)	107.3(8)	C(52B)-C(54B)-H(54F)	109.5
C(53A)-C(52A)-C(49A)	117.1(8)	H(54D)-C(54B)-H(54F)	109.5

H(54E)-C(54B)-H(54F)	109.5
C(52B)-C(55B)-H(55D)	109.5
C(52B)-C(55B)-H(55E)	109.5
H(55D)-C(55B)-H(55E)	109.5
C(52B)-C(55B)-H(55F)	109.5
H(55D)-C(55B)-H(55F)	109.5
H(55E)-C(55B)-H(55F)	109.5

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**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for DMJ19 (CCDC 194087). The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Co	460(4)	330(4)	341(4)	-15(3)	-55(3)	53(3)
P(1)	368(8)	371(8)	382(8)	-14(6)	-65(6)	52(6)
P(2)	379(8)	342(7)	310(7)	-38(6)	-60(6)	86(6)
P(3)	292(8)	375(8)	419(8)	-49(6)	57(6)	1(6)
B	300(30)	300(30)	340(30)	-70(30)	-40(30)	50(30)
C(1)	190(20)	320(30)	310(30)	-90(20)	-20(20)	50(20)
C(2)	440(30)	370(30)	260(30)	-10(20)	60(20)	-30(20)
C(3)	570(30)	470(30)	220(30)	70(30)	20(20)	-30(30)
C(4)	340(30)	350(30)	550(40)	80(30)	30(30)	20(20)
C(5)	740(40)	320(30)	820(40)	-90(30)	-410(30)	110(30)
C(6)	730(40)	410(30)	630(40)	-130(30)	-460(30)	120(30)
C(7)	320(30)	340(30)	320(30)	-70(20)	-30(20)	60(20)
C(8)	220(30)	310(30)	350(30)	-70(20)	30(20)	-40(20)
C(9)	360(30)	270(30)	200(20)	-90(20)	-40(20)	10(20)
C(10)	410(30)	290(30)	490(30)	-30(20)	-50(30)	60(30)
C(11)	590(40)	390(30)	930(40)	60(30)	-310(30)	-50(30)
C(12)	630(40)	510(40)	1280(50)	50(40)	-450(40)	-100(40)
C(13)	540(40)	410(40)	1350(50)	-60(40)	-200(40)	-90(30)
C(14)	680(40)	360(40)	1420(60)	100(40)	-190(40)	-30(30)
C(15)	540(40)	430(40)	860(40)	-20(30)	-180(30)	-10(30)
C(16)	340(30)	310(30)	330(30)	-60(20)	-110(20)	50(20)
C(17)	610(40)	310(30)	370(30)	-40(30)	-30(30)	110(30)
C(18)	650(40)	380(30)	380(30)	-20(30)	60(30)	60(30)
C(19)	530(30)	410(30)	420(30)	-60(30)	60(30)	30(30)
C(20)	480(30)	360(30)	510(30)	-70(30)	-50(30)	130(30)
C(21)	400(30)	390(30)	340(30)	-20(20)	-60(30)	30(30)
C(22)	350(30)	350(30)	300(30)	-90(20)	-120(20)	70(30)
C(23)	380(30)	400(30)	390(30)	-30(30)	-80(20)	160(30)
C(24)	360(30)	510(40)	440(30)	-70(30)	-20(30)	70(30)
C(25)	250(30)	560(40)	530(40)	-250(30)	-80(30)	110(30)
C(26)	400(30)	380(30)	540(40)	-120(30)	-180(30)	90(30)
C(27)	330(30)	420(30)	390(30)	-110(20)	-90(20)	50(30)
C(28)	270(30)	320(30)	180(30)	-20(20)	-10(20)	50(20)
C(29)	310(30)	410(30)	250(30)	20(20)	-30(20)	20(20)
C(30)	380(30)	360(30)	340(30)	-80(30)	10(20)	-30(20)
C(31)	410(30)	490(30)	280(30)	-140(30)	-80(20)	-70(30)
C(32)	360(30)	590(40)	280(30)	10(30)	-70(20)	80(30)
C(33)	350(30)	400(30)	270(30)	-20(20)	-20(20)	90(20)
C(34)	240(30)	400(30)	360(30)	20(20)	60(30)	40(20)
C(35)	360(30)	840(40)	480(40)	-30(30)	90(30)	-10(30)
C(36)	500(40)	1160(50)	430(40)	60(30)	250(30)	20(40)
C(37)	600(40)	1100(50)	330(30)	-120(30)	120(30)	80(40)
C(38)	440(30)	700(40)	320(30)	-60(30)	80(30)	-30(30)
C(39)	400(30)	550(30)	240(30)	-30(20)	120(20)	60(30)
C(40)	360(30)	290(30)	500(30)	-60(20)	80(20)	-10(30)
C(41)	360(30)	380(30)	570(30)	-80(30)	-10(30)	0(30)
C(42)	300(30)	450(40)	890(40)	-130(30)	-110(30)	0(30)

C(43)	380(40)	440(40)	1100(50)	-100(30)	10(30)	-120(30)
C(44)	440(40)	430(40)	1240(50)	100(30)	50(30)	-30(30)
C(45)	330(30)	470(40)	900(40)	90(30)	20(30)	-10(30)

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**Table 6. Hydrogen coordinates (  $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for DMJ19 (CCDC 194087).**

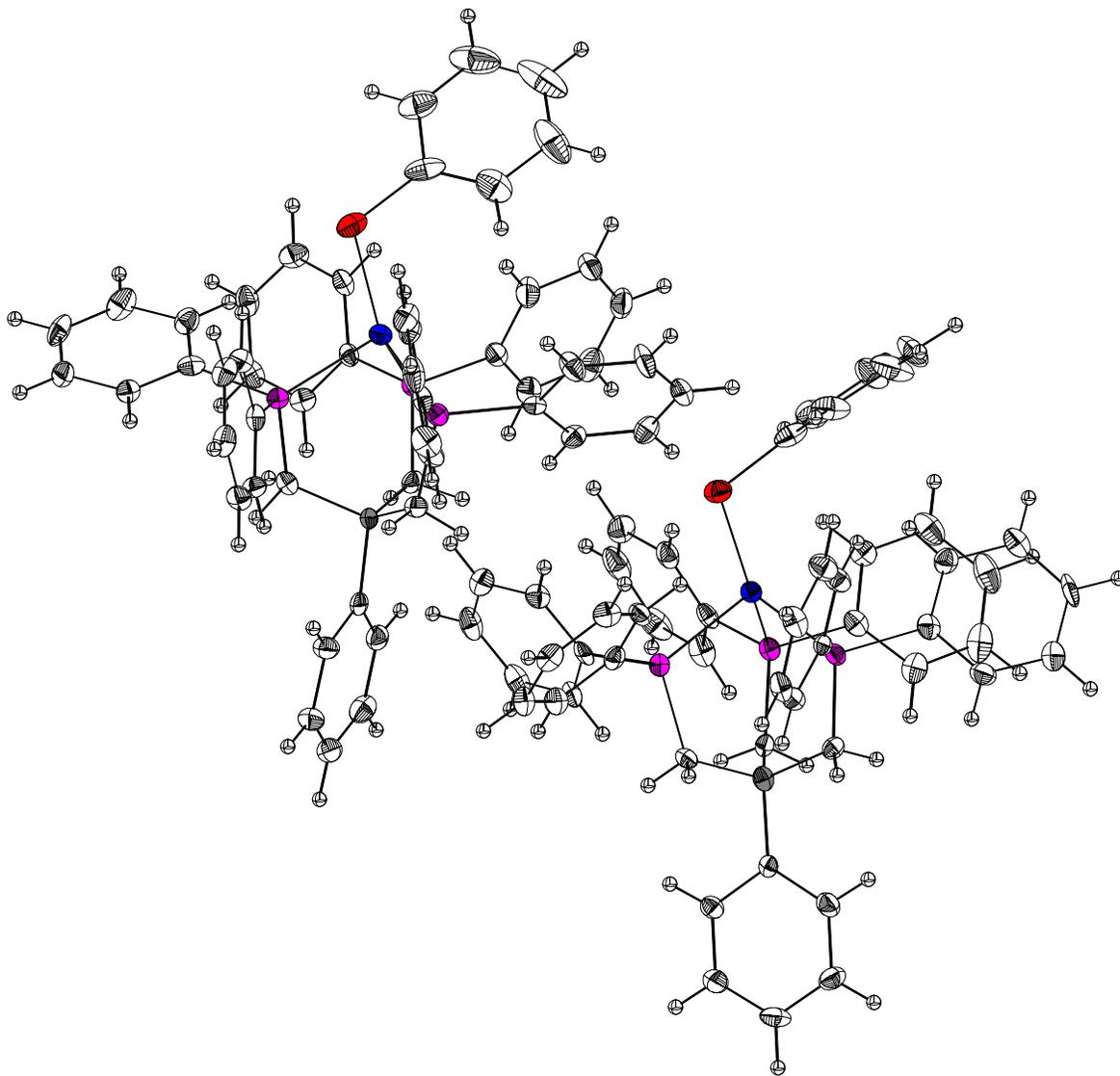
	x	y	z	$U_{\text{iso}}$
H(2)	4624	86	4583	43
H(3)	4760	-403	5588	51
H(4)	4645	-957	4925	50
H(5)	4397	-1012	3226	75
H(6)	4259	-524	2237	71
H(7A)	4726	555	2720	39
H(7B)	4495	544	3793	39
H(8A)	4251	-62	974	35
H(8B)	4650	8	1289	35
H(9A)	3801	296	3391	33
H(9B)	3767	-42	2645	33
H(11)	4974	1039	3363	76
H(12)	5346	1516	3553	97
H(13)	5171	2067	2969	92
H(14)	4619	2136	2215	98
H(15)	4246	1662	2048	73
H(17)	4076	670	4731	52
H(18)	3650	811	6007	56
H(19)	3269	1276	5712	54
H(20)	3304	1596	4104	54
H(21)	3720	1444	2811	45
H(23)	3140	181	3245	46
H(24)	2614	370	3988	52
H(25)	2388	917	3514	54
H(26)	2686	1269	2301	53
H(27)	3206	1078	1535	45
H(29)	3643	-312	1283	39
H(30)	3424	-671	-65	43
H(31)	3077	-439	-1434	47
H(32)	2946	158	-1428	50
H(33)	3166	519	-87	41
H(35)	4853	520	-1492	67
H(36)	4775	327	-3269	83
H(37)	4262	43	-3779	81
H(38)	3824	-51	-2505	59
H(39)	3900	140	-744	48
H(41)	5132	277	1003	53
H(42)	5678	542	877	65
H(43)	5727	1116	274	77
H(44)	5226	1427	-170	84
H(45)	4679	1166	-27	68
H(47A)	3792	892	-609	25
H(48A)	4100	934	-2234	50
H(50A)	4457	1891	-1355	57
H(51A)	4150	1849	270	86
H(53A)	4725	1142	-4297	170
H(53B)	4368	984	-3830	170
H(53C)	4726	937	-3174	170

H(54A)	4485	1655	-4577	121
H(54B)	4289	1886	-3686	121
H(54C)	4113	1533	-4115	121
H(55A)	4881	1846	-2883	259
H(55B)	5060	1485	-3234	259
H(55C)	4940	1542	-2012	259
H(47B)	3858	898	-1710	116
H(48B)	4228	1120	-3050	65
H(50B)	4440	1960	-1171	109
H(51B)	4071	1738	169	66
H(53D)	5082	1470	-3711	124
H(53E)	4840	1179	-3154	124
H(53F)	5057	1448	-2426	124
H(54D)	4882	2050	-2213	102
H(54E)	4565	2213	-2890	102
H(54F)	4922	2110	-3484	102
H(55D)	4258	1850	-4261	244
H(55E)	4371	1452	-4447	244
H(55F)	4632	1762	-4773	244

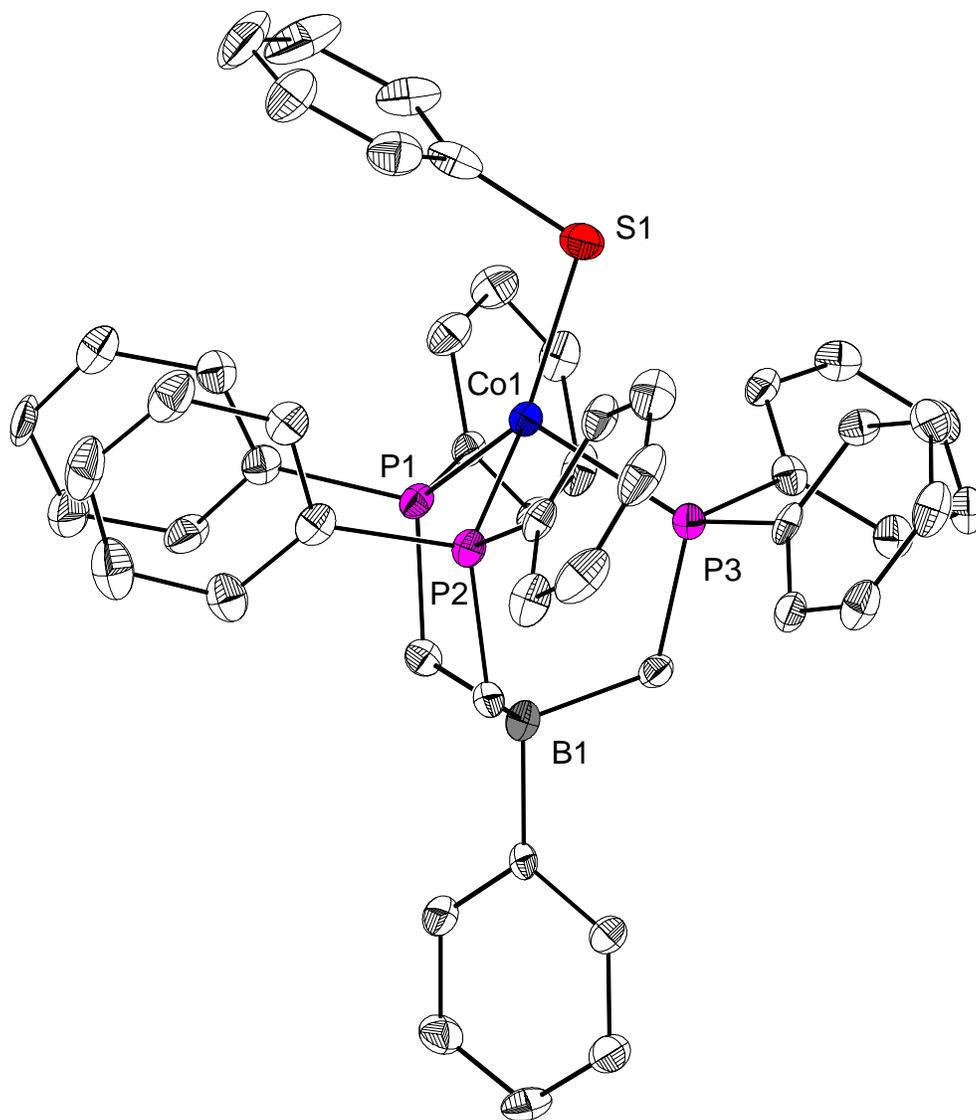
D. X-ray report for  $[\text{PhBP}_3]\text{CoSPh}$ , 5.

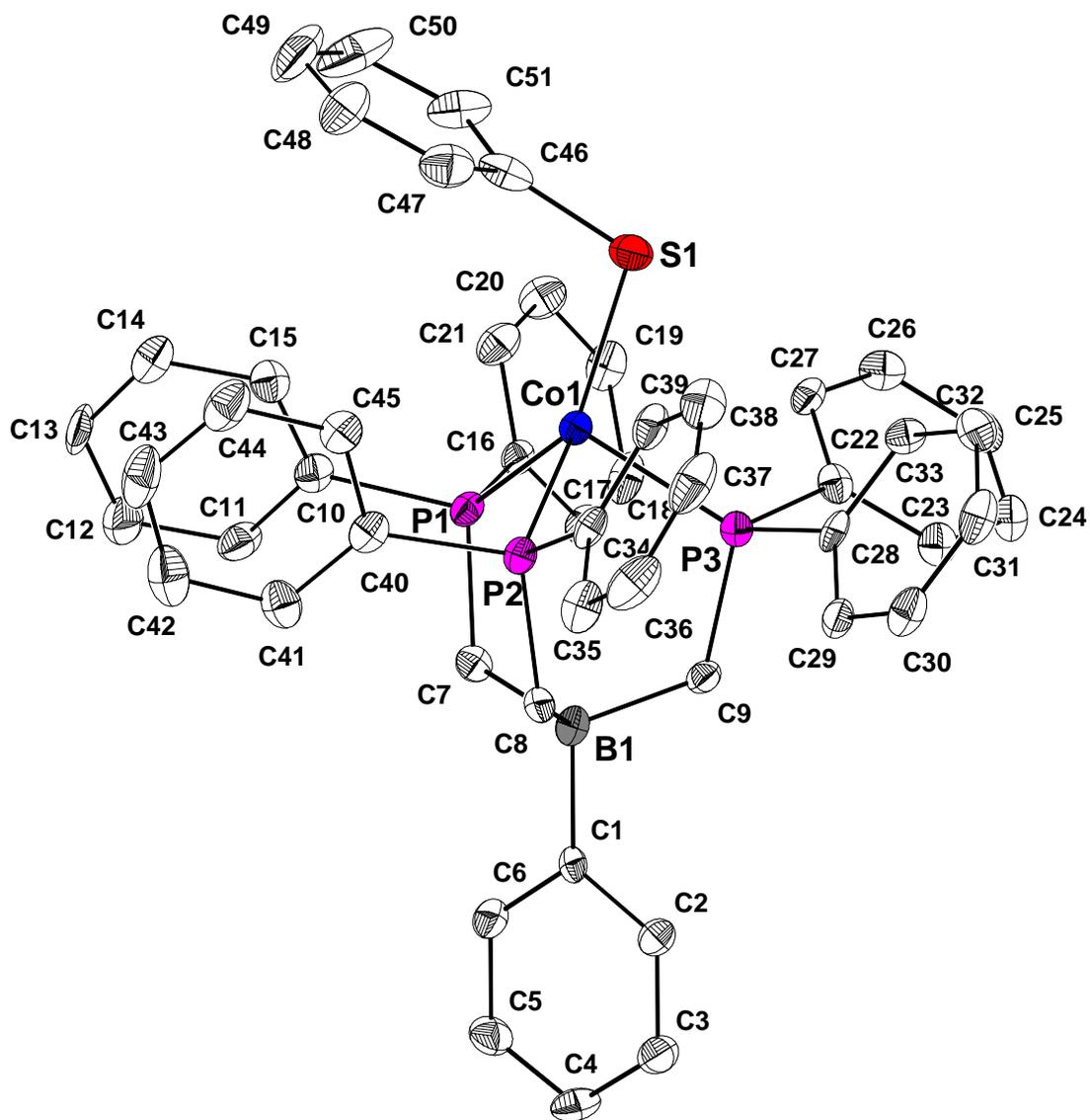
## Crystal Structure Report for

### DMJ 25, $[\text{PhBP}_3]\text{CoSPh}$

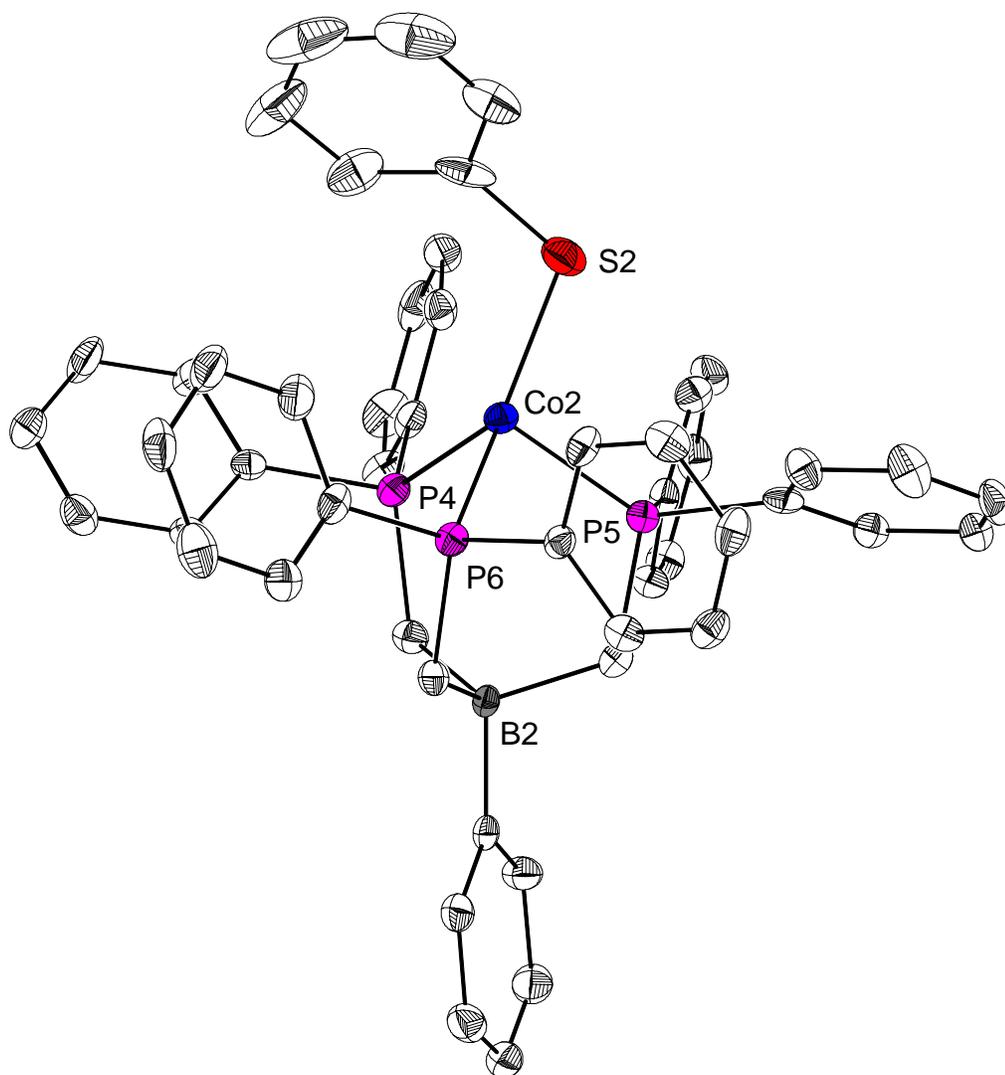


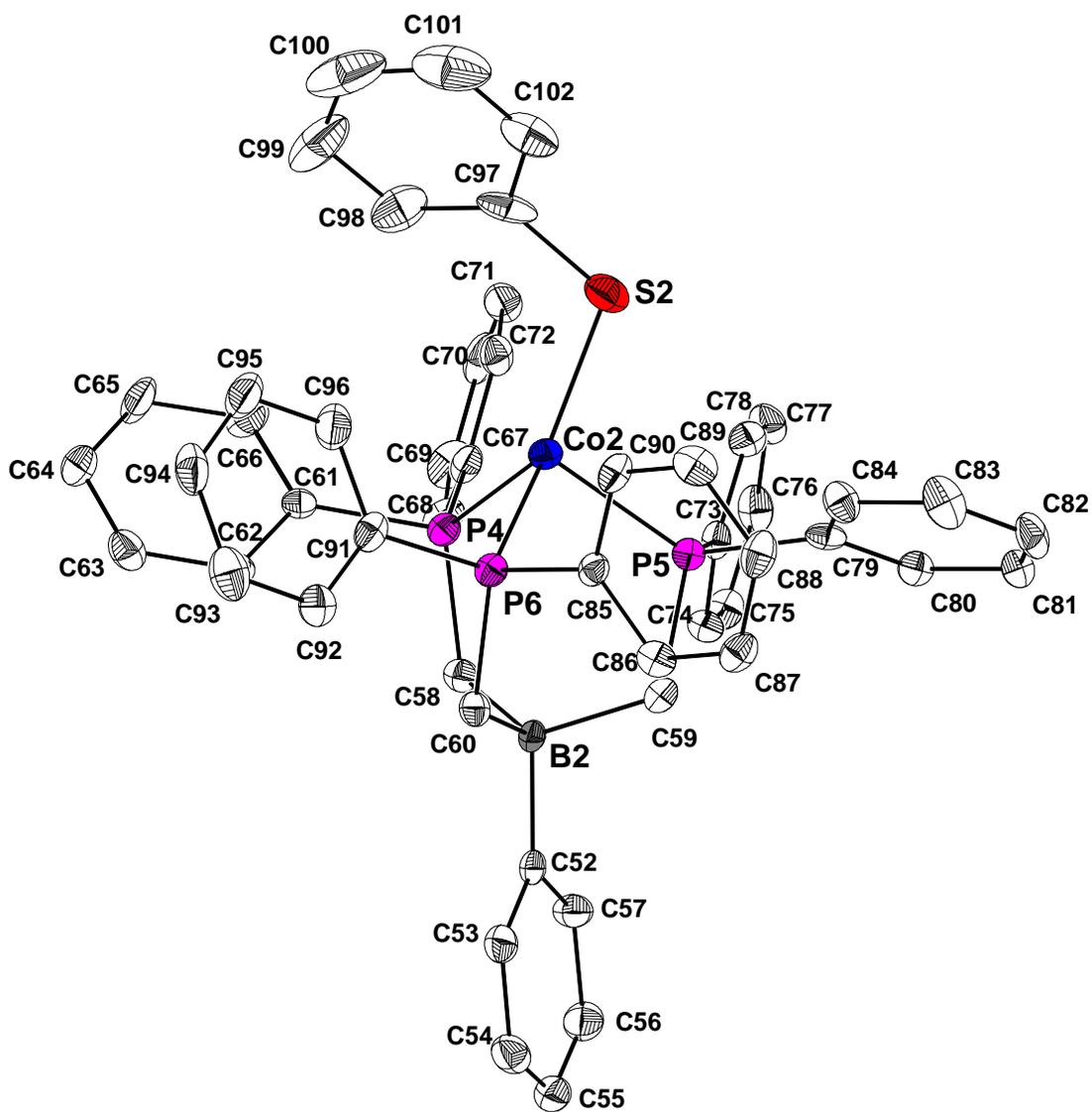
**Molecule 1:**





**Molecule 2:**





**Table 1. Crystal Data and Structure Analysis Details for dmj25, [PhBP<sub>3</sub>]CoSPh**

Empirical formula	C <sub>51</sub> H <sub>41</sub> BCoP <sub>3</sub> S
Formula weight	853.59
Crystallization solvent	benzene/petroleum ether
Crystal shape	rough block
Crystal color	dark red
Crystal size	0.15 x 0.23 x 0.26 mm

### Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoK $\alpha$	
Data collection temperature	96 K	
Theta range for 5384 reflections used in lattice determination	2.3 to 25.1°	
Unit cell dimensions	a = 16.8066(16) Å b = 14.0767(13) Å c = 19.2736(18) Å	$\alpha = 90^\circ$ $\beta = 113.801(2)^\circ$ $\gamma = 90^\circ$
Volume	4172.0(7) Å <sup>3</sup>	
Z	4	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> (# 4)	
Density (calculated)	1.359 g/cm <sup>3</sup>	
F(000)	1780	
Theta range for data collection	1.4 to 28.6°	
Completeness to theta = 28.56°	92.9%	
Index ranges	-22 ≤ h ≤ 22, -18 ≤ k ≤ 18, -25 ≤ l ≤ 25	
Reflections collected	62204	
Independent reflections	19183 [R <sub>int</sub> = 0.0832]	
Reflections > 2 $\sigma$ (I)	12994	
Average $\sigma$ (I)/(net I)	0.1139	
Absorption coefficient	0.61 mm <sup>-1</sup>	
Reflections monitored for decay	75	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	19183 / 1 / 1027
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	1.04
Final R indices [I>2σ(I), 12994 reflections]	R1 = 0.0463, wR2 = 0.0661
R indices (all data)	R1 = 0.0857, wR2 = 0.0722
Type of weighting scheme used	σ
Weighting scheme used	1/σ <sup>2</sup> (Fo <sup>2</sup> )
Max shift/error	0.080
Average shift/error	0.001
Absolute structure parameter	-0.004(9) (not in full matrix)
Largest diff. peak and hole	0.82 and -0.57 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART and SAINT
Data collection	SMART v5.054
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

## Special Refinement Details

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj25.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co(1)	2202(1)	4969(1)	-480(1)	16(1)
P(1)	2528(1)	3864(1)	380(1)	17(1)
P(2)	2462(1)	6038(1)	401(1)	16(1)
P(3)	3541(1)	5170(1)	-455(1)	16(1)
S(1)	1419(1)	4664(1)	-1655(1)	24(1)
B(1)	4079(2)	5030(3)	1219(2)	18(1)
C(1)	4967(2)	5040(2)	2004(2)	14(1)
C(2)	5645(2)	5673(2)	2114(2)	19(1)
C(3)	6399(2)	5686(3)	2774(2)	23(1)
C(4)	6507(2)	5076(3)	3354(2)	27(1)
C(5)	5852(2)	4436(3)	3268(2)	25(1)
C(6)	5103(2)	4424(3)	2607(2)	22(1)
C(7)	3481(2)	4109(2)	1226(2)	17(1)
C(8)	3517(2)	6010(2)	1184(2)	18(1)
C(9)	4378(2)	5017(3)	498(2)	17(1)
C(10)	1702(2)	3456(2)	704(2)	19(1)
C(11)	1948(2)	2915(3)	1358(2)	25(1)
C(12)	1348(2)	2649(3)	1640(2)	32(1)
C(13)	489(2)	2914(3)	1262(2)	29(1)
C(14)	230(2)	3433(3)	603(2)	28(1)
C(15)	838(2)	3707(3)	324(2)	22(1)
C(16)	2733(2)	2796(2)	-53(2)	17(1)
C(17)	3565(2)	2452(2)	113(2)	20(1)
C(18)	3684(2)	1671(3)	-269(2)	24(1)
C(19)	2992(2)	1238(3)	-830(2)	24(1)
C(20)	2159(2)	1588(3)	-1011(2)	28(1)
C(21)	2039(2)	2349(3)	-620(2)	24(1)
C(22)	3922(2)	4407(3)	-1022(2)	18(1)
C(23)	4738(2)	4566(3)	-1029(2)	22(1)
C(24)	5076(2)	3967(3)	-1405(2)	24(1)
C(25)	4603(2)	3185(3)	-1784(2)	22(1)
C(26)	3799(2)	3021(3)	-1786(2)	24(1)
C(27)	3454(2)	3621(3)	-1406(2)	20(1)
C(28)	3682(2)	6332(2)	-806(2)	17(1)
C(29)	4037(2)	7110(3)	-346(2)	20(1)
C(30)	4072(2)	7983(3)	-644(2)	26(1)
C(31)	3756(2)	8112(3)	-1422(2)	26(1)
C(32)	3404(2)	7344(3)	-1891(2)	24(1)
C(33)	3364(2)	6462(3)	-1591(2)	20(1)
C(34)	2279(2)	7220(2)	-29(2)	18(1)
C(35)	2520(2)	8022(3)	425(2)	26(1)
C(36)	2357(2)	8918(3)	88(3)	35(1)
C(37)	1969(2)	9007(3)	-678(3)	37(1)
C(38)	1730(2)	8217(3)	-1140(2)	31(1)
C(39)	1883(2)	7322(3)	-808(2)	24(1)
C(40)	1626(2)	5984(2)	780(2)	20(1)

C(41)	1779(3)	5639(3)	1494(2)	25(1)
C(42)	1100(3)	5549(3)	1716(3)	36(1)
C(43)	265(3)	5809(3)	1237(3)	38(1)
C(44)	104(3)	6167(3)	534(3)	34(1)
C(45)	779(2)	6263(2)	298(2)	22(1)
C(46)	391(2)	4421(3)	-1680(2)	27(1)
C(47)	-117(2)	5111(3)	-1536(2)	34(1)
C(48)	-902(2)	4906(4)	-1512(2)	43(1)
C(49)	-1215(3)	3992(4)	-1636(3)	53(1)
C(50)	-757(3)	3294(3)	-1814(3)	51(1)
C(51)	29(3)	3507(3)	-1852(2)	37(1)
Co(2)	2044(1)	4502(1)	4571(1)	17(1)
P(4)	2733(1)	3414(1)	5393(1)	17(1)
P(5)	3312(1)	4926(1)	4494(1)	16(1)
P(6)	2160(1)	5504(1)	5478(1)	17(1)
S(2)	1083(1)	4480(1)	3426(1)	29(1)
B(2)	3971(2)	4950(3)	6175(2)	15(1)
C(52)	4898(2)	5164(2)	6890(2)	18(1)
C(53)	4999(2)	5818(2)	7469(2)	21(1)
C(54)	5806(2)	6026(3)	8028(2)	26(1)
C(55)	6549(2)	5609(3)	8042(2)	27(1)
C(56)	6473(2)	4969(3)	7489(2)	27(1)
C(57)	5666(2)	4749(2)	6931(2)	23(1)
C(58)	3774(2)	3784(2)	6121(2)	18(1)
C(59)	4053(2)	5373(2)	5397(2)	16(1)
C(60)	3181(2)	5501(2)	6303(2)	18(1)
C(61)	2095(2)	2903(2)	5877(2)	17(1)
C(62)	2076(2)	3327(3)	6524(2)	21(1)
C(63)	1598(2)	2950(3)	6893(2)	24(1)
C(64)	1131(2)	2136(3)	6619(2)	26(1)
C(65)	1141(2)	1694(3)	5985(2)	31(1)
C(66)	1604(2)	2081(3)	5610(2)	28(1)
C(67)	2889(2)	2363(3)	4900(2)	21(1)
C(68)	3545(2)	1715(3)	5265(2)	24(1)
C(69)	3613(2)	882(3)	4920(2)	29(1)
C(70)	3027(3)	679(3)	4204(2)	29(1)
C(71)	2361(3)	1300(3)	3826(2)	27(1)
C(72)	2292(2)	2142(3)	4169(2)	21(1)
C(73)	3867(2)	3939(2)	4260(2)	17(1)
C(74)	4678(2)	3600(2)	4762(2)	20(1)
C(75)	5051(2)	2835(2)	4557(2)	21(1)
C(76)	4634(2)	2411(3)	3863(2)	25(1)
C(77)	3837(2)	2746(3)	3358(2)	24(1)
C(78)	3452(2)	3499(2)	3559(2)	20(1)
C(79)	3360(2)	5820(2)	3821(2)	18(1)
C(80)	4046(2)	5832(2)	3597(2)	19(1)
C(81)	4147(2)	6577(3)	3171(2)	25(1)
C(82)	3555(3)	7318(3)	2954(2)	27(1)
C(83)	2871(3)	7305(3)	3164(2)	31(1)
C(84)	2765(2)	6562(3)	3591(2)	23(1)
C(85)	2020(2)	6688(2)	5059(2)	16(1)
C(86)	2657(2)	7391(2)	5291(2)	20(1)
C(87)	2539(2)	8254(3)	4920(2)	23(1)
C(88)	1764(2)	8439(3)	4307(2)	26(1)

C(89)	1115(2)	7762(3)	4085(2)	25(1)
C(90)	1249(2)	6895(3)	4450(2)	22(1)
C(91)	1281(2)	5486(2)	5804(2)	20(1)
C(92)	1349(2)	5955(3)	6457(2)	25(1)
C(93)	665(3)	5962(3)	6674(2)	33(1)
C(94)	-96(2)	5494(3)	6257(2)	32(1)
C(95)	-173(2)	5019(3)	5608(2)	36(1)
C(96)	512(2)	5017(3)	5382(2)	30(1)
C(97)	67(3)	4199(3)	3397(2)	32(1)
C(98)	-73(3)	3497(3)	3856(2)	39(1)
C(99)	-892(3)	3327(3)	3852(3)	53(2)
C(100)	-1594(3)	3857(4)	3374(3)	61(2)
C(101)	-1488(3)	4533(4)	2899(3)	59(2)
C(102)	-669(3)	4704(3)	2921(2)	39(1)

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**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj25.**

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Co(1)-S(1)	2.153(1)
Co(1)-P(1)	2.175(1)
Co(1)-P(2)	2.178(1)
Co(1)-P(3)	2.249(1)
Co(2)-S(2)	2.146(1)
Co(2)-P(4)	2.172(1)
Co(2)-P(6)	2.194(1)
Co(2)-P(5)	2.275(1)
S(1)-Co(1)-P(1)	121.14(4)
S(1)-Co(1)-P(2)	143.46(4)
P(1)-Co(1)-P(2)	89.44(4)
S(1)-Co(1)-P(3)	103.24(4)
P(1)-Co(1)-P(3)	97.52(4)
P(2)-Co(1)-P(3)	90.70(4)
C(46)-S(1)-Co(1)	104.3(1)
S(2)-Co(2)-P(4)	134.33(5)
S(2)-Co(2)-P(6)	128.09(4)
P(4)-Co(2)-P(6)	91.26(4)
S(2)-Co(2)-P(5)	105.85(4)
P(4)-Co(2)-P(5)	89.73(4)
P(6)-Co(2)-P(5)	95.72(4)
C(97)-S(2)-Co(2)	111.1(1)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj25.**

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Co(1)-S(1)	2.1532(10)
Co(1)-P(1)	2.1754(11)
Co(1)-P(2)	2.1776(11)
Co(1)-P(3)	2.2490(10)
P(1)-C(7)	1.799(3)
P(1)-C(16)	1.818(4)
P(1)-C(10)	1.830(4)
P(2)-C(8)	1.807(3)
P(2)-C(40)	1.827(4)
P(2)-C(34)	1.828(4)
P(3)-C(28)	1.821(4)
P(3)-C(9)	1.821(3)
P(3)-C(22)	1.824(4)
S(1)-C(46)	1.742(4)
B(1)-C(1)	1.642(5)
B(1)-C(7)	1.643(5)
B(1)-C(8)	1.657(5)
B(1)-C(9)	1.658(5)
C(1)-C(6)	1.392(4)
C(1)-C(2)	1.393(4)
C(2)-C(3)	1.387(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.362(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.380(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.384(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(15)	1.382(5)
C(10)-C(11)	1.386(5)
C(11)-C(12)	1.375(5)
C(11)-H(11)	0.9500
C(12)-C(13)	1.381(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.375(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.387(5)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.387(5)
C(16)-C(17)	1.389(4)
C(17)-C(18)	1.383(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.370(5)

C(18)-H(18)	0.9500
C(19)-C(20)	1.389(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.371(5)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(27)	1.386(5)
C(22)-C(23)	1.394(4)
C(23)-C(24)	1.376(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.382(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.368(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.388(5)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.385(5)
C(28)-C(33)	1.398(5)
C(29)-C(30)	1.367(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.386(5)
C(30)-H(30)	0.9500
C(31)-C(32)	1.380(5)
C(31)-H(31)	0.9500
C(32)-C(33)	1.383(5)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.384(5)
C(34)-C(35)	1.384(5)
C(35)-C(36)	1.395(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.357(5)
C(36)-H(36)	0.9500
C(37)-C(38)	1.380(5)
C(37)-H(37)	0.9500
C(38)-C(39)	1.389(5)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(41)	1.381(5)
C(40)-C(45)	1.407(5)
C(41)-C(42)	1.377(5)
C(41)-H(41)	0.9500
C(42)-C(43)	1.382(5)
C(42)-H(42)	0.9500
C(43)-C(44)	1.366(6)
C(43)-H(43)	0.9500
C(44)-C(45)	1.388(5)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(47)	1.393(5)
C(46)-C(51)	1.404(5)
C(47)-C(48)	1.369(5)
C(47)-H(47)	0.9500

C(48)-C(49)	1.375(6)
C(48)-H(48)	0.9500
C(49)-C(50)	1.374(6)
C(49)-H(49)	0.9500
C(50)-C(51)	1.386(6)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
Co(2)-S(2)	2.1459(11)
Co(2)-P(4)	2.1721(11)
Co(2)-P(6)	2.1942(11)
Co(2)-P(5)	2.2748(10)
P(4)-C(58)	1.822(3)
P(4)-C(61)	1.829(4)
P(4)-C(67)	1.833(4)
P(5)-C(59)	1.796(3)
P(5)-C(73)	1.828(3)
P(5)-C(79)	1.832(4)
P(6)-C(60)	1.808(3)
P(6)-C(91)	1.823(4)
P(6)-C(85)	1.825(4)
S(2)-C(97)	1.732(4)
B(2)-C(52)	1.639(5)
B(2)-C(60)	1.640(5)
B(2)-C(58)	1.669(5)
B(2)-C(59)	1.671(5)
C(52)-C(57)	1.389(4)
C(52)-C(53)	1.403(4)
C(53)-C(54)	1.381(5)
C(53)-H(53)	0.9500
C(54)-C(55)	1.369(5)
C(54)-H(54)	0.9500
C(55)-C(56)	1.362(5)
C(55)-H(55)	0.9500
C(56)-C(57)	1.385(4)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(61)-C(66)	1.393(5)
C(61)-C(62)	1.395(5)
C(62)-C(63)	1.376(5)
C(62)-H(62)	0.9500
C(63)-C(64)	1.368(5)
C(63)-H(63)	0.9500
C(64)-C(65)	1.377(5)
C(64)-H(64)	0.9500
C(65)-C(66)	1.371(5)
C(65)-H(65)	0.9500
C(66)-H(66)	0.9500
C(67)-C(68)	1.385(5)

C(67)-C(72)	1.396(5)
C(68)-C(69)	1.375(5)
C(68)-H(68)	0.9500
C(69)-C(70)	1.363(5)
C(69)-H(69)	0.9500
C(70)-C(71)	1.375(5)
C(70)-H(70)	0.9500
C(71)-C(72)	1.385(5)
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
C(73)-C(78)	1.390(5)
C(73)-C(74)	1.399(4)
C(74)-C(75)	1.382(4)
C(74)-H(74)	0.9500
C(75)-C(76)	1.371(5)
C(75)-H(75)	0.9500
C(76)-C(77)	1.384(5)
C(76)-H(76)	0.9500
C(77)-C(78)	1.377(5)
C(77)-H(77)	0.9500
C(78)-H(78)	0.9500
C(79)-C(80)	1.384(5)
C(79)-C(84)	1.389(5)
C(80)-C(81)	1.384(5)
C(80)-H(80)	0.9500
C(81)-C(82)	1.384(5)
C(81)-H(81)	0.9500
C(82)-C(83)	1.365(5)
C(82)-H(82)	0.9500
C(83)-C(84)	1.385(5)
C(83)-H(83)	0.9500
C(84)-H(84)	0.9500
C(85)-C(90)	1.384(4)
C(85)-C(86)	1.392(4)
C(86)-C(87)	1.383(5)
C(86)-H(86)	0.9500
C(87)-C(88)	1.386(5)
C(87)-H(87)	0.9500
C(88)-C(89)	1.379(5)
C(88)-H(88)	0.9500
C(89)-C(90)	1.382(5)
C(89)-H(89)	0.9500
C(90)-H(90)	0.9500
C(91)-C(92)	1.384(5)
C(91)-C(96)	1.385(5)
C(92)-C(93)	1.375(5)
C(92)-H(92)	0.9500
C(93)-C(94)	1.373(5)
C(93)-H(93)	0.9500
C(94)-C(95)	1.379(5)
C(94)-H(94)	0.9500
C(95)-C(96)	1.386(5)
C(95)-H(95)	0.9500
C(96)-H(96)	0.9500

C(97)-C(102)	1.400(5)
C(97)-C(98)	1.408(5)
C(98)-C(99)	1.394(5)
C(98)-H(98)	0.9500
C(99)-C(100)	1.386(6)
C(99)-H(99)	0.9500
C(100)-C(101)	1.380(7)
C(100)-H(100)	0.9500
C(101)-C(102)	1.381(6)
C(101)-H(101)	0.9500
C(102)-H(102)	0.9500

S(1)-Co(1)-P(1)	121.14(4)
S(1)-Co(1)-P(2)	143.46(4)
P(1)-Co(1)-P(2)	89.44(4)
S(1)-Co(1)-P(3)	103.24(4)
P(1)-Co(1)-P(3)	97.52(4)
P(2)-Co(1)-P(3)	90.70(4)
C(7)-P(1)-C(16)	108.03(16)
C(7)-P(1)-C(10)	105.72(17)
C(16)-P(1)-C(10)	101.96(16)
C(7)-P(1)-Co(1)	114.36(12)
C(16)-P(1)-Co(1)	106.16(12)
C(10)-P(1)-Co(1)	119.46(13)
C(8)-P(2)-C(40)	108.61(17)
C(8)-P(2)-C(34)	109.10(16)
C(40)-P(2)-C(34)	101.76(16)
C(8)-P(2)-Co(1)	117.16(12)
C(40)-P(2)-Co(1)	109.76(12)
C(34)-P(2)-Co(1)	109.34(13)
C(28)-P(3)-C(9)	108.50(17)
C(28)-P(3)-C(22)	100.13(16)
C(9)-P(3)-C(22)	102.67(15)
C(28)-P(3)-Co(1)	112.60(11)
C(9)-P(3)-Co(1)	111.50(10)
C(22)-P(3)-Co(1)	120.25(12)
C(46)-S(1)-Co(1)	104.29(12)
C(1)-B(1)-C(7)	109.3(3)
C(1)-B(1)-C(8)	108.8(3)
C(7)-B(1)-C(8)	108.5(2)
C(1)-B(1)-C(9)	107.5(2)
C(7)-B(1)-C(9)	113.1(3)
C(8)-B(1)-C(9)	109.6(3)
C(6)-C(1)-C(2)	115.0(3)
C(6)-C(1)-B(1)	123.0(3)
C(2)-C(1)-B(1)	122.0(3)
C(3)-C(2)-C(1)	122.5(3)
C(3)-C(2)-H(2)	118.8
C(1)-C(2)-H(2)	118.8
C(4)-C(3)-C(2)	120.9(3)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	118.6(3)
C(3)-C(4)-H(4)	120.7

C(5)-C(4)-H(4)	120.7
C(4)-C(5)-C(6)	120.2(4)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	122.9(3)
C(5)-C(6)-H(6)	118.5
C(1)-C(6)-H(6)	118.5
B(1)-C(7)-P(1)	117.8(2)
B(1)-C(7)-H(7A)	107.8
P(1)-C(7)-H(7A)	107.8
B(1)-C(7)-H(7B)	107.8
P(1)-C(7)-H(7B)	107.8
H(7A)-C(7)-H(7B)	107.2
B(1)-C(8)-P(2)	113.8(2)
B(1)-C(8)-H(8A)	108.8
P(2)-C(8)-H(8A)	108.8
B(1)-C(8)-H(8B)	108.8
P(2)-C(8)-H(8B)	108.8
H(8A)-C(8)-H(8B)	107.7
B(1)-C(9)-P(3)	118.1(2)
B(1)-C(9)-H(9A)	107.8
P(3)-C(9)-H(9A)	107.8
B(1)-C(9)-H(9B)	107.8
P(3)-C(9)-H(9B)	107.8
H(9A)-C(9)-H(9B)	107.1
C(15)-C(10)-C(11)	119.0(3)
C(15)-C(10)-P(1)	121.3(3)
C(11)-C(10)-P(1)	119.7(3)
C(12)-C(11)-C(10)	120.8(3)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	119.7(4)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(14)-C(13)-C(12)	120.3(3)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-C(15)	119.8(4)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(10)-C(15)-C(14)	120.3(4)
C(10)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8
C(21)-C(16)-C(17)	118.1(3)
C(21)-C(16)-P(1)	118.8(3)
C(17)-C(16)-P(1)	122.8(3)
C(18)-C(17)-C(16)	120.2(3)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(19)-C(18)-C(17)	120.9(3)
C(19)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(18)-C(19)-C(20)	119.3(4)
C(18)-C(19)-H(19)	120.4

C(20)-C(19)-H(19)	120.4
C(21)-C(20)-C(19)	119.8(4)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(16)	121.6(3)
C(20)-C(21)-H(21)	119.2
C(16)-C(21)-H(21)	119.2
C(27)-C(22)-C(23)	118.2(3)
C(27)-C(22)-P(3)	122.0(3)
C(23)-C(22)-P(3)	119.7(3)
C(24)-C(23)-C(22)	121.5(3)
C(24)-C(23)-H(23)	119.2
C(22)-C(23)-H(23)	119.2
C(23)-C(24)-C(25)	119.6(3)
C(23)-C(24)-H(24)	120.2
C(25)-C(24)-H(24)	120.2
C(26)-C(25)-C(24)	119.6(3)
C(26)-C(25)-H(25)	120.2
C(24)-C(25)-H(25)	120.2
C(25)-C(26)-C(27)	121.2(4)
C(25)-C(26)-H(26)	119.4
C(27)-C(26)-H(26)	119.4
C(22)-C(27)-C(26)	120.0(3)
C(22)-C(27)-H(27)	120.0
C(26)-C(27)-H(27)	120.0
C(29)-C(28)-C(33)	117.8(3)
C(29)-C(28)-P(3)	124.0(3)
C(33)-C(28)-P(3)	118.0(3)
C(30)-C(29)-C(28)	121.5(4)
C(30)-C(29)-H(29)	119.3
C(28)-C(29)-H(29)	119.3
C(29)-C(30)-C(31)	120.7(4)
C(29)-C(30)-H(30)	119.6
C(31)-C(30)-H(30)	119.6
C(32)-C(31)-C(30)	118.7(4)
C(32)-C(31)-H(31)	120.6
C(30)-C(31)-H(31)	120.6
C(31)-C(32)-C(33)	120.7(4)
C(31)-C(32)-H(32)	119.6
C(33)-C(32)-H(32)	119.6
C(32)-C(33)-C(28)	120.5(3)
C(32)-C(33)-H(33)	119.7
C(28)-C(33)-H(33)	119.7
C(39)-C(34)-C(35)	119.4(4)
C(39)-C(34)-P(2)	120.4(3)
C(35)-C(34)-P(2)	120.2(3)
C(34)-C(35)-C(36)	119.4(4)
C(34)-C(35)-H(35)	120.3
C(36)-C(35)-H(35)	120.3
C(37)-C(36)-C(35)	120.5(4)
C(37)-C(36)-H(36)	119.7
C(35)-C(36)-H(36)	119.7
C(36)-C(37)-C(38)	121.0(4)
C(36)-C(37)-H(37)	119.5

C(38)-C(37)-H(37)	119.5
C(37)-C(38)-C(39)	118.8(4)
C(37)-C(38)-H(38)	120.6
C(39)-C(38)-H(38)	120.6
C(34)-C(39)-C(38)	120.9(4)
C(34)-C(39)-H(39)	119.6
C(38)-C(39)-H(39)	119.6
C(41)-C(40)-C(45)	119.2(3)
C(41)-C(40)-P(2)	123.3(3)
C(45)-C(40)-P(2)	117.4(3)
C(42)-C(41)-C(40)	119.8(4)
C(42)-C(41)-H(41)	120.1
C(40)-C(41)-H(41)	120.1
C(41)-C(42)-C(43)	120.9(4)
C(41)-C(42)-H(42)	119.5
C(43)-C(42)-H(42)	119.5
C(44)-C(43)-C(42)	120.1(4)
C(44)-C(43)-H(43)	120.0
C(42)-C(43)-H(43)	120.0
C(43)-C(44)-C(45)	120.0(4)
C(43)-C(44)-H(44)	120.0
C(45)-C(44)-H(44)	120.0
C(44)-C(45)-C(40)	119.9(4)
C(44)-C(45)-H(45)	120.0
C(40)-C(45)-H(45)	120.0
C(47)-C(46)-C(51)	116.3(4)
C(47)-C(46)-S(1)	122.6(3)
C(51)-C(46)-S(1)	121.1(3)
C(48)-C(47)-C(46)	122.4(4)
C(48)-C(47)-H(47)	118.8
C(46)-C(47)-H(47)	118.8
C(47)-C(48)-C(49)	119.9(4)
C(47)-C(48)-H(48)	120.1
C(49)-C(48)-H(48)	120.1
C(50)-C(49)-C(48)	119.9(4)
C(50)-C(49)-H(49)	120.0
C(48)-C(49)-H(49)	120.0
C(49)-C(50)-C(51)	120.0(4)
C(49)-C(50)-H(50)	120.0
C(51)-C(50)-H(50)	120.0
C(50)-C(51)-C(46)	121.2(4)
C(50)-C(51)-H(51)	119.4
C(46)-C(51)-H(51)	119.4
S(2)-Co(2)-P(4)	134.33(5)
S(2)-Co(2)-P(6)	128.09(4)
P(4)-Co(2)-P(6)	91.26(4)
S(2)-Co(2)-P(5)	105.85(4)
P(4)-Co(2)-P(5)	89.73(4)
P(6)-Co(2)-P(5)	95.72(4)
C(58)-P(4)-C(61)	107.38(16)
C(58)-P(4)-C(67)	109.66(16)
C(61)-P(4)-C(67)	100.53(16)
C(58)-P(4)-Co(2)	115.06(12)
C(61)-P(4)-Co(2)	113.57(11)

C(67)-P(4)-Co(2)	109.64(13)
C(59)-P(5)-C(73)	106.40(16)
C(59)-P(5)-C(79)	103.52(15)
C(73)-P(5)-C(79)	100.10(15)
C(59)-P(5)-Co(2)	109.27(11)
C(73)-P(5)-Co(2)	113.61(11)
C(79)-P(5)-Co(2)	122.44(11)
C(60)-P(6)-C(91)	108.11(17)
C(60)-P(6)-C(85)	107.37(16)
C(91)-P(6)-C(85)	100.83(15)
C(60)-P(6)-Co(2)	116.48(12)
C(91)-P(6)-Co(2)	116.24(13)
C(85)-P(6)-Co(2)	106.26(12)
C(97)-S(2)-Co(2)	111.07(14)
C(52)-B(2)-C(60)	109.9(3)
C(52)-B(2)-C(58)	109.3(3)
C(60)-B(2)-C(58)	108.8(3)
C(52)-B(2)-C(59)	107.1(3)
C(60)-B(2)-C(59)	109.3(3)
C(58)-B(2)-C(59)	112.4(3)
C(57)-C(52)-C(53)	114.8(3)
C(57)-C(52)-B(2)	121.1(3)
C(53)-C(52)-B(2)	123.9(3)
C(54)-C(53)-C(52)	121.6(3)
C(54)-C(53)-H(53)	119.2
C(52)-C(53)-H(53)	119.2
C(55)-C(54)-C(53)	121.7(4)
C(55)-C(54)-H(54)	119.1
C(53)-C(54)-H(54)	119.1
C(56)-C(55)-C(54)	118.1(4)
C(56)-C(55)-H(55)	120.9
C(54)-C(55)-H(55)	120.9
C(55)-C(56)-C(57)	120.6(3)
C(55)-C(56)-H(56)	119.7
C(57)-C(56)-H(56)	119.7
C(56)-C(57)-C(52)	123.1(3)
C(56)-C(57)-H(57)	118.4
C(52)-C(57)-H(57)	118.4
B(2)-C(58)-P(4)	115.7(2)
B(2)-C(58)-H(58A)	108.3
P(4)-C(58)-H(58A)	108.3
B(2)-C(58)-H(58B)	108.3
P(4)-C(58)-H(58B)	108.3
H(58A)-C(58)-H(58B)	107.4
B(2)-C(59)-P(5)	118.0(2)
B(2)-C(59)-H(59A)	107.8
P(5)-C(59)-H(59A)	107.8
B(2)-C(59)-H(59B)	107.8
P(5)-C(59)-H(59B)	107.8
H(59A)-C(59)-H(59B)	107.2
B(2)-C(60)-P(6)	114.1(2)
B(2)-C(60)-H(60A)	108.7
P(6)-C(60)-H(60A)	108.7
B(2)-C(60)-H(60B)	108.7

P(6)-C(60)-H(60B)	108.7
H(60A)-C(60)-H(60B)	107.6
C(66)-C(61)-C(62)	117.5(3)
C(66)-C(61)-P(4)	121.4(3)
C(62)-C(61)-P(4)	121.1(3)
C(63)-C(62)-C(61)	121.7(3)
C(63)-C(62)-H(62)	119.1
C(61)-C(62)-H(62)	119.1
C(64)-C(63)-C(62)	119.2(4)
C(64)-C(63)-H(63)	120.4
C(62)-C(63)-H(63)	120.4
C(63)-C(64)-C(65)	120.7(3)
C(63)-C(64)-H(64)	119.6
C(65)-C(64)-H(64)	119.6
C(66)-C(65)-C(64)	120.0(4)
C(66)-C(65)-H(65)	120.0
C(64)-C(65)-H(65)	120.0
C(65)-C(66)-C(61)	120.9(4)
C(65)-C(66)-H(66)	119.5
C(61)-C(66)-H(66)	119.5
C(68)-C(67)-C(72)	117.8(3)
C(68)-C(67)-P(4)	121.3(3)
C(72)-C(67)-P(4)	120.6(3)
C(69)-C(68)-C(67)	121.4(4)
C(69)-C(68)-H(68)	119.3
C(67)-C(68)-H(68)	119.3
C(70)-C(69)-C(68)	120.1(4)
C(70)-C(69)-H(69)	120.0
C(68)-C(69)-H(69)	120.0
C(69)-C(70)-C(71)	120.3(4)
C(69)-C(70)-H(70)	119.9
C(71)-C(70)-H(70)	119.9
C(70)-C(71)-C(72)	119.9(4)
C(70)-C(71)-H(71)	120.0
C(72)-C(71)-H(71)	120.0
C(71)-C(72)-C(67)	120.5(3)
C(71)-C(72)-H(72)	119.7
C(67)-C(72)-H(72)	119.7
C(78)-C(73)-C(74)	119.1(3)
C(78)-C(73)-P(5)	118.2(3)
C(74)-C(73)-P(5)	122.7(3)
C(75)-C(74)-C(73)	119.7(3)
C(75)-C(74)-H(74)	120.1
C(73)-C(74)-H(74)	120.1
C(76)-C(75)-C(74)	120.4(3)
C(76)-C(75)-H(75)	119.8
C(74)-C(75)-H(75)	119.8
C(75)-C(76)-C(77)	120.4(3)
C(75)-C(76)-H(76)	119.8
C(77)-C(76)-H(76)	119.8
C(78)-C(77)-C(76)	119.7(4)
C(78)-C(77)-H(77)	120.1
C(76)-C(77)-H(77)	120.1
C(77)-C(78)-C(73)	120.6(3)

C(77)-C(78)-H(78)	119.7
C(73)-C(78)-H(78)	119.7
C(80)-C(79)-C(84)	118.3(3)
C(80)-C(79)-P(5)	120.6(3)
C(84)-C(79)-P(5)	120.7(3)
C(81)-C(80)-C(79)	120.7(3)
C(81)-C(80)-H(80)	119.6
C(79)-C(80)-H(80)	119.6
C(80)-C(81)-C(82)	120.3(3)
C(80)-C(81)-H(81)	119.9
C(82)-C(81)-H(81)	119.9
C(83)-C(82)-C(81)	119.3(4)
C(83)-C(82)-H(82)	120.4
C(81)-C(82)-H(82)	120.4
C(82)-C(83)-C(84)	120.8(4)
C(82)-C(83)-H(83)	119.6
C(84)-C(83)-H(83)	119.6
C(83)-C(84)-C(79)	120.5(3)
C(83)-C(84)-H(84)	119.7
C(79)-C(84)-H(84)	119.7
C(90)-C(85)-C(86)	117.3(3)
C(90)-C(85)-P(6)	118.5(3)
C(86)-C(85)-P(6)	124.2(3)
C(87)-C(86)-C(85)	121.8(3)
C(87)-C(86)-H(86)	119.1
C(85)-C(86)-H(86)	119.1
C(86)-C(87)-C(88)	119.7(4)
C(86)-C(87)-H(87)	120.2
C(88)-C(87)-H(87)	120.2
C(89)-C(88)-C(87)	119.2(4)
C(89)-C(88)-H(88)	120.4
C(87)-C(88)-H(88)	120.4
C(88)-C(89)-C(90)	120.4(4)
C(88)-C(89)-H(89)	119.8
C(90)-C(89)-H(89)	119.8
C(89)-C(90)-C(85)	121.5(3)
C(89)-C(90)-H(90)	119.3
C(85)-C(90)-H(90)	119.2
C(92)-C(91)-C(96)	118.5(3)
C(92)-C(91)-P(6)	121.6(3)
C(96)-C(91)-P(6)	119.8(3)
C(93)-C(92)-C(91)	120.6(4)
C(93)-C(92)-H(92)	119.7
C(91)-C(92)-H(92)	119.7
C(94)-C(93)-C(92)	120.9(4)
C(94)-C(93)-H(93)	119.5
C(92)-C(93)-H(93)	119.5
C(93)-C(94)-C(95)	119.2(4)
C(93)-C(94)-H(94)	120.4
C(95)-C(94)-H(94)	120.4
C(94)-C(95)-C(96)	120.1(4)
C(94)-C(95)-H(95)	120.0
C(96)-C(95)-H(95)	120.0
C(91)-C(96)-C(95)	120.7(4)

C(91)-C(96)-H(96)	119.7
C(95)-C(96)-H(96)	119.7
C(102)-C(97)-C(98)	116.2(4)
C(102)-C(97)-S(2)	120.2(3)
C(98)-C(97)-S(2)	123.6(3)
C(99)-C(98)-C(97)	122.1(4)
C(99)-C(98)-H(98)	118.9
C(97)-C(98)-H(98)	118.9
C(100)-C(99)-C(98)	119.0(5)
C(100)-C(99)-H(99)	120.5
C(98)-C(99)-H(99)	120.5
C(101)-C(100)-C(99)	120.6(5)
C(101)-C(100)-H(100)	119.7
C(99)-C(100)-H(100)	119.7
C(100)-C(101)-C(102)	119.7(5)
C(100)-C(101)-H(101)	120.2
C(102)-C(101)-H(101)	120.2
C(101)-C(102)-C(97)	122.4(4)
C(101)-C(102)-H(102)	118.8
C(97)-C(102)-H(102)	118.8

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Symmetry transformations used to generate equivalent atoms:

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj25. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co(1)	151(2)	149(3)	177(3)	6(2)	69(2)	10(2)
P(1)	144(5)	161(6)	198(6)	10(5)	67(5)	-20(4)
P(2)	162(5)	147(6)	202(6)	-1(4)	91(5)	11(4)
P(3)	174(5)	146(6)	172(5)	-5(4)	84(4)	-3(4)
S(1)	232(5)	286(6)	188(5)	-21(4)	53(4)	6(4)
B(1)	190(20)	120(20)	230(20)	0(20)	107(18)	0(20)
C(1)	147(17)	143(19)	160(18)	2(18)	99(15)	43(17)
C(2)	158(19)	190(20)	220(20)	0(17)	76(18)	13(16)
C(3)	190(20)	250(20)	240(20)	4(18)	67(18)	-21(17)
C(4)	159(19)	310(20)	250(20)	10(20)	-12(16)	11(19)
C(5)	240(20)	300(20)	190(20)	63(19)	52(17)	50(19)
C(6)	171(19)	280(20)	240(20)	-15(19)	104(17)	-11(18)
C(7)	200(20)	140(20)	170(20)	32(16)	68(18)	19(16)
C(8)	190(20)	200(20)	150(20)	18(17)	81(18)	-24(17)
C(9)	125(17)	193(19)	187(19)	-17(19)	58(15)	-8(17)
C(10)	230(20)	120(20)	240(20)	-31(17)	98(18)	-51(17)
C(11)	170(20)	260(20)	280(20)	60(19)	38(19)	-14(18)
C(12)	300(20)	370(30)	320(30)	80(20)	140(20)	-60(20)
C(13)	270(20)	340(30)	380(30)	-30(20)	240(20)	-140(20)
C(14)	210(20)	270(20)	380(30)	-20(20)	150(20)	-20(19)
C(15)	250(20)	190(20)	230(20)	36(18)	104(19)	28(18)
C(16)	150(20)	160(20)	180(20)	70(17)	51(17)	-18(16)
C(17)	170(20)	170(20)	250(20)	40(17)	70(18)	6(16)
C(18)	210(20)	180(20)	390(30)	94(19)	180(20)	59(18)
C(19)	270(20)	150(20)	370(30)	-21(19)	180(20)	2(17)
C(20)	250(20)	250(20)	320(30)	-30(20)	90(20)	-36(19)
C(21)	170(20)	210(20)	330(30)	22(19)	80(20)	22(17)
C(22)	212(19)	150(20)	180(20)	58(17)	91(16)	48(17)
C(23)	250(20)	170(20)	260(20)	-1(18)	123(18)	-5(18)
C(24)	270(20)	240(20)	270(20)	4(19)	168(19)	-9(18)
C(25)	300(20)	180(20)	210(20)	11(17)	126(19)	82(18)
C(26)	260(20)	180(20)	240(20)	-8(18)	68(19)	5(18)
C(27)	130(20)	230(20)	230(20)	2(18)	82(18)	-5(17)
C(28)	88(18)	180(20)	290(20)	22(18)	117(18)	41(15)
C(29)	190(20)	220(20)	240(20)	-45(18)	129(18)	-56(17)
C(30)	250(20)	180(20)	400(30)	-92(19)	200(20)	-56(17)
C(31)	270(20)	130(20)	450(30)	40(20)	230(20)	10(17)
C(32)	280(20)	230(20)	230(20)	25(19)	118(19)	16(18)
C(33)	220(20)	140(20)	230(20)	-42(17)	74(19)	-50(16)
C(34)	132(19)	140(20)	300(20)	-3(18)	122(18)	18(16)
C(35)	270(20)	170(20)	410(30)	10(20)	200(20)	46(18)
C(36)	260(20)	200(20)	600(30)	-20(20)	170(20)	-19(19)
C(37)	230(20)	270(30)	650(40)	140(20)	220(20)	58(19)
C(38)	260(20)	310(30)	360(30)	170(20)	120(20)	109(19)
C(39)	180(20)	230(20)	330(30)	65(19)	140(20)	40(17)
C(40)	210(20)	110(20)	280(20)	-21(18)	106(19)	-16(17)

C(41)	340(20)	210(20)	260(20)	-26(19)	170(20)	17(19)
C(42)	520(30)	270(20)	410(30)	10(20)	310(30)	-20(20)
C(43)	390(30)	340(30)	570(30)	-100(20)	370(30)	-40(20)
C(44)	260(20)	320(30)	480(30)	-100(20)	210(20)	-30(20)
C(45)	220(20)	180(20)	280(30)	-4(18)	110(20)	43(17)
C(46)	370(20)	210(20)	150(20)	-13(19)	24(18)	50(20)
C(47)	350(20)	300(30)	310(30)	-40(20)	70(20)	-30(20)
C(48)	210(20)	600(30)	490(30)	0(30)	150(20)	40(30)
C(49)	170(20)	700(40)	660(40)	240(30)	120(20)	-50(30)
C(50)	240(30)	300(30)	720(40)	140(30)	-80(20)	-40(20)
C(51)	280(20)	340(30)	350(30)	-50(20)	-30(20)	0(20)
Co(2)	153(3)	172(3)	182(3)	0(2)	51(2)	0(2)
P(4)	175(5)	155(6)	190(6)	-5(5)	75(5)	-12(4)
P(5)	163(5)	145(5)	165(5)	0(5)	62(4)	11(5)
P(6)	153(5)	162(5)	190(6)	6(4)	73(4)	11(4)
S(2)	330(6)	280(6)	194(6)	25(5)	38(5)	8(5)
B(2)	155(19)	150(20)	160(20)	30(20)	69(17)	-20(20)
C(52)	203(19)	150(20)	170(20)	48(16)	78(16)	-34(16)
C(53)	240(20)	190(20)	210(20)	29(17)	94(18)	-17(17)
C(54)	360(20)	210(20)	200(20)	-14(18)	90(20)	-50(20)
C(55)	260(20)	290(20)	230(20)	43(19)	50(19)	-75(19)
C(56)	175(19)	340(20)	270(20)	70(20)	54(17)	10(20)
C(57)	190(19)	250(30)	200(20)	-20(17)	48(17)	-12(16)
C(58)	166(19)	210(20)	170(20)	-23(17)	75(17)	19(16)
C(59)	154(19)	130(20)	230(20)	-13(16)	96(17)	6(15)
C(60)	210(20)	130(20)	170(20)	50(16)	63(17)	2(16)
C(61)	132(19)	200(20)	160(20)	12(17)	31(17)	10(16)
C(62)	250(20)	170(20)	170(20)	-20(17)	51(18)	-44(17)
C(63)	320(20)	220(20)	190(20)	-9(18)	120(20)	13(19)
C(64)	190(20)	330(30)	300(20)	10(20)	139(19)	-25(18)
C(65)	300(20)	320(30)	410(30)	-60(20)	240(20)	-140(20)
C(66)	260(20)	320(20)	320(20)	-120(20)	160(20)	-101(19)
C(67)	220(20)	180(20)	260(20)	-21(18)	144(19)	-52(17)
C(68)	210(20)	200(20)	300(20)	-39(19)	95(19)	-44(18)
C(69)	290(20)	170(20)	440(30)	-10(20)	170(20)	44(18)
C(70)	420(30)	180(20)	410(30)	-80(20)	310(20)	-90(20)
C(71)	400(30)	190(20)	210(20)	-40(18)	120(20)	-92(19)
C(72)	270(20)	150(20)	220(20)	41(18)	114(19)	2(17)
C(73)	230(20)	120(20)	210(20)	-15(17)	143(18)	-3(16)
C(74)	190(20)	220(20)	160(20)	-3(17)	47(17)	-6(17)
C(75)	170(20)	190(20)	280(20)	43(18)	96(18)	61(17)
C(76)	350(20)	190(20)	280(20)	6(19)	210(20)	28(18)
C(77)	370(30)	180(20)	190(20)	-54(18)	140(20)	-30(19)
C(78)	200(20)	160(20)	230(20)	3(18)	77(18)	5(16)
C(79)	200(20)	130(20)	150(20)	-66(16)	19(17)	-11(16)
C(80)	200(20)	160(20)	190(20)	2(17)	69(18)	7(16)
C(81)	260(20)	330(30)	180(20)	-5(19)	111(19)	-53(19)
C(82)	450(30)	160(20)	210(20)	52(18)	150(20)	-19(19)
C(83)	420(30)	230(20)	300(30)	80(20)	180(20)	145(19)
C(84)	260(20)	250(20)	210(20)	18(18)	119(19)	49(18)
C(85)	160(20)	180(20)	180(20)	-25(17)	100(17)	-15(16)
C(86)	210(20)	190(20)	200(20)	-16(17)	77(18)	42(17)
C(87)	230(20)	170(20)	300(20)	-47(18)	140(20)	-29(17)
C(88)	280(20)	180(20)	360(30)	52(19)	190(20)	18(18)

C(89)	240(20)	230(20)	240(20)	20(18)	72(19)	94(18)
C(90)	180(20)	210(20)	290(20)	13(18)	127(19)	-16(17)
C(91)	163(19)	150(20)	280(20)	92(18)	83(18)	35(17)
C(92)	260(20)	250(20)	250(20)	7(19)	130(20)	5(19)
C(93)	400(30)	330(30)	330(30)	60(20)	230(20)	100(20)
C(94)	270(20)	440(30)	330(30)	160(20)	190(20)	90(20)
C(95)	210(20)	460(30)	400(30)	150(30)	101(19)	-70(20)
C(96)	330(20)	300(20)	310(20)	30(20)	176(19)	-40(20)
C(97)	380(30)	240(30)	190(20)	-132(19)	-50(20)	50(20)
C(98)	350(30)	250(30)	540(30)	-70(20)	140(20)	-50(20)
C(99)	460(30)	410(30)	840(40)	-260(30)	380(30)	-230(30)
C(100)	260(30)	700(40)	860(50)	-480(30)	220(30)	-110(30)
C(101)	280(30)	890(40)	480(30)	-260(30)	30(20)	180(30)
C(102)	420(30)	450(30)	250(20)	-70(20)	60(20)	100(20)

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**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj25.**

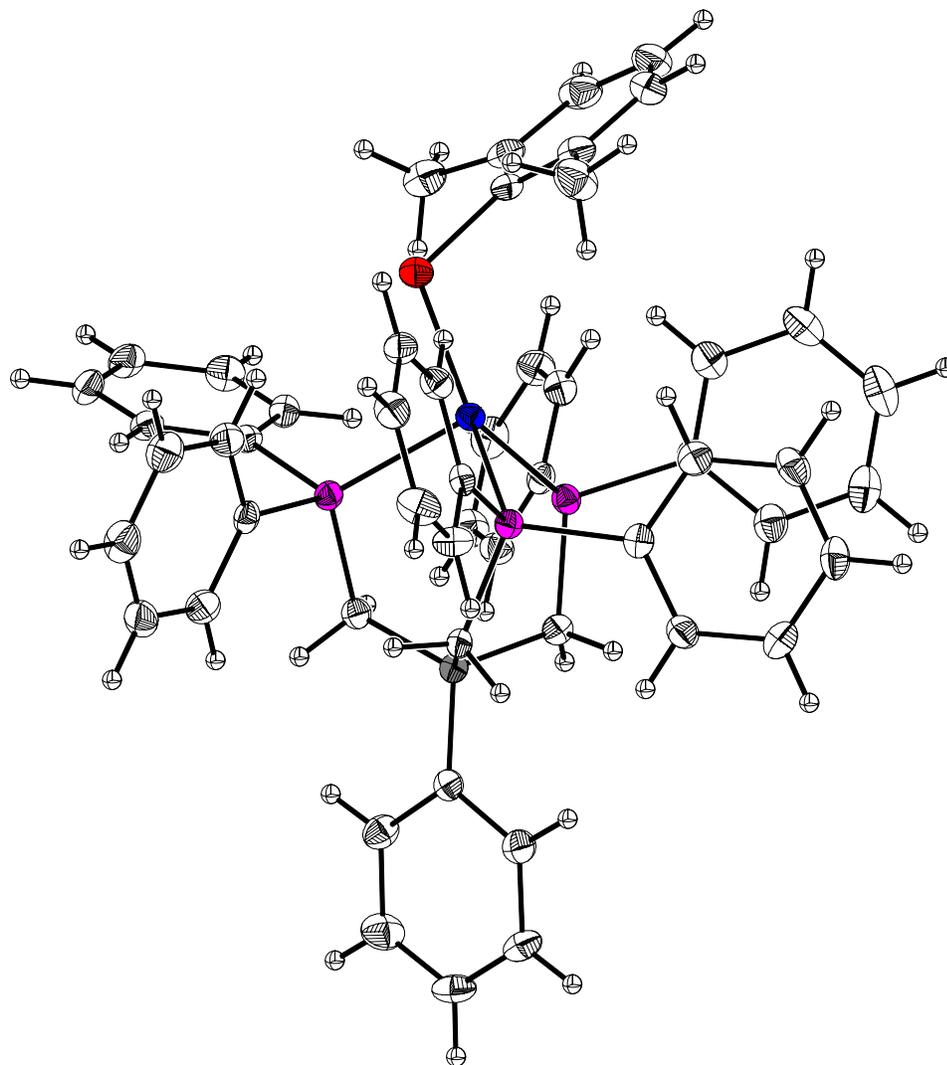
	x	y	z	$U_{\text{iso}}$
H(2)	559	611	172	23
H(3)	685	613	282	28
H(4)	702	509	381	33
H(5)	592	400	366	30
H(6)	466	398	256	27
H(7A)	329	420	165	21
H(7B)	386	354	134	21
H(8A)	386	656	114	21
H(8B)	344	607	166	21
H(9A)	467	440	51	20
H(9B)	482	552	59	20
H(11)	254	272	162	30
H(12)	153	229	209	39
H(13)	7	274	146	35
H(14)	-36	360	34	33
H(15)	66	407	-13	27
H(17)	405	276	49	24
H(18)	425	143	-14	29
H(19)	308	70	-109	29
H(20)	168	130	-140	34
H(21)	147	258	-74	29
H(23)	507	510	-77	26
H(24)	563	409	-140	29
H(25)	483	276	-204	27
H(26)	347	249	-205	29
H(27)	290	349	-141	23
H(29)	426	704	19	24
H(30)	431	851	-32	31
H(31)	378	872	-163	31
H(32)	319	742	-243	29
H(33)	312	594	-192	24
H(35)	279	796	96	32
H(36)	252	947	40	42
H(37)	186	962	-90	44
H(38)	147	828	-168	38
H(39)	171	677	-112	28
H(41)	235	547	183	30
H(42)	121	530	220	43
H(43)	-20	574	140	45
H(44)	-47	635	21	40
H(45)	67	652	-19	27
H(47)	9	575	-145	41
H(48)	-123	540	-141	52
H(49)	-175	384	-160	63
H(50)	-98	266	-191	61
H(51)	33	303	-200	44
H(53)	450	612	748	26

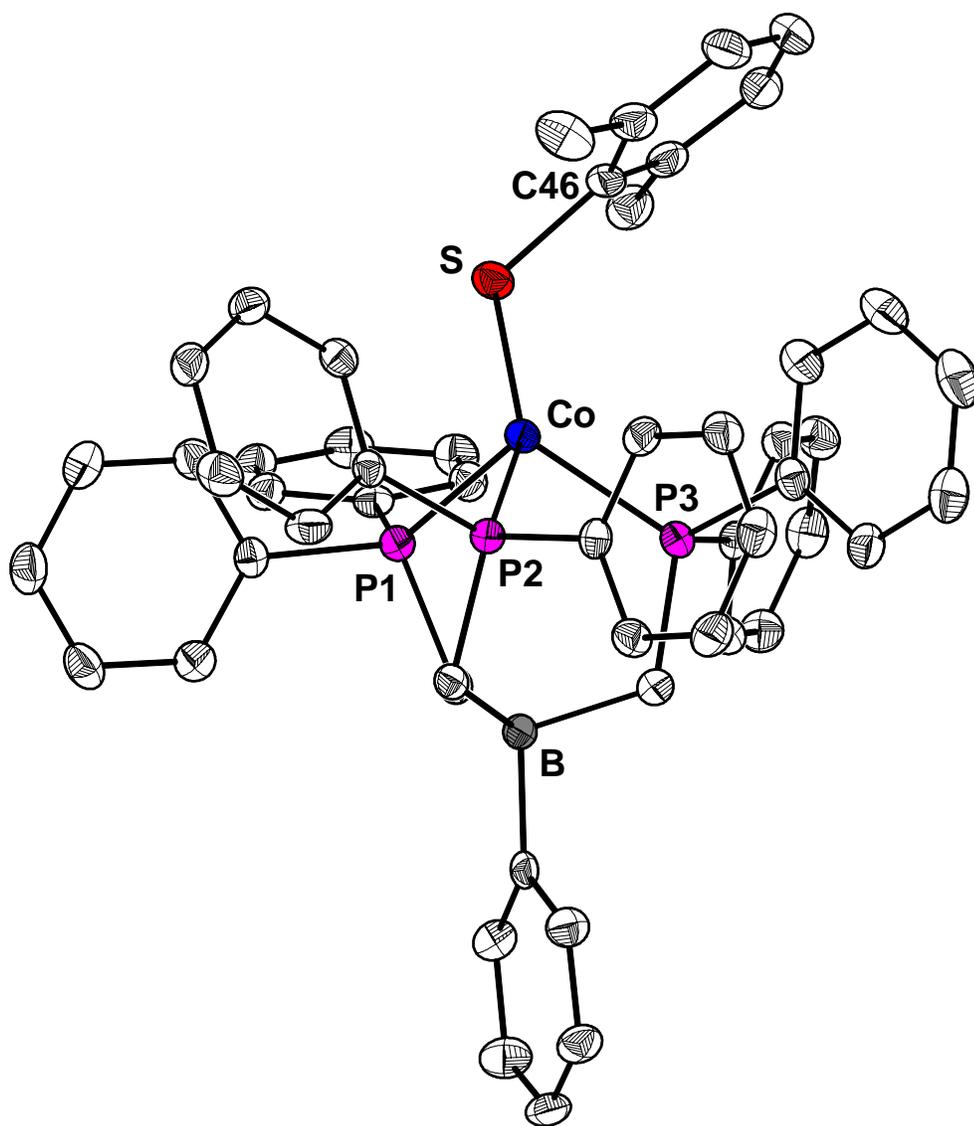
H(54)	585	647	841	32
H(55)	710	576	843	33
H(56)	698	467	749	33
H(57)	564	429	656	27
H(58A)	380	356	662	22
H(58B)	424	346	603	22
H(59A)	465	525	544	20
H(59B)	398	607	539	20
H(60A)	336	617	645	21
H(60B)	309	519	673	21
H(62)	240	389	672	25
H(63)	159	325	733	29
H(64)	80	187	687	31
H(65)	83	112	581	38
H(66)	159	178	516	34
H(68)	396	185	576	29
H(69)	407	45	518	35
H(70)	308	10	397	35
H(71)	195	115	333	32
H(72)	184	257	390	25
H(74)	497	390	524	24
H(75)	560	260	490	25
H(76)	490	188	373	30
H(77)	356	246	287	28
H(78)	290	372	322	24
H(80)	445	532	374	23
H(81)	462	658	303	30
H(82)	362	783	266	32
H(83)	246	781	302	37
H(84)	228	656	373	28
H(86)	319	727	572	24
H(87)	299	872	508	27
H(88)	168	902	404	31
H(89)	57	789	368	29
H(90)	80	643	428	26
H(92)	187	627	676	30
H(93)	72	630	712	40
H(94)	-56	550	641	39
H(95)	-70	469	531	43
H(96)	45	469	493	36
H(98)	41	313	418	47
H(99)	-97	285	417	64
H(100)	-215	375	337	73
H(101)	-198	488	256	71
H(102)	-60	518	260	47

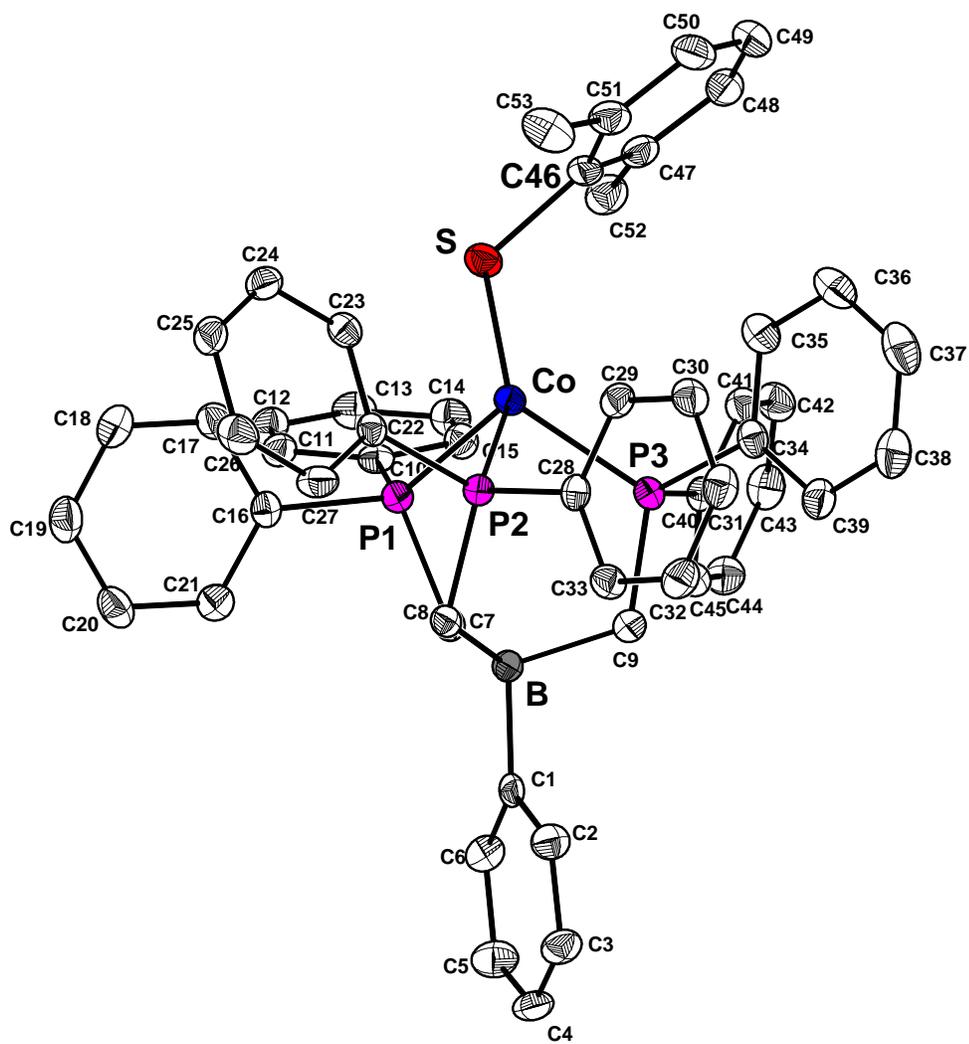
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E. X-ray report for  $[\text{PhBP}_3]\text{CoS}(2,6\text{-Me}_2\text{-Ph})$ , 6.

## Crystal Structure Report for DMJ 39, $[\text{PhBP}_3]\text{CoS}(2,6\text{-Me}_2\text{-Ph})$







**Table 1. Crystal Data and Structure Analysis Details for dmj39.**

Empirical formula	C <sub>53</sub> H <sub>50</sub> BCoP <sub>3</sub> S
Formula weight	881.64
Crystallization solvent	benzene/petroleum ether
Crystal shape	blade
Crystal color	dichroic
Crystal size	0.10 x 0.15 x 0.27 mm

**Data Collection**

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoK $\alpha$	
Data collection temperature	100(2) K	
Theta range for 6285 reflections used in lattice determination	2.26 to 28.17°	
Unit cell dimensions	a = 12.0158(9) Å b = 12.5469(9) Å c = 15.5078(12) Å	$\alpha$ = 77.7800(10)° $\beta$ = 77.5460(10)° $\gamma$ = 77.9190(10)°
Volume	2198.2(3) Å <sup>3</sup>	
Z	2	
Crystal system	triclinic	
Space group	P $\bar{1}$ (#2)	
Density (calculated)	1.332 g/cm <sup>3</sup>	
F(000)	922	
Theta range for data collection	1.4 to 28.4°	
Completeness to theta = 28.44°	91.9%	
Index ranges	-15 ≤ h ≤ 16, -16 ≤ k ≤ 16, -20 ≤ l ≤ 20	
Reflections collected	41687	
Independent reflections	10186 [R <sub>int</sub> = 0.0508]	
Reflections > 2 $\sigma$ (I)	8059	
Average $\sigma$ (I)/(net I)	0.0389	
Absorption coefficient	0.58 mm <sup>-1</sup>	
Reflections monitored for decay	380	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	10186 / 0 / 534
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	2.12
Final R indices [I>2σ(I), 8059 reflections]	R1 = 0.0405, wR2 = 0.0743
R indices (all data)	R1 = 0.0566, wR2 = 0.0762
Type of weighting scheme used	σ
Weighting scheme used	1/σ <sup>2</sup> (Fo <sup>2</sup> )
Max shift/error	0.029
Average shift/error	0.002
Largest diff. peak and hole	0.99 and -0.41 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

## Special Refinement Details

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj39.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co	8210(1)	7166(1)	2997(1)	17(1)
P(1)	8648(1)	8871(1)	2797(1)	16(1)
P(2)	6427(1)	7806(1)	3596(1)	16(1)
P(3)	7544(1)	7289(1)	1754(1)	17(1)
S	9901(1)	6261(1)	3215(1)	23(1)
B	6520(2)	9555(2)	2051(2)	17(1)
C(1)	5747(2)	10649(2)	1566(1)	17(1)
C(2)	4562(2)	10688(2)	1617(1)	24(1)
C(3)	3861(2)	11561(2)	1184(1)	26(1)
C(4)	4321(2)	12452(2)	673(1)	26(1)
C(5)	5482(2)	12457(2)	596(1)	30(1)
C(6)	6171(2)	11568(2)	1036(1)	23(1)
C(7)	7862(2)	9764(2)	1962(1)	17(1)
C(8)	5950(2)	9233(2)	3136(1)	17(1)
C(9)	6466(2)	8510(2)	1547(1)	18(1)
C(10)	10164(2)	8976(2)	2332(1)	18(1)
C(11)	10809(2)	9536(2)	2675(1)	20(1)
C(12)	11932(2)	9634(2)	2259(1)	25(1)
C(13)	12433(2)	9175(2)	1504(1)	24(1)
C(14)	11804(2)	8609(2)	1165(1)	25(1)
C(15)	10688(2)	8506(2)	1576(1)	22(1)
C(16)	8375(2)	9584(2)	3757(1)	17(1)
C(17)	8729(2)	8996(2)	4547(1)	23(1)
C(18)	8550(2)	9497(2)	5292(1)	29(1)
C(19)	8014(2)	10588(2)	5257(2)	29(1)
C(20)	7656(2)	11177(2)	4485(2)	27(1)
C(21)	7836(2)	10681(2)	3735(1)	22(1)
C(22)	6370(2)	7677(2)	4800(1)	17(1)
C(23)	7239(2)	6979(2)	5209(1)	20(1)
C(24)	7208(2)	6874(2)	6119(1)	23(1)
C(25)	6294(2)	7454(2)	6634(1)	25(1)
C(26)	5420(2)	8137(2)	6234(1)	29(1)
C(27)	5460(2)	8257(2)	5320(1)	24(1)
C(28)	5283(2)	7042(2)	3587(1)	18(1)
C(29)	5468(2)	5904(2)	3870(1)	22(1)
C(30)	4625(2)	5287(2)	3893(1)	26(1)
C(31)	3585(2)	5810(2)	3639(1)	26(1)
C(32)	3390(2)	6933(2)	3355(1)	26(1)
C(33)	4236(2)	7550(2)	3324(1)	22(1)
C(34)	6962(2)	6040(2)	1791(1)	20(1)
C(35)	7545(2)	5031(2)	2169(1)	25(1)
C(36)	7108(2)	4064(2)	2253(2)	29(1)
C(37)	6088(2)	4108(2)	1960(2)	35(1)
C(38)	5504(2)	5111(2)	1584(2)	32(1)
C(39)	5929(2)	6077(2)	1506(1)	25(1)
C(40)	8663(2)	7338(2)	742(1)	17(1)

C(41)	9502(2)	6412(2)	615(1)	22(1)
C(42)	10402(2)	6447(2)	-113(1)	26(1)
C(43)	10485(2)	7426(2)	-720(1)	27(1)
C(44)	9657(2)	8350(2)	-604(1)	25(1)
C(45)	8746(2)	8304(2)	114(1)	21(1)
C(46)	10206(2)	4881(2)	2998(1)	21(1)
C(47)	11068(2)	4635(2)	2261(1)	24(1)
C(48)	11263(2)	3585(2)	2041(2)	30(1)
C(49)	10665(2)	2774(2)	2563(2)	34(1)
C(50)	9882(2)	3000(2)	3320(2)	31(1)
C(51)	9635(2)	4047(2)	3553(2)	26(1)
C(52)	11817(2)	5459(2)	1733(1)	30(1)
C(53)	8776(2)	4254(2)	4384(2)	36(1)

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**Table 3.** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj39.

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Co-S	2.1673(6)
Co-P(2)	2.1990(6)
Co-P(3)	2.2076(6)
Co-P(1)	2.2514(6)
S-C(46)	1.781(2)
S-Co-P(2)	147.37(2)
S-Co-P(3)	123.30(2)
P(2)-Co-P(3)	86.73(2)
S-Co-P(1)	96.48(2)
P(2)-Co-P(1)	89.44(2)
P(3)-Co-P(1)	100.23(2)
C(46)-S-Co	114.64(6)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj39.**

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Co-S	2.1673(6)
Co-P(2)	2.1990(6)
Co-P(3)	2.2076(6)
Co-P(1)	2.2514(6)
P(1)-C(7)	1.8146(19)
P(1)-C(10)	1.8301(19)
P(1)-C(16)	1.832(2)
P(2)-C(8)	1.8026(18)
P(2)-C(22)	1.8257(19)
P(2)-C(28)	1.8374(18)
P(3)-C(9)	1.8072(19)
P(3)-C(34)	1.8300(19)
P(3)-C(40)	1.832(2)
S-C(46)	1.781(2)
B-C(1)	1.626(3)
B-C(7)	1.660(3)
B-C(8)	1.672(3)
B-C(9)	1.681(3)
C(1)-C(6)	1.389(3)
C(1)-C(2)	1.399(3)
C(2)-C(3)	1.381(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.371(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.376(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.389(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(15)	1.392(3)
C(10)-C(11)	1.393(3)
C(11)-C(12)	1.383(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.378(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.382(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.376(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.390(3)
C(16)-C(17)	1.392(3)
C(17)-C(18)	1.386(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.380(3)

C(18)-H(18)	0.9500
C(19)-C(20)	1.372(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.388(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(27)	1.383(3)
C(22)-C(23)	1.388(3)
C(23)-C(24)	1.382(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.380(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.379(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.385(3)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.387(3)
C(28)-C(33)	1.389(3)
C(29)-C(30)	1.388(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.381(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.369(3)
C(31)-H(31)	0.9500
C(32)-C(33)	1.389(3)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(35)	1.389(3)
C(34)-C(39)	1.394(3)
C(35)-C(36)	1.391(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.383(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.383(3)
C(37)-H(37)	0.9500
C(38)-C(39)	1.384(3)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(41)	1.388(3)
C(40)-C(45)	1.392(3)
C(41)-C(42)	1.385(3)
C(41)-H(41)	0.9500
C(42)-C(43)	1.387(3)
C(42)-H(42)	0.9500
C(43)-C(44)	1.377(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.384(3)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(51)	1.404(3)
C(46)-C(47)	1.408(3)
C(47)-C(48)	1.391(3)
C(47)-C(52)	1.504(3)

C(48)-C(49)	1.383(3)
C(48)-H(48)	0.9500
C(49)-C(50)	1.376(3)
C(49)-H(49)	0.9500
C(50)-C(51)	1.392(3)
C(50)-H(50)	0.9500
C(51)-C(53)	1.500(3)
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
S-Co-P(2)	147.37(2)
S-Co-P(3)	123.30(2)
P(2)-Co-P(3)	86.73(2)
S-Co-P(1)	96.48(2)
P(2)-Co-P(1)	89.44(2)
P(3)-Co-P(1)	100.23(2)
C(7)-P(1)-C(10)	104.06(8)
C(7)-P(1)-C(16)	107.03(9)
C(10)-P(1)-C(16)	101.72(8)
C(7)-P(1)-Co	107.93(6)
C(10)-P(1)-Co	115.20(6)
C(16)-P(1)-Co	119.60(6)
C(8)-P(2)-C(22)	109.10(9)
C(8)-P(2)-C(28)	106.94(9)
C(22)-P(2)-C(28)	101.14(8)
C(8)-P(2)-Co	113.01(6)
C(22)-P(2)-Co	107.71(6)
C(28)-P(2)-Co	118.08(6)
C(9)-P(3)-C(34)	110.45(9)
C(9)-P(3)-C(40)	105.74(9)
C(34)-P(3)-C(40)	103.87(9)
C(9)-P(3)-Co	112.86(6)
C(34)-P(3)-Co	109.79(7)
C(40)-P(3)-Co	113.71(6)
C(46)-S-Co	114.64(6)
C(1)-B-C(7)	110.36(15)
C(1)-B-C(8)	111.05(16)
C(7)-B-C(8)	109.02(15)
C(1)-B-C(9)	106.32(15)
C(7)-B-C(9)	112.32(16)
C(8)-B-C(9)	107.74(15)
C(6)-C(1)-C(2)	114.33(18)
C(6)-C(1)-B	125.44(17)
C(2)-C(1)-B	120.10(17)
C(3)-C(2)-C(1)	123.54(19)
C(3)-C(2)-H(2)	118.2
C(1)-C(2)-H(2)	118.2
C(4)-C(3)-C(2)	119.84(19)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1

C(3)-C(4)-C(5)	119.14(19)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	119.95(19)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(1)-C(6)-C(5)	123.19(19)
C(1)-C(6)-H(6)	118.4
C(5)-C(6)-H(6)	118.4
B-C(7)-P(1)	114.58(13)
B-C(7)-H(7A)	108.6
P(1)-C(7)-H(7A)	108.6
B-C(7)-H(7B)	108.6
P(1)-C(7)-H(7B)	108.6
H(7A)-C(7)-H(7B)	107.6
B-C(8)-P(2)	112.31(13)
B-C(8)-H(8A)	109.1
P(2)-C(8)-H(8A)	109.1
B-C(8)-H(8B)	109.1
P(2)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.9
B-C(9)-P(3)	114.98(12)
B-C(9)-H(9A)	108.5
P(3)-C(9)-H(9A)	108.5
B-C(9)-H(9B)	108.5
P(3)-C(9)-H(9B)	108.5
H(9A)-C(9)-H(9B)	107.5
C(15)-C(10)-C(11)	118.29(18)
C(15)-C(10)-P(1)	118.22(14)
C(11)-C(10)-P(1)	123.45(15)
C(12)-C(11)-C(10)	120.25(19)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(13)-C(12)-C(11)	120.79(19)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(12)-C(13)-C(14)	119.36(18)
C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
C(15)-C(14)-C(13)	120.25(19)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(14)-C(15)-C(10)	121.06(18)
C(14)-C(15)-H(15)	119.5
C(10)-C(15)-H(15)	119.5
C(21)-C(16)-C(17)	118.52(18)
C(21)-C(16)-P(1)	123.32(15)
C(17)-C(16)-P(1)	118.16(15)
C(18)-C(17)-C(16)	120.5(2)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	120.2(2)
C(19)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9

C(20)-C(19)-C(18)	119.9(2)
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
C(19)-C(20)-C(21)	120.2(2)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(20)-C(21)-C(16)	120.64(19)
C(20)-C(21)-H(21)	119.7
C(16)-C(21)-H(21)	119.7
C(27)-C(22)-C(23)	118.87(18)
C(27)-C(22)-P(2)	120.91(15)
C(23)-C(22)-P(2)	120.21(15)
C(24)-C(23)-C(22)	120.85(19)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	119.89(19)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(26)-C(25)-C(24)	119.62(19)
C(26)-C(25)-H(25)	120.2
C(24)-C(25)-H(25)	120.2
C(25)-C(26)-C(27)	120.5(2)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(22)-C(27)-C(26)	120.22(19)
C(22)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(29)-C(28)-C(33)	118.47(17)
C(29)-C(28)-P(2)	118.26(14)
C(33)-C(28)-P(2)	123.27(15)
C(28)-C(29)-C(30)	120.79(19)
C(28)-C(29)-H(29)	119.6
C(30)-C(29)-H(29)	119.6
C(31)-C(30)-C(29)	119.77(19)
C(31)-C(30)-H(30)	120.1
C(29)-C(30)-H(30)	120.1
C(32)-C(31)-C(30)	120.20(18)
C(32)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(31)-C(32)-C(33)	120.09(19)
C(31)-C(32)-H(32)	120.0
C(33)-C(32)-H(32)	120.0
C(32)-C(33)-C(28)	120.68(19)
C(32)-C(33)-H(33)	119.7
C(28)-C(33)-H(33)	119.7
C(35)-C(34)-C(39)	119.39(18)
C(35)-C(34)-P(3)	118.04(15)
C(39)-C(34)-P(3)	122.46(15)
C(34)-C(35)-C(36)	120.3(2)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9
C(37)-C(36)-C(35)	119.9(2)
C(37)-C(36)-H(36)	120.1
C(35)-C(36)-H(36)	120.1

C(38)-C(37)-C(36)	120.1(2)
C(38)-C(37)-H(37)	120.0
C(36)-C(37)-H(37)	120.0
C(37)-C(38)-C(39)	120.4(2)
C(37)-C(38)-H(38)	119.8
C(39)-C(38)-H(38)	119.8
C(38)-C(39)-C(34)	120.0(2)
C(38)-C(39)-H(39)	120.0
C(34)-C(39)-H(39)	120.0
C(41)-C(40)-C(45)	118.14(18)
C(41)-C(40)-P(3)	119.84(15)
C(45)-C(40)-P(3)	121.91(15)
C(42)-C(41)-C(40)	121.11(19)
C(42)-C(41)-H(41)	119.4
C(40)-C(41)-H(41)	119.4
C(41)-C(42)-C(43)	119.9(2)
C(41)-C(42)-H(42)	120.1
C(43)-C(42)-H(42)	120.1
C(44)-C(43)-C(42)	119.7(2)
C(44)-C(43)-H(43)	120.2
C(42)-C(43)-H(43)	120.2
C(43)-C(44)-C(45)	120.24(19)
C(43)-C(44)-H(44)	119.9
C(45)-C(44)-H(44)	119.9
C(44)-C(45)-C(40)	120.94(19)
C(44)-C(45)-H(45)	119.5
C(40)-C(45)-H(45)	119.5
C(51)-C(46)-C(47)	120.20(19)
C(51)-C(46)-S	121.80(16)
C(47)-C(46)-S	117.98(15)
C(48)-C(47)-C(46)	118.92(19)
C(48)-C(47)-C(52)	119.29(19)
C(46)-C(47)-C(52)	121.72(19)
C(49)-C(48)-C(47)	120.8(2)
C(49)-C(48)-H(48)	119.6
C(47)-C(48)-H(48)	119.6
C(50)-C(49)-C(48)	119.8(2)
C(50)-C(49)-H(49)	120.1
C(48)-C(49)-H(49)	120.1
C(49)-C(50)-C(51)	121.4(2)
C(49)-C(50)-H(50)	119.3
C(51)-C(50)-H(50)	119.3
C(50)-C(51)-C(46)	118.6(2)
C(50)-C(51)-C(53)	119.54(19)
C(46)-C(51)-C(53)	121.90(19)
C(47)-C(52)-H(52A)	109.5
C(47)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(47)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(51)-C(53)-H(53A)	109.5
C(51)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5

C(51)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5

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Symmetry transformations used to generate equivalent atoms:

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj39. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co	156(1)	162(2)	170(2)	-34(1)	-16(1)	-17(1)
P(1)	136(2)	176(3)	182(3)	-39(2)	-17(2)	-29(2)
P(2)	151(2)	169(3)	158(3)	-30(2)	-18(2)	-31(2)
P(3)	172(3)	164(3)	179(3)	-46(2)	-15(2)	-32(2)
S	193(3)	200(3)	289(3)	-61(2)	-49(2)	2(2)
B	160(11)	171(12)	189(13)	-34(9)	-38(9)	-32(9)
C(1)	192(10)	189(11)	151(11)	-84(8)	-28(8)	-14(8)
C(2)	227(11)	225(12)	273(13)	-11(9)	-61(9)	-57(9)
C(3)	176(10)	300(13)	279(13)	-53(10)	-73(9)	19(9)
C(4)	278(12)	262(12)	184(12)	-19(9)	-72(9)	69(10)
C(5)	327(13)	272(13)	246(13)	56(10)	-31(10)	-56(10)
C(6)	196(10)	276(12)	213(12)	-16(9)	-32(9)	-45(9)
C(7)	181(10)	175(10)	167(11)	-42(8)	-23(8)	-32(8)
C(8)	146(10)	163(10)	215(11)	-43(8)	-39(8)	-38(8)
C(9)	165(10)	196(11)	165(11)	-26(8)	-18(8)	-34(8)
C(10)	148(10)	171(10)	196(11)	0(8)	-27(8)	-20(8)
C(11)	177(10)	220(11)	212(12)	-48(9)	-46(9)	-9(9)
C(12)	180(10)	279(12)	301(13)	-37(10)	-75(9)	-65(9)
C(13)	132(10)	281(12)	290(13)	-19(10)	3(9)	-39(9)
C(14)	216(11)	275(12)	228(12)	-62(9)	16(9)	-15(9)
C(15)	198(10)	211(11)	250(12)	-57(9)	-50(9)	-42(9)
C(16)	121(9)	213(11)	202(11)	-68(8)	-7(8)	-54(8)
C(17)	210(11)	231(11)	262(12)	-59(9)	-39(9)	-29(9)
C(18)	326(13)	351(14)	227(13)	-63(10)	-88(10)	-68(11)
C(19)	277(12)	363(14)	278(13)	-167(11)	-39(10)	-39(11)
C(20)	218(11)	241(12)	356(14)	-141(10)	-19(10)	-17(9)
C(21)	192(10)	252(12)	225(12)	-42(9)	-25(9)	-34(9)
C(22)	194(10)	158(10)	170(11)	-29(8)	-26(8)	-64(8)
C(23)	204(10)	194(11)	205(12)	-58(9)	-7(9)	-20(9)
C(24)	247(11)	215(11)	226(12)	-2(9)	-82(9)	-44(9)
C(25)	345(12)	246(12)	172(12)	-32(9)	-60(10)	-68(10)
C(26)	313(12)	275(12)	236(13)	-80(10)	23(10)	8(10)
C(27)	227(11)	238(12)	229(12)	-13(9)	-44(9)	26(9)
C(28)	185(10)	218(11)	129(10)	-53(8)	2(8)	-52(9)
C(29)	250(11)	238(11)	164(11)	-24(9)	-47(9)	-44(9)
C(30)	365(13)	194(11)	211(12)	-3(9)	-39(10)	-98(10)
C(31)	293(12)	287(13)	237(12)	-33(10)	-29(10)	-162(10)
C(32)	196(11)	325(13)	273(13)	-57(10)	-64(9)	-58(10)
C(33)	244(11)	181(11)	234(12)	-24(9)	-42(9)	-49(9)
C(34)	232(11)	207(11)	157(11)	-57(8)	10(9)	-68(9)
C(35)	244(11)	234(12)	244(12)	-59(9)	14(9)	-52(9)
C(36)	349(13)	191(12)	303(13)	-50(9)	29(10)	-49(10)
C(37)	435(15)	294(13)	346(14)	-118(11)	30(11)	-174(12)
C(38)	337(13)	382(14)	293(13)	-98(11)	-56(10)	-153(11)
C(39)	292(12)	268(12)	203(12)	-58(9)	-48(9)	-74(10)
C(40)	171(10)	205(11)	164(11)	-66(8)	-33(8)	-36(9)

C(41)	247(11)	218(11)	197(12)	-33(9)	-35(9)	-59(9)
C(42)	227(11)	270(12)	286(13)	-106(10)	-14(10)	6(10)
C(43)	241(11)	355(13)	203(12)	-85(10)	29(9)	-80(10)
C(44)	296(12)	246(12)	209(12)	5(9)	-32(10)	-81(10)
C(45)	224(11)	200(11)	215(12)	-54(9)	-39(9)	-11(9)
C(46)	173(10)	187(11)	287(13)	-53(9)	-93(9)	20(9)
C(47)	197(11)	267(12)	242(12)	-52(9)	-92(9)	33(9)
C(48)	310(12)	314(13)	288(13)	-125(10)	-113(10)	72(10)
C(49)	396(14)	224(12)	433(16)	-115(11)	-179(12)	43(11)
C(50)	291(12)	202(12)	432(15)	-26(10)	-120(11)	-21(10)
C(51)	208(11)	254(12)	320(13)	-33(10)	-81(10)	8(10)
C(52)	260(12)	360(14)	271(13)	-69(10)	-59(10)	2(10)
C(53)	311(13)	275(13)	438(16)	-30(11)	41(11)	-65(11)

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**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj39.**

	x	y	z	$U_{\text{iso}}$
H(2)	422	1008	197	29
H(3)	306	1154	124	31
H(4)	384	1306	38	31
H(5)	581	1307	24	36
H(6)	697	1159	97	28
H(7A)	784	1054	201	21
H(7B)	830	965	136	21
H(8A)	510	938	321	20
H(8B)	617	972	348	20
H(9A)	656	878	89	21
H(9B)	569	830	175	21
H(11)	1048	985	320	24
H(12)	1236	1002	250	30
H(13)	1320	925	122	29
H(14)	1214	829	64	30
H(15)	1027	811	134	26
H(17)	910	824	458	28
H(18)	880	909	583	35
H(19)	789	1093	577	35
H(20)	728	1193	446	32
H(21)	759	1110	320	27
H(23)	786	657	486	24
H(24)	781	640	639	27
H(25)	627	738	726	30
H(26)	478	853	659	35
H(27)	486	874	505	29
H(29)	618	554	405	26
H(30)	476	451	408	31
H(31)	300	539	366	31
H(32)	267	729	318	31
H(33)	410	833	312	26
H(35)	824	500	237	29
H(36)	751	338	251	35
H(37)	579	345	202	42
H(38)	481	514	138	38
H(39)	552	676	126	30
H(41)	946	574	103	26
H(42)	1096	580	-20	32
H(43)	1111	746	-121	32
H(44)	971	902	-102	31
H(45)	817	894	18	26
H(48)	1181	342	153	36
H(49)	1079	206	240	41
H(50)	950	243	369	37
H(52A)	1233	515	123	45
H(52B)	1229	561	212	45
H(52C)	1133	615	151	45

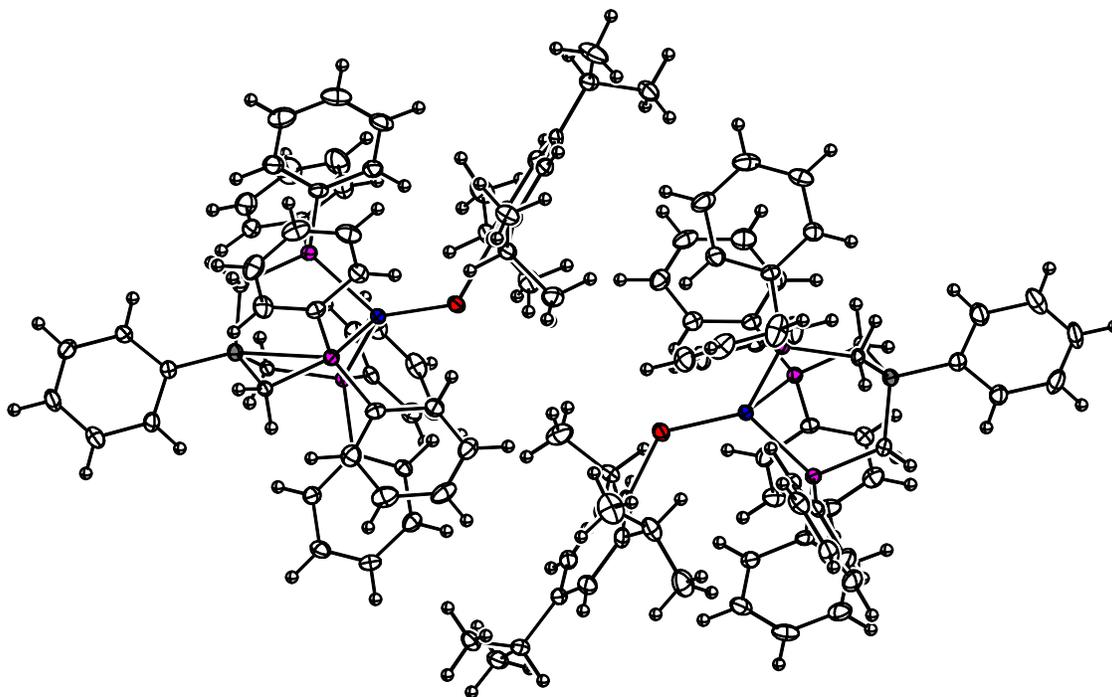
H(53A)	811	481	422	54
H(53B)	914	453	478	54
H(53C)	851	356	470	54

---

F. X-ray report for  $[\text{PhBP}_3]\text{CoS}(2,4,6\text{-}^i\text{Pr}_3\text{-Ph})$ , 7.

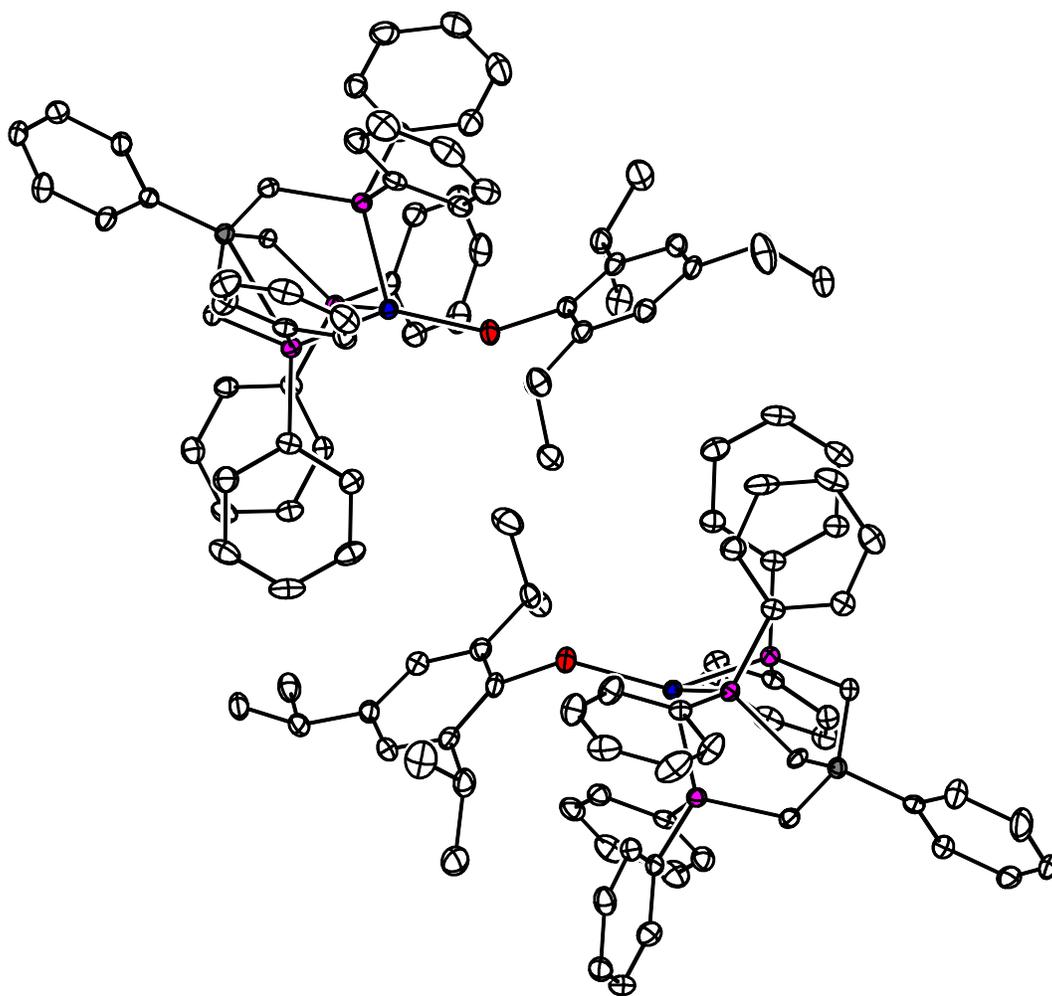
## Crystal Structure Report for

**DMJ 51,  $[\text{PhBP}_3]\text{CoS}(\text{Trip})$ , Trip = 2,4,6- $^i\text{Pr}_3\text{-Ph}$**

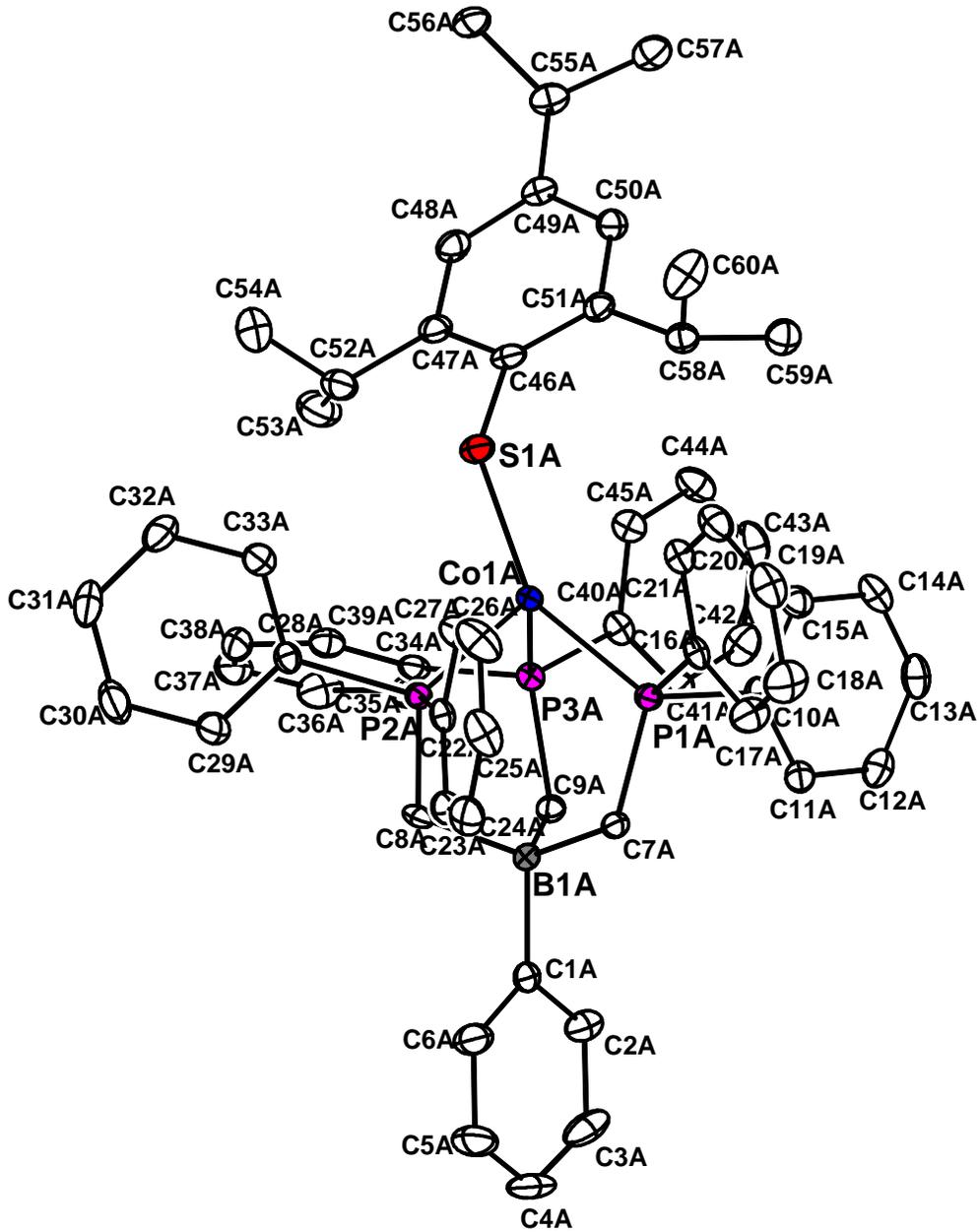


**Molecule B**

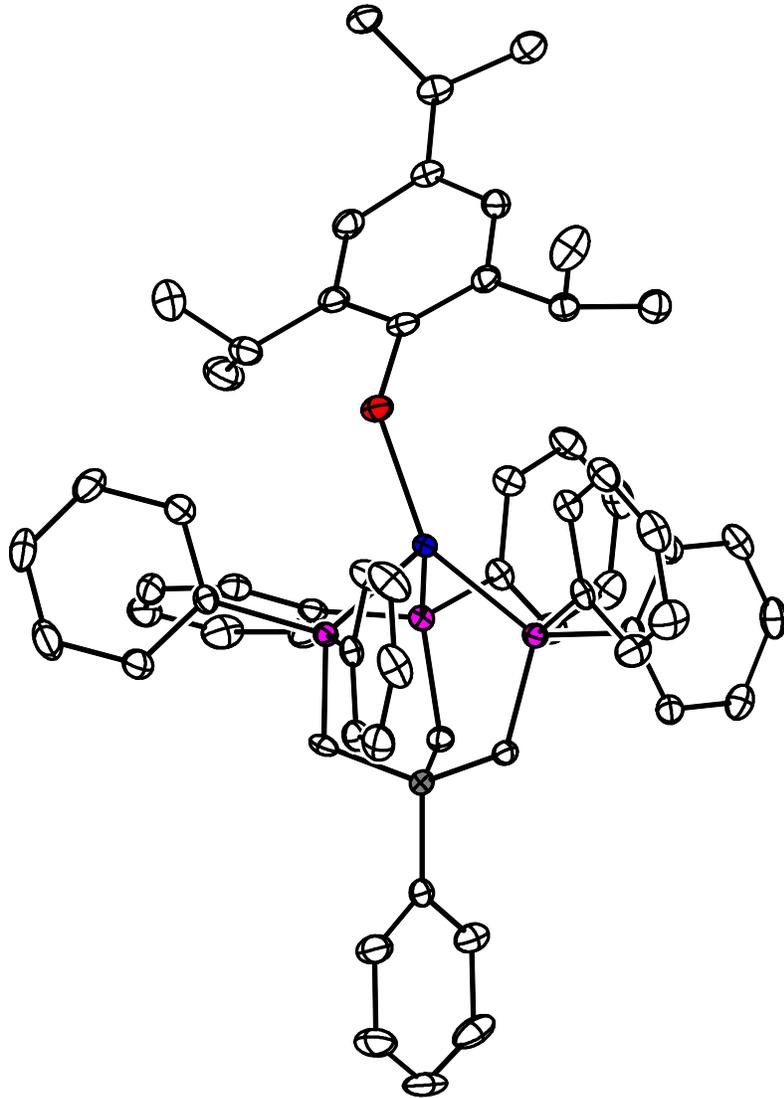
**Molecule A**



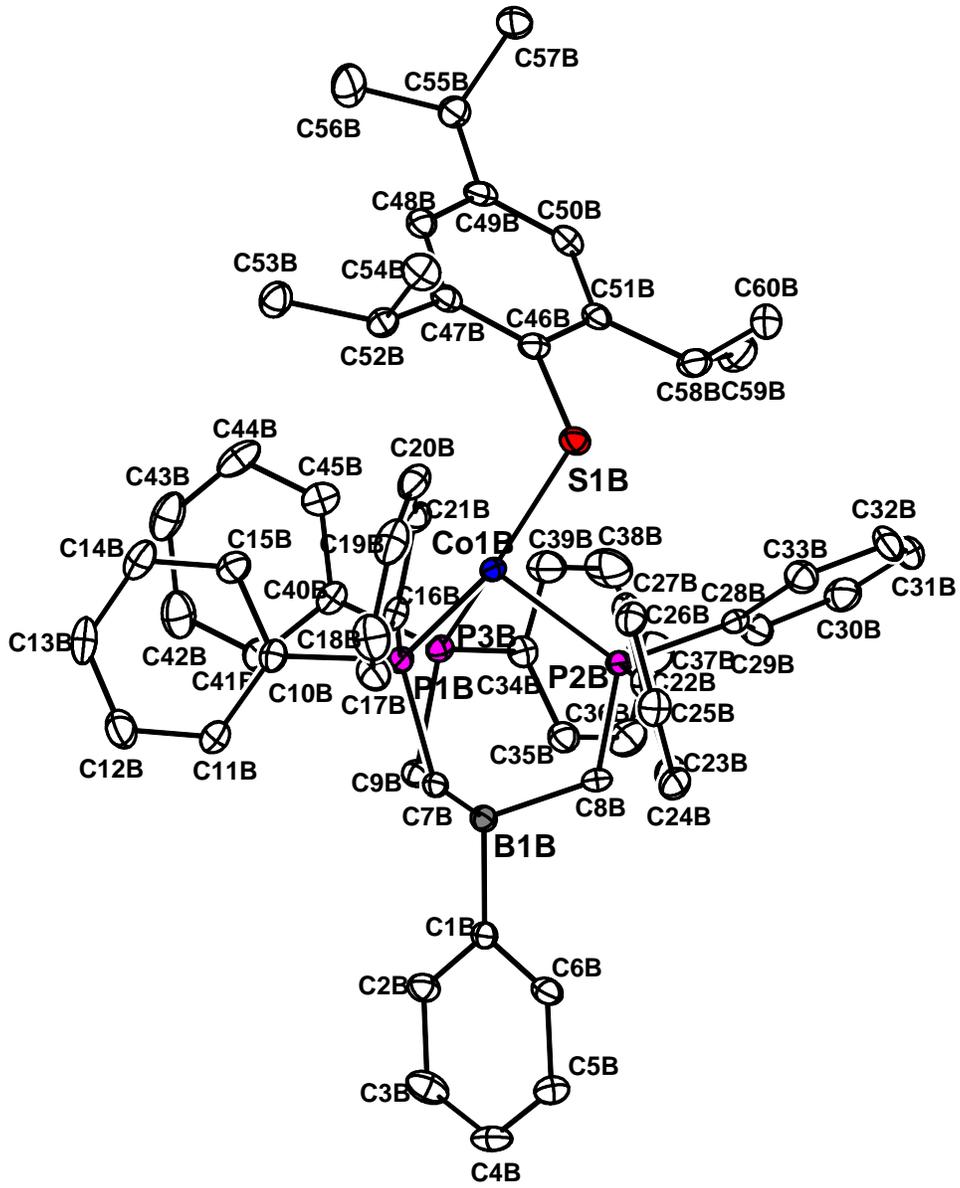
# Molecule A



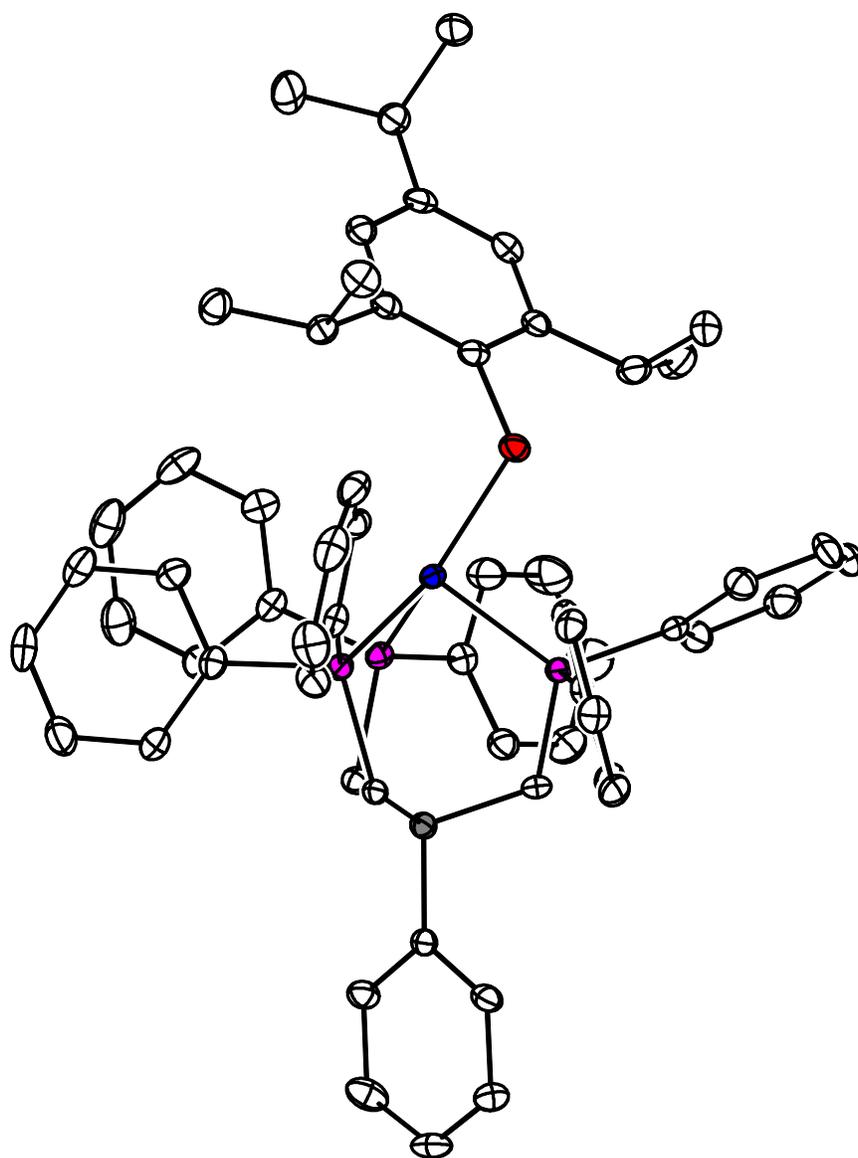
# Molecule A



# Molecule B



# Molecule B



**Table 1. Crystal Data and Structure Analysis Details for dmj51.**

Empirical formula	C <sub>60</sub> H <sub>64</sub> BCoP <sub>3</sub> S
Formula weight	979.82
Crystallization solvent	Benzene/Petroleum Ether
Crystal shape	rough block
Crystal color	purple
Crystal size	0.18 x 0.22 x 0.27 mm

**Data Collection**

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoK $\alpha$	
Data collection temperature	100 K	
Theta range for 6006 reflections used in lattice determination	2.45 to 30.60°	
Unit cell dimensions	a = 15.3738(11) Å b = 17.3171(13) Å c = 20.7953(15) Å	$\alpha$ = 65.655(1)° $\beta$ = 87.329(2)° $\gamma$ = 88.642(2)°
Volume	5038.5(6) Å <sup>3</sup>	
Z	4	
Crystal system	triclinic	
Space group	P $\bar{1}$ (#2)	
Density (calculated)	1.292 g/cm <sup>3</sup>	
F(000)	2068	
Theta range for data collection	1.7 to 31.5°	
Completeness to theta = 31.55°	84.7%	
Index ranges	-21 ≤ h ≤ 22, -24 ≤ k ≤ 23, -28 ≤ l ≤ 27	
Reflections collected	82025	
Independent reflections	28555 [R <sub>int</sub> = 0.0726]	
Reflections > 2 $\sigma$ (I)	16721	
Average $\sigma$ (I)/(net I)	0.0990	
Absorption coefficient	0.52 mm <sup>-1</sup>	
Reflections monitored for decay	395	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	28555 / 0 / 1201
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	1.10
Final R indices [I>2σ(I), 16721 reflections]	R1 = 0.0482, wR2 = 0.0836
R indices (all data)	R1 = 0.0977, wR2 = 0.0931
Type of weighting scheme used	σ
Weighting scheme used	1/[σ <sup>2</sup> (Fo <sup>2</sup> )+(0.02*P) <sup>2</sup> ] where P=(Fo <sup>2</sup> +2Fc <sup>2</sup> )/3
Max shift/error	0.033
Average shift/error	0.002
Largest diff. peak and hole	1.07 and -0.49 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

**Special Refinement Details**

Refinement of F<sup>2</sup> against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F<sup>2</sup>, conventional R-factors (R) are based on F, with F set to zero for negative F<sup>2</sup>. The threshold expression of F<sup>2</sup> > 2σ(F<sup>2</sup>) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F<sup>2</sup> are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger. The 2 4 2 and 1 0 1 reflections were omitted from the refinement due to poor correlation between the observed and calculated values.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj51.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co(1A)	4215(1)	2835(1)	2706(1)	12(1)
S(1A)	2867(1)	3108(1)	2862(1)	18(1)
P(1A)	5453(1)	3415(1)	2167(1)	13(1)
P(2A)	4861(1)	2410(1)	3764(1)	12(1)
P(3A)	4562(1)	1726(1)	2482(1)	13(1)
B(1A)	6267(2)	1837(2)	3042(1)	14(1)
C(1A)	7225(1)	1378(1)	3187(1)	15(1)
C(2A)	7634(1)	1085(1)	2711(1)	21(1)
C(3A)	8454(1)	706(1)	2819(1)	29(1)
C(4A)	8897(2)	593(1)	3409(1)	31(1)
C(5A)	8520(2)	879(2)	3887(1)	33(1)
C(6A)	7707(1)	1264(2)	3774(1)	25(1)
C(7A)	6424(1)	2884(1)	2593(1)	14(1)
C(8A)	5718(1)	1652(1)	3800(1)	14(1)
C(9A)	5718(1)	1465(1)	2560(1)	14(1)
C(10A)	5559(1)	3508(1)	1255(1)	14(1)
C(11A)	6270(1)	3191(1)	994(1)	18(1)
C(12A)	6287(1)	3238(1)	312(1)	22(1)
C(13A)	5600(2)	3604(1)	-120(1)	23(1)
C(14A)	4900(2)	3930(1)	129(1)	22(1)
C(15A)	4877(1)	3878(1)	810(1)	19(1)
C(16A)	5471(1)	4520(1)	2057(1)	15(1)
C(17A)	6252(2)	4953(1)	1934(1)	24(1)
C(18A)	6269(2)	5791(2)	1856(1)	30(1)
C(19A)	5497(2)	6199(1)	1903(1)	25(1)
C(20A)	4717(2)	5779(1)	2028(1)	22(1)
C(21A)	4702(1)	4941(1)	2105(1)	18(1)
C(22A)	5360(1)	3257(1)	3935(1)	14(1)
C(23A)	6214(1)	3238(1)	4144(1)	19(1)
C(24A)	6544(2)	3915(2)	4247(1)	24(1)
C(25A)	6033(2)	4617(1)	4153(1)	27(1)
C(26A)	5180(2)	4640(2)	3952(1)	30(1)
C(27A)	4850(2)	3966(1)	3846(1)	22(1)
C(28A)	4194(1)	1882(1)	4588(1)	14(1)
C(29A)	4548(2)	1230(2)	5166(1)	27(1)
C(30A)	4052(2)	793(2)	5778(1)	35(1)
C(31A)	3179(2)	986(1)	5817(1)	28(1)
C(32A)	2819(2)	1633(2)	5253(1)	27(1)
C(33A)	3318(1)	2081(1)	4642(1)	23(1)
C(34A)	4020(1)	742(1)	3086(1)	15(1)
C(35A)	3986(1)	42(1)	2916(1)	23(1)
C(36A)	3632(1)	-715(1)	3396(1)	28(1)
C(37A)	3313(1)	-790(1)	4054(1)	26(1)
C(38A)	3336(1)	-99(1)	4225(1)	22(1)
C(39A)	3677(1)	661(1)	3739(1)	18(1)
C(40A)	4234(1)	1814(1)	1621(1)	16(1)

C(41A)	4745(1)	1545(1)	1180(1)	20(1)
C(42A)	4446(2)	1626(2)	534(1)	25(1)
C(43A)	3641(2)	1994(1)	313(1)	25(1)
C(44A)	3132(2)	2267(1)	748(1)	23(1)
C(45A)	3418(1)	2174(1)	1396(1)	18(1)
C(46A)	2019(1)	3039(1)	2319(1)	17(1)
C(47A)	1445(1)	2338(1)	2606(1)	18(1)
C(48A)	705(1)	2357(1)	2237(1)	20(1)
C(49A)	510(1)	3022(1)	1601(1)	17(1)
C(50A)	1118(1)	3669(1)	1310(1)	17(1)
C(51A)	1876(1)	3693(1)	1653(1)	16(1)
C(52A)	1605(1)	1578(1)	3291(1)	24(1)
C(53A)	1518(2)	741(2)	3209(1)	34(1)
C(54A)	1017(2)	1604(2)	3888(1)	38(1)
C(55A)	-336(1)	3007(1)	1258(1)	20(1)
C(56A)	-1122(1)	3031(1)	1736(1)	22(1)
C(57A)	-420(1)	3707(1)	519(1)	24(1)
C(58A)	2502(1)	4427(1)	1300(1)	18(1)
C(59A)	2669(1)	4640(1)	511(1)	22(1)
C(60A)	2189(2)	5212(2)	1401(1)	33(1)
Co(1B)	579(1)	7200(1)	2378(1)	12(1)
S(1B)	1872(1)	7092(1)	1995(1)	17(1)
P(1B)	-656(1)	6574(1)	2896(1)	13(1)
P(2B)	-21(1)	7659(1)	1321(1)	12(1)
P(3B)	195(1)	8283(1)	2642(1)	14(1)
B(1B)	-1464(2)	8167(2)	2049(1)	14(1)
C(1B)	-2406(1)	8641(1)	1858(1)	14(1)
C(2B)	-2789(1)	9103(1)	2215(1)	18(1)
C(3B)	-3581(1)	9529(1)	2029(1)	24(1)
C(4B)	-4026(1)	9506(1)	1480(1)	23(1)
C(5B)	-3683(1)	9041(1)	1123(1)	23(1)
C(6B)	-2895(1)	8619(1)	1313(1)	18(1)
C(7B)	-1616(1)	7115(1)	2446(1)	13(1)
C(8B)	-875(1)	8408(1)	1295(1)	13(1)
C(9B)	-970(1)	8464(1)	2608(1)	15(1)
C(10B)	-799(1)	6439(1)	3818(1)	16(1)
C(11B)	-1576(1)	6621(1)	4106(1)	22(1)
C(12B)	-1620(2)	6553(1)	4796(1)	26(1)
C(13B)	-898(2)	6305(1)	5204(1)	26(1)
C(14B)	-134(2)	6105(1)	4933(1)	24(1)
C(15B)	-85(1)	6169(1)	4245(1)	20(1)
C(16B)	-662(1)	5469(1)	2998(1)	16(1)
C(17B)	-1441(1)	5044(1)	3061(1)	22(1)
C(18B)	-1437(2)	4207(1)	3129(1)	28(1)
C(19B)	-650(2)	3795(1)	3135(1)	27(1)
C(20B)	127(2)	4212(1)	3072(1)	24(1)
C(21B)	126(1)	5042(1)	3009(1)	19(1)
C(22B)	-526(1)	6842(1)	1116(1)	13(1)
C(23B)	-1313(1)	6953(1)	778(1)	16(1)
C(24B)	-1706(1)	6275(1)	716(1)	20(1)
C(25B)	-1312(1)	5482(1)	978(1)	20(1)
C(26B)	-517(1)	5374(1)	1289(1)	19(1)
C(27B)	-129(1)	6048(1)	1358(1)	15(1)
C(28B)	722(1)	8194(1)	554(1)	14(1)

C(29B)	1003(1)	9020(1)	394(1)	20(1)
C(30B)	1590(1)	9414(2)	-171(1)	24(1)
C(31B)	1903(1)	9007(2)	-585(1)	24(1)
C(32B)	1637(1)	8190(2)	-421(1)	26(1)
C(33B)	1055(1)	7784(1)	147(1)	21(1)
C(34B)	667(1)	9305(1)	2042(1)	16(1)
C(35B)	153(1)	9980(1)	1614(1)	19(1)
C(36B)	523(2)	10741(1)	1159(1)	26(1)
C(37B)	1412(2)	10843(2)	1133(1)	34(1)
C(38B)	1931(2)	10185(2)	1564(1)	35(1)
C(39B)	1566(1)	9418(2)	2007(1)	25(1)
C(40B)	542(1)	8194(1)	3501(1)	16(1)
C(41B)	26(1)	8477(1)	3925(1)	22(1)
C(42B)	307(2)	8390(2)	4578(1)	32(1)
C(43B)	1103(2)	8013(2)	4814(1)	31(1)
C(44B)	1621(2)	7732(1)	4394(1)	27(1)
C(45B)	1347(1)	7820(1)	3740(1)	20(1)
C(46B)	2798(1)	7199(1)	2442(1)	15(1)
C(47B)	2950(1)	6651(1)	3151(1)	16(1)
C(48B)	3704(1)	6769(1)	3452(1)	18(1)
C(49B)	4309(1)	7392(1)	3076(1)	17(1)
C(50B)	4150(1)	7912(1)	2375(1)	18(1)
C(51B)	3409(1)	7831(1)	2044(1)	16(1)
C(52B)	2348(1)	5913(1)	3567(1)	18(1)
C(53B)	2343(1)	5621(2)	4372(1)	23(1)
C(54B)	2576(1)	5172(1)	3366(1)	25(1)
C(55B)	5133(1)	7529(1)	3400(1)	19(1)
C(56B)	5114(2)	7113(2)	4202(1)	34(1)
C(57B)	5939(1)	7225(2)	3106(1)	24(1)
C(58B)	3283(1)	8390(1)	1267(1)	20(1)
C(59B)	3767(2)	9232(1)	978(1)	29(1)
C(60B)	3557(1)	7899(2)	815(1)	26(1)

---

**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj51.**

---

Co(1A)-S(1A)	2.1547(6)
Co(1A)-P(1A)	2.2019(6)
Co(1A)-P(3A)	2.2046(6)
Co(1A)-P(2A)	2.2802(6)
S(1A)-C(46A)	1.802(2)
Co(1B)-S(1B)	2.1403(6)
Co(1B)-P(1B)	2.2098(6)
Co(1B)-P(3B)	2.2209(6)
Co(1B)-P(2B)	2.2419(6)
S(1B)-C(46B)	1.790(2)
<hr/>	
S(1A)-Co(1A)-P(1A)	143.37(2)
S(1A)-Co(1A)-P(3A)	119.75(2)
P(1A)-Co(1A)-P(3A)	88.14(2)
S(1A)-Co(1A)-P(2A)	107.92(2)
P(1A)-Co(1A)-P(2A)	89.26(2)
P(3A)-Co(1A)-P(2A)	98.04(2)
C(46A)-S(1A)-Co(1A)	123.17(7)
S(1B)-Co(1B)-P(1B)	148.38(2)
S(1B)-Co(1B)-P(3B)	121.15(2)
P(1B)-Co(1B)-P(3B)	88.62(2)
S(1B)-Co(1B)-P(2B)	95.37(2)
P(1B)-Co(1B)-P(2B)	90.10(2)
P(3B)-Co(1B)-P(2B)	98.17(2)
C(46B)-S(1B)-Co(1B)	120.71(7)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj51.**

---

Co(1A)-S(1A)	2.1547(6)
Co(1A)-P(1A)	2.2019(6)
Co(1A)-P(3A)	2.2046(6)
Co(1A)-P(2A)	2.2802(6)
S(1A)-C(46A)	1.802(2)
P(1A)-C(7A)	1.8024(19)
P(1A)-C(16A)	1.831(2)
P(1A)-C(10A)	1.836(2)
P(2A)-C(8A)	1.8196(19)
P(2A)-C(22A)	1.837(2)
P(2A)-C(28A)	1.847(2)
P(3A)-C(9A)	1.8217(19)
P(3A)-C(40A)	1.827(2)
P(3A)-C(34A)	1.837(2)
B(1A)-C(1A)	1.637(3)
B(1A)-C(8A)	1.665(3)
B(1A)-C(9A)	1.665(3)
B(1A)-C(7A)	1.680(3)
C(1A)-C(6A)	1.399(3)
C(1A)-C(2A)	1.403(3)
C(2A)-C(3A)	1.392(3)
C(2A)-H(2A)	0.9500
C(3A)-C(4A)	1.372(3)
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.381(3)
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.386(3)
C(5A)-H(5A)	0.9500
C(6A)-H(6A)	0.9500
C(7A)-H(7A1)	0.9900
C(7A)-H(7A2)	0.9900
C(8A)-H(8A1)	0.9900
C(8A)-H(8A2)	0.9900
C(9A)-H(9A1)	0.9900
C(9A)-H(9A2)	0.9900
C(10A)-C(15A)	1.390(3)
C(10A)-C(11A)	1.398(3)
C(11A)-C(12A)	1.387(3)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.382(3)
C(12A)-H(12A)	0.9500
C(13A)-C(14A)	1.379(3)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.381(3)
C(14A)-H(14A)	0.9500
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.389(3)
C(16A)-C(21A)	1.395(3)
C(17A)-C(18A)	1.393(3)
C(17A)-H(17A)	0.9500
C(18A)-C(19A)	1.387(3)

C(18A)-H(18A)	0.9500
C(19A)-C(20A)	1.373(3)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.395(3)
C(20A)-H(20A)	0.9500
C(21A)-H(21A)	0.9500
C(22A)-C(27A)	1.391(3)
C(22A)-C(23A)	1.398(3)
C(23A)-C(24A)	1.387(3)
C(23A)-H(23A)	0.9500
C(24A)-C(25A)	1.381(3)
C(24A)-H(24A)	0.9500
C(25A)-C(26A)	1.389(3)
C(25A)-H(25A)	0.9500
C(26A)-C(27A)	1.385(3)
C(26A)-H(26A)	0.9500
C(27A)-H(27A)	0.9500
C(28A)-C(29A)	1.389(3)
C(28A)-C(33A)	1.393(3)
C(29A)-C(30A)	1.384(3)
C(29A)-H(29A)	0.9500
C(30A)-C(31A)	1.382(3)
C(30A)-H(30A)	0.9500
C(31A)-C(32A)	1.373(3)
C(31A)-H(31A)	0.9500
C(32A)-C(33A)	1.389(3)
C(32A)-H(32A)	0.9500
C(33A)-H(33A)	0.9500
C(34A)-C(39A)	1.388(3)
C(34A)-C(35A)	1.398(3)
C(35A)-C(36A)	1.384(3)
C(35A)-H(35A)	0.9500
C(36A)-C(37A)	1.387(3)
C(36A)-H(36A)	0.9500
C(37A)-C(38A)	1.383(3)
C(37A)-H(37A)	0.9500
C(38A)-C(39A)	1.385(3)
C(38A)-H(38A)	0.9500
C(39A)-H(39A)	0.9500
C(40A)-C(41A)	1.394(3)
C(40A)-C(45A)	1.400(3)
C(41A)-C(42A)	1.389(3)
C(41A)-H(41A)	0.9500
C(42A)-C(43A)	1.386(3)
C(42A)-H(42A)	0.9500
C(43A)-C(44A)	1.386(3)
C(43A)-H(43A)	0.9500
C(44A)-C(45A)	1.382(3)
C(44A)-H(44A)	0.9500
C(45A)-H(45A)	0.9500
C(46A)-C(51A)	1.405(3)
C(46A)-C(47A)	1.418(3)
C(47A)-C(48A)	1.394(3)
C(47A)-C(52A)	1.515(3)

C(48A)-C(49A)	1.390(3)
C(48A)-H(48A)	0.9500
C(49A)-C(50A)	1.390(3)
C(49A)-C(55A)	1.519(3)
C(50A)-C(51A)	1.405(3)
C(50A)-H(50A)	0.9500
C(51A)-C(58A)	1.518(3)
C(52A)-C(54A)	1.517(3)
C(52A)-C(53A)	1.537(3)
C(52A)-H(52A)	1.0000
C(53A)-H(53A)	0.9800
C(53A)-H(53B)	0.9800
C(53A)-H(53C)	0.9800
C(54A)-H(54A)	0.9800
C(54A)-H(54B)	0.9800
C(54A)-H(54C)	0.9800
C(55A)-C(57A)	1.523(3)
C(55A)-C(56A)	1.540(3)
C(55A)-H(55A)	1.0000
C(56A)-H(56A)	0.9800
C(56A)-H(56B)	0.9800
C(56A)-H(56C)	0.9800
C(57A)-H(57A)	0.9800
C(57A)-H(57B)	0.9800
C(57A)-H(57C)	0.9800
C(58A)-C(60A)	1.523(3)
C(58A)-C(59A)	1.536(3)
C(58A)-H(58A)	1.0000
C(59A)-H(59A)	0.9800
C(59A)-H(59B)	0.9800
C(59A)-H(59C)	0.9800
C(60A)-H(60A)	0.9800
C(60A)-H(60B)	0.9800
C(60A)-H(60C)	0.9800
Co(1B)-S(1B)	2.1403(6)
Co(1B)-P(1B)	2.2098(6)
Co(1B)-P(3B)	2.2209(6)
Co(1B)-P(2B)	2.2419(6)
S(1B)-C(46B)	1.790(2)
P(1B)-C(7B)	1.8091(19)
P(1B)-C(16B)	1.836(2)
P(1B)-C(10B)	1.837(2)
P(2B)-C(8B)	1.8115(19)
P(2B)-C(22B)	1.834(2)
P(2B)-C(28B)	1.836(2)
P(3B)-C(9B)	1.811(2)
P(3B)-C(40B)	1.832(2)
P(3B)-C(34B)	1.835(2)
B(1B)-C(1B)	1.631(3)
B(1B)-C(9B)	1.669(3)
B(1B)-C(8B)	1.673(3)
B(1B)-C(7B)	1.678(3)
C(1B)-C(2B)	1.401(3)
C(1B)-C(6B)	1.402(3)

C(2B)-C(3B)	1.394(3)
C(2B)-H(2B)	0.9500
C(3B)-C(4B)	1.374(3)
C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.383(3)
C(4B)-H(4B)	0.9500
C(5B)-C(6B)	1.386(3)
C(5B)-H(5B)	0.9500
C(6B)-H(6B)	0.9500
C(7B)-H(7B1)	0.9900
C(7B)-H(7B2)	0.9900
C(8B)-H(8B1)	0.9900
C(8B)-H(8B2)	0.9900
C(9B)-H(9B1)	0.9900
C(9B)-H(9B2)	0.9900
C(10B)-C(15B)	1.391(3)
C(10B)-C(11B)	1.398(3)
C(11B)-C(12B)	1.388(3)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.378(3)
C(12B)-H(12B)	0.9500
C(13B)-C(14B)	1.376(3)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.388(3)
C(14B)-H(14B)	0.9500
C(15B)-H(15B)	0.9500
C(16B)-C(17B)	1.394(3)
C(16B)-C(21B)	1.400(3)
C(17B)-C(18B)	1.398(3)
C(17B)-H(17B)	0.9500
C(18B)-C(19B)	1.387(3)
C(18B)-H(18B)	0.9500
C(19B)-C(20B)	1.384(3)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.387(3)
C(20B)-H(20B)	0.9500
C(21B)-H(21B)	0.9500
C(22B)-C(27B)	1.389(3)
C(22B)-C(23B)	1.398(3)
C(23B)-C(24B)	1.388(3)
C(23B)-H(23B)	0.9500
C(24B)-C(25B)	1.387(3)
C(24B)-H(24B)	0.9500
C(25B)-C(26B)	1.382(3)
C(25B)-H(25B)	0.9500
C(26B)-C(27B)	1.385(3)
C(26B)-H(26B)	0.9500
C(27B)-H(27B)	0.9500
C(28B)-C(33B)	1.384(3)
C(28B)-C(29B)	1.403(3)
C(29B)-C(30B)	1.388(3)
C(29B)-H(29B)	0.9500
C(30B)-C(31B)	1.384(3)
C(30B)-H(30B)	0.9500

C(31B)-C(32B)	1.379(3)
C(31B)-H(31B)	0.9500
C(32B)-C(33B)	1.391(3)
C(32B)-H(32B)	0.9500
C(33B)-H(33B)	0.9500
C(34B)-C(39B)	1.395(3)
C(34B)-C(35B)	1.396(3)
C(35B)-C(36B)	1.383(3)
C(35B)-H(35B)	0.9500
C(36B)-C(37B)	1.378(3)
C(36B)-H(36B)	0.9500
C(37B)-C(38B)	1.385(3)
C(37B)-H(37B)	0.9500
C(38B)-C(39B)	1.381(3)
C(38B)-H(38B)	0.9500
C(39B)-H(39B)	0.9500
C(40B)-C(41B)	1.386(3)
C(40B)-C(45B)	1.397(3)
C(41B)-C(42B)	1.391(3)
C(41B)-H(41B)	0.9500
C(42B)-C(43B)	1.385(3)
C(42B)-H(42B)	0.9500
C(43B)-C(44B)	1.380(3)
C(43B)-H(43B)	0.9500
C(44B)-C(45B)	1.389(3)
C(44B)-H(44B)	0.9500
C(45B)-H(45B)	0.9500
C(46B)-C(51B)	1.413(3)
C(46B)-C(47B)	1.413(3)
C(47B)-C(48B)	1.401(3)
C(47B)-C(52B)	1.520(3)
C(48B)-C(49B)	1.388(3)
C(48B)-H(48B)	0.9500
C(49B)-C(50B)	1.392(3)
C(49B)-C(55B)	1.531(3)
C(50B)-C(51B)	1.397(3)
C(50B)-H(50B)	0.9500
C(51B)-C(58B)	1.521(3)
C(52B)-C(54B)	1.533(3)
C(52B)-C(53B)	1.537(3)
C(52B)-H(52B)	1.0000
C(53B)-H(53D)	0.9800
C(53B)-H(53E)	0.9800
C(53B)-H(53F)	0.9800
C(54B)-H(54D)	0.9800
C(54B)-H(54E)	0.9800
C(54B)-H(54F)	0.9800
C(55B)-C(56B)	1.518(3)
C(55B)-C(57B)	1.533(3)
C(55B)-H(55B)	1.0000
C(56B)-H(56D)	0.9800
C(56B)-H(56E)	0.9800
C(56B)-H(56F)	0.9800
C(57B)-H(57D)	0.9800

C(57B)-H(57E)	0.9800
C(57B)-H(57F)	0.9800
C(58B)-C(59B)	1.525(3)
C(58B)-C(60B)	1.546(3)
C(58B)-H(58B)	1.0000
C(59B)-H(59D)	0.9800
C(59B)-H(59E)	0.9800
C(59B)-H(59F)	0.9800
C(60B)-H(60D)	0.9800
C(60B)-H(60E)	0.9800
C(60B)-H(60F)	0.9800
S(1A)-Co(1A)-P(1A)	143.37(2)
S(1A)-Co(1A)-P(3A)	119.75(2)
P(1A)-Co(1A)-P(3A)	88.14(2)
S(1A)-Co(1A)-P(2A)	107.92(2)
P(1A)-Co(1A)-P(2A)	89.26(2)
P(3A)-Co(1A)-P(2A)	98.04(2)
C(46A)-S(1A)-Co(1A)	123.17(7)
C(7A)-P(1A)-C(16A)	109.14(10)
C(7A)-P(1A)-C(10A)	106.35(9)
C(16A)-P(1A)-C(10A)	103.08(9)
C(7A)-P(1A)-Co(1A)	115.51(7)
C(16A)-P(1A)-Co(1A)	109.04(7)
C(10A)-P(1A)-Co(1A)	112.94(7)
C(8A)-P(2A)-C(22A)	107.29(10)
C(8A)-P(2A)-C(28A)	105.07(9)
C(22A)-P(2A)-C(28A)	100.61(9)
C(8A)-P(2A)-Co(1A)	108.40(7)
C(22A)-P(2A)-Co(1A)	115.42(7)
C(28A)-P(2A)-Co(1A)	119.03(7)
C(9A)-P(3A)-C(40A)	108.37(9)
C(9A)-P(3A)-C(34A)	104.18(9)
C(40A)-P(3A)-C(34A)	101.96(10)
C(9A)-P(3A)-Co(1A)	113.11(7)
C(40A)-P(3A)-Co(1A)	114.22(7)
C(34A)-P(3A)-Co(1A)	113.97(7)
C(1A)-B(1A)-C(8A)	110.86(17)
C(1A)-B(1A)-C(9A)	108.62(17)
C(8A)-B(1A)-C(9A)	110.02(16)
C(1A)-B(1A)-C(7A)	107.77(16)
C(8A)-B(1A)-C(7A)	109.64(17)
C(9A)-B(1A)-C(7A)	109.91(17)
C(6A)-C(1A)-C(2A)	114.94(19)
C(6A)-C(1A)-B(1A)	123.44(19)
C(2A)-C(1A)-B(1A)	121.61(19)
C(3A)-C(2A)-C(1A)	122.4(2)
C(3A)-C(2A)-H(2A)	118.8
C(1A)-C(2A)-H(2A)	118.8
C(4A)-C(3A)-C(2A)	120.7(2)
C(4A)-C(3A)-H(3A)	119.6
C(2A)-C(3A)-H(3A)	119.6
C(3A)-C(4A)-C(5A)	118.6(2)
C(3A)-C(4A)-H(4A)	120.7

C(5A)-C(4A)-H(4A)	120.7
C(4A)-C(5A)-C(6A)	120.5(2)
C(4A)-C(5A)-H(5A)	119.7
C(6A)-C(5A)-H(5A)	119.7
C(5A)-C(6A)-C(1A)	122.8(2)
C(5A)-C(6A)-H(6A)	118.6
C(1A)-C(6A)-H(6A)	118.6
B(1A)-C(7A)-P(1A)	111.59(13)
B(1A)-C(7A)-H(7A1)	109.3
P(1A)-C(7A)-H(7A1)	109.3
B(1A)-C(7A)-H(7A2)	109.3
P(1A)-C(7A)-H(7A2)	109.3
H(7A1)-C(7A)-H(7A2)	108.0
B(1A)-C(8A)-P(2A)	115.96(13)
B(1A)-C(8A)-H(8A1)	108.3
P(2A)-C(8A)-H(8A1)	108.3
B(1A)-C(8A)-H(8A2)	108.3
P(2A)-C(8A)-H(8A2)	108.3
H(8A1)-C(8A)-H(8A2)	107.4
B(1A)-C(9A)-P(3A)	116.12(14)
B(1A)-C(9A)-H(9A1)	108.3
P(3A)-C(9A)-H(9A1)	108.3
B(1A)-C(9A)-H(9A2)	108.3
P(3A)-C(9A)-H(9A2)	108.3
H(9A1)-C(9A)-H(9A2)	107.4
C(15A)-C(10A)-C(11A)	118.31(19)
C(15A)-C(10A)-P(1A)	118.22(16)
C(11A)-C(10A)-P(1A)	123.40(16)
C(12A)-C(11A)-C(10A)	120.5(2)
C(12A)-C(11A)-H(11A)	119.7
C(10A)-C(11A)-H(11A)	119.7
C(13A)-C(12A)-C(11A)	120.1(2)
C(13A)-C(12A)-H(12A)	119.9
C(11A)-C(12A)-H(12A)	119.9
C(14A)-C(13A)-C(12A)	119.8(2)
C(14A)-C(13A)-H(13A)	120.1
C(12A)-C(13A)-H(13A)	120.1
C(13A)-C(14A)-C(15A)	120.2(2)
C(13A)-C(14A)-H(14A)	119.9
C(15A)-C(14A)-H(14A)	119.9
C(14A)-C(15A)-C(10A)	121.0(2)
C(14A)-C(15A)-H(15A)	119.5
C(10A)-C(15A)-H(15A)	119.5
C(17A)-C(16A)-C(21A)	118.49(19)
C(17A)-C(16A)-P(1A)	120.65(16)
C(21A)-C(16A)-P(1A)	120.85(16)
C(16A)-C(17A)-C(18A)	120.8(2)
C(16A)-C(17A)-H(17A)	119.6
C(18A)-C(17A)-H(17A)	119.6
C(19A)-C(18A)-C(17A)	119.7(2)
C(19A)-C(18A)-H(18A)	120.2
C(17A)-C(18A)-H(18A)	120.2
C(20A)-C(19A)-C(18A)	120.4(2)
C(20A)-C(19A)-H(19A)	119.8

C(18A)-C(19A)-H(19A)	119.8
C(19A)-C(20A)-C(21A)	119.8(2)
C(19A)-C(20A)-H(20A)	120.1
C(21A)-C(20A)-H(20A)	120.1
C(20A)-C(21A)-C(16A)	120.8(2)
C(20A)-C(21A)-H(21A)	119.6
C(16A)-C(21A)-H(21A)	119.6
C(27A)-C(22A)-C(23A)	118.0(2)
C(27A)-C(22A)-P(2A)	117.52(16)
C(23A)-C(22A)-P(2A)	124.45(16)
C(24A)-C(23A)-C(22A)	120.7(2)
C(24A)-C(23A)-H(23A)	119.7
C(22A)-C(23A)-H(23A)	119.7
C(25A)-C(24A)-C(23A)	120.6(2)
C(25A)-C(24A)-H(24A)	119.7
C(23A)-C(24A)-H(24A)	119.7
C(24A)-C(25A)-C(26A)	119.3(2)
C(24A)-C(25A)-H(25A)	120.4
C(26A)-C(25A)-H(25A)	120.4
C(27A)-C(26A)-C(25A)	120.1(2)
C(27A)-C(26A)-H(26A)	119.9
C(25A)-C(26A)-H(26A)	119.9
C(26A)-C(27A)-C(22A)	121.3(2)
C(26A)-C(27A)-H(27A)	119.4
C(22A)-C(27A)-H(27A)	119.4
C(29A)-C(28A)-C(33A)	117.67(19)
C(29A)-C(28A)-P(2A)	120.05(16)
C(33A)-C(28A)-P(2A)	122.18(16)
C(30A)-C(29A)-C(28A)	121.4(2)
C(30A)-C(29A)-H(29A)	119.3
C(28A)-C(29A)-H(29A)	119.3
C(31A)-C(30A)-C(29A)	120.1(2)
C(31A)-C(30A)-H(30A)	119.9
C(29A)-C(30A)-H(30A)	119.9
C(32A)-C(31A)-C(30A)	119.2(2)
C(32A)-C(31A)-H(31A)	120.4
C(30A)-C(31A)-H(31A)	120.4
C(31A)-C(32A)-C(33A)	120.8(2)
C(31A)-C(32A)-H(32A)	119.6
C(33A)-C(32A)-H(32A)	119.6
C(32A)-C(33A)-C(28A)	120.7(2)
C(32A)-C(33A)-H(33A)	119.6
C(28A)-C(33A)-H(33A)	119.6
C(39A)-C(34A)-C(35A)	118.3(2)
C(39A)-C(34A)-P(3A)	120.56(16)
C(35A)-C(34A)-P(3A)	121.04(16)
C(36A)-C(35A)-C(34A)	120.5(2)
C(36A)-C(35A)-H(35A)	119.8
C(34A)-C(35A)-H(35A)	119.8
C(35A)-C(36A)-C(37A)	120.3(2)
C(35A)-C(36A)-H(36A)	119.8
C(37A)-C(36A)-H(36A)	119.8
C(38A)-C(37A)-C(36A)	119.7(2)
C(38A)-C(37A)-H(37A)	120.1

C(36A)-C(37A)-H(37A)	120.1
C(37A)-C(38A)-C(39A)	119.8(2)
C(37A)-C(38A)-H(38A)	120.1
C(39A)-C(38A)-H(38A)	120.1
C(38A)-C(39A)-C(34A)	121.3(2)
C(38A)-C(39A)-H(39A)	119.3
C(34A)-C(39A)-H(39A)	119.3
C(41A)-C(40A)-C(45A)	118.5(2)
C(41A)-C(40A)-P(3A)	124.11(16)
C(45A)-C(40A)-P(3A)	117.40(16)
C(42A)-C(41A)-C(40A)	120.7(2)
C(42A)-C(41A)-H(41A)	119.7
C(40A)-C(41A)-H(41A)	119.7
C(43A)-C(42A)-C(41A)	120.3(2)
C(43A)-C(42A)-H(42A)	119.9
C(41A)-C(42A)-H(42A)	119.9
C(42A)-C(43A)-C(44A)	119.3(2)
C(42A)-C(43A)-H(43A)	120.4
C(44A)-C(43A)-H(43A)	120.4
C(45A)-C(44A)-C(43A)	120.8(2)
C(45A)-C(44A)-H(44A)	119.6
C(43A)-C(44A)-H(44A)	119.6
C(44A)-C(45A)-C(40A)	120.4(2)
C(44A)-C(45A)-H(45A)	119.8
C(40A)-C(45A)-H(45A)	119.8
C(51A)-C(46A)-C(47A)	120.19(19)
C(51A)-C(46A)-S(1A)	121.39(17)
C(47A)-C(46A)-S(1A)	118.20(16)
C(48A)-C(47A)-C(46A)	118.12(19)
C(48A)-C(47A)-C(52A)	119.1(2)
C(46A)-C(47A)-C(52A)	122.77(19)
C(49A)-C(48A)-C(47A)	123.2(2)
C(49A)-C(48A)-H(48A)	118.4
C(47A)-C(48A)-H(48A)	118.4
C(48A)-C(49A)-C(50A)	117.13(19)
C(48A)-C(49A)-C(55A)	119.35(19)
C(50A)-C(49A)-C(55A)	123.52(19)
C(49A)-C(50A)-C(51A)	122.7(2)
C(49A)-C(50A)-H(50A)	118.7
C(51A)-C(50A)-H(50A)	118.7
C(50A)-C(51A)-C(46A)	118.4(2)
C(50A)-C(51A)-C(58A)	119.24(19)
C(46A)-C(51A)-C(58A)	122.35(19)
C(47A)-C(52A)-C(54A)	111.01(18)
C(47A)-C(52A)-C(53A)	111.64(19)
C(54A)-C(52A)-C(53A)	111.9(2)
C(47A)-C(52A)-H(52A)	107.3
C(54A)-C(52A)-H(52A)	107.3
C(53A)-C(52A)-H(52A)	107.3
C(52A)-C(53A)-H(53A)	109.5
C(52A)-C(53A)-H(53B)	109.5
H(53A)-C(53A)-H(53B)	109.5
C(52A)-C(53A)-H(53C)	109.5
H(53A)-C(53A)-H(53C)	109.5

H(53B)-C(53A)-H(53C)	109.5
C(52A)-C(54A)-H(54A)	109.5
C(52A)-C(54A)-H(54B)	109.5
H(54A)-C(54A)-H(54B)	109.5
C(52A)-C(54A)-H(54C)	109.5
H(54A)-C(54A)-H(54C)	109.5
H(54B)-C(54A)-H(54C)	109.5
C(49A)-C(55A)-C(57A)	114.28(18)
C(49A)-C(55A)-C(56A)	110.48(18)
C(57A)-C(55A)-C(56A)	110.10(17)
C(49A)-C(55A)-H(55A)	107.2
C(57A)-C(55A)-H(55A)	107.2
C(56A)-C(55A)-H(55A)	107.2
C(55A)-C(56A)-H(56A)	109.5
C(55A)-C(56A)-H(56B)	109.5
H(56A)-C(56A)-H(56B)	109.5
C(55A)-C(56A)-H(56C)	109.5
H(56A)-C(56A)-H(56C)	109.5
H(56B)-C(56A)-H(56C)	109.5
C(55A)-C(57A)-H(57A)	109.5
C(55A)-C(57A)-H(57B)	109.5
H(57A)-C(57A)-H(57B)	109.5
C(55A)-C(57A)-H(57C)	109.5
H(57A)-C(57A)-H(57C)	109.5
H(57B)-C(57A)-H(57C)	109.5
C(51A)-C(58A)-C(60A)	111.58(17)
C(51A)-C(58A)-C(59A)	112.27(18)
C(60A)-C(58A)-C(59A)	110.31(18)
C(51A)-C(58A)-H(58A)	107.5
C(60A)-C(58A)-H(58A)	107.5
C(59A)-C(58A)-H(58A)	107.5
C(58A)-C(59A)-H(59A)	109.5
C(58A)-C(59A)-H(59B)	109.5
H(59A)-C(59A)-H(59B)	109.5
C(58A)-C(59A)-H(59C)	109.5
H(59A)-C(59A)-H(59C)	109.5
H(59B)-C(59A)-H(59C)	109.5
C(58A)-C(60A)-H(60A)	109.5
C(58A)-C(60A)-H(60B)	109.5
H(60A)-C(60A)-H(60B)	109.5
C(58A)-C(60A)-H(60C)	109.5
H(60A)-C(60A)-H(60C)	109.5
H(60B)-C(60A)-H(60C)	109.5
S(1B)-Co(1B)-P(1B)	148.38(2)
S(1B)-Co(1B)-P(3B)	121.15(2)
P(1B)-Co(1B)-P(3B)	88.62(2)
S(1B)-Co(1B)-P(2B)	95.37(2)
P(1B)-Co(1B)-P(2B)	90.10(2)
P(3B)-Co(1B)-P(2B)	98.17(2)
C(46B)-S(1B)-Co(1B)	120.71(7)
C(7B)-P(1B)-C(16B)	109.40(10)
C(7B)-P(1B)-C(10B)	107.13(9)
C(16B)-P(1B)-C(10B)	101.48(9)
C(7B)-P(1B)-Co(1B)	113.81(7)

C(16B)-P(1B)-Co(1B)	110.82(7)
C(10B)-P(1B)-Co(1B)	113.42(7)
C(8B)-P(2B)-C(22B)	106.52(9)
C(8B)-P(2B)-C(28B)	107.24(9)
C(22B)-P(2B)-C(28B)	103.21(9)
C(8B)-P(2B)-Co(1B)	107.90(7)
C(22B)-P(2B)-Co(1B)	115.70(7)
C(28B)-P(2B)-Co(1B)	115.64(7)
C(9B)-P(3B)-C(40B)	108.17(10)
C(9B)-P(3B)-C(34B)	104.65(9)
C(40B)-P(3B)-C(34B)	101.76(10)
C(9B)-P(3B)-Co(1B)	111.83(7)
C(40B)-P(3B)-Co(1B)	114.85(7)
C(34B)-P(3B)-Co(1B)	114.62(7)
C(1B)-B(1B)-C(9B)	109.87(17)
C(1B)-B(1B)-C(8B)	108.17(16)
C(9B)-B(1B)-C(8B)	111.88(16)
C(1B)-B(1B)-C(7B)	109.27(16)
C(9B)-B(1B)-C(7B)	108.17(16)
C(8B)-B(1B)-C(7B)	109.46(16)
C(2B)-C(1B)-C(6B)	114.73(18)
C(2B)-C(1B)-B(1B)	123.35(19)
C(6B)-C(1B)-B(1B)	121.91(18)
C(3B)-C(2B)-C(1B)	122.7(2)
C(3B)-C(2B)-H(2B)	118.7
C(1B)-C(2B)-H(2B)	118.7
C(4B)-C(3B)-C(2B)	120.4(2)
C(4B)-C(3B)-H(3B)	119.8
C(2B)-C(3B)-H(3B)	119.8
C(3B)-C(4B)-C(5B)	118.9(2)
C(3B)-C(4B)-H(4B)	120.5
C(5B)-C(4B)-H(4B)	120.5
C(4B)-C(5B)-C(6B)	120.1(2)
C(4B)-C(5B)-H(5B)	120.0
C(6B)-C(5B)-H(5B)	120.0
C(5B)-C(6B)-C(1B)	123.2(2)
C(5B)-C(6B)-H(6B)	118.4
C(1B)-C(6B)-H(6B)	118.4
B(1B)-C(7B)-P(1B)	111.26(13)
B(1B)-C(7B)-H(7B1)	109.4
P(1B)-C(7B)-H(7B1)	109.4
B(1B)-C(7B)-H(7B2)	109.4
P(1B)-C(7B)-H(7B2)	109.4
H(7B1)-C(7B)-H(7B2)	108.0
B(1B)-C(8B)-P(2B)	115.46(13)
B(1B)-C(8B)-H(8B1)	108.4
P(2B)-C(8B)-H(8B1)	108.4
B(1B)-C(8B)-H(8B2)	108.4
P(2B)-C(8B)-H(8B2)	108.4
H(8B1)-C(8B)-H(8B2)	107.5
B(1B)-C(9B)-P(3B)	114.63(14)
B(1B)-C(9B)-H(9B1)	108.6
P(3B)-C(9B)-H(9B1)	108.6
B(1B)-C(9B)-H(9B2)	108.6

P(3B)-C(9B)-H(9B2)	108.6
H(9B1)-C(9B)-H(9B2)	107.6
C(15B)-C(10B)-C(11B)	118.4(2)
C(15B)-C(10B)-P(1B)	117.98(16)
C(11B)-C(10B)-P(1B)	123.53(16)
C(12B)-C(11B)-C(10B)	120.3(2)
C(12B)-C(11B)-H(11B)	119.9
C(10B)-C(11B)-H(11B)	119.9
C(13B)-C(12B)-C(11B)	120.4(2)
C(13B)-C(12B)-H(12B)	119.8
C(11B)-C(12B)-H(12B)	119.8
C(14B)-C(13B)-C(12B)	120.1(2)
C(14B)-C(13B)-H(13B)	120.0
C(12B)-C(13B)-H(13B)	120.0
C(13B)-C(14B)-C(15B)	120.0(2)
C(13B)-C(14B)-H(14B)	120.0
C(15B)-C(14B)-H(14B)	120.0
C(14B)-C(15B)-C(10B)	120.8(2)
C(14B)-C(15B)-H(15B)	119.6
C(10B)-C(15B)-H(15B)	119.6
C(17B)-C(16B)-C(21B)	118.9(2)
C(17B)-C(16B)-P(1B)	121.12(16)
C(21B)-C(16B)-P(1B)	120.00(16)
C(16B)-C(17B)-C(18B)	120.6(2)
C(16B)-C(17B)-H(17B)	119.7
C(18B)-C(17B)-H(17B)	119.7
C(19B)-C(18B)-C(17B)	119.6(2)
C(19B)-C(18B)-H(18B)	120.2
C(17B)-C(18B)-H(18B)	120.2
C(20B)-C(19B)-C(18B)	120.2(2)
C(20B)-C(19B)-H(19B)	119.9
C(18B)-C(19B)-H(19B)	119.9
C(19B)-C(20B)-C(21B)	120.3(2)
C(19B)-C(20B)-H(20B)	119.9
C(21B)-C(20B)-H(20B)	119.9
C(20B)-C(21B)-C(16B)	120.4(2)
C(20B)-C(21B)-H(21B)	119.8
C(16B)-C(21B)-H(21B)	119.8
C(27B)-C(22B)-C(23B)	118.37(19)
C(27B)-C(22B)-P(2B)	117.61(15)
C(23B)-C(22B)-P(2B)	123.86(15)
C(24B)-C(23B)-C(22B)	120.47(19)
C(24B)-C(23B)-H(23B)	119.8
C(22B)-C(23B)-H(23B)	119.8
C(25B)-C(24B)-C(23B)	120.2(2)
C(25B)-C(24B)-H(24B)	119.9
C(23B)-C(24B)-H(24B)	119.9
C(26B)-C(25B)-C(24B)	119.6(2)
C(26B)-C(25B)-H(25B)	120.2
C(24B)-C(25B)-H(25B)	120.2
C(25B)-C(26B)-C(27B)	120.1(2)
C(25B)-C(26B)-H(26B)	119.9
C(27B)-C(26B)-H(26B)	119.9
C(26B)-C(27B)-C(22B)	121.06(19)

C(26B)-C(27B)-H(27B)	119.5
C(22B)-C(27B)-H(27B)	119.5
C(33B)-C(28B)-C(29B)	118.55(19)
C(33B)-C(28B)-P(2B)	121.56(16)
C(29B)-C(28B)-P(2B)	119.79(16)
C(30B)-C(29B)-C(28B)	119.9(2)
C(30B)-C(29B)-H(29B)	120.0
C(28B)-C(29B)-H(29B)	120.0
C(31B)-C(30B)-C(29B)	121.1(2)
C(31B)-C(30B)-H(30B)	119.5
C(29B)-C(30B)-H(30B)	119.5
C(32B)-C(31B)-C(30B)	118.9(2)
C(32B)-C(31B)-H(31B)	120.5
C(30B)-C(31B)-H(31B)	120.5
C(31B)-C(32B)-C(33B)	120.6(2)
C(31B)-C(32B)-H(32B)	119.7
C(33B)-C(32B)-H(32B)	119.7
C(28B)-C(33B)-C(32B)	120.9(2)
C(28B)-C(33B)-H(33B)	119.6
C(32B)-C(33B)-H(33B)	119.6
C(39B)-C(34B)-C(35B)	118.4(2)
C(39B)-C(34B)-P(3B)	119.63(16)
C(35B)-C(34B)-P(3B)	121.98(16)
C(36B)-C(35B)-C(34B)	121.1(2)
C(36B)-C(35B)-H(35B)	119.5
C(34B)-C(35B)-H(35B)	119.5
C(37B)-C(36B)-C(35B)	119.8(2)
C(37B)-C(36B)-H(36B)	120.1
C(35B)-C(36B)-H(36B)	120.1
C(36B)-C(37B)-C(38B)	119.9(2)
C(36B)-C(37B)-H(37B)	120.0
C(38B)-C(37B)-H(37B)	120.0
C(39B)-C(38B)-C(37B)	120.4(2)
C(39B)-C(38B)-H(38B)	119.8
C(37B)-C(38B)-H(38B)	119.8
C(38B)-C(39B)-C(34B)	120.4(2)
C(38B)-C(39B)-H(39B)	119.8
C(34B)-C(39B)-H(39B)	119.8
C(41B)-C(40B)-C(45B)	118.9(2)
C(41B)-C(40B)-P(3B)	122.04(16)
C(45B)-C(40B)-P(3B)	119.07(16)
C(40B)-C(41B)-C(42B)	120.5(2)
C(40B)-C(41B)-H(41B)	119.8
C(42B)-C(41B)-H(41B)	119.8
C(43B)-C(42B)-C(41B)	120.3(2)
C(43B)-C(42B)-H(42B)	119.9
C(41B)-C(42B)-H(42B)	119.9
C(44B)-C(43B)-C(42B)	119.6(2)
C(44B)-C(43B)-H(43B)	120.2
C(42B)-C(43B)-H(43B)	120.2
C(43B)-C(44B)-C(45B)	120.4(2)
C(43B)-C(44B)-H(44B)	119.8
C(45B)-C(44B)-H(44B)	119.8
C(44B)-C(45B)-C(40B)	120.4(2)

C(44B)-C(45B)-H(45B)	119.8
C(40B)-C(45B)-H(45B)	119.8
C(51B)-C(46B)-C(47B)	120.38(19)
C(51B)-C(46B)-S(1B)	117.17(16)
C(47B)-C(46B)-S(1B)	122.36(16)
C(48B)-C(47B)-C(46B)	118.4(2)
C(48B)-C(47B)-C(52B)	120.12(19)
C(46B)-C(47B)-C(52B)	121.32(19)
C(49B)-C(48B)-C(47B)	122.3(2)
C(49B)-C(48B)-H(48B)	118.8
C(47B)-C(48B)-H(48B)	118.8
C(48B)-C(49B)-C(50B)	118.0(2)
C(48B)-C(49B)-C(55B)	122.8(2)
C(50B)-C(49B)-C(55B)	119.2(2)
C(49B)-C(50B)-C(51B)	122.6(2)
C(49B)-C(50B)-H(50B)	118.7
C(51B)-C(50B)-H(50B)	118.7
C(50B)-C(51B)-C(46B)	118.31(19)
C(50B)-C(51B)-C(58B)	120.58(19)
C(46B)-C(51B)-C(58B)	121.07(19)
C(47B)-C(52B)-C(54B)	109.21(17)
C(47B)-C(52B)-C(53B)	114.77(18)
C(54B)-C(52B)-C(53B)	110.58(18)
C(47B)-C(52B)-H(52B)	107.3
C(54B)-C(52B)-H(52B)	107.3
C(53B)-C(52B)-H(52B)	107.3
C(52B)-C(53B)-H(53D)	109.5
C(52B)-C(53B)-H(53E)	109.5
H(53D)-C(53B)-H(53E)	109.5
C(52B)-C(53B)-H(53F)	109.5
H(53D)-C(53B)-H(53F)	109.5
H(53E)-C(53B)-H(53F)	109.5
C(52B)-C(54B)-H(54D)	109.5
C(52B)-C(54B)-H(54E)	109.5
H(54D)-C(54B)-H(54E)	109.5
C(52B)-C(54B)-H(54F)	109.5
H(54D)-C(54B)-H(54F)	109.5
H(54E)-C(54B)-H(54F)	109.5
C(56B)-C(55B)-C(49B)	114.25(18)
C(56B)-C(55B)-C(57B)	109.63(18)
C(49B)-C(55B)-C(57B)	110.44(17)
C(56B)-C(55B)-H(55B)	107.4
C(49B)-C(55B)-H(55B)	107.4
C(57B)-C(55B)-H(55B)	107.4
C(55B)-C(56B)-H(56D)	109.5
C(55B)-C(56B)-H(56E)	109.5
H(56D)-C(56B)-H(56E)	109.5
C(55B)-C(56B)-H(56F)	109.5
H(56D)-C(56B)-H(56F)	109.5
H(56E)-C(56B)-H(56F)	109.5
C(55B)-C(57B)-H(57D)	109.5
C(55B)-C(57B)-H(57E)	109.5
H(57D)-C(57B)-H(57E)	109.5
C(55B)-C(57B)-H(57F)	109.5

H(57D)-C(57B)-H(57F)	109.5
H(57E)-C(57B)-H(57F)	109.5
C(51B)-C(58B)-C(59B)	115.19(19)
C(51B)-C(58B)-C(60B)	109.78(17)
C(59B)-C(58B)-C(60B)	108.78(18)
C(51B)-C(58B)-H(58B)	107.6
C(59B)-C(58B)-H(58B)	107.6
C(60B)-C(58B)-H(58B)	107.6
C(58B)-C(59B)-H(59D)	109.5
C(58B)-C(59B)-H(59E)	109.5
H(59D)-C(59B)-H(59E)	109.5
C(58B)-C(59B)-H(59F)	109.5
H(59D)-C(59B)-H(59F)	109.5
H(59E)-C(59B)-H(59F)	109.5
C(58B)-C(60B)-H(60D)	109.5
C(58B)-C(60B)-H(60E)	109.5
H(60D)-C(60B)-H(60E)	109.5
C(58B)-C(60B)-H(60F)	109.5
H(60D)-C(60B)-H(60F)	109.5
H(60E)-C(60B)-H(60F)	109.5

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Symmetry transformations used to generate equivalent atoms:

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj51. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co(1A)	120(1)	122(2)	121(2)	-48(1)	-17(1)	11(1)
S(1A)	136(3)	251(3)	191(3)	-117(2)	-17(2)	17(2)
P(1A)	128(3)	129(3)	128(3)	-53(2)	-11(2)	9(2)
P(2A)	126(3)	132(3)	116(3)	-50(2)	-12(2)	12(2)
P(3A)	139(3)	125(3)	135(3)	-58(2)	-17(2)	4(2)
B(1A)	119(12)	143(13)	137(12)	-52(10)	5(9)	-3(9)
C(1A)	157(11)	91(11)	178(12)	-23(9)	13(9)	-19(8)
C(2A)	167(12)	202(12)	292(13)	-123(11)	13(10)	-1(9)
C(3A)	198(13)	230(13)	495(17)	-216(13)	116(12)	-21(10)
C(4A)	118(12)	183(13)	571(18)	-109(13)	-37(12)	33(9)
C(5A)	178(13)	377(16)	395(16)	-114(13)	-95(11)	42(11)
C(6A)	172(12)	316(14)	276(14)	-135(11)	-12(10)	33(10)
C(7A)	112(10)	164(11)	135(11)	-61(9)	-3(8)	0(8)
C(8A)	144(11)	130(11)	148(11)	-58(9)	-50(8)	61(8)
C(9A)	141(11)	135(11)	155(11)	-60(9)	6(9)	17(8)
C(10A)	169(11)	119(11)	120(11)	-46(9)	5(9)	-30(8)
C(11A)	173(11)	184(12)	154(11)	-52(9)	-5(9)	-8(9)
C(12A)	241(12)	220(13)	194(12)	-98(10)	55(10)	-31(10)
C(13A)	340(14)	220(13)	125(12)	-75(10)	8(10)	-68(10)
C(14A)	296(13)	162(12)	174(12)	-34(10)	-81(10)	-5(10)
C(15A)	213(12)	168(12)	188(12)	-69(10)	-12(9)	24(9)
C(16A)	215(12)	128(11)	95(10)	-39(9)	-24(9)	-2(9)
C(17A)	216(12)	177(12)	325(14)	-116(11)	13(10)	-9(10)
C(18A)	274(14)	226(14)	410(16)	-138(12)	8(12)	-89(11)
C(19A)	411(15)	137(12)	218(13)	-80(10)	-41(11)	-15(11)
C(20A)	292(13)	187(12)	186(12)	-74(10)	-36(10)	49(10)
C(21A)	222(12)	160(12)	156(11)	-52(9)	-19(9)	3(9)
C(22A)	195(11)	136(11)	94(10)	-45(9)	-10(9)	-13(9)
C(23A)	205(12)	192(12)	156(11)	-64(10)	-20(9)	-2(9)
C(24A)	247(13)	303(14)	178(12)	-103(11)	-49(10)	-53(11)
C(25A)	410(15)	180(13)	229(13)	-71(11)	-90(11)	-65(11)
C(26A)	452(16)	163(13)	307(14)	-126(11)	-136(12)	71(11)
C(27A)	233(12)	194(12)	240(13)	-91(10)	-77(10)	31(10)
C(28A)	177(11)	131(11)	121(11)	-54(9)	-7(9)	1(9)
C(29A)	250(13)	310(14)	183(13)	-53(11)	3(10)	107(11)
C(30A)	473(17)	274(14)	184(13)	8(11)	31(12)	137(12)
C(31A)	393(15)	209(13)	203(13)	-60(11)	122(11)	-47(11)
C(32A)	210(13)	365(15)	241(13)	-132(12)	65(10)	12(11)
C(33A)	219(12)	262(13)	182(12)	-60(10)	-13(10)	56(10)
C(34A)	113(10)	137(11)	186(12)	-47(9)	-40(9)	11(8)
C(35A)	215(12)	230(13)	275(13)	-134(11)	25(10)	15(10)
C(36A)	245(13)	169(13)	444(16)	-152(12)	-7(12)	-3(10)
C(37A)	194(12)	145(12)	350(15)	-11(11)	-16(11)	-16(9)
C(38A)	172(12)	245(13)	188(12)	-32(10)	1(9)	-32(10)
C(39A)	153(11)	184(12)	221(12)	-93(10)	-38(9)	7(9)
C(40A)	200(11)	114(11)	160(11)	-57(9)	-33(9)	-25(9)

C(41A)	186(12)	228(13)	202(12)	-109(10)	-15(9)	-7(9)
C(42A)	279(13)	313(14)	231(13)	-180(11)	29(10)	-48(11)
C(43A)	340(14)	259(14)	163(12)	-78(11)	-71(10)	-77(11)
C(44A)	231(12)	173(12)	268(13)	-66(10)	-106(10)	-15(10)
C(45A)	193(12)	172(12)	189(12)	-95(10)	-32(9)	4(9)
C(46A)	102(10)	240(12)	201(12)	-126(10)	-15(9)	26(9)
C(47A)	142(11)	174(12)	220(12)	-82(10)	13(9)	25(9)
C(48A)	148(11)	180(12)	250(13)	-81(10)	19(9)	-41(9)
C(49A)	130(11)	212(12)	213(12)	-133(10)	-8(9)	4(9)
C(50A)	173(11)	189(12)	158(11)	-72(9)	-9(9)	12(9)
C(51A)	150(11)	189(12)	167(11)	-89(10)	16(9)	8(9)
C(52A)	171(12)	235(13)	260(13)	-33(11)	-47(10)	14(10)
C(53A)	272(14)	246(14)	410(16)	-47(12)	-65(12)	29(11)
C(54A)	364(15)	426(17)	233(14)	-27(12)	4(12)	13(13)
C(55A)	157(11)	220(12)	266(13)	-150(11)	-27(10)	-15(9)
C(56A)	133(11)	267(13)	263(13)	-117(11)	-17(9)	-16(9)
C(57A)	183(12)	336(14)	236(13)	-167(11)	-22(10)	-19(10)
C(58A)	144(11)	206(12)	185(12)	-72(10)	-33(9)	-19(9)
C(59A)	212(12)	233(13)	225(13)	-99(10)	-9(10)	-28(10)
C(60A)	344(15)	327(15)	386(16)	-230(13)	103(12)	-117(12)
Co(1B)	118(1)	129(2)	125(2)	-52(1)	-21(1)	9(1)
S(1B)	125(3)	241(3)	186(3)	-117(2)	-14(2)	-3(2)
P(1B)	140(3)	130(3)	122(3)	-50(2)	-14(2)	11(2)
P(2B)	115(3)	123(3)	124(3)	-51(2)	-12(2)	8(2)
P(3B)	140(3)	135(3)	140(3)	-66(2)	-23(2)	6(2)
B(1B)	126(12)	132(12)	142(12)	-47(10)	3(9)	2(9)
C(1B)	128(10)	111(11)	137(11)	-21(9)	12(8)	-9(8)
C(2B)	139(11)	220(12)	209(12)	-115(10)	-15(9)	4(9)
C(3B)	188(12)	236(13)	378(15)	-201(12)	19(11)	-3(10)
C(4B)	123(11)	194(12)	332(14)	-77(11)	-42(10)	24(9)
C(5B)	155(12)	284(13)	226(13)	-89(11)	-45(10)	26(10)
C(6B)	145(11)	215(12)	204(12)	-105(10)	6(9)	30(9)
C(7B)	110(10)	161(11)	119(11)	-68(9)	-8(8)	7(8)
C(8B)	106(10)	119(11)	164(11)	-60(9)	-31(8)	14(8)
C(9B)	149(11)	125(11)	166(11)	-54(9)	-4(9)	10(8)
C(10B)	210(12)	105(11)	135(11)	-34(9)	-4(9)	-14(9)
C(11B)	236(12)	216(13)	155(12)	-34(10)	-27(9)	35(10)
C(12B)	318(14)	259(14)	210(13)	-98(11)	57(11)	36(11)
C(13B)	428(15)	214(13)	119(12)	-59(10)	31(11)	-71(11)
C(14B)	299(14)	239(13)	163(12)	-41(10)	-71(10)	-50(10)
C(15B)	193(12)	164(12)	201(12)	-46(10)	-28(9)	-16(9)
C(16B)	219(12)	142(11)	104(11)	-42(9)	-17(9)	-14(9)
C(17B)	215(12)	226(13)	230(13)	-93(10)	32(10)	-10(10)
C(18B)	338(14)	217(13)	283(14)	-100(11)	56(11)	-112(11)
C(19B)	481(16)	139(12)	196(13)	-72(10)	-44(11)	28(11)
C(20B)	336(14)	204(13)	176(12)	-87(10)	-68(10)	94(11)
C(21B)	204(12)	209(12)	165(12)	-83(10)	-46(9)	25(9)
C(22B)	154(11)	151(11)	101(10)	-57(9)	18(8)	-20(9)
C(23B)	200(11)	140(11)	148(11)	-51(9)	-33(9)	17(9)
C(24B)	192(12)	247(13)	169(12)	-95(10)	-43(9)	-6(10)
C(25B)	242(12)	187(12)	198(12)	-111(10)	-13(10)	-43(10)
C(26B)	252(12)	141(11)	169(12)	-55(9)	-12(10)	22(9)
C(27B)	137(11)	181(12)	116(11)	-55(9)	-12(8)	-5(9)
C(28B)	113(10)	168(11)	128(11)	-39(9)	-26(8)	17(8)

C(29B)	189(12)	193(12)	216(12)	-80(10)	8(9)	5(9)
C(30B)	217(12)	200(13)	246(13)	-19(10)	-13(10)	-5(10)
C(31B)	163(12)	309(14)	170(12)	-16(11)	48(9)	-18(10)
C(32B)	195(12)	389(15)	209(13)	-159(11)	55(10)	13(11)
C(33B)	203(12)	207(12)	217(12)	-85(10)	3(10)	-9(10)
C(34B)	182(11)	145(11)	171(11)	-83(9)	0(9)	-10(9)
C(35B)	177(11)	209(12)	190(12)	-99(10)	-8(9)	11(9)
C(36B)	312(14)	168(12)	270(14)	-60(10)	-44(11)	20(10)
C(37B)	323(15)	166(13)	431(17)	-23(12)	6(12)	-69(11)
C(38B)	218(13)	348(16)	453(17)	-127(13)	22(12)	-79(11)
C(39B)	207(12)	229(13)	293(14)	-83(11)	-16(10)	21(10)
C(40B)	202(11)	116(11)	152(11)	-53(9)	-40(9)	-27(9)
C(41B)	211(12)	244(13)	228(13)	-124(11)	-14(10)	-18(10)
C(42B)	396(16)	372(16)	241(14)	-190(12)	23(12)	-60(12)
C(43B)	423(16)	317(15)	197(13)	-102(12)	-85(12)	-100(12)
C(44B)	309(14)	210(13)	283(14)	-82(11)	-174(11)	7(10)
C(45B)	209(12)	163(12)	255(13)	-99(10)	-47(10)	-12(9)
C(46B)	127(10)	186(12)	187(12)	-123(10)	-28(9)	24(9)
C(47B)	140(11)	193(12)	193(12)	-111(10)	6(9)	20(9)
C(48B)	164(11)	205(12)	175(12)	-100(10)	-12(9)	21(9)
C(49B)	114(11)	233(12)	230(12)	-155(10)	-27(9)	40(9)
C(50B)	148(11)	205(12)	201(12)	-107(10)	33(9)	-12(9)
C(51B)	136(11)	196(12)	168(11)	-100(10)	3(9)	35(9)
C(52B)	158(11)	201(12)	175(12)	-84(10)	-29(9)	-3(9)
C(53B)	218(12)	261(13)	193(12)	-66(10)	-25(10)	-45(10)
C(54B)	233(13)	248(13)	292(14)	-132(11)	-4(10)	-38(10)
C(55B)	177(11)	227(12)	195(12)	-111(10)	-23(9)	-4(9)
C(56B)	234(13)	608(19)	226(14)	-205(13)	-31(11)	-108(12)
C(57B)	152(11)	327(14)	243(13)	-124(11)	-19(10)	-21(10)
C(58B)	155(11)	212(12)	215(12)	-67(10)	-36(9)	16(9)
C(59B)	264(13)	269(14)	260(14)	-28(11)	-48(11)	-26(11)
C(60B)	229(13)	355(15)	179(12)	-99(11)	-2(10)	23(11)

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**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj51.**

	x	y	z	$U_{\text{iso}}$
H(2A)	734	115	230	26
H(3A)	871	52	248	35
H(4A)	945	32	349	37
H(5A)	882	81	430	39
H(6A)	747	146	411	30
H(7A1)	690	298	223	16
H(7A2)	660	313	292	16
H(8A1)	614	164	415	17
H(8A2)	545	108	397	17
H(9A1)	578	84	277	17
H(9A2)	599	168	208	17
H(11A)	675	294	129	21
H(12A)	677	302	14	26
H(13A)	561	363	-59	27
H(14A)	443	419	-17	26
H(15A)	439	410	98	23
H(17A)	678	467	190	28
H(18A)	681	608	177	36
H(19A)	551	677	185	30
H(20A)	419	606	206	27
H(21A)	416	465	219	22
H(23A)	657	276	422	22
H(24A)	713	390	438	29
H(25A)	626	508	423	33
H(26A)	482	512	389	35
H(27A)	427	399	371	26
H(29A)	514	108	514	32
H(30A)	431	36	617	42
H(31A)	283	68	623	34
H(32A)	222	178	528	33
H(33A)	306	253	426	28
H(35A)	421	9	247	28
H(36A)	361	-119	327	33
H(37A)	308	-131	438	31
H(38A)	312	-15	468	26
H(39A)	368	114	386	22
H(41A)	530	130	132	24
H(42A)	480	143	24	30
H(43A)	344	206	-13	30
H(44A)	258	252	60	27
H(45A)	306	236	169	21
H(48A)	32	189	243	23
H(50A)	102	411	86	21
H(52A)	222	161	342	29
H(53A)	162	26	366	51
H(53B)	195	72	286	51
H(53C)	93	70	306	51

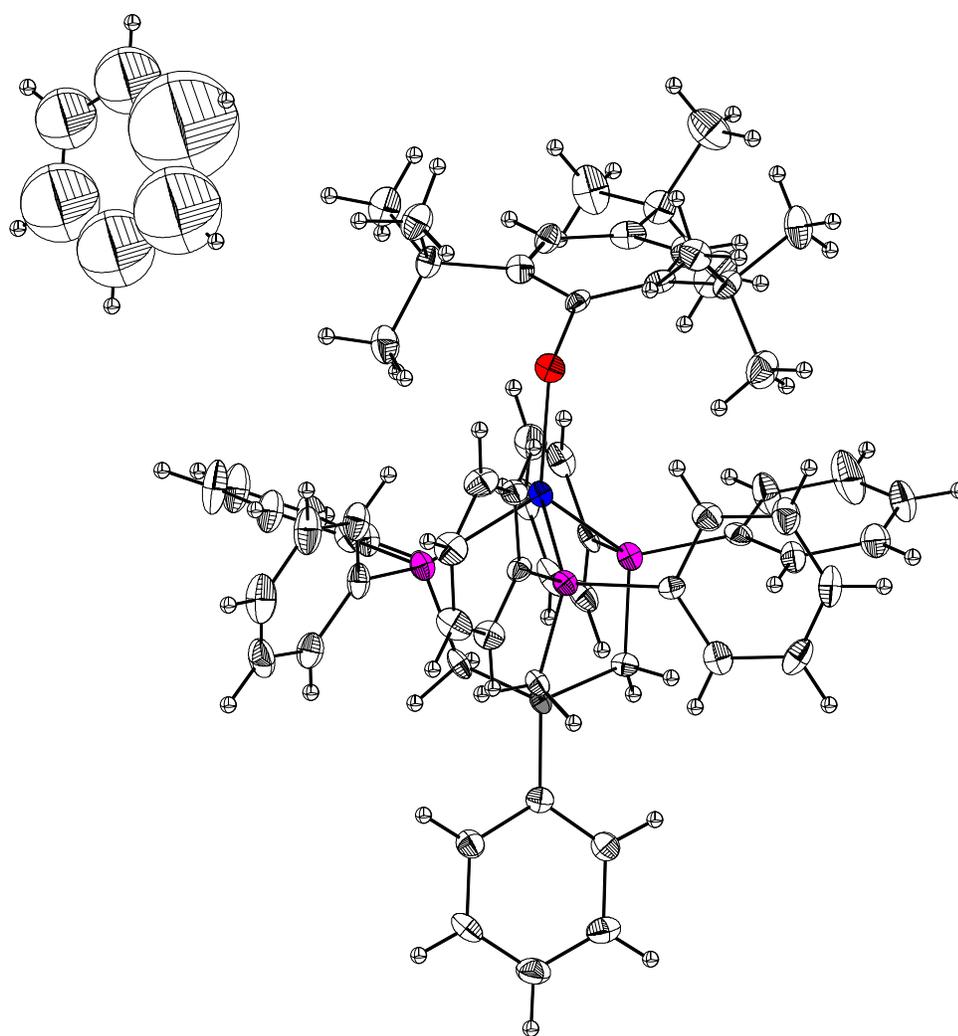
H(54A)	112	213	394	57
H(54B)	114	112	433	57
H(54C)	41	158	378	57
H(55A)	-36	245	121	24
H(56A)	-108	256	220	33
H(56B)	-166	299	152	33
H(56C)	-112	356	179	33
H(57A)	-36	426	54	35
H(57B)	-99	367	34	35
H(57C)	4	364	20	35
H(58A)	307	425	153	22
H(59A)	284	412	45	33
H(59B)	314	506	32	33
H(59C)	214	488	26	33
H(60A)	166	543	114	49
H(60B)	264	565	122	49
H(60C)	207	506	191	49
H(2B)	-250	913	260	22
H(3B)	-382	984	228	29
H(4B)	-456	980	135	27
H(5B)	-399	901	75	27
H(6B)	-268	830	106	22
H(7B1)	-176	690	209	15
H(7B2)	-212	699	279	15
H(8B1)	-61	897	116	15
H(8B2)	-127	846	92	15
H(9B1)	-124	815	309	18
H(9B2)	-108	908	247	18
H(11B)	-208	679	383	26
H(12B)	-215	668	499	32
H(13B)	-93	627	567	31
H(14B)	36	592	522	29
H(15B)	44	603	406	23
H(17B)	-198	533	306	27
H(18B)	-197	392	317	34
H(19B)	-64	323	318	32
H(20B)	66	393	307	28
H(21B)	66	532	297	23
H(23B)	-158	750	59	20
H(24B)	-225	635	49	24
H(25B)	-159	502	94	24
H(26B)	-24	484	146	23
H(27B)	42	597	157	18
H(29B)	79	931	67	24
H(30B)	178	997	-27	29
H(31B)	230	929	-98	29
H(32B)	185	790	-70	31
H(33B)	88	722	26	25
H(35B)	-46	992	164	22
H(36B)	16	1119	86	31
H(37B)	167	1136	82	41
H(38B)	254	1026	155	42
H(39B)	193	896	229	30
H(41B)	-52	873	377	26

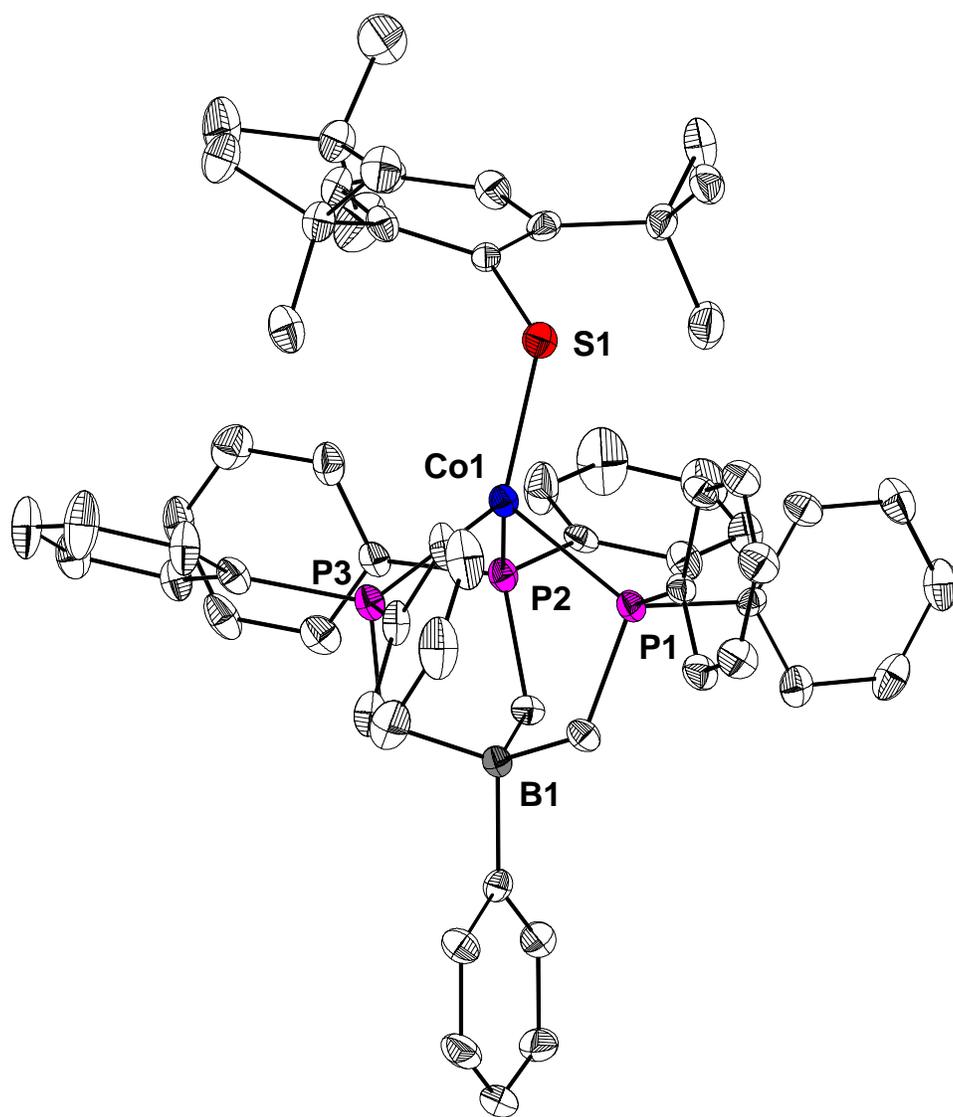
H(42B)	-5	859	486	38
H(43B)	129	795	526	37
H(44B)	217	748	455	32
H(45B)	171	762	345	24
H(48B)	380	641	393	21
H(50B)	456	834	211	21
H(52B)	174	610	342	21
H(53D)	291	536	455	35
H(53E)	188	520	459	35
H(53F)	224	611	449	35
H(54D)	253	536	286	38
H(54E)	217	471	361	38
H(54F)	317	498	350	38
H(55B)	520	815	325	23
H(56D)	459	729	439	51
H(56E)	563	728	437	51
H(56F)	511	650	436	51
H(57D)	646	733	331	36
H(57E)	598	753	259	36
H(57F)	589	662	323	36
H(58B)	265	852	121	24
H(59D)	367	951	130	43
H(59E)	355	960	51	43
H(59F)	439	913	93	43
H(60D)	417	773	89	39
H(60E)	348	826	32	39
H(60F)	319	740	95	39

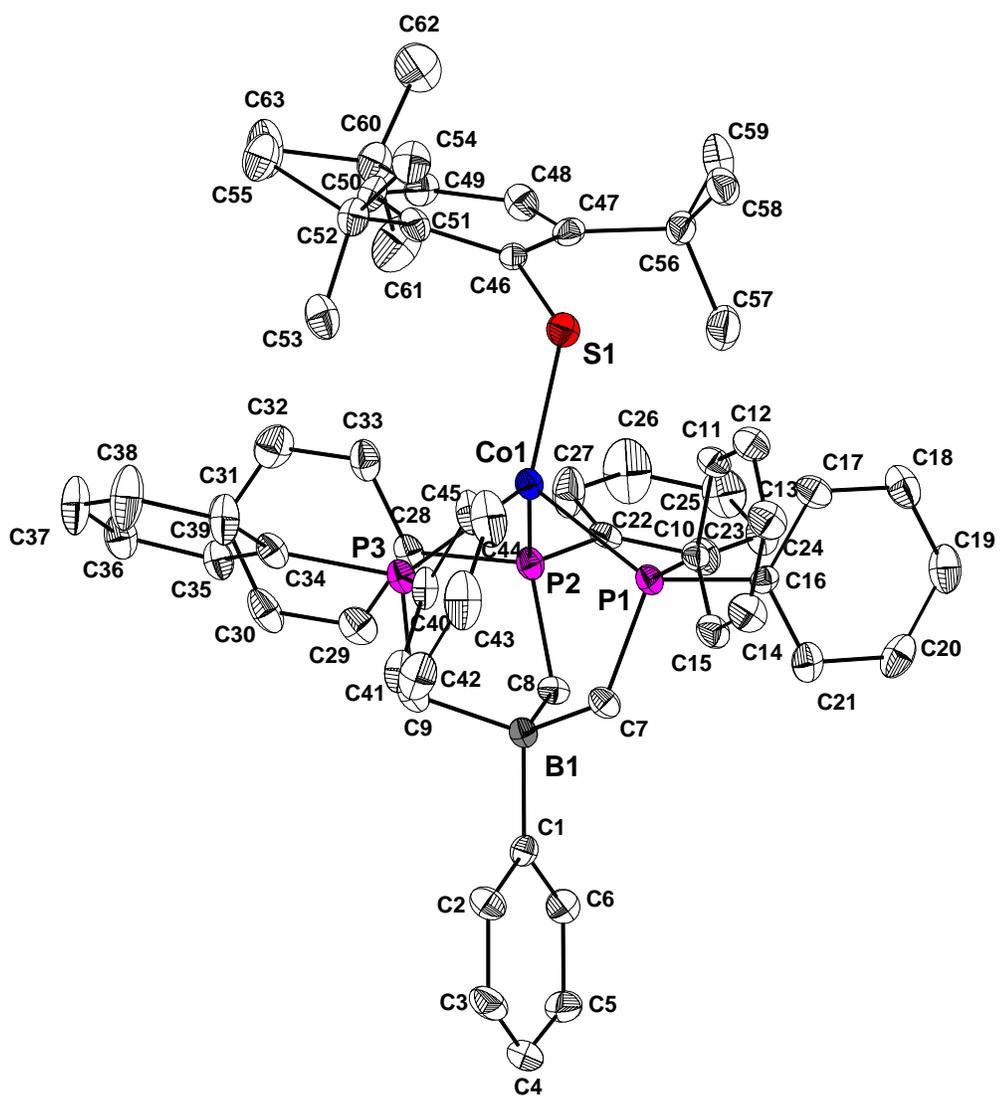
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G. X-ray report for  $[\text{PhBP}_3]\text{CoS}(2,4,6\text{-}^t\text{Bu}_3\text{-Ph})$ , **8**.

## Crystal Structure Report for DMJ 31, $[\text{PhBP}_3]\text{CoS}(2,4,6\text{-}^t\text{Bu}_3\text{-Ph})$







**Table 1. Crystal Data and Structure Analysis Details for dmj31, [PhBP<sub>3</sub>]CoS(2,4,6-<sup>t</sup>Bu-Ph).**

Empirical formula	C <sub>63</sub> H <sub>70</sub> BCoP <sub>3</sub> S · C <sub>6</sub> H <sub>6</sub>
Formula weight	1100.01
Crystallization solvent	benzene/petroleum ether
Crystal shape	blade
Crystal color	green
Crystal size	0.05 x 0.11 x 0.15 mm

### Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoKα	
Data collection temperature	96 K	
Theta range for 5547 reflections used in lattice determination	2.26 to 22.31°	
Unit cell dimensions	a = 13.8333(10) Å b = 13.9539(10) Å c = 17.5922(13) Å	α = 99.1450(10)° β = 106.5870(10)° γ = 107.0290(10)°
Volume	3000.8(4) Å <sup>3</sup>	
Z	2	
Crystal system	triclinic	
Space group	P $\bar{1}$ (#2)	
Density (calculated)	1.217 g/cm <sup>3</sup>	
F(000)	1166	
Theta range for data collection	1.2 to 28.6°	
Completeness to theta = 28.59°	92.1%	
Index ranges	-18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -23 ≤ l ≤ 23	
Reflections collected	63510	
Independent reflections	14141 [R <sub>int</sub> = 0.1354]	
Reflections > 2σ(I)	6625	
Average σ(I)/(net I)	0.1677	
Absorption coefficient	0.44 mm <sup>-1</sup>	
Reflections monitored for decay	87	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	14141 / 0 / 643
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	1.58
Final R indices [I>2σ(I), 6625 reflections]	R1 = 0.0663, wR2 = 0.1133
R indices (all data)	R1 = 0.1759, wR2 = 0.1318
Type of weighting scheme used	σ
Weighting scheme used	1/σ <sup>2</sup> (Fo <sup>2</sup> )
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	1.61 and -0.72 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINTE v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

## Special Refinement Details

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

The solvent benzene was refined isotropically. To prevent solvent disorder during refinement, the benzene molecule was fixed using the AFIX 66 command. Two difference peaks greater than 1 were found near the ring suggesting solvent disorder.

**Table 2. Atomic coordinates (  $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj31.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co(1)	8386(1)	8223(1)	2389(1)	17(1)
P(1)	10020(1)	8254(1)	2217(1)	17(1)
P(2)	7627(1)	8551(1)	1125(1)	18(1)
P(3)	7597(1)	6373(1)	1913(1)	19(1)
S(1)	8733(1)	9225(1)	3612(1)	22(1)
B(1)	8429(4)	6872(4)	587(3)	16(1)
C(1)	8512(3)	6234(4)	-240(3)	18(1)
C(2)	8632(4)	5263(4)	-277(3)	23(1)
C(3)	8723(4)	4701(4)	-957(3)	28(1)
C(4)	8695(4)	5084(4)	-1637(3)	29(1)
C(5)	8608(4)	6048(4)	-1616(3)	27(1)
C(6)	8527(3)	6599(4)	-924(3)	22(1)
C(7)	9664(3)	7233(3)	1301(3)	18(1)
C(8)	8094(3)	7894(3)	401(3)	16(1)
C(9)	7498(3)	6085(3)	854(3)	19(1)
C(10)	11122(4)	8120(4)	3020(3)	17(1)
C(11)	11394(4)	8633(4)	3837(3)	20(1)
C(12)	12246(4)	8557(4)	4442(3)	26(1)
C(13)	12803(4)	7935(4)	4231(3)	28(1)
C(14)	12525(4)	7412(4)	3432(3)	27(1)
C(15)	11698(3)	7510(4)	2823(3)	22(1)
C(16)	10772(3)	9469(4)	2053(3)	15(1)
C(17)	11133(4)	10379(4)	2682(3)	24(1)
C(18)	11755(4)	11316(4)	2624(3)	31(1)
C(19)	12026(4)	11364(4)	1938(3)	29(1)
C(20)	11665(4)	10490(4)	1301(3)	28(1)
C(21)	11038(3)	9537(4)	1354(3)	22(1)
C(22)	7757(4)	9825(4)	915(3)	18(1)
C(23)	8735(4)	10447(4)	907(3)	24(1)
C(24)	8855(4)	11414(4)	754(3)	28(1)
C(25)	8012(4)	11765(4)	617(3)	38(2)
C(26)	7044(5)	11156(4)	633(4)	52(2)
C(27)	6920(4)	10191(4)	784(3)	36(2)
C(28)	6172(4)	7931(3)	822(3)	18(1)
C(29)	5495(4)	7346(4)	36(3)	25(1)
C(30)	4391(4)	6903(4)	-145(3)	28(1)
C(31)	3962(4)	7042(4)	468(3)	28(1)
C(32)	4621(4)	7628(4)	1239(3)	32(1)
C(33)	5720(4)	8068(4)	1435(3)	26(1)
C(34)	6329(4)	5519(4)	1930(3)	21(1)
C(35)	5351(4)	5484(4)	1396(3)	22(1)
C(36)	4375(4)	4875(4)	1424(3)	28(1)
C(37)	4372(4)	4279(4)	1979(3)	40(2)
C(38)	5331(4)	4284(4)	2500(4)	45(2)
C(39)	6306(4)	4904(4)	2480(3)	30(1)
C(40)	8541(4)	5839(4)	2470(3)	22(1)

C(41)	8644(4)	4914(4)	2112(3)	26(1)
C(42)	9361(4)	4533(4)	2566(4)	33(1)
C(43)	10005(4)	5060(4)	3372(4)	39(2)
C(44)	9922(4)	5960(4)	3735(4)	37(2)
C(45)	9193(4)	6352(4)	3286(3)	28(1)
C(46)	7678(4)	9713(4)	3615(3)	17(1)
C(47)	7758(4)	10694(4)	3473(3)	20(1)
C(48)	6809(4)	10918(4)	3215(3)	24(1)
C(49)	5809(4)	10241(4)	3161(3)	23(1)
C(50)	5807(4)	9401(4)	3473(3)	22(1)
C(51)	6714(4)	9122(4)	3721(3)	20(1)
C(52)	6629(4)	8221(4)	4138(3)	22(1)
C(53)	6610(4)	7233(4)	3589(3)	32(1)
C(54)	7578(4)	8574(4)	4957(3)	31(1)
C(55)	5608(4)	7912(4)	4365(3)	31(1)
C(56)	8824(4)	11592(4)	3626(3)	22(1)
C(57)	9189(4)	11470(4)	2889(3)	35(1)
C(58)	9719(4)	11662(4)	4415(3)	27(1)
C(59)	8699(4)	12661(4)	3772(3)	32(1)
C(60)	4800(4)	10519(4)	2828(3)	26(1)
C(61)	4671(4)	10616(5)	1943(3)	46(2)
C(62)	4945(4)	11567(4)	3363(3)	44(2)
C(63)	3780(4)	9708(4)	2826(3)	41(2)
C(64)	2130(4)	4488(6)	4968(4)	108(3)
C(65)	2810(6)	5517(6)	5338(3)	129(4)
C(66)	3635(6)	5965(4)	5060(5)	351(10)
C(67)	3781(5)	5384(7)	4412(5)	222(6)
C(68)	3101(7)	4355(7)	4041(3)	173(5)
C(69)	2275(6)	3907(4)	4319(4)	180(5)

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**Table 3.** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj31.

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Co(1)-S(1)	2.207(1)
Co(1)-P(2)	2.351(1)
Co(1)-P(1)	2.354(1)
Co(1)-P(3)	2.387(1)
S(1)-C(46)	1.784(5)
<hr/>	
S(1)-Co(1)-P(2)	125.24(5)
S(1)-Co(1)-P(1)	109.46(5)
P(2)-Co(1)-P(1)	96.11(5)
S(1)-Co(1)-P(3)	128.37(6)
P(2)-Co(1)-P(3)	96.30(5)
P(1)-Co(1)-P(3)	92.81(5)
C(46)-S(1)-Co(1)	111.3(2)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj31.**

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Co(1)-S(1)	2.2070(14)
Co(1)-P(2)	2.3511(14)
Co(1)-P(1)	2.3537(14)
Co(1)-P(3)	2.3867(14)
P(1)-C(7)	1.810(4)
P(1)-C(16)	1.826(5)
P(1)-C(10)	1.838(5)
P(2)-C(28)	1.818(5)
P(2)-C(8)	1.823(4)
P(2)-C(22)	1.842(5)
P(3)-C(9)	1.800(5)
P(3)-C(40)	1.815(5)
P(3)-C(34)	1.821(5)
S(1)-C(46)	1.784(5)
B(1)-C(1)	1.633(7)
B(1)-C(9)	1.663(7)
B(1)-C(8)	1.673(6)
B(1)-C(7)	1.679(6)
C(1)-C(6)	1.382(6)
C(1)-C(2)	1.407(6)
C(2)-C(3)	1.381(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.380(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.380(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.383(6)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.389(6)
C(10)-C(15)	1.393(6)
C(11)-C(12)	1.388(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.393(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.362(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.384(6)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.391(6)
C(16)-C(17)	1.396(6)
C(17)-C(18)	1.376(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.367(6)

C(18)-H(18)	0.9500
C(19)-C(20)	1.373(7)
C(19)-H(19)	0.9500
C(20)-C(21)	1.392(6)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(27)	1.373(6)
C(22)-C(23)	1.381(6)
C(23)-C(24)	1.390(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.368(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.371(7)
C(25)-H(25)	0.9500
C(26)-C(27)	1.385(7)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.382(6)
C(28)-C(33)	1.406(6)
C(29)-C(30)	1.387(6)
C(29)-H(29)	0.9500
C(30)-C(31)	1.385(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.358(7)
C(31)-H(31)	0.9500
C(32)-C(33)	1.376(6)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(35)	1.391(6)
C(34)-C(39)	1.393(6)
C(35)-C(36)	1.388(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.380(6)
C(36)-H(36)	0.9500
C(37)-C(38)	1.378(7)
C(37)-H(37)	0.9500
C(38)-C(39)	1.387(6)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(45)	1.394(6)
C(40)-C(41)	1.408(6)
C(41)-C(42)	1.377(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.382(7)
C(42)-H(42)	0.9500
C(43)-C(44)	1.367(7)
C(43)-H(43)	0.9500
C(44)-C(45)	1.394(6)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(47)	1.408(6)
C(46)-C(51)	1.427(6)
C(47)-C(48)	1.406(6)
C(47)-C(56)	1.549(6)

C(48)-C(49)	1.395(6)
C(48)-H(48)	0.9500
C(49)-C(50)	1.371(6)
C(49)-C(60)	1.537(6)
C(50)-C(51)	1.396(6)
C(50)-H(50)	0.9500
C(51)-C(52)	1.546(6)
C(52)-C(54)	1.535(6)
C(52)-C(55)	1.536(6)
C(52)-C(53)	1.542(6)
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-C(57)	1.524(6)
C(56)-C(58)	1.541(6)
C(56)-C(59)	1.542(6)
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(60)-C(63)	1.527(6)
C(60)-C(62)	1.533(6)
C(60)-C(61)	1.547(7)
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-C(65)	1.3900
C(64)-C(69)	1.3900
C(64)-H(64)	0.9500
C(65)-C(66)	1.3900
C(65)-H(65)	0.9500
C(66)-C(67)	1.3900
C(66)-H(66)	0.9500
C(67)-C(68)	1.3900
C(67)-H(67)	0.9500
C(68)-C(69)	1.3900
C(68)-H(68)	0.9500

C(69)-H(69)	0.9500
S(1)-Co(1)-P(2)	125.24(5)
S(1)-Co(1)-P(1)	109.46(5)
P(2)-Co(1)-P(1)	96.11(5)
S(1)-Co(1)-P(3)	128.37(6)
P(2)-Co(1)-P(3)	96.30(5)
P(1)-Co(1)-P(3)	92.81(5)
C(7)-P(1)-C(16)	107.2(2)
C(7)-P(1)-C(10)	107.1(2)
C(16)-P(1)-C(10)	99.0(2)
C(7)-P(1)-Co(1)	106.38(15)
C(16)-P(1)-Co(1)	113.79(14)
C(10)-P(1)-Co(1)	122.39(16)
C(28)-P(2)-C(8)	109.2(2)
C(28)-P(2)-C(22)	102.0(2)
C(8)-P(2)-C(22)	105.4(2)
C(28)-P(2)-Co(1)	106.33(16)
C(8)-P(2)-Co(1)	105.73(14)
C(22)-P(2)-Co(1)	127.38(15)
C(9)-P(3)-C(40)	108.0(2)
C(9)-P(3)-C(34)	105.4(2)
C(40)-P(3)-C(34)	101.0(2)
C(9)-P(3)-Co(1)	104.63(15)
C(40)-P(3)-Co(1)	108.14(16)
C(34)-P(3)-Co(1)	128.47(16)
C(46)-S(1)-Co(1)	111.27(15)
C(1)-B(1)-C(9)	109.1(4)
C(1)-B(1)-C(8)	109.5(4)
C(9)-B(1)-C(8)	110.1(4)
C(1)-B(1)-C(7)	104.5(3)
C(9)-B(1)-C(7)	111.2(4)
C(8)-B(1)-C(7)	112.2(4)
C(6)-C(1)-C(2)	115.0(4)
C(6)-C(1)-B(1)	124.7(4)
C(2)-C(1)-B(1)	120.2(4)
C(3)-C(2)-C(1)	122.4(5)
C(3)-C(2)-H(2)	118.8
C(1)-C(2)-H(2)	118.8
C(4)-C(3)-C(2)	120.3(5)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	119.0(5)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	119.5(5)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(1)-C(6)-C(5)	123.7(5)
C(1)-C(6)-H(6)	118.2
C(5)-C(6)-H(6)	118.2
B(1)-C(7)-P(1)	117.9(3)
B(1)-C(7)-H(7A)	107.8
P(1)-C(7)-H(7A)	107.8

B(1)-C(7)-H(7B)	107.8
P(1)-C(7)-H(7B)	107.8
H(7A)-C(7)-H(7B)	107.2
B(1)-C(8)-P(2)	118.4(3)
B(1)-C(8)-H(8A)	107.7
P(2)-C(8)-H(8A)	107.7
B(1)-C(8)-H(8B)	107.7
P(2)-C(8)-H(8B)	107.7
H(8A)-C(8)-H(8B)	107.1
B(1)-C(9)-P(3)	118.2(3)
B(1)-C(9)-H(9A)	107.8
P(3)-C(9)-H(9A)	107.8
B(1)-C(9)-H(9B)	107.8
P(3)-C(9)-H(9B)	107.8
H(9A)-C(9)-H(9B)	107.1
C(11)-C(10)-C(15)	119.0(4)
C(11)-C(10)-P(1)	120.0(4)
C(15)-C(10)-P(1)	121.0(4)
C(12)-C(11)-C(10)	120.1(5)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	119.8(5)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(14)-C(13)-C(12)	120.3(5)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(13)-C(14)-C(15)	120.2(5)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-C(10)	120.6(5)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.7
C(21)-C(16)-C(17)	118.2(5)
C(21)-C(16)-P(1)	123.9(4)
C(17)-C(16)-P(1)	117.8(4)
C(18)-C(17)-C(16)	121.3(5)
C(18)-C(17)-H(17)	119.3
C(16)-C(17)-H(17)	119.3
C(19)-C(18)-C(17)	119.7(5)
C(19)-C(18)-H(18)	120.1
C(17)-C(18)-H(18)	120.1
C(18)-C(19)-C(20)	120.5(5)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(19)-C(20)-C(21)	120.3(5)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(16)-C(21)-C(20)	120.0(5)
C(16)-C(21)-H(21)	120.0
C(20)-C(21)-H(21)	120.0
C(27)-C(22)-C(23)	118.7(5)
C(27)-C(22)-P(2)	122.1(4)
C(23)-C(22)-P(2)	119.2(4)

C(22)-C(23)-C(24)	120.3(5)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(25)-C(24)-C(23)	120.5(5)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	119.5(5)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(25)-C(26)-C(27)	120.2(5)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(22)-C(27)-C(26)	120.9(5)
C(22)-C(27)-H(27)	119.6
C(26)-C(27)-H(27)	119.6
C(29)-C(28)-C(33)	118.8(4)
C(29)-C(28)-P(2)	124.2(4)
C(33)-C(28)-P(2)	117.0(4)
C(28)-C(29)-C(30)	120.6(5)
C(28)-C(29)-H(29)	119.7
C(30)-C(29)-H(29)	119.7
C(31)-C(30)-C(29)	119.8(5)
C(31)-C(30)-H(30)	120.1
C(29)-C(30)-H(30)	120.1
C(32)-C(31)-C(30)	119.9(5)
C(32)-C(31)-H(31)	120.0
C(30)-C(31)-H(31)	120.0
C(31)-C(32)-C(33)	121.3(5)
C(31)-C(32)-H(32)	119.4
C(33)-C(32)-H(32)	119.4
C(32)-C(33)-C(28)	119.6(5)
C(32)-C(33)-H(33)	120.2
C(28)-C(33)-H(33)	120.2
C(35)-C(34)-C(39)	118.3(4)
C(35)-C(34)-P(3)	120.1(4)
C(39)-C(34)-P(3)	121.5(4)
C(36)-C(35)-C(34)	121.1(5)
C(36)-C(35)-H(35)	119.5
C(34)-C(35)-H(35)	119.5
C(37)-C(36)-C(35)	119.6(5)
C(37)-C(36)-H(36)	120.2
C(35)-C(36)-H(36)	120.2
C(38)-C(37)-C(36)	120.3(5)
C(38)-C(37)-H(37)	119.9
C(36)-C(37)-H(37)	119.9
C(37)-C(38)-C(39)	120.1(5)
C(37)-C(38)-H(38)	119.9
C(39)-C(38)-H(38)	119.9
C(38)-C(39)-C(34)	120.6(5)
C(38)-C(39)-H(39)	119.7
C(34)-C(39)-H(39)	119.7
C(45)-C(40)-C(41)	117.9(4)
C(45)-C(40)-P(3)	119.5(4)
C(41)-C(40)-P(3)	122.6(4)

C(42)-C(41)-C(40)	120.3(5)
C(42)-C(41)-H(41)	119.9
C(40)-C(41)-H(41)	119.9
C(41)-C(42)-C(43)	120.7(5)
C(41)-C(42)-H(42)	119.7
C(43)-C(42)-H(42)	119.7
C(44)-C(43)-C(42)	120.2(5)
C(44)-C(43)-H(43)	119.9
C(42)-C(43)-H(43)	119.9
C(43)-C(44)-C(45)	119.8(5)
C(43)-C(44)-H(44)	120.1
C(45)-C(44)-H(44)	120.1
C(44)-C(45)-C(40)	121.1(5)
C(44)-C(45)-H(45)	119.5
C(40)-C(45)-H(45)	119.5
C(47)-C(46)-C(51)	117.8(4)
C(47)-C(46)-S(1)	119.9(3)
C(51)-C(46)-S(1)	122.2(4)
C(48)-C(47)-C(46)	118.5(4)
C(48)-C(47)-C(56)	115.9(4)
C(46)-C(47)-C(56)	125.5(4)
C(49)-C(48)-C(47)	122.4(5)
C(49)-C(48)-H(48)	118.8
C(47)-C(48)-H(48)	118.8
C(50)-C(49)-C(48)	116.9(4)
C(50)-C(49)-C(60)	123.9(4)
C(48)-C(49)-C(60)	119.0(5)
C(49)-C(50)-C(51)	123.0(5)
C(49)-C(50)-H(50)	118.5
C(51)-C(50)-H(50)	118.5
C(50)-C(51)-C(46)	118.6(4)
C(50)-C(51)-C(52)	117.4(4)
C(46)-C(51)-C(52)	123.9(4)
C(54)-C(52)-C(55)	105.4(4)
C(54)-C(52)-C(53)	110.0(4)
C(55)-C(52)-C(53)	107.0(4)
C(54)-C(52)-C(51)	109.4(4)
C(55)-C(52)-C(51)	112.4(4)
C(53)-C(52)-C(51)	112.4(4)
C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(52)-C(54)-H(54A)	109.5
C(52)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(52)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(52)-C(55)-H(55A)	109.5
C(52)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5

C(52)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(57)-C(56)-C(58)	110.6(4)
C(57)-C(56)-C(59)	107.0(4)
C(58)-C(56)-C(59)	104.7(4)
C(57)-C(56)-C(47)	111.0(4)
C(58)-C(56)-C(47)	111.3(4)
C(59)-C(56)-C(47)	112.0(4)
C(56)-C(57)-H(57A)	109.5
C(56)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(56)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(56)-C(58)-H(58A)	109.5
C(56)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(56)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(56)-C(59)-H(59A)	109.5
C(56)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(56)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(63)-C(60)-C(62)	107.9(4)
C(63)-C(60)-C(49)	112.2(4)
C(62)-C(60)-C(49)	109.8(4)
C(63)-C(60)-C(61)	110.0(4)
C(62)-C(60)-C(61)	108.6(4)
C(49)-C(60)-C(61)	108.3(4)
C(60)-C(61)-H(61A)	109.5
C(60)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(60)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(60)-C(62)-H(62A)	109.5
C(60)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(60)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(60)-C(63)-H(63A)	109.5
C(60)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(60)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
C(65)-C(64)-C(69)	120.0
C(65)-C(64)-H(64)	120.0
C(69)-C(64)-H(64)	120.0

C(66)-C(65)-C(64)	120.0
C(66)-C(65)-H(65)	120.0
C(64)-C(65)-H(65)	120.0
C(65)-C(66)-C(67)	120.0
C(65)-C(66)-H(66)	120.0
C(67)-C(66)-H(66)	120.0
C(68)-C(67)-C(66)	120.0
C(68)-C(67)-H(67)	120.0
C(66)-C(67)-H(67)	120.0
C(69)-C(68)-C(67)	120.0
C(69)-C(68)-H(68)	120.0
C(67)-C(68)-H(68)	120.0
C(68)-C(69)-C(64)	120.0
C(68)-C(69)-H(69)	120.0
C(64)-C(69)-H(69)	120.0

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Symmetry transformations used to generate equivalent atoms:

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj31. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co(1)	147(4)	165(4)	193(4)	45(3)	41(3)	59(3)
P(1)	145(7)	153(7)	171(7)	23(6)	29(6)	41(6)
P(2)	147(7)	165(7)	200(8)	43(6)	31(6)	52(6)
P(3)	163(7)	161(7)	210(8)	47(6)	30(6)	47(6)
S(1)	172(7)	244(8)	226(8)	45(6)	43(6)	84(6)
B(1)	150(30)	130(30)	200(30)	40(30)	50(30)	70(20)
C(1)	120(30)	210(30)	200(30)	40(20)	50(20)	70(20)
C(2)	260(30)	210(30)	180(30)	40(20)	30(20)	80(20)
C(3)	320(30)	170(30)	310(30)	-10(30)	90(30)	90(30)
C(4)	310(30)	250(30)	250(30)	-40(30)	110(30)	50(30)
C(5)	270(30)	320(30)	200(30)	30(30)	100(30)	80(30)
C(6)	200(30)	220(30)	240(30)	60(30)	60(20)	100(20)
C(7)	200(30)	140(30)	200(30)	40(20)	40(20)	70(20)
C(8)	130(20)	210(30)	120(30)	30(20)	0(20)	90(20)
C(9)	170(30)	120(30)	260(30)	40(20)	20(20)	80(20)
C(10)	170(30)	180(30)	120(30)	30(20)	40(20)	30(20)
C(11)	220(30)	190(30)	150(30)	30(20)	30(20)	70(20)
C(12)	230(30)	330(30)	140(30)	20(30)	0(20)	60(30)
C(13)	250(30)	310(30)	230(30)	60(30)	20(30)	110(30)
C(14)	180(30)	310(30)	300(30)	40(30)	10(20)	140(30)
C(15)	180(30)	240(30)	180(30)	20(20)	0(20)	60(20)
C(16)	110(20)	200(30)	150(30)	40(20)	40(20)	80(20)
C(17)	250(30)	240(30)	180(30)	30(30)	30(20)	90(30)
C(18)	310(30)	220(30)	290(30)	70(30)	40(30)	20(30)
C(19)	240(30)	250(30)	360(40)	180(30)	50(30)	50(30)
C(20)	210(30)	420(40)	260(30)	210(30)	100(30)	120(30)
C(21)	130(30)	240(30)	300(30)	90(30)	40(20)	100(20)
C(22)	200(30)	170(30)	130(30)	-10(20)	20(20)	60(20)
C(23)	260(30)	180(30)	250(30)	80(20)	70(30)	70(20)
C(24)	250(30)	240(30)	310(30)	70(30)	90(30)	40(30)
C(25)	450(40)	240(30)	490(40)	190(30)	140(30)	170(30)
C(26)	390(40)	370(40)	890(50)	310(40)	150(40)	270(30)
C(27)	260(30)	230(30)	620(40)	160(30)	170(30)	90(30)
C(28)	160(30)	100(30)	260(30)	50(20)	40(20)	80(20)
C(29)	260(30)	190(30)	300(30)	50(30)	50(30)	130(30)
C(30)	220(30)	160(30)	370(40)	20(30)	-30(30)	70(20)
C(31)	130(30)	210(30)	470(40)	120(30)	30(30)	60(20)
C(32)	280(30)	330(40)	420(40)	150(30)	160(30)	170(30)
C(33)	170(30)	200(30)	370(40)	70(30)	60(30)	60(20)
C(34)	200(30)	160(30)	230(30)	30(20)	20(20)	60(20)
C(35)	190(30)	200(30)	250(30)	80(20)	30(20)	40(20)
C(36)	190(30)	240(30)	370(40)	100(30)	30(30)	80(20)
C(37)	230(30)	370(40)	540(40)	260(30)	90(30)	-10(30)
C(38)	290(30)	430(40)	660(50)	400(40)	130(30)	60(30)
C(39)	180(30)	320(30)	370(40)	190(30)	40(30)	30(30)
C(40)	140(30)	200(30)	290(30)	130(30)	50(20)	40(20)

C(41)	190(30)	270(30)	300(30)	130(30)	80(30)	50(20)
C(42)	310(30)	250(30)	550(40)	210(30)	210(30)	180(30)
C(43)	230(30)	400(40)	520(40)	270(30)	30(30)	100(30)
C(44)	280(30)	340(40)	410(40)	220(30)	-10(30)	40(30)
C(45)	200(30)	240(30)	280(30)	100(30)	20(30)	-20(20)
C(46)	170(30)	190(30)	110(30)	30(20)	50(20)	30(20)
C(47)	170(30)	270(30)	140(30)	30(20)	60(20)	80(20)
C(48)	270(30)	200(30)	230(30)	80(20)	70(30)	70(20)
C(49)	120(30)	340(30)	210(30)	30(30)	20(20)	110(20)
C(50)	170(30)	260(30)	250(30)	110(30)	100(20)	70(20)
C(51)	170(30)	210(30)	160(30)	30(20)	0(20)	40(20)
C(52)	200(30)	240(30)	240(30)	120(30)	70(20)	80(20)
C(53)	310(30)	230(30)	360(40)	100(30)	80(30)	30(30)
C(54)	290(30)	370(40)	270(30)	140(30)	70(30)	100(30)
C(55)	210(30)	390(40)	390(40)	190(30)	100(30)	130(30)
C(56)	190(30)	260(30)	180(30)	70(20)	60(20)	40(20)
C(57)	300(30)	330(40)	380(40)	110(30)	140(30)	30(30)
C(58)	210(30)	250(30)	270(30)	20(30)	40(30)	40(20)
C(59)	220(30)	240(30)	430(40)	130(30)	30(30)	20(30)
C(60)	170(30)	320(30)	290(30)	110(30)	50(20)	120(30)
C(61)	290(30)	740(50)	460(40)	320(40)	90(30)	300(30)
C(62)	330(30)	400(40)	580(40)	50(30)	100(30)	200(30)
C(63)	140(30)	390(40)	640(40)	180(30)	30(30)	120(30)

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**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj31.**

	x	y	z	$U_{\text{iso}}$
H(2)	865	498	18	27
H(3)	880	405	-96	33
H(4)	874	469	-211	35
H(5)	860	633	-207	32
H(6)	848	726	-92	26
H(7A)	1020	746	103	22
H(7B)	974	661	147	22
H(8A)	752	766	-15	19
H(8B)	873	842	37	19
H(9A)	751	538	70	23
H(9B)	678	607	51	23
H(11)	1100	904	398	24
H(12)	1245	893	500	32
H(13)	1338	788	465	34
H(14)	1290	698	329	32
H(15)	1152	716	227	26
H(17)	1094	1035	316	29
H(18)	1200	1193	306	37
H(19)	1247	1201	190	35
H(20)	1184	1054	82	33
H(21)	1079	893	91	27
H(23)	933	1021	101	28
H(24)	953	1184	75	34
H(25)	810	1243	51	45
H(26)	646	1140	54	62
H(27)	625	978	80	43
H(29)	579	725	-38	30
H(30)	393	650	-69	34
H(31)	321	673	35	34
H(32)	432	774	165	38
H(33)	617	846	198	31
H(35)	535	588	101	27
H(36)	371	487	106	34
H(37)	371	386	200	48
H(38)	532	386	287	54
H(39)	696	491	284	36
H(41)	822	455	155	31
H(42)	941	390	232	39
H(43)	1051	480	368	47
H(44)	1036	632	429	45
H(45)	914	698	354	33
H(48)	685	1155	307	29
H(50)	516	899	352	26
H(53A)	647	666	385	48
H(53B)	731	736	352	48
H(53C)	604	705	305	48
H(54A)	753	914	533	47

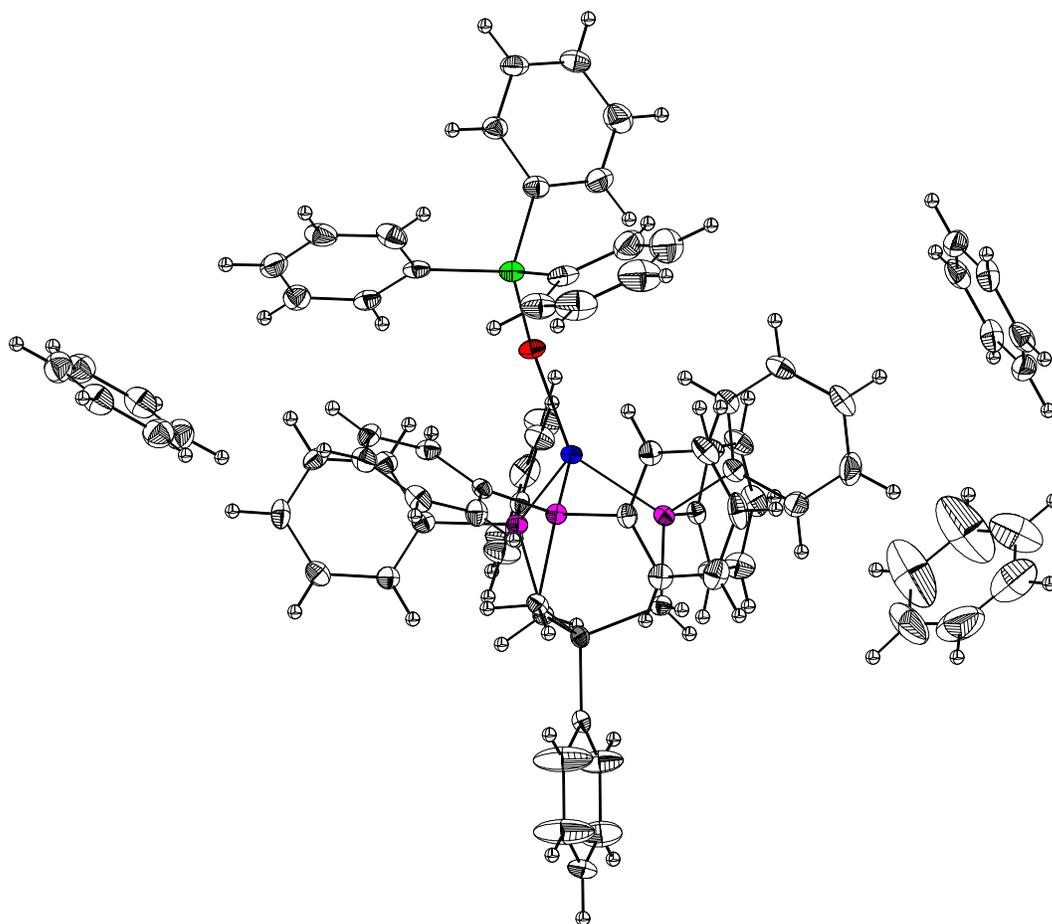
H(54B)	826	882	486	47
H(54C)	755	799	520	47
H(55A)	555	854	466	47
H(55B)	565	743	472	47
H(55C)	497	757	386	47
H(57A)	987	1204	300	53
H(57B)	863	1148	240	53
H(57C)	930	1081	279	53
H(58A)	986	1101	436	40
H(58B)	949	1179	489	40
H(58C)	1038	1224	450	40
H(59A)	833	1271	417	49
H(59B)	828	1274	325	49
H(59C)	942	1321	399	49
H(61A)	458	995	160	69
H(61B)	531	1116	195	69
H(61C)	403	1080	172	69
H(62A)	433	1177	312	66
H(62B)	561	1210	339	66
H(62C)	499	1151	392	66
H(63A)	387	965	339	61
H(63B)	365	904	247	61
H(63C)	316	992	262	61
H(64)	157	418	516	130
H(65)	271	591	578	155
H(66)	410	667	531	421
H(67)	435	569	422	266
H(68)	320	396	360	208
H(69)	181	320	407	216

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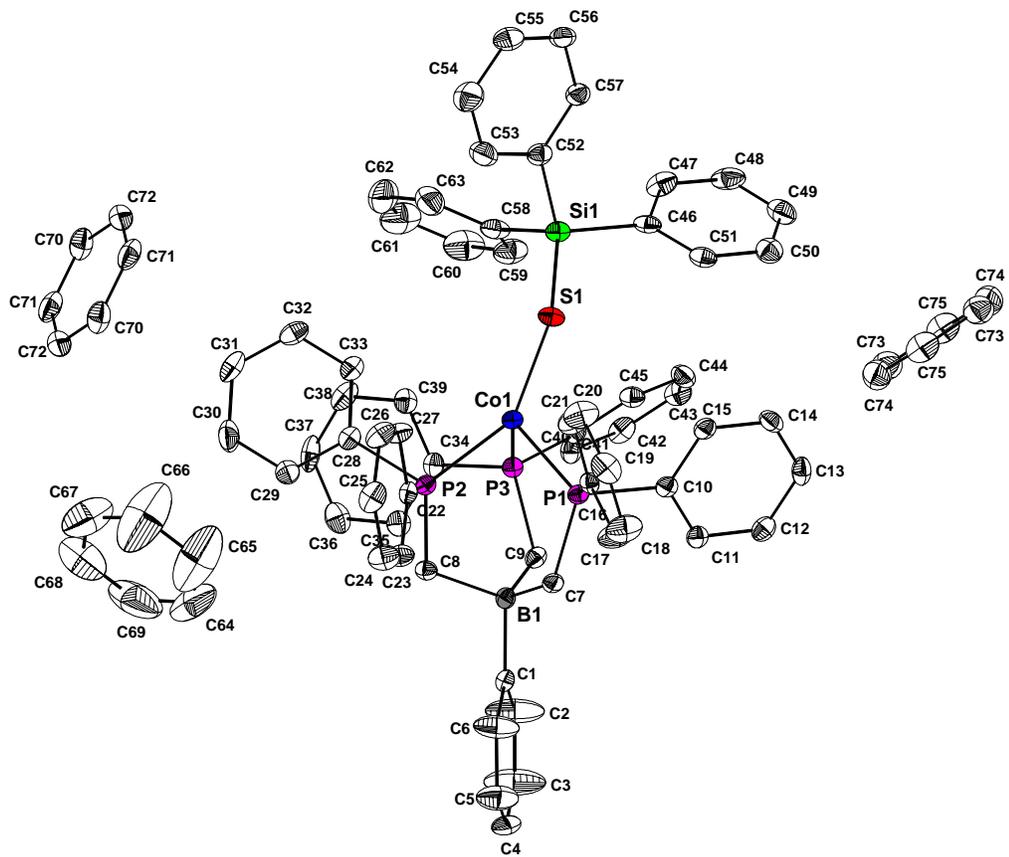
H. X-ray report for  $[\text{PhBP}_3]\text{CoSSiPh}_3$ , **9**.

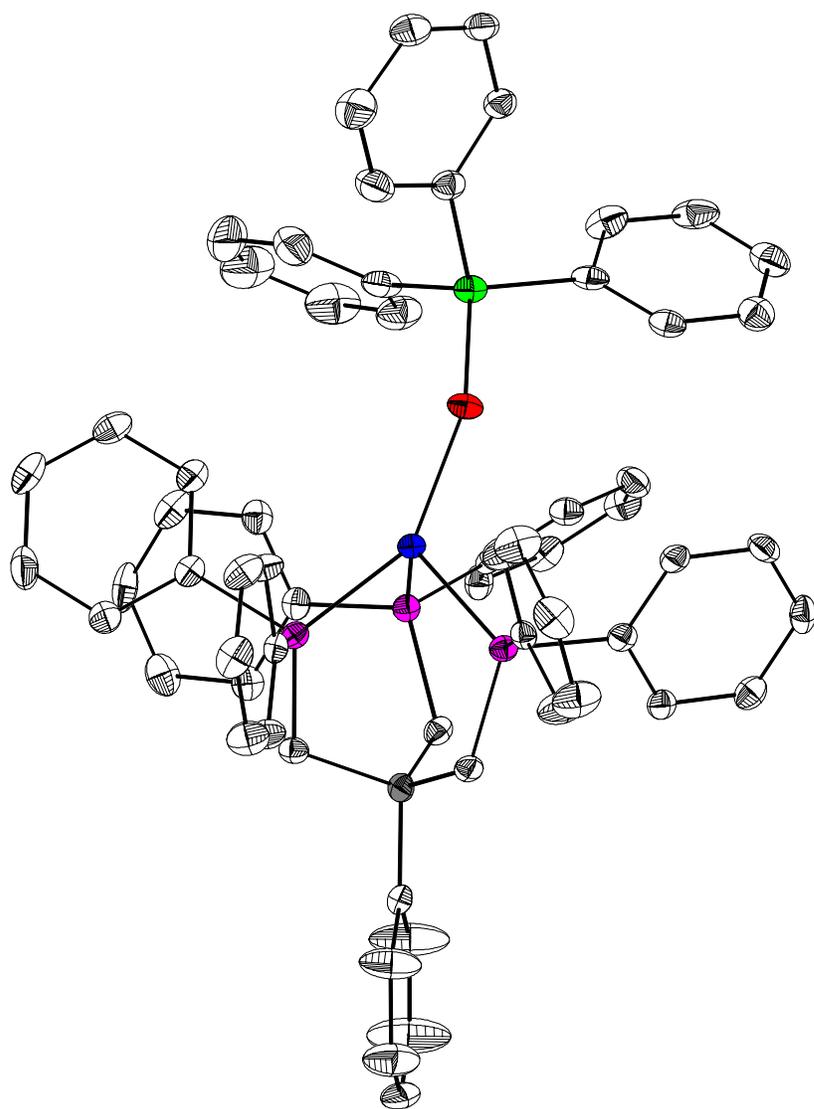
## Crystal Structure Report for

### DMJ 26, $[\text{PhBP}_3]\text{CoSSiPh}_3$



Note: Two half benzenes created by symmetry.





**Table 1. Crystal Data and Structure Analysis Details for dmj26, [PhBP<sub>3</sub>]CoSSiPh<sub>3</sub>.**

Empirical formula	C <sub>63</sub> H <sub>56</sub> BCoP <sub>3</sub> SSi · 2 C <sub>6</sub> H <sub>6</sub>
Formula weight	1192.09
Crystallization solvent	benzene/petroleum ether
Crystal shape	rough block
Crystal color	green
Crystal size	0.16 x 0.25 x 0.33 mm

### Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoKα	
Data collection temperature	96 K	
Theta range for 7903 reflections used in lattice determination	2.16 to 26.82°	
Unit cell dimensions	a = 11.0416(8) Å b = 12.8426(9) Å c = 22.3975(15) Å	α = 87.2280(10)° β = 81.4350(10)° γ = 73.0240(10)°
Volume	3003.7(4) Å <sup>3</sup>	
Z	2	
Crystal system	triclinic	
Space group	P $\bar{1}$ (#2)	
Density (calculated)	1.318 g/cm <sup>3</sup>	
F(000)	1250	
Theta range for data collection	1.7 to 28.6°	
Completeness to theta = 28.62°	90.8%	
Index ranges	-14 ≤ h ≤ 14, -16 ≤ k ≤ 17, -29 ≤ l ≤ 29	
Reflections collected	45903	
Independent reflections	13979 [R <sub>int</sub> = 0.0868]	
Reflections > 2σ(I)	8221	
Average σ(I)/(net I)	0.1095	
Absorption coefficient	0.47 mm <sup>-1</sup>	
Reflections monitored for decay	167	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	13979 / 0 / 739
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	1.22
Final R indices [I>2σ(I), 8221 reflections]	R1 = 0.0529, wR2 = 0.0777
R indices (all data)	R1 = 0.1081, wR2 = 0.0863
Type of weighting scheme used	σ
Weighting scheme used	1/σ <sup>2</sup> (Fo <sup>2</sup> )
Max shift/error	0.031
Average shift/error	0.001
Largest diff. peak and hole	0.69 and -0.63 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

## Special Refinement Details

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj26.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co(1)	4948(1)	7888(1)	7751(1)	15(1)
P(1)	5500(1)	6481(1)	8360(1)	16(1)
P(2)	4578(1)	6801(1)	7137(1)	16(1)
P(3)	6834(1)	7708(1)	7169(1)	16(1)
S(1)	3927(1)	9323(1)	8305(1)	19(1)
Si(1)	4030(1)	10941(1)	8165(1)	19(1)
B(1)	7081(3)	5362(3)	7267(1)	16(1)
C(1)	8086(3)	4190(2)	7064(1)	17(1)
C(2)	9312(3)	4053(3)	6780(2)	62(1)
C(3)	10156(4)	3036(3)	6617(2)	72(1)
C(4)	9816(3)	2121(2)	6740(1)	30(1)
C(5)	8623(3)	2215(3)	7023(2)	45(1)
C(6)	7777(3)	3232(3)	7177(2)	44(1)
C(7)	6375(3)	5225(2)	7968(1)	17(1)
C(8)	5924(2)	5704(2)	6827(1)	16(1)
C(9)	7825(2)	6311(2)	7225(1)	17(1)
C(10)	6560(3)	6741(2)	8855(1)	17(1)
C(11)	7862(3)	6191(2)	8795(1)	18(1)
C(12)	8633(3)	6421(2)	9168(1)	22(1)
C(13)	8123(3)	7198(2)	9617(1)	23(1)
C(14)	6820(3)	7737(2)	9683(1)	22(1)
C(15)	6052(3)	7519(2)	9307(1)	19(1)
C(16)	4239(3)	6182(2)	8904(1)	16(1)
C(17)	4449(3)	5184(2)	9195(1)	33(1)
C(18)	3510(3)	4935(3)	9604(1)	35(1)
C(19)	2335(3)	5687(2)	9727(1)	28(1)
C(20)	2113(3)	6691(3)	9450(1)	32(1)
C(21)	3055(3)	6937(2)	9039(1)	26(1)
C(22)	3282(3)	6219(2)	7441(1)	17(1)
C(23)	3405(3)	5109(2)	7444(1)	22(1)
C(24)	2369(3)	4734(2)	7651(1)	28(1)
C(25)	1189(3)	5457(2)	7843(1)	27(1)
C(26)	1062(3)	6552(2)	7845(1)	26(1)
C(27)	2104(3)	6930(2)	7646(1)	22(1)
C(28)	3873(2)	7660(2)	6531(1)	17(1)
C(29)	3818(3)	7198(2)	5993(1)	28(1)
C(30)	3227(3)	7843(3)	5545(1)	35(1)
C(31)	2721(3)	8952(3)	5625(1)	28(1)
C(32)	2799(3)	9414(2)	6150(1)	24(1)
C(33)	3359(3)	8777(2)	6601(1)	22(1)
C(34)	6846(2)	8015(2)	6362(1)	17(1)
C(35)	7452(3)	7250(2)	5908(1)	21(1)
C(36)	7375(3)	7523(3)	5310(1)	28(1)
C(37)	6719(3)	8567(3)	5148(1)	30(1)
C(38)	6125(3)	9329(3)	5588(1)	27(1)
C(39)	6183(3)	9055(2)	6191(1)	21(1)

C(40)	7829(2)	8512(2)	7384(1)	15(1)
C(41)	8883(3)	8613(2)	6990(1)	21(1)
C(42)	9695(3)	9137(2)	7166(1)	24(1)
C(43)	9459(3)	9569(2)	7743(1)	25(1)
C(44)	8415(3)	9477(2)	8136(1)	25(1)
C(45)	7600(3)	8943(2)	7957(1)	20(1)
C(46)	5144(3)	11217(2)	8651(1)	20(1)
C(47)	5636(3)	12109(2)	8540(1)	29(1)
C(48)	6462(3)	12311(2)	8900(2)	33(1)
C(49)	6796(3)	11642(3)	9384(2)	31(1)
C(50)	6310(3)	10769(2)	9510(1)	26(1)
C(51)	5510(3)	10555(2)	9144(1)	22(1)
C(52)	2364(3)	11825(2)	8426(1)	21(1)
C(53)	1305(3)	11616(2)	8240(1)	31(1)
C(54)	84(3)	12274(3)	8414(2)	35(1)
C(55)	-120(3)	13157(2)	8778(1)	32(1)
C(56)	891(3)	13397(2)	8956(1)	26(1)
C(57)	2127(3)	12740(2)	8778(1)	22(1)
C(58)	4476(3)	11360(2)	7366(1)	26(1)
C(59)	5701(3)	11355(2)	7126(1)	34(1)
C(60)	5985(4)	11726(3)	6542(2)	45(1)
C(61)	5056(4)	12089(3)	6184(2)	52(1)
C(62)	3839(4)	12098(3)	6405(2)	50(1)
C(63)	3532(3)	11745(3)	6991(1)	38(1)
C(64)	3191(6)	4811(4)	5527(4)	97(2)
C(65)	2060(6)	5192(5)	5893(3)	109(2)
C(66)	1045(4)	5759(5)	5638(2)	124(2)
C(67)	1120(4)	5970(3)	5038(2)	75(1)
C(68)	2215(5)	5622(4)	4679(2)	74(1)
C(69)	3230(5)	5072(5)	4926(3)	107(2)
C(70)	357(3)	10854(3)	4711(1)	30(1)
C(71)	645(3)	9878(3)	4423(1)	31(1)
C(72)	291(3)	9022(3)	4710(1)	32(1)
C(74)	9622(3)	9339(3)	9648(2)	35(1)
C(73)	10540(3)	9828(3)	9400(2)	34(1)
C(75)	9087(3)	9508(3)	10244(2)	34(1)

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**Table 3.** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj26.

---

Co(1)-P(2)	2.1667(8)
Co(1)-S(1)	2.1904(8)
Co(1)-P(1)	2.2057(8)
Co(1)-P(3)	2.2432(8)
S(1)-Si(1)	2.120(1)
Si(1)-C(46)	1.874(3)
P(2)-Co(1)-S(1)	139.91(3)
P(2)-Co(1)-P(1)	87.79(3)
S(1)-Co(1)-P(1)	108.15(3)
P(2)-Co(1)-P(3)	87.65(3)
S(1)-Co(1)-P(3)	123.62(3)
P(1)-Co(1)-P(3)	99.63(3)
Si(1)-S(1)-Co(1)	128.04(4)
C(46)-Si(1)-S(1)	110.0(1)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj26.**

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Co(1)-P(2)	2.1667(8)
Co(1)-S(1)	2.1904(8)
Co(1)-P(1)	2.2057(8)
Co(1)-P(3)	2.2432(8)
P(1)-C(7)	1.811(3)
P(1)-C(16)	1.825(3)
P(1)-C(10)	1.833(3)
P(2)-C(8)	1.800(3)
P(2)-C(28)	1.826(3)
P(2)-C(22)	1.831(3)
P(3)-C(9)	1.818(3)
P(3)-C(34)	1.830(3)
P(3)-C(40)	1.835(3)
S(1)-Si(1)	2.1199(10)
Si(1)-C(46)	1.874(3)
Si(1)-C(58)	1.881(3)
Si(1)-C(52)	1.881(3)
B(1)-C(1)	1.627(4)
B(1)-C(9)	1.649(4)
B(1)-C(7)	1.671(4)
B(1)-C(8)	1.675(4)
C(1)-C(6)	1.372(4)
C(1)-C(2)	1.373(4)
C(2)-C(3)	1.394(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.339(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.348(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.390(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.393(4)
C(10)-C(15)	1.393(3)
C(11)-C(12)	1.377(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.388(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.392(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.371(4)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.382(4)
C(16)-C(17)	1.383(4)

C(17)-C(18)	1.378(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.371(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.375(4)
C(19)-H(19)	0.9500
C(20)-C(21)	1.382(4)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(27)	1.380(4)
C(22)-C(23)	1.393(4)
C(23)-C(24)	1.377(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.382(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.372(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.382(4)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.385(4)
C(28)-C(33)	1.387(4)
C(29)-C(30)	1.384(4)
C(29)-H(29)	0.9500
C(30)-C(31)	1.379(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.368(4)
C(31)-H(31)	0.9500
C(32)-C(33)	1.372(4)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.390(4)
C(34)-C(35)	1.398(4)
C(35)-C(36)	1.377(4)
C(35)-H(35)	0.9500
C(36)-C(37)	1.385(4)
C(36)-H(36)	0.9500
C(37)-C(38)	1.372(4)
C(37)-H(37)	0.9500
C(38)-C(39)	1.384(4)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(45)	1.383(4)
C(40)-C(41)	1.385(3)
C(41)-C(42)	1.378(4)
C(41)-H(41)	0.9500
C(42)-C(43)	1.388(4)
C(42)-H(42)	0.9500
C(43)-C(44)	1.373(4)
C(43)-H(43)	0.9500
C(44)-C(45)	1.392(4)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(51)	1.395(4)

C(46)-C(47)	1.402(4)
C(47)-C(48)	1.388(4)
C(47)-H(47)	0.9500
C(48)-C(49)	1.375(4)
C(48)-H(48)	0.9500
C(49)-C(50)	1.378(4)
C(49)-H(49)	0.9500
C(50)-C(51)	1.381(4)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-C(57)	1.386(4)
C(52)-C(53)	1.397(4)
C(53)-C(54)	1.376(4)
C(53)-H(53)	0.9500
C(54)-C(55)	1.374(4)
C(54)-H(54)	0.9500
C(55)-C(56)	1.357(4)
C(55)-H(55)	0.9500
C(56)-C(57)	1.390(4)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(59)	1.377(4)
C(58)-C(63)	1.397(4)
C(59)-C(60)	1.394(4)
C(59)-H(59)	0.9500
C(60)-C(61)	1.357(5)
C(60)-H(60)	0.9500
C(61)-C(62)	1.358(5)
C(61)-H(61)	0.9500
C(62)-C(63)	1.394(4)
C(62)-H(62)	0.9500
C(63)-H(63)	0.9500
C(64)-C(65)	1.358(7)
C(64)-C(69)	1.369(7)
C(64)-H(64)	0.9500
C(65)-C(66)	1.335(6)
C(65)-H(65)	0.9500
C(66)-C(67)	1.354(6)
C(66)-H(66)	0.9500
C(67)-C(68)	1.319(5)
C(67)-H(67)	0.9500
C(68)-C(69)	1.322(6)
C(68)-H(68)	0.9500
C(69)-H(69)	0.9500
C(70)-C(71)	1.369(4)
C(70)-C(72)#1	1.377(4)
C(70)-H(70)	0.9500
C(71)-C(72)	1.372(4)
C(71)-H(71)	0.9500
C(72)-C(70)#1	1.377(4)
C(72)-H(72)	0.9500
C(74)-C(75)	1.377(4)
C(74)-C(73)	1.379(4)
C(74)-H(74)	0.9500

C(73)-C(75)#2	1.378(4)
C(73)-H(73)	0.9500
C(75)-C(73)#2	1.378(4)
C(75)-H(75)	0.9500
P(2)-Co(1)-S(1)	139.91(3)
P(2)-Co(1)-P(1)	87.79(3)
S(1)-Co(1)-P(1)	108.15(3)
P(2)-Co(1)-P(3)	87.65(3)
S(1)-Co(1)-P(3)	123.62(3)
P(1)-Co(1)-P(3)	99.63(3)
C(7)-P(1)-C(16)	107.05(13)
C(7)-P(1)-C(10)	106.28(13)
C(16)-P(1)-C(10)	101.96(12)
C(7)-P(1)-Co(1)	113.56(9)
C(16)-P(1)-Co(1)	117.67(9)
C(10)-P(1)-Co(1)	109.17(9)
C(8)-P(2)-C(28)	110.19(12)
C(8)-P(2)-C(22)	107.78(13)
C(28)-P(2)-C(22)	100.89(12)
C(8)-P(2)-Co(1)	116.76(9)
C(28)-P(2)-Co(1)	105.96(9)
C(22)-P(2)-Co(1)	114.05(9)
C(9)-P(3)-C(34)	106.31(13)
C(9)-P(3)-C(40)	103.40(12)
C(34)-P(3)-C(40)	101.92(12)
C(9)-P(3)-Co(1)	108.62(9)
C(34)-P(3)-Co(1)	118.57(9)
C(40)-P(3)-Co(1)	116.57(9)
Si(1)-S(1)-Co(1)	128.04(4)
C(46)-Si(1)-C(58)	109.15(14)
C(46)-Si(1)-C(52)	108.68(12)
C(58)-Si(1)-C(52)	106.71(13)
C(46)-Si(1)-S(1)	110.03(10)
C(58)-Si(1)-S(1)	116.99(10)
C(52)-Si(1)-S(1)	104.91(10)
C(1)-B(1)-C(9)	110.4(2)
C(1)-B(1)-C(7)	107.7(2)
C(9)-B(1)-C(7)	111.9(2)
C(1)-B(1)-C(8)	110.2(2)
C(9)-B(1)-C(8)	109.8(2)
C(7)-B(1)-C(8)	106.8(2)
C(6)-C(1)-C(2)	113.7(3)
C(6)-C(1)-B(1)	122.0(3)
C(2)-C(1)-B(1)	124.3(3)
C(1)-C(2)-C(3)	122.9(3)
C(1)-C(2)-H(2)	118.5
C(3)-C(2)-H(2)	118.5
C(4)-C(3)-C(2)	121.3(3)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
C(3)-C(4)-C(5)	117.9(3)
C(3)-C(4)-H(4)	121.1
C(5)-C(4)-H(4)	121.1

C(4)-C(5)-C(6)	120.7(3)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(1)-C(6)-C(5)	123.5(3)
C(1)-C(6)-H(6)	118.2
C(5)-C(6)-H(6)	118.2
B(1)-C(7)-P(1)	115.78(18)
B(1)-C(7)-H(7A)	108.3
P(1)-C(7)-H(7A)	108.3
B(1)-C(7)-H(7B)	108.3
P(1)-C(7)-H(7B)	108.3
H(7A)-C(7)-H(7B)	107.4
B(1)-C(8)-P(2)	112.38(18)
B(1)-C(8)-H(8A)	109.1
P(2)-C(8)-H(8A)	109.1
B(1)-C(8)-H(8B)	109.1
P(2)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.9
B(1)-C(9)-P(3)	116.24(18)
B(1)-C(9)-H(9A)	108.2
P(3)-C(9)-H(9A)	108.2
B(1)-C(9)-H(9B)	108.2
P(3)-C(9)-H(9B)	108.2
H(9A)-C(9)-H(9B)	107.4
C(11)-C(10)-C(15)	118.6(3)
C(11)-C(10)-P(1)	122.4(2)
C(15)-C(10)-P(1)	119.0(2)
C(12)-C(11)-C(10)	120.8(3)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	120.5(3)
C(11)-C(12)-H(12)	119.7
C(13)-C(12)-H(12)	119.7
C(12)-C(13)-C(14)	118.7(3)
C(12)-C(13)-H(13)	120.6
C(14)-C(13)-H(13)	120.6
C(15)-C(14)-C(13)	120.9(3)
C(15)-C(14)-H(14)	119.6
C(13)-C(14)-H(14)	119.6
C(14)-C(15)-C(10)	120.5(3)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.7
C(21)-C(16)-C(17)	118.0(3)
C(21)-C(16)-P(1)	121.6(2)
C(17)-C(16)-P(1)	120.4(2)
C(18)-C(17)-C(16)	121.6(3)
C(18)-C(17)-H(17)	119.2
C(16)-C(17)-H(17)	119.2
C(19)-C(18)-C(17)	119.7(3)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(18)-C(19)-C(20)	119.7(3)
C(18)-C(19)-H(19)	120.2
C(20)-C(19)-H(19)	120.2

C(19)-C(20)-C(21)	120.5(3)
C(19)-C(20)-H(20)	119.8
C(21)-C(20)-H(20)	119.8
C(20)-C(21)-C(16)	120.6(3)
C(20)-C(21)-H(21)	119.7
C(16)-C(21)-H(21)	119.7
C(27)-C(22)-C(23)	118.6(3)
C(27)-C(22)-P(2)	117.8(2)
C(23)-C(22)-P(2)	123.5(2)
C(24)-C(23)-C(22)	120.4(3)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(23)-C(24)-C(25)	120.3(3)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(26)-C(25)-C(24)	119.7(3)
C(26)-C(25)-H(25)	120.1
C(24)-C(25)-H(25)	120.2
C(25)-C(26)-C(27)	120.0(3)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(22)-C(27)-C(26)	121.0(3)
C(22)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.5
C(29)-C(28)-C(33)	118.6(3)
C(29)-C(28)-P(2)	120.1(2)
C(33)-C(28)-P(2)	121.3(2)
C(30)-C(29)-C(28)	120.1(3)
C(30)-C(29)-H(29)	119.9
C(28)-C(29)-H(29)	119.9
C(31)-C(30)-C(29)	120.3(3)
C(31)-C(30)-H(30)	119.8
C(29)-C(30)-H(30)	119.8
C(32)-C(31)-C(30)	119.7(3)
C(32)-C(31)-H(31)	120.1
C(30)-C(31)-H(31)	120.1
C(31)-C(32)-C(33)	120.2(3)
C(31)-C(32)-H(32)	119.9
C(33)-C(32)-H(32)	119.9
C(32)-C(33)-C(28)	121.0(3)
C(32)-C(33)-H(33)	119.5
C(28)-C(33)-H(33)	119.5
C(39)-C(34)-C(35)	118.2(3)
C(39)-C(34)-P(3)	118.2(2)
C(35)-C(34)-P(3)	123.6(2)
C(36)-C(35)-C(34)	120.5(3)
C(36)-C(35)-H(35)	119.7
C(34)-C(35)-H(35)	119.7
C(35)-C(36)-C(37)	120.5(3)
C(35)-C(36)-H(36)	119.8
C(37)-C(36)-H(36)	119.8
C(38)-C(37)-C(36)	119.7(3)
C(38)-C(37)-H(37)	120.2
C(36)-C(37)-H(37)	120.2

C(37)-C(38)-C(39)	120.2(3)
C(37)-C(38)-H(38)	119.9
C(39)-C(38)-H(38)	119.9
C(38)-C(39)-C(34)	121.0(3)
C(38)-C(39)-H(39)	119.5
C(34)-C(39)-H(39)	119.5
C(45)-C(40)-C(41)	119.2(3)
C(45)-C(40)-P(3)	120.4(2)
C(41)-C(40)-P(3)	120.2(2)
C(42)-C(41)-C(40)	120.6(3)
C(42)-C(41)-H(41)	119.7
C(40)-C(41)-H(41)	119.7
C(41)-C(42)-C(43)	119.9(3)
C(41)-C(42)-H(42)	120.1
C(43)-C(42)-H(42)	120.1
C(44)-C(43)-C(42)	120.1(3)
C(44)-C(43)-H(43)	120.0
C(42)-C(43)-H(43)	120.0
C(43)-C(44)-C(45)	119.8(3)
C(43)-C(44)-H(44)	120.1
C(45)-C(44)-H(44)	120.1
C(40)-C(45)-C(44)	120.4(3)
C(40)-C(45)-H(45)	119.8
C(44)-C(45)-H(45)	119.8
C(51)-C(46)-C(47)	116.8(3)
C(51)-C(46)-Si(1)	121.7(2)
C(47)-C(46)-Si(1)	121.5(2)
C(48)-C(47)-C(46)	121.3(3)
C(48)-C(47)-H(47)	119.3
C(46)-C(47)-H(47)	119.3
C(49)-C(48)-C(47)	120.1(3)
C(49)-C(48)-H(48)	119.9
C(47)-C(48)-H(48)	119.9
C(48)-C(49)-C(50)	119.8(3)
C(48)-C(49)-H(49)	120.1
C(50)-C(49)-H(49)	120.1
C(49)-C(50)-C(51)	120.0(3)
C(49)-C(50)-H(50)	120.0
C(51)-C(50)-H(50)	120.0
C(50)-C(51)-C(46)	121.8(3)
C(50)-C(51)-H(51)	119.1
C(46)-C(51)-H(51)	119.1
C(57)-C(52)-C(53)	116.9(3)
C(57)-C(52)-Si(1)	122.3(2)
C(53)-C(52)-Si(1)	120.7(2)
C(54)-C(53)-C(52)	121.3(3)
C(54)-C(53)-H(53)	119.4
C(52)-C(53)-H(53)	119.4
C(55)-C(54)-C(53)	120.3(3)
C(55)-C(54)-H(54)	119.8
C(53)-C(54)-H(54)	119.8
C(56)-C(55)-C(54)	119.9(3)
C(56)-C(55)-H(55)	120.1
C(54)-C(55)-H(55)	120.1

C(55)-C(56)-C(57)	120.1(3)
C(55)-C(56)-H(56)	119.9
C(57)-C(56)-H(56)	119.9
C(52)-C(57)-C(56)	121.5(3)
C(52)-C(57)-H(57)	119.3
C(56)-C(57)-H(57)	119.3
C(59)-C(58)-C(63)	116.7(3)
C(59)-C(58)-Si(1)	123.3(2)
C(63)-C(58)-Si(1)	120.0(2)
C(58)-C(59)-C(60)	121.7(3)
C(58)-C(59)-H(59)	119.1
C(60)-C(59)-H(59)	119.1
C(61)-C(60)-C(59)	120.7(4)
C(61)-C(60)-H(60)	119.7
C(59)-C(60)-H(60)	119.7
C(60)-C(61)-C(62)	119.1(3)
C(60)-C(61)-H(61)	120.4
C(62)-C(61)-H(61)	120.4
C(61)-C(62)-C(63)	121.1(4)
C(61)-C(62)-H(62)	119.5
C(63)-C(62)-H(62)	119.5
C(62)-C(63)-C(58)	120.7(3)
C(62)-C(63)-H(63)	119.6
C(58)-C(63)-H(63)	119.6
C(65)-C(64)-C(69)	117.9(5)
C(65)-C(64)-H(64)	121.0
C(69)-C(64)-H(64)	121.0
C(66)-C(65)-C(64)	117.9(6)
C(66)-C(65)-H(65)	121.0
C(64)-C(65)-H(65)	121.0
C(65)-C(66)-C(67)	122.1(5)
C(65)-C(66)-H(66)	118.9
C(67)-C(66)-H(66)	118.9
C(68)-C(67)-C(66)	120.7(5)
C(68)-C(67)-H(67)	119.6
C(66)-C(67)-H(67)	119.6
C(67)-C(68)-C(69)	117.7(5)
C(67)-C(68)-H(68)	121.1
C(69)-C(68)-H(68)	121.1
C(68)-C(69)-C(64)	123.5(6)
C(68)-C(69)-H(69)	118.2
C(64)-C(69)-H(69)	118.2
C(71)-C(70)-C(72)#1	119.9(3)
C(71)-C(70)-H(70)	120.1
C(72)#1-C(70)-H(70)	120.1
C(70)-C(71)-C(72)	120.1(3)
C(70)-C(71)-H(71)	119.9
C(72)-C(71)-H(71)	119.9
C(71)-C(72)-C(70)#1	120.0(3)
C(71)-C(72)-H(72)	120.0
C(70)#1-C(72)-H(72)	120.0
C(75)-C(74)-C(73)	120.4(3)
C(75)-C(74)-H(74)	119.8
C(73)-C(74)-H(74)	119.8

C(75)#2-C(73)-C(74)	119.2(3)
C(75)#2-C(73)-H(73)	120.4
C(74)-C(73)-H(73)	120.4
C(74)-C(75)-C(73)#2	120.4(3)
C(74)-C(75)-H(75)	119.8
C(73)#2-C(75)-H(75)	119.8

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Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 -x+2,-y+2,-z+2

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj26. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co(1)	142(2)	134(2)	160(2)	3(2)	-6(2)	-34(2)
P(1)	160(4)	142(4)	160(4)	8(3)	-15(3)	-41(3)
P(2)	140(4)	156(4)	171(4)	13(3)	-25(3)	-41(3)
P(3)	163(4)	155(4)	158(4)	10(3)	-17(3)	-55(3)
S(1)	189(4)	140(4)	220(4)	-19(3)	36(3)	-54(3)
Si(1)	189(4)	163(4)	210(5)	-2(4)	3(4)	-37(4)
B(1)	125(17)	185(18)	185(19)	-12(15)	-35(14)	-50(14)
C(1)	165(15)	182(16)	155(16)	25(13)	-48(13)	-49(13)
C(2)	520(30)	190(20)	990(30)	10(20)	380(20)	-92(18)
C(3)	380(20)	340(20)	1220(40)	-120(30)	400(30)	-30(20)
C(4)	230(18)	212(18)	390(20)	-52(16)	-52(16)	59(15)
C(5)	530(20)	201(19)	550(30)	26(18)	70(20)	-67(18)
C(6)	360(20)	236(19)	590(30)	-68(18)	227(19)	-38(16)
C(7)	198(16)	116(15)	220(17)	20(13)	-67(13)	-61(12)
C(8)	152(15)	142(15)	196(16)	-8(13)	-15(13)	-55(12)
C(9)	144(15)	187(16)	173(16)	17(13)	-20(12)	-25(12)
C(10)	214(16)	142(15)	159(16)	38(13)	-18(13)	-60(13)
C(11)	220(16)	187(16)	128(15)	26(13)	-6(13)	-43(13)
C(12)	197(16)	232(17)	213(17)	57(14)	-29(14)	-55(14)
C(13)	293(18)	256(18)	204(17)	58(14)	-112(14)	-164(15)
C(14)	326(19)	176(16)	156(16)	-31(13)	-7(14)	-66(14)
C(15)	220(16)	154(15)	179(16)	40(13)	-36(13)	-49(13)
C(16)	197(16)	149(15)	151(16)	11(12)	-38(13)	-85(13)
C(17)	298(19)	260(19)	340(20)	66(16)	78(16)	0(15)
C(18)	400(20)	242(19)	380(20)	121(16)	38(17)	-101(16)
C(19)	307(19)	350(20)	227(18)	3(15)	77(15)	-198(16)
C(20)	213(18)	330(20)	380(20)	39(17)	77(16)	-73(15)
C(21)	241(18)	228(17)	307(19)	60(15)	-14(15)	-69(14)
C(22)	176(16)	197(16)	143(16)	18(13)	-50(13)	-51(13)
C(23)	178(16)	191(17)	272(18)	1(14)	2(14)	-44(13)
C(24)	292(19)	204(17)	360(20)	53(15)	-12(16)	-115(15)
C(25)	190(17)	340(20)	314(19)	91(16)	-39(15)	-150(15)
C(26)	134(16)	281(19)	334(19)	70(15)	-6(14)	-44(14)
C(27)	185(16)	153(16)	304(18)	28(14)	-6(14)	-27(13)
C(28)	127(15)	211(16)	170(16)	31(13)	2(13)	-55(13)
C(29)	370(20)	197(17)	264(19)	12(15)	-116(16)	-58(15)
C(30)	490(20)	380(20)	218(19)	19(16)	-168(17)	-135(18)
C(31)	183(17)	360(20)	296(19)	127(16)	-91(15)	-66(15)
C(32)	157(16)	228(17)	317(19)	54(15)	-6(14)	-24(13)
C(33)	187(16)	232(17)	218(17)	30(14)	-36(14)	-47(14)
C(34)	139(15)	217(16)	190(16)	13(13)	-28(13)	-93(13)
C(35)	215(17)	241(17)	188(17)	20(14)	-1(14)	-92(14)
C(36)	281(18)	390(20)	196(18)	-31(16)	26(15)	-149(16)
C(37)	270(18)	520(20)	152(17)	105(16)	-83(15)	-176(17)
C(38)	203(17)	310(19)	289(19)	116(16)	-54(15)	-62(15)
C(39)	193(16)	265(17)	177(17)	-2(14)	-4(13)	-73(14)

C(40)	140(15)	126(15)	189(16)	34(13)	-49(13)	-42(12)
C(41)	242(17)	243(17)	173(16)	43(13)	-48(14)	-105(14)
C(42)	190(17)	232(17)	312(19)	88(15)	-50(14)	-100(14)
C(43)	180(16)	206(17)	410(20)	5(15)	-89(15)	-94(14)
C(44)	228(17)	229(17)	312(19)	-93(15)	-66(15)	-51(14)
C(45)	173(16)	175(16)	235(17)	-14(14)	1(13)	-41(13)
C(46)	146(15)	145(16)	280(18)	-50(14)	34(14)	-21(12)
C(47)	223(17)	223(18)	410(20)	65(16)	-47(16)	-59(14)
C(48)	238(18)	167(17)	600(30)	-31(17)	-80(18)	-63(14)
C(49)	202(17)	311(19)	430(20)	-161(17)	-31(16)	-54(15)
C(50)	231(17)	273(18)	261(18)	-26(15)	0(15)	-61(15)
C(51)	186(16)	185(16)	245(18)	-48(14)	38(14)	-37(13)
C(52)	237(17)	172(16)	209(17)	31(13)	-13(14)	-50(13)
C(53)	292(19)	268(19)	340(20)	-92(16)	-31(16)	-49(15)
C(54)	216(18)	380(20)	460(20)	-25(18)	-69(17)	-73(16)
C(55)	198(18)	297(19)	370(20)	-67(16)	0(16)	40(15)
C(56)	321(19)	182(17)	216(18)	-6(14)	-22(15)	22(15)
C(57)	252(17)	179(16)	213(17)	20(14)	-34(14)	-41(14)
C(58)	320(19)	158(16)	253(18)	-27(14)	40(15)	-21(14)
C(59)	410(20)	231(18)	310(20)	70(16)	41(17)	-39(16)
C(60)	470(20)	380(20)	390(20)	27(19)	160(20)	-69(19)
C(61)	670(30)	390(20)	340(20)	112(19)	80(20)	-30(20)
C(62)	690(30)	480(20)	250(20)	63(18)	-120(20)	-10(20)
C(63)	500(20)	340(20)	290(20)	-47(17)	-54(18)	-86(18)
C(64)	770(40)	340(30)	2070(70)	90(40)	-1030(50)	-170(30)
C(65)	840(40)	1350(50)	1380(50)	860(40)	-560(40)	-720(40)
C(66)	390(30)	2210(70)	820(40)	620(40)	130(30)	-130(40)
C(67)	540(30)	680(30)	840(40)	250(30)	60(30)	10(20)
C(68)	750(40)	760(40)	760(40)	-290(30)	120(30)	-360(30)
C(69)	440(30)	1000(50)	1690(70)	-910(50)	-130(40)	40(30)
C(70)	306(19)	360(20)	300(20)	70(17)	-128(16)	-158(16)
C(71)	243(18)	430(20)	179(18)	63(16)	-45(14)	-1(16)
C(72)	440(20)	248(19)	270(20)	-20(16)	-138(17)	-51(16)
C(74)	400(20)	310(20)	380(20)	21(17)	-116(18)	-142(17)
C(73)	380(20)	290(20)	360(20)	28(17)	-57(17)	-95(17)
C(75)	249(19)	330(20)	440(20)	82(17)	-34(17)	-127(16)

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**Table 6. Hydrogen coordinates (  $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj26.**

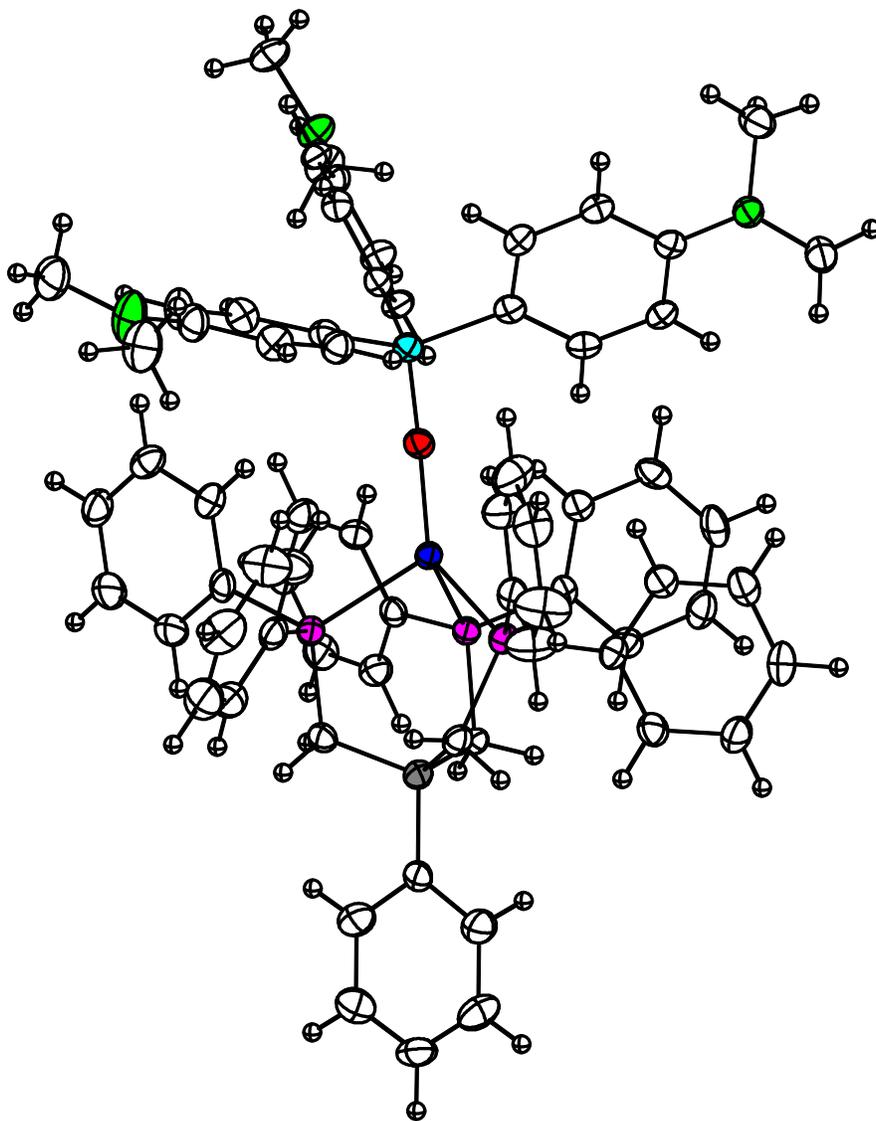
	x	y	z	$U_{\text{iso}}$
H(2)	960	468	669	75
H(3)	1099	299	641	86
H(4)	1040	143	663	36
H(5)	836	158	712	54
H(6)	694	327	737	52
H(7A)	704	481	821	21
H(7B)	578	479	795	21
H(8A)	563	506	677	19
H(8B)	628	592	642	19
H(9A)	850	616	687	21
H(9B)	826	625	759	21
H(11)	822	565	849	22
H(12)	952	604	912	26
H(13)	865	736	988	27
H(14)	646	826	999	27
H(15)	517	790	936	22
H(17)	526	466	911	40
H(18)	368	424	980	42
H(19)	168	552	1000	34
H(20)	131	722	954	39
H(21)	289	763	885	32
H(23)	421	461	730	26
H(24)	246	397	766	34
H(25)	47	520	797	32
H(26)	26	705	798	31
H(27)	201	769	765	27
H(29)	419	644	593	33
H(30)	317	752	518	42
H(31)	232	939	532	34
H(32)	246	1018	620	29
H(33)	339	910	697	26
H(35)	792	654	601	25
H(36)	777	699	501	34
H(37)	668	876	474	36
H(38)	567	1004	548	33
H(39)	576	959	649	25
H(41)	905	832	660	25
H(42)	1042	920	689	29
H(43)	1002	993	787	30
H(44)	825	978	853	30
H(45)	688	887	823	24
H(47)	540	1259	821	35
H(48)	680	1291	881	40
H(49)	736	1178	963	38
H(50)	653	1031	985	31
H(51)	520	994	923	26
H(53)	143	1101	799	37

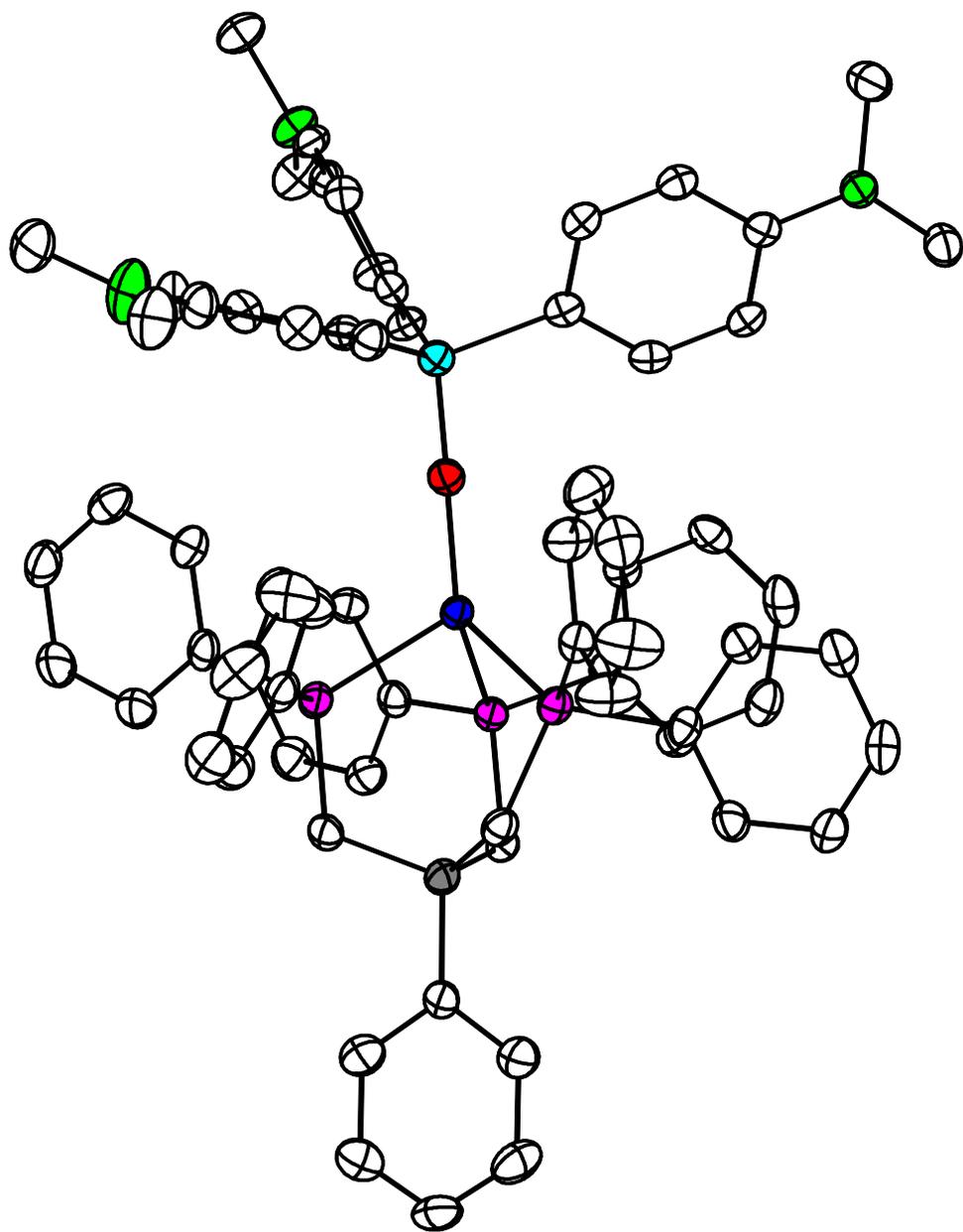
H(54)	-62	1212	828	42
H(55)	-97	1360	890	38
H(56)	75	1401	920	31
H(57)	283	1292	890	26
H(59)	637	1109	737	41
H(60)	684	1172	639	54
H(61)	526	1233	578	62
H(62)	319	1235	616	60
H(63)	267	1177	714	46
H(64)	393	438	568	117
H(65)	199	506	632	131
H(66)	24	602	589	148
H(67)	38	637	487	90
H(68)	227	576	426	89
H(69)	403	484	467	128
H(70)	60	1145	451	36
H(71)	109	979	402	37
H(72)	49	835	451	38
H(74)	936	888	941	42
H(73)	1091	971	899	41
H(75)	846	917	1041	40

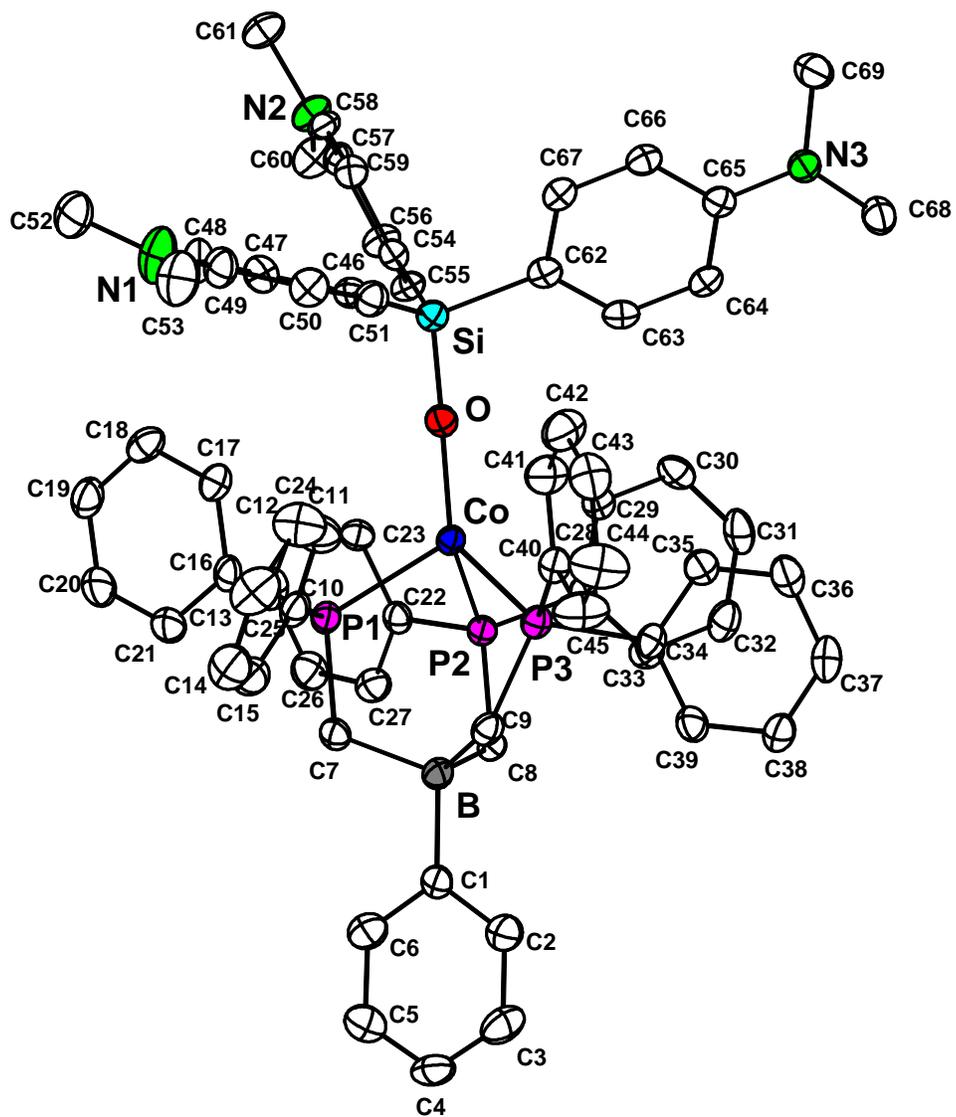
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I. X-ray report for  $[\text{PhBP}_3]\text{CoO}(4\text{-NMe}_2\text{-Ph})_3$ , 10.

## Crystal Structure Report for DMJ 47, $[\text{PhBP}_3]\text{CoOSi}(\text{Ph-}i>p\text{-NMe}_2)_3$







**Table 1. Crystal Data and Structure Analysis Details for dmj47.**

Empirical formula	C <sub>69</sub> H <sub>71</sub> BCoN <sub>3</sub> OP <sub>3</sub> Si
Formula weight	1149.03
Crystallization solvent	Toluene/Petroleum Ether
Crystal shape	Block
Crystal color	Red/Purple
Crystal size	0.25 x 0.30 x 0.33 mm

**Data Collection**

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoK $\alpha$	
Data collection temperature	100 K	
Theta range for 8144 reflections used in lattice determination	2.14 to 27.80°	
Unit cell dimensions	a = 12.1092(11) Å b = 12.3919(11) Å c = 21.3227(19) Å	$\alpha$ = 80.696(2)° $\beta$ = 75.993(2)° $\gamma$ = 72.962(1)°
Volume	2954.0(5) Å <sup>3</sup>	
Z	2	
Crystal system	triclinic	
Space group	P $\bar{1}$ (#2)	
Density (calculated)	1.292 g/cm <sup>3</sup>	
F(000)	1210	
Theta range for data collection	1.7 to 28.4°	
Completeness to theta = 28.36°	92.0%	
Index ranges	-15 ≤ h ≤ 16, -16 ≤ k ≤ 16, -28 ≤ l ≤ 28	
Reflections collected	60978	
Independent reflections	13620 [R <sub>int</sub> = 0.0640]	
Reflections > 2 $\sigma$ (I)	9064	
Average $\sigma$ (I)/(net I)	0.0622	
Absorption coefficient	0.44 mm <sup>-1</sup>	
Reflections monitored for decay	236	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	13620 / 0 / 718
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	1.73
Final R indices [I>2σ(I), 9064 reflections]	R1 = 0.0485, wR2 = 0.0712
R indices (all data)	R1 = 0.0877, wR2 = 0.0751
Type of weighting scheme used	σ
Weighting scheme used	1/σ <sup>2</sup> (Fo <sup>2</sup> )
Max shift/error	0.027
Average shift/error	0.002
Largest diff. peak and hole	1.26 and -0.65 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

## Special Refinement Details

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj47.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co	4709(1)	1854(1)	2534(1)	19(1)
O	5960(1)	854(1)	2810(1)	23(1)
P(1)	4597(1)	1877(1)	1487(1)	24(1)
P(2)	2885(1)	1866(1)	2846(1)	19(1)
P(3)	4106(1)	3704(1)	2540(1)	22(1)
Si	7252(1)	188(1)	2956(1)	21(1)
B	2412(2)	3629(2)	1797(1)	24(1)
N(1)	11037(2)	380(2)	481(1)	46(1)
N(2)	7515(2)	-4796(2)	3897(1)	27(1)
N(3)	7893(2)	2063(2)	5298(1)	24(1)
C(4)	-643(2)	5862(2)	975(1)	35(1)
C(5)	-154(2)	4769(2)	823(1)	39(1)
C(6)	811(2)	4100(2)	1075(1)	37(1)
C(1)	1318(2)	4478(2)	1489(1)	22(1)
C(2)	774(2)	5589(2)	1634(1)	35(1)
C(3)	-179(2)	6272(2)	1381(1)	39(1)
C(7)	3156(2)	2598(2)	1324(1)	23(1)
C(8)	1824(2)	3019(2)	2508(1)	20(1)
C(9)	3313(2)	4353(2)	1903(1)	24(1)
C(10)	5637(2)	2584(2)	922(1)	26(1)
C(11)	6676(2)	2557(2)	1097(1)	39(1)
C(12)	7476(2)	3100(2)	702(1)	48(1)
C(13)	7262(2)	3673(2)	114(1)	46(1)
C(14)	6236(2)	3701(2)	-74(1)	44(1)
C(15)	5425(2)	3169(2)	331(1)	36(1)
C(16)	5039(2)	454(2)	1215(1)	24(1)
C(17)	6050(2)	-302(2)	1379(1)	26(1)
C(18)	6392(2)	-1408(2)	1224(1)	29(1)
C(19)	5724(2)	-1779(2)	904(1)	33(1)
C(20)	4726(2)	-1047(2)	742(1)	43(1)
C(21)	4385(2)	67(2)	895(1)	39(1)
C(22)	2745(2)	520(2)	2670(1)	20(1)
C(23)	3708(2)	-430(2)	2679(1)	24(1)
C(24)	3633(2)	-1480(2)	2574(1)	30(1)
C(25)	2606(2)	-1589(2)	2450(1)	32(1)
C(26)	1652(2)	-661(2)	2435(1)	31(1)
C(27)	1719(2)	393(2)	2548(1)	27(1)
C(28)	2490(2)	1777(2)	3731(1)	18(1)
C(29)	3336(2)	1145(2)	4084(1)	23(1)
C(30)	3083(2)	1102(2)	4755(1)	27(1)
C(31)	1995(2)	1692(2)	5077(1)	31(1)
C(32)	1155(2)	2314(2)	4735(1)	31(1)
C(33)	1395(2)	2362(2)	4063(1)	25(1)
C(34)	3211(2)	4296(2)	3292(1)	21(1)
C(35)	3613(2)	3861(2)	3866(1)	26(1)
C(36)	2978(2)	4236(2)	4453(1)	33(1)

C(37)	1921(2)	5068(2)	4483(1)	36(1)
C(38)	1510(2)	5518(2)	3924(1)	34(1)
C(39)	2150(2)	5138(2)	3331(1)	27(1)
C(40)	5384(2)	4267(2)	2431(1)	24(1)
C(41)	6411(2)	3586(2)	2602(1)	37(1)
C(42)	7369(2)	4010(2)	2549(1)	45(1)
C(43)	7309(2)	5128(2)	2329(1)	39(1)
C(44)	6287(3)	5813(2)	2167(1)	50(1)
C(45)	5327(2)	5388(2)	2212(1)	45(1)
C(46)	8455(2)	233(2)	2220(1)	22(1)
C(47)	8872(2)	-623(2)	1801(1)	27(1)
C(48)	9718(2)	-592(2)	1242(1)	32(1)
C(49)	10192(2)	333(2)	1049(1)	31(1)
C(50)	9781(2)	1215(2)	1452(1)	30(1)
C(51)	8945(2)	1147(2)	2020(1)	27(1)
C(52)	11647(2)	-623(2)	157(1)	42(1)
C(53)	11345(2)	1412(2)	235(1)	48(1)
C(54)	7336(2)	-1338(2)	3229(1)	20(1)
C(55)	6338(2)	-1716(2)	3525(1)	24(1)
C(56)	6383(2)	-2840(2)	3746(1)	24(1)
C(57)	7465(2)	-3671(2)	3679(1)	21(1)
C(58)	8480(2)	-3313(2)	3390(1)	22(1)
C(59)	8406(2)	-2186(2)	3176(1)	23(1)
C(60)	6439(2)	-5161(2)	4090(1)	33(1)
C(61)	8644(2)	-5640(2)	3794(1)	33(1)
C(62)	7493(2)	851(2)	3627(1)	20(1)
C(63)	6526(2)	1388(2)	4079(1)	21(1)
C(64)	6626(2)	1778(2)	4628(1)	21(1)
C(65)	7740(2)	1657(2)	4754(1)	20(1)
C(66)	8722(2)	1148(2)	4298(1)	22(1)
C(67)	8593(2)	755(2)	3756(1)	23(1)
C(68)	6824(2)	2610(2)	5736(1)	30(1)
C(69)	8736(2)	1275(2)	5660(1)	32(1)

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**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj47.**

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Co-O	1.809(1)
Co-P(2)	2.1436(7)
Co-P(3)	2.1936(7)
Co-P(1)	2.2645(7)
O-Si	1.618(2)
O-Co-P(2)	127.61(5)
O-Co-P(3)	129.77(5)
P(2)-Co-P(3)	86.47(2)
O-Co-P(1)	117.36(5)
P(2)-Co-P(1)	90.43(2)
P(3)-Co-P(1)	94.56(2)
Si-O-Co	165.66(9)

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**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj47.**

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Co-O	1.8095(14)
Co-P(2)	2.1436(7)
Co-P(3)	2.1936(7)
Co-P(1)	2.2645(7)
O-Si	1.6181(15)
P(1)-C(7)	1.801(2)
P(1)-C(16)	1.833(2)
P(1)-C(10)	1.838(2)
P(2)-C(8)	1.804(2)
P(2)-C(28)	1.823(2)
P(2)-C(22)	1.830(2)
P(3)-C(9)	1.800(2)
P(3)-C(40)	1.828(2)
P(3)-C(34)	1.832(2)
Si-C(54)	1.866(2)
Si-C(46)	1.871(2)
Si-C(62)	1.879(2)
B-C(1)	1.635(3)
B-C(7)	1.663(3)
B-C(8)	1.673(3)
B-C(9)	1.675(3)
N(1)-C(49)	1.389(3)
N(1)-C(53)	1.421(3)
N(1)-C(52)	1.435(3)
N(2)-C(57)	1.384(3)
N(2)-C(60)	1.448(3)
N(2)-C(61)	1.451(3)
N(3)-C(65)	1.408(3)
N(3)-C(68)	1.452(3)
N(3)-C(69)	1.464(3)
C(4)-C(3)	1.366(3)
C(4)-C(5)	1.367(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.390(3)
C(5)-H(5)	0.9500
C(6)-C(1)	1.392(3)
C(6)-H(6)	0.9500
C(1)-C(2)	1.390(3)
C(2)-C(3)	1.387(3)
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.386(3)
C(10)-C(15)	1.390(3)
C(11)-C(12)	1.380(3)
C(11)-H(11)	0.9500

C(12)-C(13)	1.380(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.384(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.390(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.383(3)
C(16)-C(17)	1.388(3)
C(17)-C(18)	1.382(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.385(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.363(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.389(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(27)	1.385(3)
C(22)-C(23)	1.395(3)
C(23)-C(24)	1.388(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.379(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.373(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.394(3)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(33)	1.390(3)
C(28)-C(29)	1.395(3)
C(29)-C(30)	1.384(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.379(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.371(3)
C(31)-H(31)	0.9500
C(32)-C(33)	1.385(3)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.392(3)
C(34)-C(35)	1.395(3)
C(35)-C(36)	1.375(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.383(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.374(3)
C(37)-H(37)	0.9500
C(38)-C(39)	1.389(3)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(41)	1.377(3)
C(40)-C(45)	1.379(3)
C(41)-C(42)	1.382(3)

C(41)-H(41)	0.9500
C(42)-C(43)	1.376(3)
C(42)-H(42)	0.9500
C(43)-C(44)	1.366(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.388(3)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(51)	1.390(3)
C(46)-C(47)	1.398(3)
C(47)-C(48)	1.374(3)
C(47)-H(47)	0.9500
C(48)-C(49)	1.390(3)
C(48)-H(48)	0.9500
C(49)-C(50)	1.399(3)
C(50)-C(51)	1.388(3)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-C(55)	1.395(3)
C(54)-C(59)	1.403(3)
C(55)-C(56)	1.386(3)
C(55)-H(55)	0.9500
C(56)-C(57)	1.402(3)
C(56)-H(56)	0.9500
C(57)-C(58)	1.398(3)
C(58)-C(59)	1.381(3)
C(58)-H(58)	0.9500
C(59)-H(59)	0.9500
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-C(67)	1.393(3)
C(62)-C(63)	1.396(3)
C(63)-C(64)	1.380(3)
C(63)-H(63)	0.9500
C(64)-C(65)	1.399(3)
C(64)-H(64)	0.9500
C(65)-C(66)	1.399(3)
C(66)-C(67)	1.382(3)
C(66)-H(66)	0.9500
C(67)-H(67)	0.9500
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(69)-H(69A)	0.9800

C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
O-Co-P(2)	127.61(5)
O-Co-P(3)	129.77(5)
P(2)-Co-P(3)	86.47(2)
O-Co-P(1)	117.36(5)
P(2)-Co-P(1)	90.43(2)
P(3)-Co-P(1)	94.56(2)
Si-O-Co	165.66(9)
C(7)-P(1)-C(16)	108.59(10)
C(7)-P(1)-C(10)	106.38(10)
C(16)-P(1)-C(10)	103.00(10)
C(7)-P(1)-Co	113.39(7)
C(16)-P(1)-Co	112.80(7)
C(10)-P(1)-Co	111.97(8)
C(8)-P(2)-C(28)	109.86(10)
C(8)-P(2)-C(22)	109.17(10)
C(28)-P(2)-C(22)	102.83(9)
C(8)-P(2)-Co	117.36(7)
C(28)-P(2)-Co	109.22(7)
C(22)-P(2)-Co	107.38(7)
C(9)-P(3)-C(40)	109.12(10)
C(9)-P(3)-C(34)	107.23(10)
C(40)-P(3)-C(34)	100.51(10)
C(9)-P(3)-Co	111.47(7)
C(40)-P(3)-Co	109.23(8)
C(34)-P(3)-Co	118.53(7)
O-Si-C(54)	110.66(9)
O-Si-C(46)	112.26(9)
C(54)-Si-C(46)	107.08(10)
O-Si-C(62)	108.02(9)
C(54)-Si-C(62)	108.48(9)
C(46)-Si-C(62)	110.29(10)
C(1)-B-C(7)	110.59(18)
C(1)-B-C(8)	107.16(18)
C(7)-B-C(8)	107.21(17)
C(1)-B-C(9)	110.67(18)
C(7)-B-C(9)	110.45(18)
C(8)-B-C(9)	110.65(18)
C(49)-N(1)-C(53)	120.0(2)
C(49)-N(1)-C(52)	120.4(2)
C(53)-N(1)-C(52)	119.5(2)
C(57)-N(2)-C(60)	119.95(18)
C(57)-N(2)-C(61)	119.29(18)
C(60)-N(2)-C(61)	119.35(18)
C(65)-N(3)-C(68)	116.45(18)
C(65)-N(3)-C(69)	115.62(18)
C(68)-N(3)-C(69)	111.10(17)
C(3)-C(4)-C(5)	119.0(2)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	119.8(2)
C(4)-C(5)-H(5)	120.1

C(6)-C(5)-H(5)	120.1
C(5)-C(6)-C(1)	123.4(2)
C(5)-C(6)-H(6)	118.3
C(1)-C(6)-H(6)	118.3
C(2)-C(1)-C(6)	114.3(2)
C(2)-C(1)-B	124.6(2)
C(6)-C(1)-B	121.0(2)
C(3)-C(2)-C(1)	123.0(2)
C(3)-C(2)-H(2)	118.5
C(1)-C(2)-H(2)	118.5
C(4)-C(3)-C(2)	120.4(2)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
B-C(7)-P(1)	113.57(14)
B-C(7)-H(7A)	108.9
P(1)-C(7)-H(7A)	108.9
B-C(7)-H(7B)	108.9
P(1)-C(7)-H(7B)	108.9
H(7A)-C(7)-H(7B)	107.7
B-C(8)-P(2)	113.09(14)
B-C(8)-H(8A)	109.0
P(2)-C(8)-H(8A)	109.0
B-C(8)-H(8B)	109.0
P(2)-C(8)-H(8B)	109.0
H(8A)-C(8)-H(8B)	107.8
B-C(9)-P(3)	113.61(15)
B-C(9)-H(9A)	108.8
P(3)-C(9)-H(9A)	108.8
B-C(9)-H(9B)	108.8
P(3)-C(9)-H(9B)	108.8
H(9A)-C(9)-H(9B)	107.7
C(11)-C(10)-C(15)	118.0(2)
C(11)-C(10)-P(1)	118.70(18)
C(15)-C(10)-P(1)	123.29(19)
C(12)-C(11)-C(10)	121.4(2)
C(12)-C(11)-H(11)	119.3
C(10)-C(11)-H(11)	119.3
C(11)-C(12)-C(13)	120.2(3)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	119.4(3)
C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
C(13)-C(14)-C(15)	120.1(2)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-C(10)	120.9(2)
C(14)-C(15)-H(15)	119.6
C(10)-C(15)-H(15)	119.6
C(21)-C(16)-C(17)	118.2(2)
C(21)-C(16)-P(1)	123.86(18)
C(17)-C(16)-P(1)	117.78(17)
C(18)-C(17)-C(16)	120.7(2)
C(18)-C(17)-H(17)	119.7

C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	120.2(2)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(20)-C(19)-C(18)	119.8(2)
C(20)-C(19)-H(19)	120.1
C(18)-C(19)-H(19)	120.1
C(19)-C(20)-C(21)	120.1(2)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(16)-C(21)-C(20)	121.1(2)
C(16)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
C(27)-C(22)-C(23)	118.6(2)
C(27)-C(22)-P(2)	123.18(17)
C(23)-C(22)-P(2)	118.19(17)
C(24)-C(23)-C(22)	120.5(2)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(25)-C(24)-C(23)	120.1(2)
C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(26)-C(25)-C(24)	120.1(2)
C(26)-C(25)-H(25)	120.0
C(24)-C(25)-H(25)	120.0
C(25)-C(26)-C(27)	120.0(2)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(22)-C(27)-C(26)	120.7(2)
C(22)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7
C(33)-C(28)-C(29)	118.91(19)
C(33)-C(28)-P(2)	122.29(16)
C(29)-C(28)-P(2)	118.73(16)
C(30)-C(29)-C(28)	120.2(2)
C(30)-C(29)-H(29)	119.9
C(28)-C(29)-H(29)	119.9
C(31)-C(30)-C(29)	120.1(2)
C(31)-C(30)-H(30)	119.9
C(29)-C(30)-H(30)	119.9
C(32)-C(31)-C(30)	120.1(2)
C(32)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(31)-C(32)-C(33)	120.3(2)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(32)-C(33)-C(28)	120.3(2)
C(32)-C(33)-H(33)	119.9
C(28)-C(33)-H(33)	119.9
C(39)-C(34)-C(35)	117.8(2)
C(39)-C(34)-P(3)	124.52(17)
C(35)-C(34)-P(3)	117.65(17)
C(36)-C(35)-C(34)	121.3(2)
C(36)-C(35)-H(35)	119.3

C(34)-C(35)-H(35)	119.3
C(35)-C(36)-C(37)	120.0(2)
C(35)-C(36)-H(36)	120.0
C(37)-C(36)-H(36)	120.0
C(38)-C(37)-C(36)	119.8(2)
C(38)-C(37)-H(37)	120.1
C(36)-C(37)-H(37)	120.1
C(37)-C(38)-C(39)	120.2(2)
C(37)-C(38)-H(38)	119.9
C(39)-C(38)-H(38)	119.9
C(38)-C(39)-C(34)	120.8(2)
C(38)-C(39)-H(39)	119.6
C(34)-C(39)-H(39)	119.6
C(41)-C(40)-C(45)	118.5(2)
C(41)-C(40)-P(3)	120.04(17)
C(45)-C(40)-P(3)	121.37(19)
C(40)-C(41)-C(42)	120.9(2)
C(40)-C(41)-H(41)	119.6
C(42)-C(41)-H(41)	119.6
C(43)-C(42)-C(41)	120.4(3)
C(43)-C(42)-H(42)	119.8
C(41)-C(42)-H(42)	119.8
C(44)-C(43)-C(42)	119.1(2)
C(44)-C(43)-H(43)	120.5
C(42)-C(43)-H(43)	120.5
C(43)-C(44)-C(45)	120.7(2)
C(43)-C(44)-H(44)	119.6
C(45)-C(44)-H(44)	119.6
C(40)-C(45)-C(44)	120.4(2)
C(40)-C(45)-H(45)	119.8
C(44)-C(45)-H(45)	119.8
C(51)-C(46)-C(47)	114.6(2)
C(51)-C(46)-Si	123.17(17)
C(47)-C(46)-Si	122.07(17)
C(48)-C(47)-C(46)	123.5(2)
C(48)-C(47)-H(47)	118.2
C(46)-C(47)-H(47)	118.2
C(47)-C(48)-C(49)	120.9(2)
C(47)-C(48)-H(48)	119.5
C(49)-C(48)-H(48)	119.5
N(1)-C(49)-C(48)	121.4(2)
N(1)-C(49)-C(50)	121.4(2)
C(48)-C(49)-C(50)	117.2(2)
C(51)-C(50)-C(49)	120.5(2)
C(51)-C(50)-H(50)	119.7
C(49)-C(50)-H(50)	119.7
C(50)-C(51)-C(46)	123.3(2)
C(50)-C(51)-H(51)	118.4
C(46)-C(51)-H(51)	118.4
N(1)-C(52)-H(52A)	109.5
N(1)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
N(1)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5

H(52B)-C(52)-H(52C)	109.5
N(1)-C(53)-H(53A)	109.5
N(1)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
N(1)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(55)-C(54)-C(59)	114.7(2)
C(55)-C(54)-Si	122.41(17)
C(59)-C(54)-Si	122.86(17)
C(56)-C(55)-C(54)	123.4(2)
C(56)-C(55)-H(55)	118.3
C(54)-C(55)-H(55)	118.3
C(55)-C(56)-C(57)	120.6(2)
C(55)-C(56)-H(56)	119.7
C(57)-C(56)-H(56)	119.7
N(2)-C(57)-C(58)	121.93(19)
N(2)-C(57)-C(56)	120.9(2)
C(58)-C(57)-C(56)	117.2(2)
C(59)-C(58)-C(57)	120.8(2)
C(59)-C(58)-H(58)	119.6
C(57)-C(58)-H(58)	119.6
C(58)-C(59)-C(54)	123.3(2)
C(58)-C(59)-H(59)	118.3
C(54)-C(59)-H(59)	118.3
N(2)-C(60)-H(60A)	109.5
N(2)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
N(2)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
N(2)-C(61)-H(61A)	109.5
N(2)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
N(2)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(67)-C(62)-C(63)	115.22(19)
C(67)-C(62)-Si	124.61(16)
C(63)-C(62)-Si	119.83(16)
C(64)-C(63)-C(62)	123.5(2)
C(64)-C(63)-H(63)	118.2
C(62)-C(63)-H(63)	118.2
C(63)-C(64)-C(65)	120.3(2)
C(63)-C(64)-H(64)	119.8
C(65)-C(64)-H(64)	119.8
C(64)-C(65)-C(66)	117.1(2)
C(64)-C(65)-N(3)	122.6(2)
C(66)-C(65)-N(3)	120.2(2)
C(67)-C(66)-C(65)	121.2(2)
C(67)-C(66)-H(66)	119.4
C(65)-C(66)-H(66)	119.4
C(66)-C(67)-C(62)	122.6(2)
C(66)-C(67)-H(67)	118.7

C(62)-C(67)-H(67)	118.7
N(3)-C(68)-H(68A)	109.5
N(3)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
N(3)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
N(3)-C(69)-H(69A)	109.5
N(3)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
N(3)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5

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Symmetry transformations used to generate equivalent atoms:

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj47. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co	211(2)	170(2)	182(2)	-9(1)	-28(1)	-40(1)
O	270(9)	195(8)	220(9)	9(7)	-66(7)	-66(7)
P(1)	281(4)	211(3)	188(3)	-25(3)	-42(3)	-6(3)
P(2)	213(3)	174(3)	177(3)	-3(3)	-35(3)	-48(3)
P(3)	245(4)	174(3)	229(3)	-17(3)	-35(3)	-62(3)
Si	225(4)	186(4)	210(4)	2(3)	-41(3)	-60(3)
B	264(16)	189(15)	233(15)	-22(12)	-60(13)	-24(12)
N(1)	560(16)	402(14)	346(13)	-85(11)	161(12)	-217(12)
N(2)	243(12)	169(11)	350(12)	9(9)	5(9)	-56(9)
N(3)	206(11)	280(11)	237(11)	-40(9)	-34(9)	-60(9)
C(4)	283(15)	341(16)	351(16)	72(13)	-89(12)	4(13)
C(5)	358(17)	450(18)	395(16)	-45(14)	-151(13)	-95(14)
C(6)	408(17)	259(15)	407(16)	-36(12)	-136(14)	-8(13)
C(1)	279(14)	193(13)	170(12)	23(10)	-28(10)	-64(11)
C(2)	358(16)	311(15)	406(16)	-98(12)	-140(13)	-28(13)
C(3)	362(17)	216(14)	544(18)	-47(13)	-93(14)	-12(12)
C(7)	285(14)	208(13)	172(12)	11(10)	-54(10)	-52(11)
C(8)	211(13)	163(12)	225(13)	-40(10)	-63(10)	-9(10)
C(9)	267(14)	180(12)	226(13)	-5(10)	-20(11)	-31(10)
C(10)	325(15)	182(13)	232(13)	-39(10)	-19(11)	-10(11)
C(11)	392(17)	407(17)	360(16)	63(13)	-102(14)	-117(14)
C(12)	419(18)	516(19)	516(19)	77(15)	-101(15)	-196(15)
C(13)	424(19)	367(17)	505(19)	45(14)	48(15)	-136(14)
C(14)	540(20)	379(17)	289(15)	59(13)	-5(14)	-74(15)
C(15)	366(16)	337(16)	317(15)	-32(13)	-52(13)	-26(13)
C(16)	315(15)	217(13)	147(12)	-23(10)	5(11)	-48(11)
C(17)	246(14)	237(14)	268(14)	-53(11)	9(11)	-73(11)
C(18)	254(14)	246(14)	285(14)	13(11)	20(11)	-29(11)
C(19)	437(17)	224(14)	299(15)	-70(11)	-48(13)	-30(13)
C(20)	570(19)	326(16)	428(17)	-153(13)	-255(15)	4(14)
C(21)	527(18)	292(15)	339(15)	-77(12)	-222(14)	54(13)
C(22)	254(14)	199(13)	151(12)	-1(10)	-33(10)	-65(11)
C(23)	251(14)	217(13)	231(13)	10(10)	-66(11)	-56(11)
C(24)	361(16)	200(14)	293(14)	-11(11)	-40(12)	-31(12)
C(25)	432(17)	205(14)	334(15)	-53(11)	-61(13)	-122(13)
C(26)	319(15)	312(15)	346(15)	-55(12)	-86(12)	-128(13)
C(27)	263(14)	251(14)	276(14)	-14(11)	-53(11)	-53(11)
C(28)	254(13)	135(12)	170(12)	-7(9)	-40(10)	-96(10)
C(29)	274(14)	188(13)	227(13)	7(10)	-55(11)	-78(11)
C(30)	373(16)	206(13)	249(14)	62(11)	-139(12)	-107(12)
C(31)	542(18)	253(14)	145(13)	14(11)	-17(13)	-171(13)
C(32)	341(15)	271(14)	243(14)	-46(11)	42(12)	-62(12)
C(33)	252(14)	241(13)	243(14)	1(11)	-49(11)	-55(11)
C(34)	236(13)	166(12)	261(13)	-56(10)	-29(11)	-86(10)
C(35)	339(15)	189(13)	270(14)	1(11)	-83(12)	-81(11)
C(36)	463(17)	301(15)	252(14)	-35(12)	-98(13)	-131(13)

C(37)	432(17)	352(16)	303(15)	-152(12)	-8(13)	-124(14)
C(38)	332(16)	306(15)	370(16)	-147(12)	-75(13)	-19(12)
C(39)	327(15)	252(14)	276(14)	-59(11)	-100(12)	-83(12)
C(40)	294(14)	206(13)	213(13)	-11(10)	-16(11)	-76(11)
C(41)	405(17)	210(14)	566(18)	-59(13)	-194(14)	-102(13)
C(42)	359(17)	357(17)	710(20)	-211(15)	-178(15)	-57(14)
C(43)	365(17)	465(18)	389(16)	-53(14)	-16(13)	-236(14)
C(44)	550(20)	348(17)	680(20)	218(15)	-224(17)	-285(16)
C(45)	399(18)	309(16)	680(20)	124(14)	-201(15)	-147(14)
C(46)	225(13)	216(13)	222(13)	4(10)	-54(10)	-51(11)
C(47)	301(15)	277(14)	270(14)	-20(11)	-58(12)	-130(12)
C(48)	385(16)	331(15)	260(14)	-104(12)	2(12)	-118(13)
C(49)	330(15)	333(15)	233(14)	-37(12)	13(12)	-87(12)
C(50)	326(15)	268(14)	297(14)	28(12)	-28(12)	-115(12)
C(51)	285(14)	244(14)	274(14)	-25(11)	-45(12)	-66(11)
C(52)	358(17)	525(18)	327(16)	-101(14)	59(13)	-95(14)
C(53)	470(18)	546(19)	386(17)	-70(14)	120(14)	-238(15)
C(54)	227(13)	214(13)	186(12)	-20(10)	-56(10)	-68(11)
C(55)	188(13)	221(13)	264(13)	-17(11)	-34(11)	-13(11)
C(56)	180(13)	224(13)	299(14)	9(11)	-8(11)	-72(11)
C(57)	241(14)	172(13)	199(12)	-19(10)	-22(10)	-42(11)
C(58)	179(13)	206(13)	248(13)	-31(10)	-38(10)	5(10)
C(59)	197(13)	255(14)	236(13)	-25(11)	-19(10)	-90(11)
C(60)	343(16)	226(14)	389(16)	16(12)	5(12)	-114(12)
C(61)	325(15)	183(13)	420(16)	4(11)	-65(12)	-11(12)
C(62)	213(13)	168(12)	197(12)	54(10)	-19(10)	-68(10)
C(63)	188(13)	175(12)	269(13)	42(10)	-65(11)	-69(10)
C(64)	187(13)	158(12)	234(13)	14(10)	-5(10)	-40(10)
C(65)	250(14)	126(12)	242(13)	20(10)	-69(11)	-69(10)
C(66)	182(13)	199(13)	296(14)	-10(11)	-49(11)	-64(10)
C(67)	212(13)	191(13)	251(13)	-7(10)	-10(11)	-54(10)
C(68)	296(15)	358(15)	252(14)	-62(11)	-42(12)	-98(12)
C(69)	290(15)	393(16)	284(14)	-4(12)	-92(12)	-87(12)

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**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj47.**

	x	y	z	$U_{\text{iso}}$
H(4)	-130	633	80	42
H(5)	-47	447	55	47
H(6)	114	335	96	44
H(2)	107	589	192	42
H(3)	-51	703	149	47
H(7A)	324	292	86	27
H(7B)	269	204	138	27
H(8A)	118	273	245	24
H(8B)	147	360	282	24
H(9A)	284	513	200	29
H(9B)	389	442	149	29
H(11)	684	216	150	47
H(12)	818	308	83	58
H(13)	781	404	-16	55
H(14)	609	408	-48	52
H(15)	472	321	20	43
H(17)	651	-6	160	31
H(18)	709	-192	134	35
H(19)	596	-254	80	40
H(20)	426	-130	52	51
H(21)	369	57	78	47
H(23)	442	-36	276	28
H(24)	429	-212	259	36
H(25)	256	-231	238	38
H(26)	95	-74	235	37
H(27)	105	103	254	32
H(29)	409	74	386	27
H(30)	366	66	499	32
H(31)	183	167	554	37
H(32)	40	272	496	37
H(33)	81	280	383	30
H(35)	434	329	385	32
H(36)	326	392	484	39
H(37)	148	533	489	43
H(38)	79	609	394	40
H(39)	186	546	295	33
H(41)	646	281	276	44
H(42)	807	353	267	54
H(43)	797	542	229	47
H(44)	623	659	202	60
H(45)	463	587	209	55
H(47)	855	-126	191	33
H(48)	998	-121	98	39
H(50)	1008	187	134	36
H(51)	869	176	229	32
H(52A)	1199	-123	47	64
H(52B)	1228	-46	-20	64

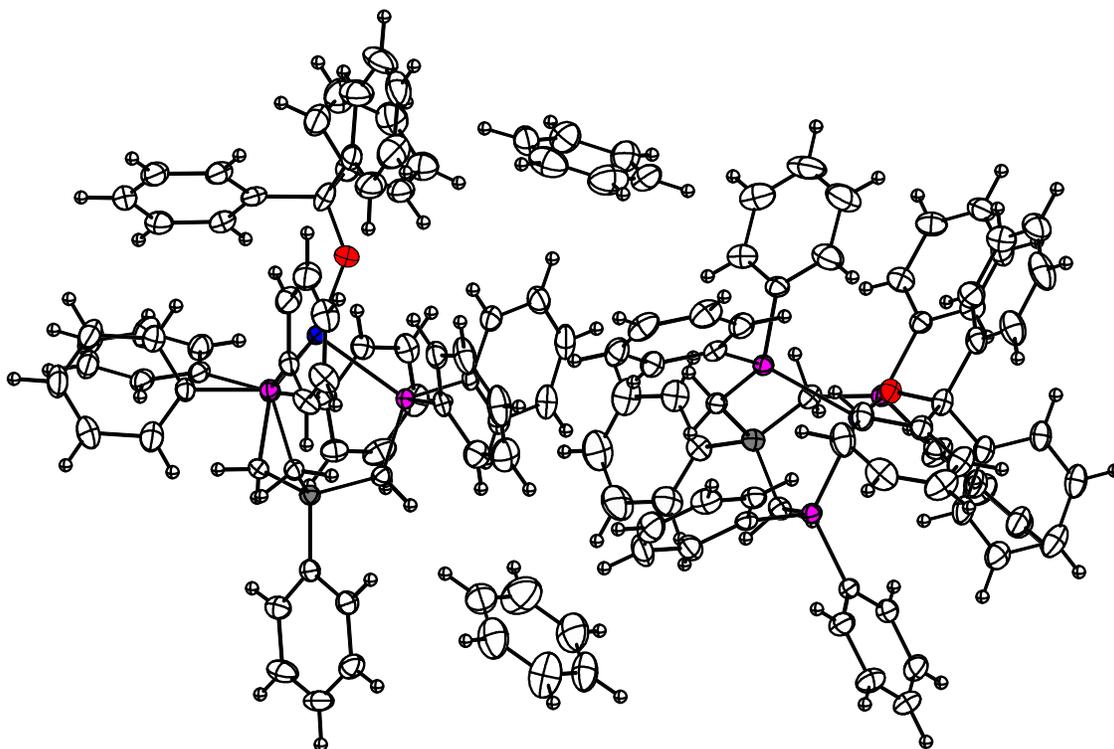
H(52C)	1109	-87	-2	64
H(53A)	1062	204	25	72
H(53B)	1178	136	-22	72
H(53C)	1184	155	50	72
H(55)	559	-118	358	28
H(56)	567	-305	394	29
H(58)	923	-385	334	27
H(59)	912	-198	298	27
H(60A)	597	-484	449	50
H(60B)	664	-599	416	50
H(60C)	598	-490	375	50
H(61A)	895	-569	333	49
H(61B)	854	-638	401	49
H(61C)	920	-542	398	49
H(63)	576	149	401	25
H(64)	594	213	492	25
H(66)	949	107	436	27
H(67)	928	40	346	27
H(68A)	635	324	549	45
H(68B)	703	290	608	45
H(68C)	637	206	593	45
H(69A)	842	64	588	48
H(69B)	888	167	598	48
H(69C)	948	99	536	48

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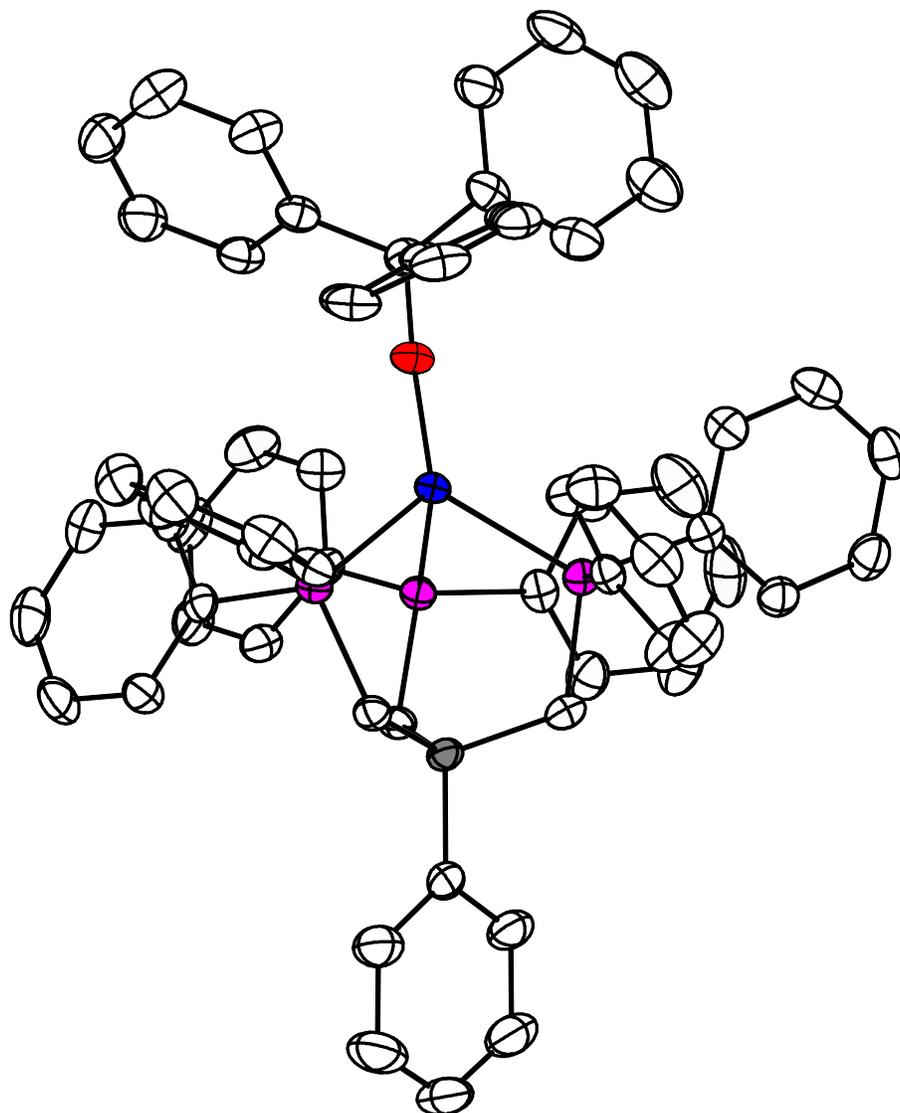
J. X-ray report for  $[\text{PhBP}_3]\text{CoOCPh}_3$ , 12.

## Crystal Structure Report for

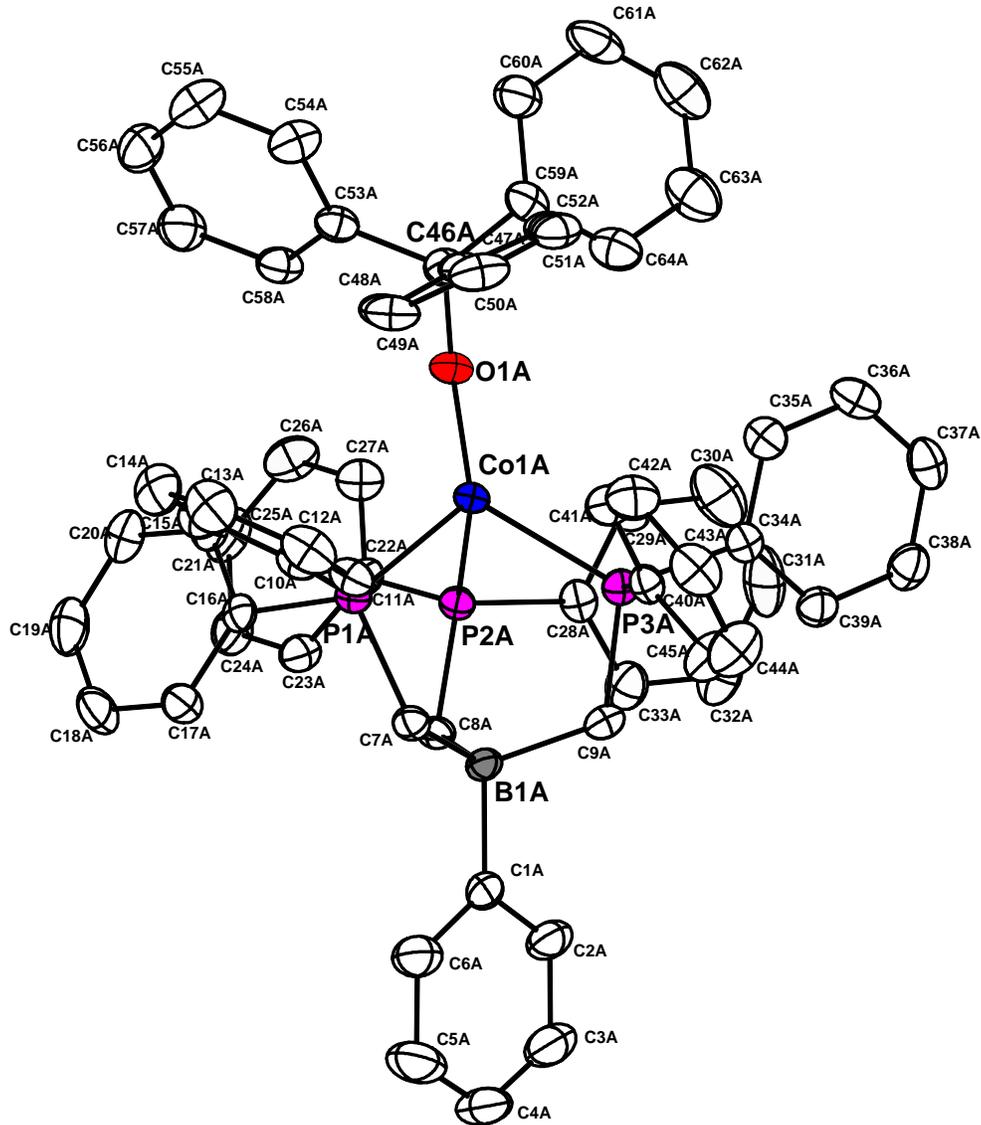
### DMJ 49, $[\text{PhBP}_3]\text{CoOCPh}_3$



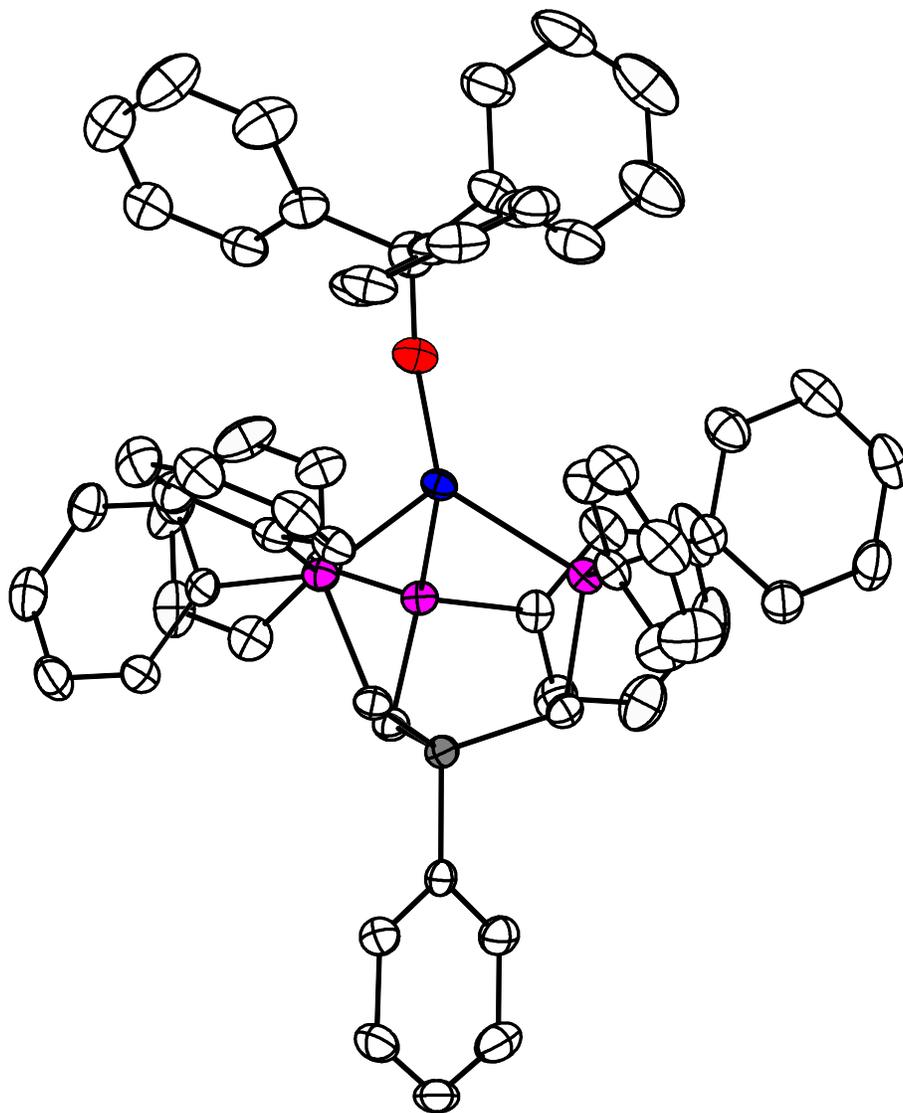
# Molecule A



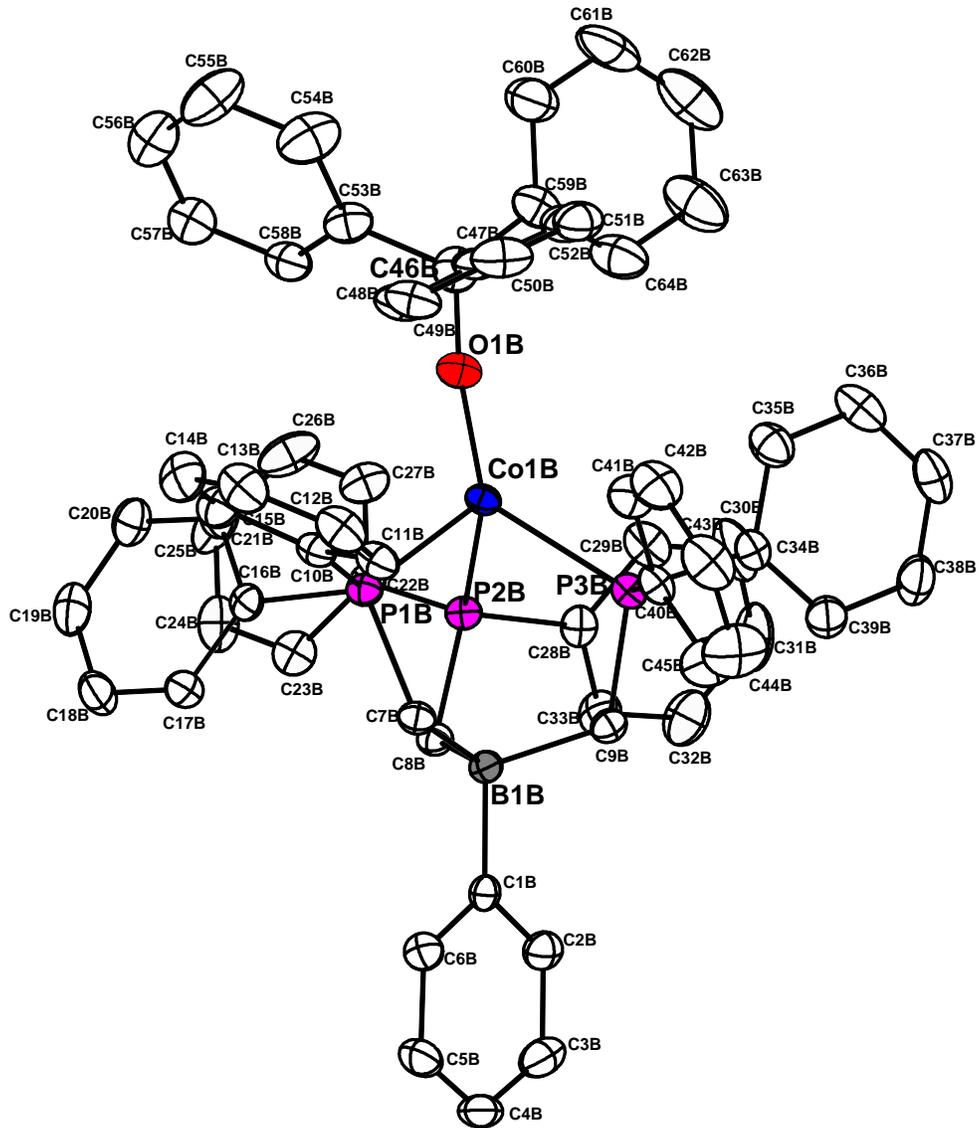
# Molecule A



# Molecule B



# Molecule B



**Table 1. Crystal Data and Structure Analysis Details for dmj49.**

Empirical formula	$C_{64}H_{56}BCoOP_3 \cdot C_6H_6$
Formula weight	1081.85
Crystallization solvent	Benzene/Petroleum Ether
Crystal shape	Block
Crystal color	Blue/Purple
Crystal size	0.07 x 0.30 x 0.33 mm

**Data Collection**

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoK $\alpha$	
Data collection temperature	100 K	
Theta range for 7298 reflections used in lattice determination	2.31 to 28.11°	
Unit cell dimensions	a = 12.9420(10) Å b = 20.8485(15) Å c = 21.5457(16) Å	$\alpha = 77.5290(10)^\circ$ $\beta = 82.1430(10)^\circ$ $\gamma = 88.6260(10)^\circ$
Volume	5622.9(7) Å <sup>3</sup>	
Z	4	
Crystal system	triclinic	
Space group	P $\bar{1}$ (# 2)	
Density (calculated)	1.278 g/cm <sup>3</sup>	
F(000)	2268	
Theta range for data collection	1.5 to 28.5°	
Completeness to theta = 28.45°	92.1%	
Index ranges	-17 ≤ h ≤ 17, -27 ≤ k ≤ 27, -28 ≤ l ≤ 28	
Reflections collected	117501	
Independent reflections	26130 [R <sub>int</sub> = 0.0703]	
Reflections > 2σ(I)	17673	
Average σ(I)/(net I)	0.0609	
Absorption coefficient	0.44 mm <sup>-1</sup>	
Reflections monitored for decay	419	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	26130 / 0 / 1369
Treatment of hydrogen atoms	Calculated positions and Uiso
Goodness-of-fit on F <sup>2</sup>	1.41
Final R indices [I>2σ(I), 17673 reflections]	R1 = 0.0457, wR2 = 0.0867
R indices (all data)	R1 = 0.0797, wR2 = 0.0930
Type of weighting scheme used	σ
Weighting scheme used	1/σ <sup>2</sup> (Fo <sup>2</sup> )
Max shift/error	0.023
Average shift/error	0.002
Largest diff. peak and hole	1.17 and -0.42 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINTE v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

**Special Refinement Details**

Refinement of F<sup>2</sup> against ALL reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F<sup>2</sup>, conventional R-factors (R) are based on F, with F set to zero for negative F<sup>2</sup>. The threshold expression of F<sup>2</sup> > 2σ(F<sup>2</sup>) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F<sup>2</sup> are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj49.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co(1A)	8311(1)	8510(1)	2281(1)	19(1)
P(1A)	6609(1)	8191(1)	2211(1)	19(1)
P(2A)	7951(1)	8413(1)	3402(1)	19(1)
P(3A)	7973(1)	9662(1)	2072(1)	21(1)
O(1A)	9507(1)	8025(1)	2192(1)	26(1)
B(1A)	6103(2)	9178(1)	3010(1)	21(1)
C(1A)	5077(2)	9447(1)	3414(1)	26(1)
C(2A)	5221(2)	9815(1)	3864(1)	34(1)
C(3A)	4416(2)	10022(1)	4264(1)	44(1)
C(4A)	3419(2)	9855(1)	4244(1)	51(1)
C(5A)	3228(2)	9476(1)	3831(1)	52(1)
C(6A)	4048(2)	9279(1)	3423(1)	40(1)
C(7A)	5751(2)	8825(1)	2449(1)	22(1)
C(8A)	6613(2)	8644(1)	3581(1)	21(1)
C(9A)	6922(2)	9804(1)	2682(1)	23(1)
C(10A)	6163(2)	7997(1)	1502(1)	23(1)
C(11A)	5912(2)	8493(1)	1000(1)	28(1)
C(12A)	5582(2)	8339(1)	461(1)	38(1)
C(13A)	5511(2)	7688(1)	418(1)	42(1)
C(14A)	5777(2)	7196(1)	906(1)	40(1)
C(15A)	6102(2)	7345(1)	1442(1)	31(1)
C(16A)	6302(2)	7438(1)	2815(1)	21(1)
C(17A)	5326(2)	7293(1)	3177(1)	31(1)
C(18A)	5164(2)	6716(1)	3637(1)	42(1)
C(19A)	5973(2)	6273(1)	3733(1)	41(1)
C(20A)	6940(2)	6405(1)	3375(1)	35(1)
C(21A)	7105(2)	6984(1)	2922(1)	26(1)
C(22A)	8176(2)	7655(1)	3975(1)	22(1)
C(23A)	7418(2)	7382(1)	4480(1)	27(1)
C(24A)	7623(2)	6812(1)	4913(1)	32(1)
C(25A)	8569(2)	6514(1)	4844(1)	37(1)
C(26A)	9325(2)	6776(1)	4344(1)	38(1)
C(27A)	9132(2)	7346(1)	3911(1)	30(1)
C(28A)	8768(2)	8997(1)	3638(1)	24(1)
C(29A)	9795(2)	9048(1)	3352(1)	44(1)
C(30A)	10482(2)	9479(2)	3489(2)	59(1)
C(31A)	10140(2)	9856(1)	3929(2)	53(1)
C(32A)	9124(2)	9823(1)	4209(1)	42(1)
C(33A)	8438(2)	9390(1)	4066(1)	34(1)
C(34A)	9074(2)	10198(1)	2073(1)	22(1)
C(35A)	10016(2)	10100(1)	1712(1)	30(1)
C(36A)	10896(2)	10466(1)	1714(1)	35(1)
C(37A)	10839(2)	10946(1)	2071(1)	34(1)
C(38A)	9905(2)	11059(1)	2418(1)	33(1)
C(39A)	9029(2)	10685(1)	2426(1)	28(1)
C(40A)	7561(2)	10034(1)	1293(1)	22(1)

C(41A)	7821(2)	9738(1)	780(1)	31(1)
C(42A)	7576(2)	10031(1)	175(1)	38(1)
C(43A)	7066(2)	10626(1)	81(1)	37(1)
C(44A)	6805(2)	10928(1)	588(1)	44(1)
C(45A)	7045(2)	10632(1)	1189(1)	38(1)
C(46A)	10167(2)	7828(1)	1698(1)	26(1)
C(47A)	9770(2)	8110(1)	1053(1)	26(1)
C(48A)	8840(2)	7863(1)	939(1)	30(1)
C(49A)	8440(2)	8088(1)	373(1)	34(1)
C(50A)	8964(2)	8580(1)	-99(1)	38(1)
C(51A)	9873(2)	8841(1)	9(1)	33(1)
C(52A)	10277(2)	8604(1)	582(1)	28(1)
C(53A)	10164(2)	7069(1)	1822(1)	26(1)
C(54A)	10452(2)	6735(1)	1333(1)	36(1)
C(55A)	10441(2)	6053(1)	1448(1)	43(1)
C(56A)	10138(2)	5694(1)	2061(1)	42(1)
C(57A)	9873(2)	6014(1)	2553(1)	40(1)
C(58A)	9891(2)	6698(1)	2433(1)	30(1)
C(59A)	11285(2)	8074(1)	1708(1)	27(1)
C(60A)	12181(2)	7765(1)	1488(1)	39(1)
C(61A)	13165(2)	8011(1)	1511(1)	47(1)
C(62A)	13265(2)	8566(2)	1736(1)	46(1)
C(63A)	12388(2)	8882(2)	1950(1)	47(1)
C(64A)	11410(2)	8631(1)	1939(1)	37(1)
C(65A)	2197(2)	7299(2)	3437(1)	50(1)
C(66A)	2160(2)	7835(2)	3698(2)	61(1)
C(67A)	2098(3)	7772(2)	4352(2)	73(1)
C(68A)	2050(2)	7164(2)	4748(1)	52(1)
C(69A)	2082(2)	6622(2)	4486(2)	57(1)
C(70A)	2154(3)	6692(2)	3829(2)	65(1)
Co(1B)	4368(1)	6446(1)	7665(1)	18(1)
P(1B)	2645(1)	6818(1)	7726(1)	19(1)
P(2B)	4509(1)	6512(1)	6541(1)	19(1)
P(3B)	3921(1)	5314(1)	7896(1)	20(1)
O(1B)	5471(1)	6933(1)	7773(1)	30(1)
B(1B)	2484(2)	5833(1)	6931(1)	19(1)
C(1B)	1620(2)	5565(1)	6554(1)	20(1)
C(2B)	1938(2)	5194(1)	6095(1)	26(1)
C(3B)	1259(2)	4976(1)	5738(1)	33(1)
C(4B)	214(2)	5134(1)	5826(1)	34(1)
C(5B)	-127(2)	5508(1)	6262(1)	35(1)
C(6B)	560(2)	5713(1)	6620(1)	28(1)
C(7B)	1894(2)	6216(1)	7479(1)	21(1)
C(8B)	3240(2)	6345(1)	6355(1)	20(1)
C(9B)	3182(2)	5190(1)	7268(1)	20(1)
C(10B)	1870(2)	7015(1)	8435(1)	22(1)
C(11B)	1445(2)	6516(1)	8939(1)	27(1)
C(12B)	862(2)	6667(1)	9481(1)	34(1)
C(13B)	699(2)	7317(1)	9520(1)	38(1)
C(14B)	1117(2)	7811(1)	9027(1)	38(1)
C(15B)	1702(2)	7664(1)	8490(1)	30(1)
C(16B)	2621(2)	7583(1)	7127(1)	20(1)
C(17B)	1822(2)	7765(1)	6756(1)	28(1)
C(18B)	1888(2)	8348(1)	6297(1)	37(1)

C(19B)	2745(2)	8757(1)	6216(1)	36(1)
C(20B)	3529(2)	8591(1)	6588(1)	31(1)
C(21B)	3473(2)	8005(1)	7040(1)	24(1)
C(22B)	4994(2)	7274(1)	6004(1)	21(1)
C(23B)	4479(2)	7594(1)	5498(1)	29(1)
C(24B)	4851(2)	8194(1)	5122(1)	35(1)
C(25B)	5726(2)	8469(1)	5254(1)	39(1)
C(26B)	6259(2)	8149(1)	5742(1)	41(1)
C(27B)	5891(2)	7550(1)	6118(1)	30(1)
C(28B)	5400(2)	5909(1)	6256(1)	22(1)
C(29B)	6226(2)	5689(1)	6589(1)	31(1)
C(30B)	6941(2)	5243(1)	6383(1)	42(1)
C(31B)	6832(2)	5027(1)	5835(1)	44(1)
C(32B)	6023(2)	5245(1)	5499(1)	42(1)
C(33B)	5308(2)	5680(1)	5706(1)	32(1)
C(34B)	5022(2)	4746(1)	7927(1)	22(1)
C(35B)	5827(2)	4868(1)	8257(1)	33(1)
C(36B)	6722(2)	4488(1)	8261(1)	39(1)
C(37B)	6814(2)	3973(1)	7944(1)	37(1)
C(38B)	6011(2)	3838(1)	7634(1)	36(1)
C(39B)	5124(2)	4223(1)	7622(1)	30(1)
C(40B)	3132(2)	4980(1)	8669(1)	22(1)
C(41B)	3251(2)	5246(1)	9189(1)	31(1)
C(42B)	2726(2)	4981(1)	9795(1)	38(1)
C(43B)	2080(2)	4447(1)	9882(1)	41(1)
C(44B)	1958(2)	4174(1)	9368(1)	51(1)
C(45B)	2480(2)	4439(1)	8763(1)	42(1)
C(46B)	5889(2)	7122(1)	8264(1)	31(1)
C(47B)	5221(2)	6860(1)	8910(1)	29(1)
C(48B)	4236(2)	7126(1)	9021(1)	35(1)
C(49B)	3589(2)	6922(1)	9592(1)	38(1)
C(50B)	3920(2)	6433(1)	10073(1)	41(1)
C(51B)	4883(2)	6147(1)	9966(1)	37(1)
C(52B)	5530(2)	6365(1)	9390(1)	33(1)
C(53B)	5946(2)	7883(1)	8135(1)	31(1)
C(54B)	5985(2)	8223(1)	8626(1)	50(1)
C(55B)	6047(2)	8908(1)	8491(1)	56(1)
C(56B)	6075(2)	9267(1)	7874(1)	48(1)
C(57B)	6053(2)	8941(1)	7387(1)	42(1)
C(58B)	6001(2)	8258(1)	7516(1)	32(1)
C(59B)	7018(2)	6858(1)	8268(1)	31(1)
C(60B)	7782(2)	7130(1)	8537(1)	47(1)
C(61B)	8775(2)	6865(2)	8532(2)	57(1)
C(62B)	9030(2)	6332(2)	8275(1)	55(1)
C(63B)	8295(2)	6059(2)	8010(1)	57(1)
C(64B)	7301(2)	6326(1)	8004(1)	44(1)
C(65B)	9479(2)	8038(2)	5461(1)	56(1)
C(66B)	9082(2)	8563(1)	5706(1)	49(1)
C(67B)	8671(2)	8466(1)	6345(1)	45(1)
C(68B)	8644(2)	7851(1)	6729(1)	43(1)
C(69B)	9046(2)	7334(1)	6474(2)	54(1)
C(70B)	9469(2)	7430(2)	5844(2)	60(1)

**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj49.**

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Co(1A)-O(1A)	1.8390(14)
Co(1A)-P(1A)	2.3494(6)
Co(1A)-P(2A)	2.3608(6)
Co(1A)-P(3A)	2.3874(6)
O(1A)-C(46A)	1.398(2)
Co(1B)-O(1B)	1.8386(15)
Co(1B)-P(1B)	2.3392(6)
Co(1B)-P(3B)	2.3745(6)
Co(1B)-P(2B)	2.3774(6)
O(1B)-C(46B)	1.384(3)
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O(1A)-Co(1A)-P(1A)	126.83(5)
O(1A)-Co(1A)-P(2A)	102.99(5)
P(1A)-Co(1A)-P(2A)	92.56(2)
O(1A)-Co(1A)-P(3A)	133.18(5)
P(1A)-Co(1A)-P(3A)	95.67(2)
P(2A)-Co(1A)-P(3A)	92.40(2)
C(46A)-O(1A)-Co(1A)	138.00(13)
O(1B)-Co(1B)-P(1B)	123.45(5)
O(1B)-Co(1B)-P(3B)	135.85(5)
P(1B)-Co(1B)-P(3B)	95.20(2)
O(1B)-Co(1B)-P(2B)	105.19(5)
P(1B)-Co(1B)-P(2B)	92.88(2)
P(3B)-Co(1B)-P(2B)	91.92(2)
C(46B)-O(1B)-Co(1B)	139.05(14)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj49.**

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Co(1A)-O(1A)	1.8390(14)
Co(1A)-P(1A)	2.3494(6)
Co(1A)-P(2A)	2.3608(6)
Co(1A)-P(3A)	2.3874(6)
P(1A)-C(7A)	1.820(2)
P(1A)-C(16A)	1.822(2)
P(1A)-C(10A)	1.829(2)
P(2A)-C(8A)	1.799(2)
P(2A)-C(28A)	1.827(2)
P(2A)-C(22A)	1.828(2)
P(3A)-C(9A)	1.824(2)
P(3A)-C(34A)	1.833(2)
P(3A)-C(40A)	1.834(2)
O(1A)-C(46A)	1.398(2)
B(1A)-C(1A)	1.642(3)
B(1A)-C(7A)	1.662(3)
B(1A)-C(8A)	1.668(3)
B(1A)-C(9A)	1.671(3)
C(1A)-C(6A)	1.381(3)
C(1A)-C(2A)	1.393(3)
C(2A)-C(3A)	1.382(3)
C(2A)-H(2A)	0.9500
C(3A)-C(4A)	1.353(4)
C(3A)-H(3A)	0.9500
C(4A)-C(5A)	1.359(4)
C(4A)-H(4A)	0.9500
C(5A)-C(6A)	1.396(3)
C(5A)-H(5A)	0.9500
C(6A)-H(6A)	0.9500
C(7A)-H(7A1)	0.9900
C(7A)-H(7A2)	0.9900
C(8A)-H(8A1)	0.9900
C(8A)-H(8A2)	0.9900
C(9A)-H(9A1)	0.9900
C(9A)-H(9A2)	0.9900
C(10A)-C(11A)	1.393(3)
C(10A)-C(15A)	1.399(3)
C(11A)-C(12A)	1.391(3)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.388(3)
C(12A)-H(12A)	0.9500
C(13A)-C(14A)	1.376(3)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.379(3)
C(14A)-H(14A)	0.9500
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.393(3)
C(16A)-C(21A)	1.398(3)
C(17A)-C(18A)	1.384(3)
C(17A)-H(17A)	0.9500
C(18A)-C(19A)	1.385(4)

C(18A)-H(18A)	0.9500
C(19A)-C(20A)	1.377(3)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.381(3)
C(20A)-H(20A)	0.9500
C(21A)-H(21A)	0.9500
C(22A)-C(27A)	1.385(3)
C(22A)-C(23A)	1.392(3)
C(23A)-C(24A)	1.387(3)
C(23A)-H(23A)	0.9500
C(24A)-C(25A)	1.365(3)
C(24A)-H(24A)	0.9500
C(25A)-C(26A)	1.378(3)
C(25A)-H(25A)	0.9500
C(26A)-C(27A)	1.385(3)
C(26A)-H(26A)	0.9500
C(27A)-H(27A)	0.9500
C(28A)-C(33A)	1.379(3)
C(28A)-C(29A)	1.382(3)
C(29A)-C(30A)	1.383(4)
C(29A)-H(29A)	0.9500
C(30A)-C(31A)	1.379(4)
C(30A)-H(30A)	0.9500
C(31A)-C(32A)	1.367(4)
C(31A)-H(31A)	0.9500
C(32A)-C(33A)	1.390(3)
C(32A)-H(32A)	0.9500
C(33A)-H(33A)	0.9500
C(34A)-C(39A)	1.389(3)
C(34A)-C(35A)	1.390(3)
C(35A)-C(36A)	1.388(3)
C(35A)-H(35A)	0.9500
C(36A)-C(37A)	1.383(3)
C(36A)-H(36A)	0.9500
C(37A)-C(38A)	1.375(3)
C(37A)-H(37A)	0.9500
C(38A)-C(39A)	1.389(3)
C(38A)-H(38A)	0.9500
C(39A)-H(39A)	0.9500
C(40A)-C(41A)	1.379(3)
C(40A)-C(45A)	1.390(3)
C(41A)-C(42A)	1.389(3)
C(41A)-H(41A)	0.9500
C(42A)-C(43A)	1.380(3)
C(42A)-H(42A)	0.9500
C(43A)-C(44A)	1.376(3)
C(43A)-H(43A)	0.9500
C(44A)-C(45A)	1.382(3)
C(44A)-H(44A)	0.9500
C(45A)-H(45A)	0.9500
C(46A)-C(47A)	1.539(3)
C(46A)-C(53A)	1.547(3)
C(46A)-C(59A)	1.550(3)
C(47A)-C(52A)	1.386(3)

C(47A)-C(48A)	1.392(3)
C(48A)-C(49A)	1.375(3)
C(48A)-H(48A)	0.9500
C(49A)-C(50A)	1.393(3)
C(49A)-H(49A)	0.9500
C(50A)-C(51A)	1.377(3)
C(50A)-H(50A)	0.9500
C(51A)-C(52A)	1.392(3)
C(51A)-H(51A)	0.9500
C(52A)-H(52A)	0.9500
C(53A)-C(58A)	1.378(3)
C(53A)-C(54A)	1.390(3)
C(54A)-C(55A)	1.389(3)
C(54A)-H(54A)	0.9500
C(55A)-C(56A)	1.381(3)
C(55A)-H(55A)	0.9500
C(56A)-C(57A)	1.372(3)
C(56A)-H(56A)	0.9500
C(57A)-C(58A)	1.394(3)
C(57A)-H(57A)	0.9500
C(58A)-H(58A)	0.9500
C(59A)-C(64A)	1.380(3)
C(59A)-C(60A)	1.389(3)
C(60A)-C(61A)	1.396(3)
C(60A)-H(60A)	0.9500
C(61A)-C(62A)	1.363(4)
C(61A)-H(61A)	0.9500
C(62A)-C(63A)	1.373(4)
C(62A)-H(62A)	0.9500
C(63A)-C(64A)	1.386(3)
C(63A)-H(63A)	0.9500
C(64A)-H(64A)	0.9500
C(65A)-C(66A)	1.352(4)
C(65A)-C(70A)	1.359(4)
C(65A)-H(65A)	0.9500
C(66A)-C(67A)	1.378(4)
C(66A)-H(66A)	0.9500
C(67A)-C(68A)	1.364(4)
C(67A)-H(67A)	0.9500
C(68A)-C(69A)	1.364(4)
C(68A)-H(68A)	0.9500
C(69A)-C(70A)	1.383(4)
C(69A)-H(69A)	0.9500
C(70A)-H(70A)	0.9500
Co(1B)-O(1B)	1.8386(15)
Co(1B)-P(1B)	2.3392(6)
Co(1B)-P(3B)	2.3745(6)
Co(1B)-P(2B)	2.3774(6)
P(1B)-C(7B)	1.814(2)
P(1B)-C(16B)	1.825(2)
P(1B)-C(10B)	1.829(2)
P(2B)-C(8B)	1.802(2)
P(2B)-C(22B)	1.822(2)
P(2B)-C(28B)	1.831(2)

P(3B)-C(9B)	1.823(2)
P(3B)-C(34B)	1.830(2)
P(3B)-C(40B)	1.836(2)
O(1B)-C(46B)	1.384(3)
B(1B)-C(1B)	1.642(3)
B(1B)-C(7B)	1.657(3)
B(1B)-C(8B)	1.668(3)
B(1B)-C(9B)	1.686(3)
C(1B)-C(6B)	1.395(3)
C(1B)-C(2B)	1.397(3)
C(2B)-C(3B)	1.387(3)
C(2B)-H(2B)	0.9500
C(3B)-C(4B)	1.381(3)
C(3B)-H(3B)	0.9500
C(4B)-C(5B)	1.367(3)
C(4B)-H(4B)	0.9500
C(5B)-C(6B)	1.384(3)
C(5B)-H(5B)	0.9500
C(6B)-H(6B)	0.9500
C(7B)-H(7B1)	0.9900
C(7B)-H(7B2)	0.9900
C(8B)-H(8B1)	0.9900
C(8B)-H(8B2)	0.9900
C(9B)-H(9B1)	0.9900
C(9B)-H(9B2)	0.9900
C(10B)-C(11B)	1.392(3)
C(10B)-C(15B)	1.393(3)
C(11B)-C(12B)	1.393(3)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.384(3)
C(12B)-H(12B)	0.9500
C(13B)-C(14B)	1.371(3)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.382(3)
C(14B)-H(14B)	0.9500
C(15B)-H(15B)	0.9500
C(16B)-C(17B)	1.389(3)
C(16B)-C(21B)	1.395(3)
C(17B)-C(18B)	1.388(3)
C(17B)-H(17B)	0.9500
C(18B)-C(19B)	1.385(3)
C(18B)-H(18B)	0.9500
C(19B)-C(20B)	1.371(3)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.384(3)
C(20B)-H(20B)	0.9500
C(21B)-H(21B)	0.9500
C(22B)-C(27B)	1.381(3)
C(22B)-C(23B)	1.393(3)
C(23B)-C(24B)	1.392(3)
C(23B)-H(23B)	0.9500
C(24B)-C(25B)	1.372(3)
C(24B)-H(24B)	0.9500
C(25B)-C(26B)	1.379(4)

C(25B)-H(25B)	0.9500
C(26B)-C(27B)	1.388(3)
C(26B)-H(26B)	0.9500
C(27B)-H(27B)	0.9500
C(28B)-C(29B)	1.383(3)
C(28B)-C(33B)	1.389(3)
C(29B)-C(30B)	1.393(3)
C(29B)-H(29B)	0.9500
C(30B)-C(31B)	1.375(4)
C(30B)-H(30B)	0.9500
C(31B)-C(32B)	1.369(4)
C(31B)-H(31B)	0.9500
C(32B)-C(33B)	1.378(3)
C(32B)-H(32B)	0.9500
C(33B)-H(33B)	0.9500
C(34B)-C(39B)	1.384(3)
C(34B)-C(35B)	1.396(3)
C(35B)-C(36B)	1.387(3)
C(35B)-H(35B)	0.9500
C(36B)-C(37B)	1.386(3)
C(36B)-H(36B)	0.9500
C(37B)-C(38B)	1.375(3)
C(37B)-H(37B)	0.9500
C(38B)-C(39B)	1.385(3)
C(38B)-H(38B)	0.9500
C(39B)-H(39B)	0.9500
C(40B)-C(41B)	1.380(3)
C(40B)-C(45B)	1.388(3)
C(41B)-C(42B)	1.391(3)
C(41B)-H(41B)	0.9500
C(42B)-C(43B)	1.373(3)
C(42B)-H(42B)	0.9500
C(43B)-C(44B)	1.378(4)
C(43B)-H(43B)	0.9500
C(44B)-C(45B)	1.388(3)
C(44B)-H(44B)	0.9500
C(45B)-H(45B)	0.9500
C(46B)-C(47B)	1.534(3)
C(46B)-C(59B)	1.550(3)
C(46B)-C(53B)	1.552(3)
C(47B)-C(52B)	1.387(3)
C(47B)-C(48B)	1.390(3)
C(48B)-C(49B)	1.380(3)
C(48B)-H(48B)	0.9500
C(49B)-C(50B)	1.392(3)
C(49B)-H(49B)	0.9500
C(50B)-C(51B)	1.381(3)
C(50B)-H(50B)	0.9500
C(51B)-C(52B)	1.393(3)
C(51B)-H(51B)	0.9500
C(52B)-H(52B)	0.9500
C(53B)-C(58B)	1.385(3)
C(53B)-C(54B)	1.401(3)
C(54B)-C(55B)	1.396(4)

C(54B)-H(54B)	0.9500
C(55B)-C(56B)	1.373(4)
C(55B)-H(55B)	0.9500
C(56B)-C(57B)	1.373(3)
C(56B)-H(56B)	0.9500
C(57B)-C(58B)	1.392(3)
C(57B)-H(57B)	0.9500
C(58B)-H(58B)	0.9500
C(59B)-C(64B)	1.372(3)
C(59B)-C(60B)	1.400(3)
C(60B)-C(61B)	1.386(4)
C(60B)-H(60B)	0.9500
C(61B)-C(62B)	1.359(4)
C(61B)-H(61B)	0.9500
C(62B)-C(63B)	1.366(4)
C(62B)-H(62B)	0.9500
C(63B)-C(64B)	1.390(3)
C(63B)-H(63B)	0.9500
C(64B)-H(64B)	0.9500
C(65B)-C(70B)	1.354(4)
C(65B)-C(66B)	1.375(4)
C(65B)-H(65B)	0.9500
C(66B)-C(67B)	1.381(4)
C(66B)-H(66B)	0.9500
C(67B)-C(68B)	1.366(3)
C(67B)-H(67B)	0.9500
C(68B)-C(69B)	1.372(4)
C(68B)-H(68B)	0.9500
C(69B)-C(70B)	1.367(4)
C(69B)-H(69B)	0.9500
C(70B)-H(70B)	0.9500

O(1A)-Co(1A)-P(1A)	126.83(5)
O(1A)-Co(1A)-P(2A)	102.99(5)
P(1A)-Co(1A)-P(2A)	92.56(2)
O(1A)-Co(1A)-P(3A)	133.18(5)
P(1A)-Co(1A)-P(3A)	95.67(2)
P(2A)-Co(1A)-P(3A)	92.40(2)
C(7A)-P(1A)-C(16A)	106.87(10)
C(7A)-P(1A)-C(10A)	106.96(10)
C(16A)-P(1A)-C(10A)	102.40(10)
C(7A)-P(1A)-Co(1A)	106.12(7)
C(16A)-P(1A)-Co(1A)	107.57(7)
C(10A)-P(1A)-Co(1A)	125.70(7)
C(8A)-P(2A)-C(28A)	107.67(10)
C(8A)-P(2A)-C(22A)	107.69(10)
C(28A)-P(2A)-C(22A)	101.59(9)
C(8A)-P(2A)-Co(1A)	107.57(7)
C(28A)-P(2A)-Co(1A)	108.99(7)
C(22A)-P(2A)-Co(1A)	122.50(7)
C(9A)-P(3A)-C(34A)	108.39(10)
C(9A)-P(3A)-C(40A)	106.53(10)
C(34A)-P(3A)-C(40A)	100.51(9)
C(9A)-P(3A)-Co(1A)	107.27(7)

C(34A)-P(3A)-Co(1A)	116.27(7)
C(40A)-P(3A)-Co(1A)	117.22(7)
C(46A)-O(1A)-Co(1A)	138.00(13)
C(1A)-B(1A)-C(7A)	110.68(17)
C(1A)-B(1A)-C(8A)	102.52(17)
C(7A)-B(1A)-C(8A)	112.47(17)
C(1A)-B(1A)-C(9A)	109.19(17)
C(7A)-B(1A)-C(9A)	110.68(17)
C(8A)-B(1A)-C(9A)	111.00(17)
C(6A)-C(1A)-C(2A)	113.7(2)
C(6A)-C(1A)-B(1A)	126.7(2)
C(2A)-C(1A)-B(1A)	119.09(19)
C(3A)-C(2A)-C(1A)	123.8(2)
C(3A)-C(2A)-H(2A)	118.1
C(1A)-C(2A)-H(2A)	118.1
C(4A)-C(3A)-C(2A)	120.1(3)
C(4A)-C(3A)-H(3A)	119.9
C(2A)-C(3A)-H(3A)	119.9
C(3A)-C(4A)-C(5A)	118.9(3)
C(3A)-C(4A)-H(4A)	120.5
C(5A)-C(4A)-H(4A)	120.5
C(4A)-C(5A)-C(6A)	120.3(3)
C(4A)-C(5A)-H(5A)	119.8
C(6A)-C(5A)-H(5A)	119.8
C(1A)-C(6A)-C(5A)	123.1(2)
C(1A)-C(6A)-H(6A)	118.5
C(5A)-C(6A)-H(6A)	118.5
B(1A)-C(7A)-P(1A)	116.67(14)
B(1A)-C(7A)-H(7A1)	108.1
P(1A)-C(7A)-H(7A1)	108.1
B(1A)-C(7A)-H(7A2)	108.1
P(1A)-C(7A)-H(7A2)	108.1
H(7A1)-C(7A)-H(7A2)	107.3
B(1A)-C(8A)-P(2A)	117.21(14)
B(1A)-C(8A)-H(8A1)	108.0
P(2A)-C(8A)-H(8A1)	108.0
B(1A)-C(8A)-H(8A2)	108.0
P(2A)-C(8A)-H(8A2)	108.0
H(8A1)-C(8A)-H(8A2)	107.2
B(1A)-C(9A)-P(3A)	116.71(14)
B(1A)-C(9A)-H(9A1)	108.1
P(3A)-C(9A)-H(9A1)	108.1
B(1A)-C(9A)-H(9A2)	108.1
P(3A)-C(9A)-H(9A2)	108.1
H(9A1)-C(9A)-H(9A2)	107.3
C(11A)-C(10A)-C(15A)	118.3(2)
C(11A)-C(10A)-P(1A)	121.19(17)
C(15A)-C(10A)-P(1A)	120.51(17)
C(12A)-C(11A)-C(10A)	120.6(2)
C(12A)-C(11A)-H(11A)	119.7
C(10A)-C(11A)-H(11A)	119.7
C(13A)-C(12A)-C(11A)	119.9(2)
C(13A)-C(12A)-H(12A)	120.0
C(11A)-C(12A)-H(12A)	120.0

C(14A)-C(13A)-C(12A)	119.8(2)
C(14A)-C(13A)-H(13A)	120.1
C(12A)-C(13A)-H(13A)	120.1
C(13A)-C(14A)-C(15A)	120.4(2)
C(13A)-C(14A)-H(14A)	119.8
C(15A)-C(14A)-H(14A)	119.8
C(14A)-C(15A)-C(10A)	120.9(2)
C(14A)-C(15A)-H(15A)	119.6
C(10A)-C(15A)-H(15A)	119.6
C(17A)-C(16A)-C(21A)	118.5(2)
C(17A)-C(16A)-P(1A)	124.20(17)
C(21A)-C(16A)-P(1A)	117.27(16)
C(18A)-C(17A)-C(16A)	120.5(2)
C(18A)-C(17A)-H(17A)	119.7
C(16A)-C(17A)-H(17A)	119.7
C(17A)-C(18A)-C(19A)	119.9(2)
C(17A)-C(18A)-H(18A)	120.1
C(19A)-C(18A)-H(18A)	120.1
C(20A)-C(19A)-C(18A)	120.4(2)
C(20A)-C(19A)-H(19A)	119.8
C(18A)-C(19A)-H(19A)	119.8
C(19A)-C(20A)-C(21A)	119.7(2)
C(19A)-C(20A)-H(20A)	120.2
C(21A)-C(20A)-H(20A)	120.2
C(20A)-C(21A)-C(16A)	120.9(2)
C(20A)-C(21A)-H(21A)	119.5
C(16A)-C(21A)-H(21A)	119.5
C(27A)-C(22A)-C(23A)	118.8(2)
C(27A)-C(22A)-P(2A)	119.22(17)
C(23A)-C(22A)-P(2A)	121.98(16)
C(24A)-C(23A)-C(22A)	120.4(2)
C(24A)-C(23A)-H(23A)	119.8
C(22A)-C(23A)-H(23A)	119.8
C(25A)-C(24A)-C(23A)	120.1(2)
C(25A)-C(24A)-H(24A)	120.0
C(23A)-C(24A)-H(24A)	120.0
C(24A)-C(25A)-C(26A)	120.2(2)
C(24A)-C(25A)-H(25A)	119.9
C(26A)-C(25A)-H(25A)	119.9
C(25A)-C(26A)-C(27A)	120.2(2)
C(25A)-C(26A)-H(26A)	119.9
C(27A)-C(26A)-H(26A)	119.9
C(26A)-C(27A)-C(22A)	120.3(2)
C(26A)-C(27A)-H(27A)	119.9
C(22A)-C(27A)-H(27A)	119.9
C(33A)-C(28A)-C(29A)	118.6(2)
C(33A)-C(28A)-P(2A)	125.30(17)
C(29A)-C(28A)-P(2A)	116.13(18)
C(28A)-C(29A)-C(30A)	121.2(3)
C(28A)-C(29A)-H(29A)	119.4
C(30A)-C(29A)-H(29A)	119.4
C(31A)-C(30A)-C(29A)	119.3(3)
C(31A)-C(30A)-H(30A)	120.4
C(29A)-C(30A)-H(30A)	120.4

C(32A)-C(31A)-C(30A)	120.5(3)
C(32A)-C(31A)-H(31A)	119.8
C(30A)-C(31A)-H(31A)	119.8
C(31A)-C(32A)-C(33A)	119.8(3)
C(31A)-C(32A)-H(32A)	120.1
C(33A)-C(32A)-H(32A)	120.1
C(28A)-C(33A)-C(32A)	120.7(2)
C(28A)-C(33A)-H(33A)	119.7
C(32A)-C(33A)-H(33A)	119.7
C(39A)-C(34A)-C(35A)	118.2(2)
C(39A)-C(34A)-P(3A)	123.85(17)
C(35A)-C(34A)-P(3A)	117.92(16)
C(36A)-C(35A)-C(34A)	121.1(2)
C(36A)-C(35A)-H(35A)	119.5
C(34A)-C(35A)-H(35A)	119.5
C(37A)-C(36A)-C(35A)	119.9(2)
C(37A)-C(36A)-H(36A)	120.0
C(35A)-C(36A)-H(36A)	120.0
C(38A)-C(37A)-C(36A)	119.5(2)
C(38A)-C(37A)-H(37A)	120.2
C(36A)-C(37A)-H(37A)	120.2
C(37A)-C(38A)-C(39A)	120.6(2)
C(37A)-C(38A)-H(38A)	119.7
C(39A)-C(38A)-H(38A)	119.7
C(38A)-C(39A)-C(34A)	120.6(2)
C(38A)-C(39A)-H(39A)	119.7
C(34A)-C(39A)-H(39A)	119.7
C(41A)-C(40A)-C(45A)	118.1(2)
C(41A)-C(40A)-P(3A)	119.76(17)
C(45A)-C(40A)-P(3A)	122.00(17)
C(40A)-C(41A)-C(42A)	120.9(2)
C(40A)-C(41A)-H(41A)	119.6
C(42A)-C(41A)-H(41A)	119.6
C(43A)-C(42A)-C(41A)	120.2(2)
C(43A)-C(42A)-H(42A)	119.9
C(41A)-C(42A)-H(42A)	119.9
C(44A)-C(43A)-C(42A)	119.6(2)
C(44A)-C(43A)-H(43A)	120.2
C(42A)-C(43A)-H(43A)	120.2
C(43A)-C(44A)-C(45A)	120.0(2)
C(43A)-C(44A)-H(44A)	120.0
C(45A)-C(44A)-H(44A)	120.0
C(44A)-C(45A)-C(40A)	121.2(2)
C(44A)-C(45A)-H(45A)	119.4
C(40A)-C(45A)-H(45A)	119.4
O(1A)-C(46A)-C(47A)	109.38(17)
O(1A)-C(46A)-C(53A)	108.88(17)
C(47A)-C(46A)-C(53A)	109.38(18)
O(1A)-C(46A)-C(59A)	108.08(17)
C(47A)-C(46A)-C(59A)	111.80(17)
C(53A)-C(46A)-C(59A)	109.28(17)
C(52A)-C(47A)-C(48A)	117.9(2)
C(52A)-C(47A)-C(46A)	123.7(2)
C(48A)-C(47A)-C(46A)	118.3(2)

C(49A)-C(48A)-C(47A)	121.6(2)
C(49A)-C(48A)-H(48A)	119.2
C(47A)-C(48A)-H(48A)	119.2
C(48A)-C(49A)-C(50A)	119.7(2)
C(48A)-C(49A)-H(49A)	120.1
C(50A)-C(49A)-H(49A)	120.1
C(51A)-C(50A)-C(49A)	119.6(2)
C(51A)-C(50A)-H(50A)	120.2
C(49A)-C(50A)-H(50A)	120.2
C(50A)-C(51A)-C(52A)	120.1(2)
C(50A)-C(51A)-H(51A)	119.9
C(52A)-C(51A)-H(51A)	119.9
C(47A)-C(52A)-C(51A)	121.0(2)
C(47A)-C(52A)-H(52A)	119.5
C(51A)-C(52A)-H(52A)	119.5
C(58A)-C(53A)-C(54A)	117.6(2)
C(58A)-C(53A)-C(46A)	120.5(2)
C(54A)-C(53A)-C(46A)	121.9(2)
C(55A)-C(54A)-C(53A)	121.5(2)
C(55A)-C(54A)-H(54A)	119.2
C(53A)-C(54A)-H(54A)	119.2
C(56A)-C(55A)-C(54A)	119.7(2)
C(56A)-C(55A)-H(55A)	120.1
C(54A)-C(55A)-H(55A)	120.1
C(57A)-C(56A)-C(55A)	119.6(2)
C(57A)-C(56A)-H(56A)	120.2
C(55A)-C(56A)-H(56A)	120.2
C(56A)-C(57A)-C(58A)	120.2(2)
C(56A)-C(57A)-H(57A)	119.9
C(58A)-C(57A)-H(57A)	119.9
C(53A)-C(58A)-C(57A)	121.3(2)
C(53A)-C(58A)-H(58A)	119.3
C(57A)-C(58A)-H(58A)	119.3
C(64A)-C(59A)-C(60A)	117.5(2)
C(64A)-C(59A)-C(46A)	119.2(2)
C(60A)-C(59A)-C(46A)	123.3(2)
C(59A)-C(60A)-C(61A)	120.6(3)
C(59A)-C(60A)-H(60A)	119.7
C(61A)-C(60A)-H(60A)	119.7
C(62A)-C(61A)-C(60A)	120.6(2)
C(62A)-C(61A)-H(61A)	119.7
C(60A)-C(61A)-H(61A)	119.7
C(61A)-C(62A)-C(63A)	119.7(3)
C(61A)-C(62A)-H(62A)	120.1
C(63A)-C(62A)-H(62A)	120.1
C(62A)-C(63A)-C(64A)	119.7(3)
C(62A)-C(63A)-H(63A)	120.1
C(64A)-C(63A)-H(63A)	120.1
C(59A)-C(64A)-C(63A)	121.9(2)
C(59A)-C(64A)-H(64A)	119.1
C(63A)-C(64A)-H(64A)	119.1
C(66A)-C(65A)-C(70A)	119.2(3)
C(66A)-C(65A)-H(65A)	120.4
C(70A)-C(65A)-H(65A)	120.4

C(65A)-C(66A)-C(67A)	120.9(3)
C(65A)-C(66A)-H(66A)	119.6
C(67A)-C(66A)-H(66A)	119.6
C(68A)-C(67A)-C(66A)	120.2(3)
C(68A)-C(67A)-H(67A)	119.9
C(66A)-C(67A)-H(67A)	119.9
C(67A)-C(68A)-C(69A)	119.1(3)
C(67A)-C(68A)-H(68A)	120.5
C(69A)-C(68A)-H(68A)	120.5
C(68A)-C(69A)-C(70A)	120.1(3)
C(68A)-C(69A)-H(69A)	119.9
C(70A)-C(69A)-H(69A)	119.9
C(65A)-C(70A)-C(69A)	120.5(3)
C(65A)-C(70A)-H(70A)	119.7
C(69A)-C(70A)-H(70A)	119.7
O(1B)-Co(1B)-P(1B)	123.45(5)
O(1B)-Co(1B)-P(3B)	135.85(5)
P(1B)-Co(1B)-P(3B)	95.20(2)
O(1B)-Co(1B)-P(2B)	105.19(5)
P(1B)-Co(1B)-P(2B)	92.88(2)
P(3B)-Co(1B)-P(2B)	91.92(2)
C(7B)-P(1B)-C(16B)	107.31(10)
C(7B)-P(1B)-C(10B)	106.17(9)
C(16B)-P(1B)-C(10B)	102.78(9)
C(7B)-P(1B)-Co(1B)	106.36(7)
C(16B)-P(1B)-Co(1B)	107.38(7)
C(10B)-P(1B)-Co(1B)	125.74(7)
C(8B)-P(2B)-C(22B)	107.97(10)
C(8B)-P(2B)-C(28B)	106.55(10)
C(22B)-P(2B)-C(28B)	101.57(9)
C(8B)-P(2B)-Co(1B)	107.99(7)
C(22B)-P(2B)-Co(1B)	118.13(7)
C(28B)-P(2B)-Co(1B)	113.92(7)
C(9B)-P(3B)-C(34B)	108.52(10)
C(9B)-P(3B)-C(40B)	107.29(10)
C(34B)-P(3B)-C(40B)	100.95(9)
C(9B)-P(3B)-Co(1B)	106.82(7)
C(34B)-P(3B)-Co(1B)	115.46(7)
C(40B)-P(3B)-Co(1B)	117.31(7)
C(46B)-O(1B)-Co(1B)	139.05(14)
C(1B)-B(1B)-C(7B)	110.25(17)
C(1B)-B(1B)-C(8B)	104.40(16)
C(7B)-B(1B)-C(8B)	111.60(17)
C(1B)-B(1B)-C(9B)	108.74(16)
C(7B)-B(1B)-C(9B)	111.12(17)
C(8B)-B(1B)-C(9B)	110.50(17)
C(6B)-C(1B)-C(2B)	114.58(19)
C(6B)-C(1B)-B(1B)	125.07(18)
C(2B)-C(1B)-B(1B)	120.20(19)
C(3B)-C(2B)-C(1B)	123.3(2)
C(3B)-C(2B)-H(2B)	118.3
C(1B)-C(2B)-H(2B)	118.3
C(4B)-C(3B)-C(2B)	119.6(2)
C(4B)-C(3B)-H(3B)	120.2

C(2B)-C(3B)-H(3B)	120.2
C(5B)-C(4B)-C(3B)	119.1(2)
C(5B)-C(4B)-H(4B)	120.5
C(3B)-C(4B)-H(4B)	120.5
C(4B)-C(5B)-C(6B)	120.5(2)
C(4B)-C(5B)-H(5B)	119.7
C(6B)-C(5B)-H(5B)	119.7
C(5B)-C(6B)-C(1B)	122.9(2)
C(5B)-C(6B)-H(6B)	118.5
C(1B)-C(6B)-H(6B)	118.5
B(1B)-C(7B)-P(1B)	117.64(14)
B(1B)-C(7B)-H(7B1)	107.9
P(1B)-C(7B)-H(7B1)	107.9
B(1B)-C(7B)-H(7B2)	107.9
P(1B)-C(7B)-H(7B2)	107.9
H(7B1)-C(7B)-H(7B2)	107.2
B(1B)-C(8B)-P(2B)	115.71(14)
B(1B)-C(8B)-H(8B1)	108.4
P(2B)-C(8B)-H(8B1)	108.4
B(1B)-C(8B)-H(8B2)	108.4
P(2B)-C(8B)-H(8B2)	108.4
H(8B1)-C(8B)-H(8B2)	107.4
B(1B)-C(9B)-P(3B)	116.79(14)
B(1B)-C(9B)-H(9B1)	108.1
P(3B)-C(9B)-H(9B1)	108.1
B(1B)-C(9B)-H(9B2)	108.1
P(3B)-C(9B)-H(9B2)	108.1
H(9B1)-C(9B)-H(9B2)	107.3
C(11B)-C(10B)-C(15B)	118.4(2)
C(11B)-C(10B)-P(1B)	120.45(16)
C(15B)-C(10B)-P(1B)	121.13(17)
C(10B)-C(11B)-C(12B)	120.4(2)
C(10B)-C(11B)-H(11B)	119.8
C(12B)-C(11B)-H(11B)	119.8
C(13B)-C(12B)-C(11B)	120.0(2)
C(13B)-C(12B)-H(12B)	120.0
C(11B)-C(12B)-H(12B)	120.0
C(14B)-C(13B)-C(12B)	120.0(2)
C(14B)-C(13B)-H(13B)	120.0
C(12B)-C(13B)-H(13B)	120.0
C(13B)-C(14B)-C(15B)	120.3(2)
C(13B)-C(14B)-H(14B)	119.8
C(15B)-C(14B)-H(14B)	119.8
C(14B)-C(15B)-C(10B)	120.9(2)
C(14B)-C(15B)-H(15B)	119.5
C(10B)-C(15B)-H(15B)	119.5
C(17B)-C(16B)-C(21B)	118.7(2)
C(17B)-C(16B)-P(1B)	124.45(17)
C(21B)-C(16B)-P(1B)	116.84(16)
C(18B)-C(17B)-C(16B)	120.4(2)
C(18B)-C(17B)-H(17B)	119.8
C(16B)-C(17B)-H(17B)	119.8
C(19B)-C(18B)-C(17B)	119.9(2)
C(19B)-C(18B)-H(18B)	120.1

C(17B)-C(18B)-H(18B)	120.1
C(20B)-C(19B)-C(18B)	120.4(2)
C(20B)-C(19B)-H(19B)	119.8
C(18B)-C(19B)-H(19B)	119.8
C(19B)-C(20B)-C(21B)	119.8(2)
C(19B)-C(20B)-H(20B)	120.1
C(21B)-C(20B)-H(20B)	120.1
C(20B)-C(21B)-C(16B)	120.8(2)
C(20B)-C(21B)-H(21B)	119.6
C(16B)-C(21B)-H(21B)	119.6
C(27B)-C(22B)-C(23B)	119.4(2)
C(27B)-C(22B)-P(2B)	118.25(17)
C(23B)-C(22B)-P(2B)	122.37(17)
C(24B)-C(23B)-C(22B)	120.2(2)
C(24B)-C(23B)-H(23B)	119.9
C(22B)-C(23B)-H(23B)	119.9
C(25B)-C(24B)-C(23B)	119.6(2)
C(25B)-C(24B)-H(24B)	120.2
C(23B)-C(24B)-H(24B)	120.2
C(24B)-C(25B)-C(26B)	120.8(2)
C(24B)-C(25B)-H(25B)	119.6
C(26B)-C(25B)-H(25B)	119.6
C(25B)-C(26B)-C(27B)	119.7(2)
C(25B)-C(26B)-H(26B)	120.1
C(27B)-C(26B)-H(26B)	120.1
C(22B)-C(27B)-C(26B)	120.3(2)
C(22B)-C(27B)-H(27B)	119.8
C(26B)-C(27B)-H(27B)	119.8
C(29B)-C(28B)-C(33B)	118.2(2)
C(29B)-C(28B)-P(2B)	118.70(17)
C(33B)-C(28B)-P(2B)	123.08(17)
C(28B)-C(29B)-C(30B)	121.0(2)
C(28B)-C(29B)-H(29B)	119.5
C(30B)-C(29B)-H(29B)	119.5
C(31B)-C(30B)-C(29B)	119.6(2)
C(31B)-C(30B)-H(30B)	120.2
C(29B)-C(30B)-H(30B)	120.2
C(32B)-C(31B)-C(30B)	120.1(2)
C(32B)-C(31B)-H(31B)	119.9
C(30B)-C(31B)-H(31B)	119.9
C(31B)-C(32B)-C(33B)	120.4(2)
C(31B)-C(32B)-H(32B)	119.8
C(33B)-C(32B)-H(32B)	119.8
C(32B)-C(33B)-C(28B)	120.8(2)
C(32B)-C(33B)-H(33B)	119.6
C(28B)-C(33B)-H(33B)	119.6
C(39B)-C(34B)-C(35B)	118.3(2)
C(39B)-C(34B)-P(3B)	124.05(17)
C(35B)-C(34B)-P(3B)	117.55(17)
C(36B)-C(35B)-C(34B)	120.7(2)
C(36B)-C(35B)-H(35B)	119.6
C(34B)-C(35B)-H(35B)	119.6
C(37B)-C(36B)-C(35B)	119.9(2)
C(37B)-C(36B)-H(36B)	120.0

C(35B)-C(36B)-H(36B)	120.0
C(38B)-C(37B)-C(36B)	119.6(2)
C(38B)-C(37B)-H(37B)	120.2
C(36B)-C(37B)-H(37B)	120.2
C(37B)-C(38B)-C(39B)	120.5(2)
C(37B)-C(38B)-H(38B)	119.7
C(39B)-C(38B)-H(38B)	119.7
C(34B)-C(39B)-C(38B)	120.8(2)
C(34B)-C(39B)-H(39B)	119.6
C(38B)-C(39B)-H(39B)	119.6
C(41B)-C(40B)-C(45B)	118.5(2)
C(41B)-C(40B)-P(3B)	118.77(17)
C(45B)-C(40B)-P(3B)	122.50(17)
C(40B)-C(41B)-C(42B)	121.0(2)
C(40B)-C(41B)-H(41B)	119.5
C(42B)-C(41B)-H(41B)	119.5
C(43B)-C(42B)-C(41B)	119.8(2)
C(43B)-C(42B)-H(42B)	120.1
C(41B)-C(42B)-H(42B)	120.1
C(42B)-C(43B)-C(44B)	119.9(2)
C(42B)-C(43B)-H(43B)	120.0
C(44B)-C(43B)-H(43B)	120.0
C(43B)-C(44B)-C(45B)	120.2(3)
C(43B)-C(44B)-H(44B)	119.9
C(45B)-C(44B)-H(44B)	119.9
C(40B)-C(45B)-C(44B)	120.5(2)
C(40B)-C(45B)-H(45B)	119.7
C(44B)-C(45B)-H(45B)	119.7
O(1B)-C(46B)-C(47B)	110.52(19)
O(1B)-C(46B)-C(59B)	108.42(18)
C(47B)-C(46B)-C(59B)	110.85(18)
O(1B)-C(46B)-C(53B)	109.69(18)
C(47B)-C(46B)-C(53B)	109.49(18)
C(59B)-C(46B)-C(53B)	107.81(19)
C(52B)-C(47B)-C(48B)	117.7(2)
C(52B)-C(47B)-C(46B)	124.2(2)
C(48B)-C(47B)-C(46B)	118.1(2)
C(49B)-C(48B)-C(47B)	121.7(2)
C(49B)-C(48B)-H(48B)	119.1
C(47B)-C(48B)-H(48B)	119.1
C(48B)-C(49B)-C(50B)	119.8(2)
C(48B)-C(49B)-H(49B)	120.1
C(50B)-C(49B)-H(49B)	120.1
C(51B)-C(50B)-C(49B)	119.5(2)
C(51B)-C(50B)-H(50B)	120.3
C(49B)-C(50B)-H(50B)	120.3
C(50B)-C(51B)-C(52B)	120.0(2)
C(50B)-C(51B)-H(51B)	120.0
C(52B)-C(51B)-H(51B)	120.0
C(47B)-C(52B)-C(51B)	121.3(2)
C(47B)-C(52B)-H(52B)	119.3
C(51B)-C(52B)-H(52B)	119.3
C(58B)-C(53B)-C(54B)	116.8(2)
C(58B)-C(53B)-C(46B)	120.7(2)

C(54B)-C(53B)-C(46B)	122.4(2)
C(55B)-C(54B)-C(53B)	120.8(3)
C(55B)-C(54B)-H(54B)	119.6
C(53B)-C(54B)-H(54B)	119.6
C(56B)-C(55B)-C(54B)	121.1(3)
C(56B)-C(55B)-H(55B)	119.5
C(54B)-C(55B)-H(55B)	119.5
C(55B)-C(56B)-C(57B)	118.8(3)
C(55B)-C(56B)-H(56B)	120.6
C(57B)-C(56B)-H(56B)	120.6
C(56B)-C(57B)-C(58B)	120.5(3)
C(56B)-C(57B)-H(57B)	119.8
C(58B)-C(57B)-H(57B)	119.8
C(53B)-C(58B)-C(57B)	122.0(2)
C(53B)-C(58B)-H(58B)	119.0
C(57B)-C(58B)-H(58B)	119.0
C(64B)-C(59B)-C(60B)	117.1(2)
C(64B)-C(59B)-C(46B)	119.6(2)
C(60B)-C(59B)-C(46B)	123.3(2)
C(61B)-C(60B)-C(59B)	120.4(3)
C(61B)-C(60B)-H(60B)	119.8
C(59B)-C(60B)-H(60B)	119.8
C(62B)-C(61B)-C(60B)	121.2(3)
C(62B)-C(61B)-H(61B)	119.4
C(60B)-C(61B)-H(61B)	119.4
C(61B)-C(62B)-C(63B)	119.2(3)
C(61B)-C(62B)-H(62B)	120.4
C(63B)-C(62B)-H(62B)	120.4
C(62B)-C(63B)-C(64B)	120.2(3)
C(62B)-C(63B)-H(63B)	119.9
C(64B)-C(63B)-H(63B)	119.9
C(59B)-C(64B)-C(63B)	121.9(3)
C(59B)-C(64B)-H(64B)	119.1
C(63B)-C(64B)-H(64B)	119.1
C(70B)-C(65B)-C(66B)	120.2(3)
C(70B)-C(65B)-H(65B)	119.9
C(66B)-C(65B)-H(65B)	119.9
C(65B)-C(66B)-C(67B)	119.6(3)
C(65B)-C(66B)-H(66B)	120.2
C(67B)-C(66B)-H(66B)	120.2
C(68B)-C(67B)-C(66B)	120.2(3)
C(68B)-C(67B)-H(67B)	119.9
C(66B)-C(67B)-H(67B)	119.9
C(67B)-C(68B)-C(69B)	119.3(3)
C(67B)-C(68B)-H(68B)	120.4
C(69B)-C(68B)-H(68B)	120.4
C(70B)-C(69B)-C(68B)	120.7(3)
C(70B)-C(69B)-H(69B)	119.7
C(68B)-C(69B)-H(69B)	119.7
C(65B)-C(70B)-C(69B)	120.1(3)
C(65B)-C(70B)-H(70B)	119.9
C(69B)-C(70B)-H(70B)	119.9

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Symmetry transformations used to generate equivalent atoms:



**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj49. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co(1A)	162(2)	217(2)	173(2)	-39(1)	-15(1)	15(1)
P(1A)	177(3)	230(3)	181(3)	-55(2)	-32(2)	10(2)
P(2A)	179(3)	219(3)	186(3)	-42(2)	-32(2)	12(2)
P(3A)	213(3)	216(3)	201(3)	-32(2)	-46(2)	19(2)
O(1A)	199(8)	318(9)	251(9)	-53(7)	-11(6)	61(7)
B(1A)	190(13)	207(13)	247(14)	-71(11)	-35(10)	36(10)
C(1A)	245(13)	207(12)	309(13)	-41(10)	-39(10)	35(9)
C(2A)	379(15)	270(13)	367(15)	-73(11)	-8(12)	96(11)
C(3A)	554(19)	326(15)	416(16)	-90(13)	42(14)	126(13)
C(4A)	457(19)	462(18)	580(20)	-165(15)	130(15)	128(14)
C(5A)	282(15)	640(20)	620(20)	-155(17)	28(13)	76(14)
C(6A)	320(15)	428(16)	477(17)	-164(13)	-27(12)	55(12)
C(7A)	180(11)	224(12)	258(12)	-29(10)	-40(9)	30(9)
C(8A)	186(11)	259(12)	204(12)	-88(9)	-15(9)	5(9)
C(9A)	259(12)	223(12)	213(12)	-62(9)	-40(9)	62(9)
C(10A)	177(11)	345(13)	183(11)	-79(10)	-18(9)	-22(10)
C(11A)	224(12)	390(14)	237(13)	-81(11)	-14(10)	-22(10)
C(12A)	326(14)	566(18)	223(13)	-15(12)	-68(11)	-22(12)
C(13A)	473(17)	585(19)	257(14)	-174(13)	-70(12)	-124(14)
C(14A)	496(17)	439(16)	323(15)	-191(13)	-76(12)	-78(13)
C(15A)	329(14)	355(14)	263(13)	-105(11)	-69(10)	-5(11)
C(16A)	241(12)	217(12)	202(12)	-81(9)	-53(9)	-29(9)
C(17A)	262(13)	326(14)	339(14)	-103(11)	4(11)	-33(10)
C(18A)	398(16)	409(16)	392(16)	-69(13)	127(12)	-160(13)
C(19A)	612(19)	262(14)	331(15)	8(11)	-60(13)	-94(13)
C(20A)	449(16)	234(13)	385(15)	-54(11)	-148(12)	0(11)
C(21A)	283(13)	243(12)	268(13)	-77(10)	-73(10)	-16(10)
C(22A)	263(12)	215(12)	188(11)	-63(9)	-70(9)	18(9)
C(23A)	287(13)	271(13)	259(13)	-71(10)	-19(10)	37(10)
C(24A)	445(16)	264(13)	240(13)	-19(10)	-32(11)	-17(11)
C(25A)	588(18)	253(13)	288(14)	-27(11)	-174(13)	65(12)
C(26A)	381(15)	405(16)	384(16)	-97(13)	-157(12)	156(12)
C(27A)	294(13)	353(14)	265(13)	-60(11)	-61(10)	44(11)
C(28A)	226(12)	236(12)	238(12)	1(10)	-100(9)	-5(9)
C(29A)	299(15)	539(18)	511(18)	-151(14)	-79(13)	-60(13)
C(30A)	371(17)	730(20)	660(20)	-78(18)	-138(15)	-171(16)
C(31A)	540(20)	421(17)	660(20)	-22(15)	-324(17)	-180(14)
C(32A)	556(19)	297(15)	462(17)	-81(12)	-232(14)	30(13)
C(33A)	341(14)	312(14)	385(15)	-94(12)	-129(11)	2(11)
C(34A)	233(12)	222(12)	203(12)	3(9)	-71(9)	11(9)
C(35A)	294(13)	329(14)	278(13)	-67(11)	-46(10)	-10(11)
C(36A)	268(14)	451(16)	288(14)	-33(12)	20(11)	-11(11)
C(37A)	306(14)	332(14)	381(15)	-12(12)	-108(11)	-87(11)
C(38A)	333(14)	279(14)	426(15)	-113(11)	-126(12)	18(11)
C(39A)	245(13)	260(13)	355(14)	-69(11)	-65(10)	37(10)
C(40A)	205(12)	220(12)	234(12)	-4(9)	-48(9)	-20(9)

C(41A)	331(14)	316(14)	242(13)	-20(11)	-25(10)	51(11)
C(42A)	427(16)	471(17)	219(13)	-71(12)	-21(11)	36(13)
C(43A)	375(15)	463(16)	230(13)	64(12)	-106(11)	-19(12)
C(44A)	575(18)	366(15)	379(16)	-14(13)	-194(13)	129(13)
C(45A)	545(17)	334(14)	276(14)	-81(11)	-138(12)	106(12)
C(46A)	290(13)	270(13)	197(12)	-21(10)	-6(10)	27(10)
C(47A)	255(13)	274(13)	220(12)	-63(10)	26(9)	81(10)
C(48A)	260(13)	393(15)	231(13)	-59(11)	31(10)	70(11)
C(49A)	263(13)	489(16)	289(14)	-128(12)	-11(11)	94(12)
C(50A)	412(16)	487(17)	222(13)	-76(12)	-56(11)	221(13)
C(51A)	371(15)	330(14)	249(13)	-22(11)	52(11)	107(11)
C(52A)	284(13)	293(13)	245(13)	-48(10)	46(10)	66(10)
C(53A)	215(12)	312(13)	230(12)	-37(10)	-28(9)	35(10)
C(54A)	418(15)	375(15)	275(14)	-71(11)	-58(11)	111(12)
C(55A)	519(17)	404(16)	405(16)	-160(13)	-134(13)	147(13)
C(56A)	398(16)	281(14)	550(18)	-44(13)	-74(13)	53(12)
C(57A)	396(16)	341(15)	373(15)	44(12)	23(12)	34(12)
C(58A)	267(13)	347(14)	259(13)	-46(11)	20(10)	41(11)
C(59A)	247(13)	298(13)	223(12)	61(10)	-24(10)	16(10)
C(60A)	327(15)	328(15)	445(16)	30(12)	43(12)	46(12)
C(61A)	219(14)	500(18)	545(18)	127(15)	40(12)	93(12)
C(62A)	287(15)	630(20)	409(17)	76(14)	-122(12)	-80(14)
C(63A)	364(16)	670(20)	401(16)	-137(15)	-72(13)	-107(14)
C(64A)	278(14)	510(17)	349(15)	-129(13)	-36(11)	7(12)
C(65A)	441(17)	570(20)	391(17)	19(15)	61(13)	151(14)
C(66A)	780(20)	460(19)	500(20)	104(16)	-74(17)	-62(17)
C(67A)	1090(30)	530(20)	610(20)	-123(18)	-220(20)	-80(20)
C(68A)	391(17)	720(20)	414(18)	35(16)	-154(13)	-14(15)
C(69A)	590(20)	486(19)	510(20)	133(16)	-22(15)	74(15)
C(70A)	840(20)	500(20)	530(20)	-36(16)	49(17)	185(17)
Co(1B)	164(2)	233(2)	157(2)	-50(1)	-24(1)	1(1)
P(1B)	178(3)	227(3)	177(3)	-66(2)	-17(2)	-1(2)
P(2B)	171(3)	221(3)	168(3)	-56(2)	2(2)	-10(2)
P(3B)	183(3)	229(3)	182(3)	-33(2)	-14(2)	8(2)
O(1B)	242(9)	354(10)	300(9)	-71(7)	-61(7)	-38(7)
B(1B)	184(13)	189(13)	192(13)	-54(10)	-25(10)	-5(10)
C(1B)	235(12)	150(11)	201(11)	2(9)	-33(9)	-20(9)
C(2B)	292(13)	233(12)	247(13)	-16(10)	-39(10)	-49(10)
C(3B)	477(16)	271(13)	250(13)	-56(11)	-66(11)	-94(11)
C(4B)	411(16)	288(14)	354(15)	-7(11)	-204(12)	-101(11)
C(5B)	280(14)	337(14)	454(16)	-32(12)	-169(12)	-21(11)
C(6B)	275(13)	255(13)	309(13)	-52(10)	-73(10)	-15(10)
C(7B)	167(11)	241(12)	211(12)	-48(9)	-22(9)	-19(9)
C(8B)	202(11)	227(12)	182(11)	-71(9)	-27(9)	5(9)
C(9B)	212(11)	197(11)	189(11)	-43(9)	-9(9)	-28(9)
C(10B)	180(11)	306(13)	194(12)	-91(10)	-35(9)	38(9)
C(11B)	235(12)	361(14)	228(12)	-78(11)	-56(10)	36(10)
C(12B)	294(14)	496(17)	202(13)	-29(11)	-4(10)	26(12)
C(13B)	351(15)	554(18)	247(14)	-177(13)	2(11)	147(13)
C(14B)	446(16)	399(16)	317(15)	-169(12)	-7(12)	98(12)
C(15B)	320(14)	339(14)	269(13)	-120(11)	-15(10)	25(11)
C(16B)	207(11)	212(12)	205(11)	-90(9)	-3(9)	48(9)
C(17B)	270(13)	279(13)	317(14)	-95(11)	-97(10)	38(10)
C(18B)	447(16)	347(15)	362(15)	-100(12)	-205(12)	154(12)

C(19B)	473(16)	240(13)	323(14)	-25(11)	-21(12)	61(12)
C(20B)	306(14)	248(13)	347(14)	-71(11)	32(11)	18(10)
C(21B)	213(12)	254(12)	271(13)	-82(10)	-12(10)	41(10)
C(22B)	215(12)	221(12)	174(11)	-73(9)	61(9)	-14(9)
C(23B)	297(13)	312(13)	238(13)	-57(10)	29(10)	-11(10)
C(24B)	396(15)	305(14)	268(14)	2(11)	80(11)	52(12)
C(25B)	559(18)	254(14)	289(14)	-71(11)	174(13)	-93(12)
C(26B)	455(16)	448(16)	323(15)	-160(13)	100(12)	-227(13)
C(27B)	328(14)	358(14)	226(13)	-99(11)	29(10)	-70(11)
C(28B)	186(11)	211(12)	214(12)	-4(9)	54(9)	-25(9)
C(29B)	227(13)	413(15)	252(13)	-8(11)	16(10)	1(11)
C(30B)	246(14)	462(17)	419(17)	139(13)	60(12)	85(12)
C(31B)	420(16)	315(15)	475(18)	3(13)	177(13)	108(12)
C(32B)	479(17)	372(16)	419(16)	-176(13)	56(13)	48(13)
C(33B)	312(14)	326(14)	337(14)	-118(11)	-8(11)	37(11)
C(34B)	199(12)	229(12)	205(12)	0(9)	1(9)	6(9)
C(35B)	301(14)	406(15)	278(13)	-88(11)	-51(11)	71(11)
C(36B)	280(14)	537(17)	327(15)	-35(13)	-95(11)	76(12)
C(37B)	270(14)	358(15)	424(16)	13(12)	-27(12)	116(11)
C(38B)	301(14)	242(13)	514(17)	-88(12)	-12(12)	37(11)
C(39B)	226(13)	264(13)	406(15)	-44(11)	-39(11)	-30(10)
C(40B)	184(11)	259(12)	193(12)	6(9)	-11(9)	19(9)
C(41B)	331(14)	345(14)	236(13)	-16(11)	-15(10)	-31(11)
C(42B)	430(16)	494(17)	205(13)	-55(12)	-29(11)	40(13)
C(43B)	353(15)	532(18)	244(14)	63(13)	40(11)	-5(13)
C(44B)	495(18)	578(19)	379(17)	10(14)	71(13)	-252(15)
C(45B)	476(17)	485(17)	272(14)	-65(12)	39(12)	-120(13)
C(46B)	417(15)	349(14)	153(12)	-44(10)	-11(10)	17(11)
C(47B)	321(14)	353(14)	238(13)	-88(11)	-109(10)	-58(11)
C(48B)	332(15)	492(16)	254(14)	-78(12)	-100(11)	-61(12)
C(49B)	266(14)	557(18)	342(15)	-127(13)	-88(11)	-32(12)
C(50B)	373(16)	576(18)	273(14)	-102(13)	-2(12)	-182(13)
C(51B)	451(16)	365(15)	292(14)	-36(11)	-122(12)	-91(12)
C(52B)	367(15)	372(15)	269(13)	-85(11)	-103(11)	-34(11)
C(53B)	299(13)	376(14)	271(13)	-113(11)	-2(10)	-44(11)
C(54B)	640(20)	543(19)	291(15)	-112(14)	27(13)	-171(15)
C(55B)	740(20)	481(19)	481(19)	-254(16)	83(16)	-163(16)
C(56B)	507(18)	380(16)	543(19)	-126(15)	-10(14)	-28(13)
C(57B)	405(16)	401(16)	453(17)	-89(13)	-115(13)	9(12)
C(58B)	283(13)	396(15)	310(14)	-105(12)	-83(11)	16(11)
C(59B)	274(13)	413(15)	199(12)	-1(11)	-19(10)	-28(11)
C(60B)	477(18)	442(17)	491(18)	13(14)	-220(14)	-90(14)
C(61B)	354(17)	670(20)	600(20)	175(17)	-262(15)	-200(15)
C(62B)	247(15)	880(30)	403(17)	122(17)	-3(13)	24(16)
C(63B)	331(16)	940(30)	456(18)	-233(17)	-72(14)	213(16)
C(64B)	297(15)	660(20)	409(16)	-205(15)	-80(12)	43(13)
C(65B)	469(18)	930(30)	347(17)	-268(18)	-63(14)	-107(17)
C(66B)	586(19)	495(18)	370(17)	-2(14)	-81(14)	-125(15)
C(67B)	500(18)	436(17)	418(17)	-112(14)	-66(13)	28(13)
C(68B)	350(15)	551(19)	337(15)	16(14)	-29(12)	-82(13)
C(69B)	490(19)	373(17)	750(20)	-20(16)	-227(17)	-30(14)
C(70B)	580(20)	630(20)	700(20)	-370(20)	-175(18)	51(17)

**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj49.**

	x	y	z	$U_{\text{iso}}$
H(2A)	591	993	390	41
H(3A)	456	1028	455	53
H(4A)	286	1000	451	61
H(5A)	253	935	382	62
H(6A)	389	902	314	48
H(7A1)	569	917	206	27
H(7A2)	505	863	260	27
H(8A1)	618	824	369	25
H(8A2)	655	883	397	25
H(9A1)	724	993	303	28
H(9A2)	651	1018	249	28
H(11A)	597	894	102	34
H(12A)	540	868	12	45
H(13A)	528	758	5	51
H(14A)	574	675	87	48
H(15A)	629	700	177	37
H(17A)	477	759	311	37
H(18A)	450	662	389	50
H(19A)	586	588	405	49
H(20A)	749	610	344	42
H(21A)	778	708	268	31
H(23A)	676	759	453	33
H(24A)	710	663	526	39
H(25A)	871	612	514	45
H(26A)	998	656	430	46
H(27A)	966	752	357	36
H(29A)	1003	878	306	53
H(30A)	1118	952	328	71
H(31A)	1061	1014	404	64
H(32A)	889	1010	450	51
H(33A)	773	936	426	40
H(35A)	1006	978	146	36
H(36A)	1154	1039	147	42
H(37A)	1144	1120	208	41
H(38A)	986	1140	266	40
H(39A)	839	1076	268	34
H(41A)	817	933	84	37
H(42A)	776	982	-17	45
H(43A)	690	1083	-33	44
H(44A)	646	1134	53	53
H(45A)	686	1084	154	45
H(48A)	847	753	126	36
H(49A)	781	791	30	41
H(50A)	870	874	-49	45
H(51A)	1023	918	-31	40
H(52A)	1091	878	65	34
H(54A)	1066	698	91	43

H(55A)	1064	584	111	51
H(56A)	1011	523	214	50
H(57A)	968	577	298	48
H(58A)	971	691	278	36
H(60A)	1212	738	132	47
H(61A)	1377	779	137	56
H(62A)	1394	873	175	55
H(63A)	1245	927	210	57
H(64A)	1081	885	210	45
H(65A)	225	735	299	60
H(66A)	218	826	343	73
H(67A)	209	815	453	88
H(68A)	199	712	520	63
H(69A)	206	620	476	69
H(70A)	217	631	365	78
H(2B)	266	508	602	31
H(3B)	151	472	544	40
H(4B)	-26	498	559	41
H(5B)	-84	563	632	42
H(6B)	30	597	692	33
H(7B1)	164	588	787	25
H(7B2)	127	644	731	25
H(8B1)	287	677	625	24
H(8B2)	334	616	596	24
H(9B1)	368	506	692	24
H(9B2)	270	482	745	24
H(11B)	156	607	891	32
H(12B)	58	632	982	41
H(13B)	30	742	989	45
H(14B)	100	826	906	45
H(15B)	199	801	815	36
H(17B)	123	749	682	33
H(18B)	134	847	604	44
H(19B)	279	915	590	43
H(20B)	411	888	654	37
H(21B)	402	789	729	29
H(23B)	387	740	541	35
H(24B)	450	841	478	41
H(25B)	597	889	501	46
H(26B)	688	834	582	49
H(27B)	626	733	645	36
H(29B)	631	584	696	37
H(30B)	750	509	662	51
H(31B)	732	473	569	53
H(32B)	595	510	512	51
H(33B)	475	583	547	39
H(35B)	576	522	848	39
H(36B)	727	458	848	46
H(37B)	743	371	794	44
H(38B)	607	348	743	43
H(39B)	458	413	740	36
H(41B)	370	562	913	38
H(42B)	282	517	1015	46
H(43B)	172	427	1030	49

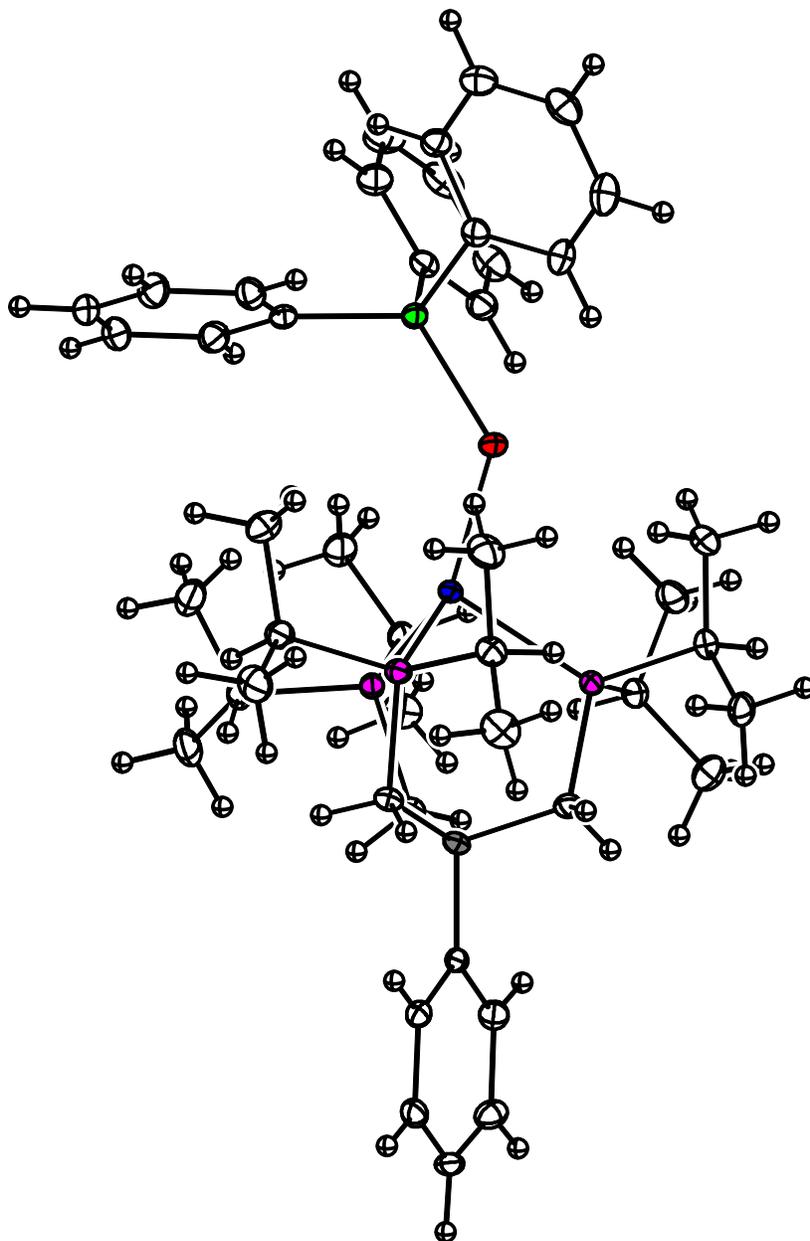
H(44B)	151	380	943	61
H(45B)	239	425	841	50
H(48B)	400	746	870	42
H(49B)	292	711	966	45
H(50B)	349	630	1047	49
H(51B)	510	580	1028	44
H(52B)	620	617	932	39
H(54B)	597	798	906	59
H(55B)	607	913	883	67
H(56B)	611	973	779	57
H(57B)	607	918	696	50
H(58B)	600	804	717	39
H(60B)	762	750	872	57
H(61B)	929	706	871	68
H(62B)	971	615	828	66
H(63B)	846	569	783	68
H(64B)	680	614	781	53
H(65B)	976	810	502	67
H(66B)	909	899	544	59
H(67B)	841	883	652	54
H(68B)	835	778	717	52
H(69B)	903	690	674	65
H(70B)	976	707	568	72

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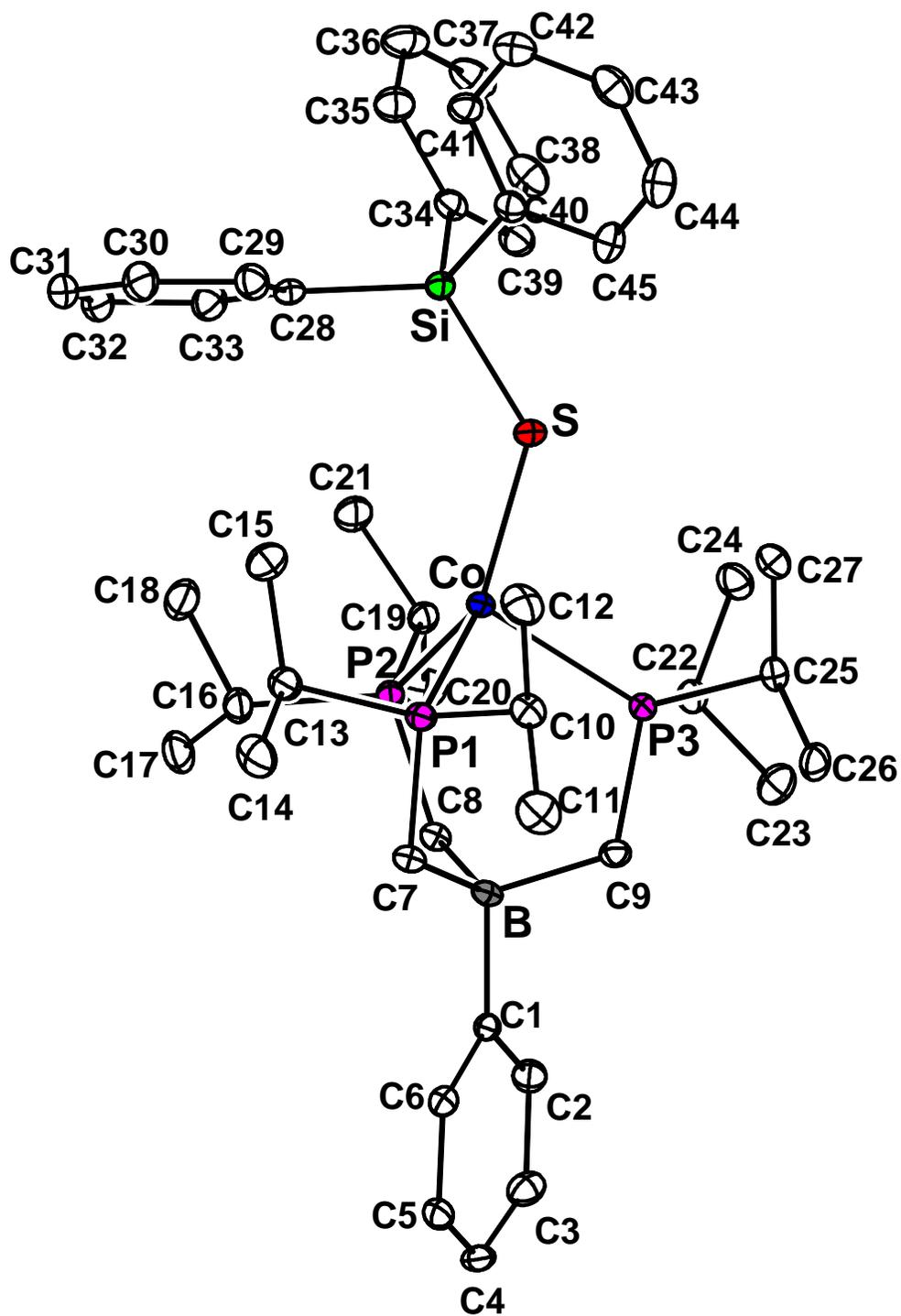
K. X-ray report for  $[\text{PhBP}^{i\text{Pr}}_3]\text{CoSSiPh}_3$ , 15.

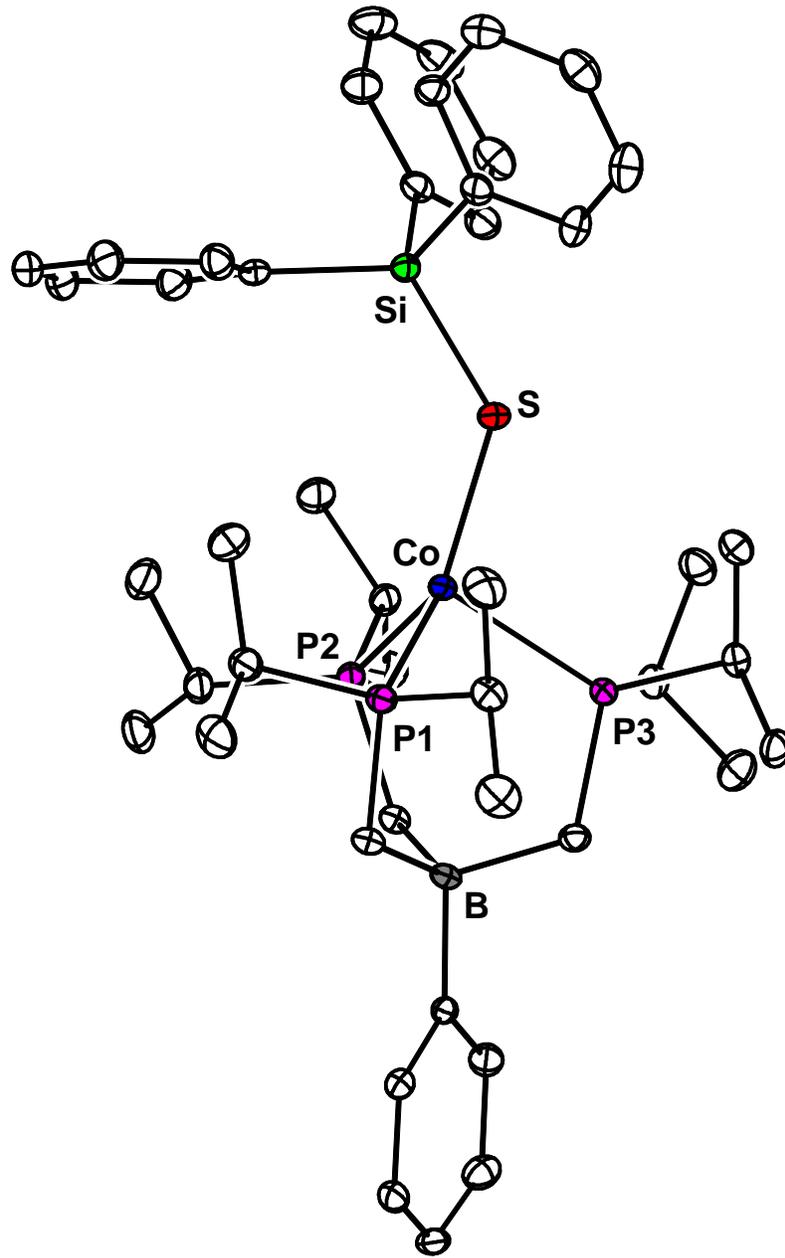
## Crystal Structure Report for

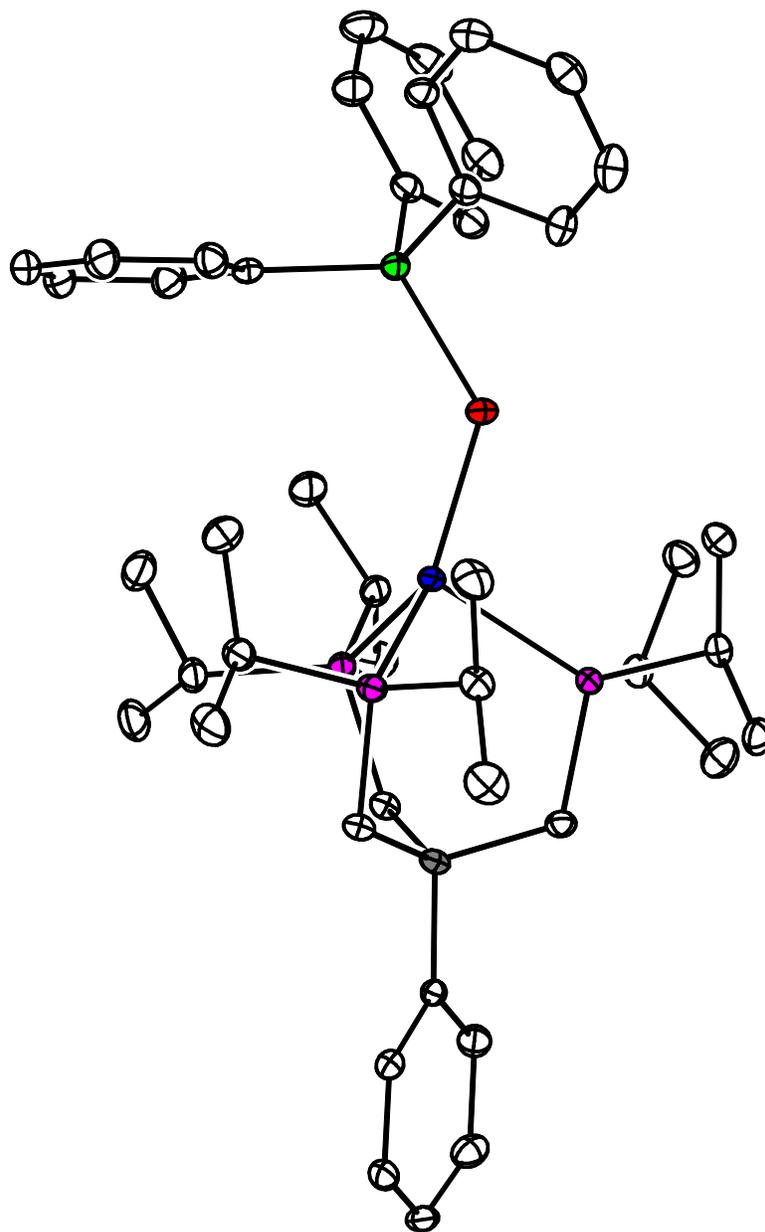
## DMJ 52, $[\text{PhBP}^{i\text{Pr}}_3]\text{CoSSiPh}_3$

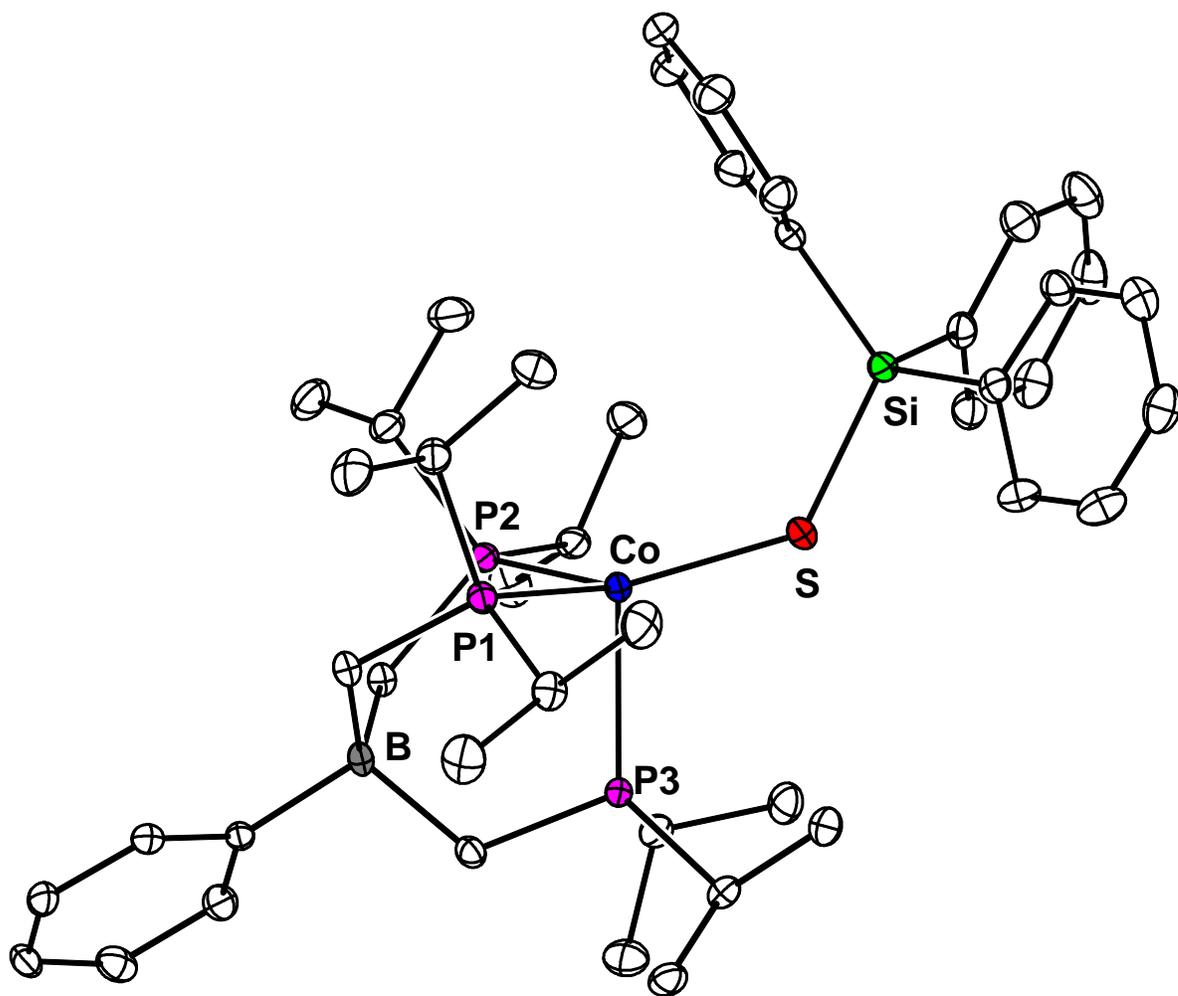












**Table 1. Crystal Data and Structure Analysis Details for dmj52.**

Empirical formula	C <sub>45</sub> H <sub>68</sub> BCoP <sub>3</sub> SSi
Formula weight	831.79
Crystallization solvent	Benzene/Petroleum Ether
Crystal shape	irregular block
Crystal color	forest green
Crystal size	0.25 x 0.27 x 0.43 mm

### Data Collection

Preliminary photograph(s)	rotation
Type of diffractometer	SMART 1000 CCD
Wavelength	0.71073 Å MoK $\alpha$
Data collection temperature	100 K
Theta range for 7178 reflections used in lattice determination	2.40 to 34.13°
Unit cell dimensions	a = 10.3161(4) Å $\alpha = 90^\circ$ b = 14.4678(6) Å $\beta = 90^\circ$ c = 29.9630(13) Å $\gamma = 90^\circ$
Volume	4472.0(3) Å <sup>3</sup>
Z	4
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (# 19)
Density (calculated)	1.235 g/cm <sup>3</sup>
F(000)	1780
Theta range for data collection	2.0 to 36.0°
Completeness to theta = 36.04°	95.6%
Index ranges	-16 ≤ h ≤ 15, -22 ≤ k ≤ 23, -49 ≤ l ≤ 47
Reflections collected	80179
Independent reflections	19688 [R <sub>int</sub> = 0.0662]
Reflections > 2 $\sigma$ (I)	15879
Average $\sigma$ (I)/(net I)	0.0660
Absorption coefficient	0.60 mm <sup>-1</sup>
Reflections monitored for decay	604
Decay of standards	0

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	19688 / 0 / 481
Treatment of hydrogen atoms	Calculated positions and $U_{\text{iso}}$
Goodness-of-fit on $F^2$	1.37
Final R indices [ $I > 2\sigma(I)$ , 15879 reflections]	$R1 = 0.0431$ , $wR2 = 0.0606$
R indices (all data)	$R1 = 0.0587$ , $wR2 = 0.0622$
Type of weighting scheme used	$\sigma$
Weighting scheme used	$1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Absolute structure parameter	-0.010(6)
Largest diff. peak and hole	1.70 and -0.66 $e \cdot \text{\AA}^{-3}$

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

**Special Refinement Details**

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger. The 0 0 2 reflection has been omitted during refinement due to poor agreement between experimental and observed intensities.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj52.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co	8335(1)	9512(1)	8639(1)	11(1)
S	7557(1)	9161(1)	9293(1)	16(1)
P(1)	7560(1)	9949(1)	7996(1)	12(1)
P(2)	10124(1)	10265(1)	8507(1)	11(1)
P(3)	9151(1)	8118(1)	8344(1)	11(1)
Si	6606(1)	9972(1)	9780(1)	12(1)
B	10050(2)	9355(1)	7624(1)	12(1)
C(1)	10898(1)	9307(1)	7163(1)	11(1)
C(2)	12166(1)	8952(1)	7159(1)	16(1)
C(3)	12936(2)	8941(1)	6779(1)	19(1)
C(4)	12470(2)	9303(1)	6381(1)	18(1)
C(5)	11214(1)	9638(1)	6367(1)	17(1)
C(6)	10457(1)	9633(1)	6750(1)	14(1)
C(7)	8735(1)	10000(1)	7548(1)	13(1)
C(8)	10979(1)	9834(1)	8019(1)	12(1)
C(9)	9640(1)	8289(1)	7762(1)	13(1)
C(10)	6366(1)	9025(1)	7850(1)	16(1)
C(11)	6093(2)	8884(1)	7351(1)	25(1)
C(12)	5102(2)	9100(1)	8120(1)	24(1)
C(13)	6720(2)	11089(1)	7980(1)	17(1)
C(14)	6026(2)	11279(1)	7537(1)	24(1)
C(15)	5834(2)	11282(1)	8381(1)	26(1)
C(16)	10041(2)	11535(1)	8415(1)	16(1)
C(17)	11355(2)	12036(1)	8408(1)	23(1)
C(18)	9092(2)	12038(1)	8726(1)	23(1)
C(19)	11102(1)	10042(1)	9020(1)	14(1)
C(20)	12576(2)	10028(1)	8945(1)	21(1)
C(21)	10737(2)	10670(1)	9413(1)	21(1)
C(22)	10651(1)	7737(1)	8646(1)	14(1)
C(23)	11458(2)	7001(1)	8401(1)	22(1)
C(24)	10323(2)	7425(1)	9120(1)	19(1)
C(25)	8190(1)	7011(1)	8361(1)	14(1)
C(26)	7779(2)	6621(1)	7908(1)	18(1)
C(27)	7032(2)	7051(1)	8680(1)	21(1)
C(28)	6257(1)	11227(1)	9665(1)	14(1)
C(29)	5053(2)	11523(1)	9507(1)	18(1)
C(30)	4781(2)	12452(1)	9440(1)	21(1)
C(31)	5716(2)	13115(1)	9535(1)	23(1)
C(32)	6922(2)	12844(1)	9689(1)	22(1)
C(33)	7193(2)	11911(1)	9754(1)	18(1)
C(34)	7604(1)	9938(1)	10307(1)	14(1)
C(35)	7238(1)	10453(1)	10686(1)	20(1)
C(36)	7934(2)	10406(1)	11083(1)	24(1)
C(37)	9016(2)	9840(1)	11112(1)	23(1)
C(38)	9396(2)	9337(1)	10746(1)	22(1)
C(39)	8712(1)	9386(1)	10347(1)	18(1)

C(40)	4996(1)	9384(1)	9886(1)	14(1)
C(41)	4069(1)	9795(1)	10166(1)	16(1)
C(42)	2885(1)	9382(1)	10248(1)	20(1)
C(43)	2582(2)	8540(1)	10050(1)	22(1)
C(44)	3477(2)	8120(1)	9774(1)	23(1)
C(45)	4678(2)	8533(1)	9692(1)	18(1)

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**Table 3.** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj52.

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Co-S	2.1783(4)
Co-P(1)	2.1787(4)
Co-P(2)	2.1792(4)
Co-P(3)	2.3569(4)
S-Si	2.1134(5)
S-Co-P(1)	136.692(17)
S-Co-P(2)	126.303(17)
P(1)-Co-P(2)	90.303(16)
S-Co-P(3)	105.643(16)
P(1)-Co-P(3)	92.753(16)
P(2)-Co-P(3)	93.267(15)
Si-S-Co	131.53(2)

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Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj52.**

---

Co-S	2.1783(4)
Co-P(1)	2.1787(4)
Co-P(2)	2.1792(4)
Co-P(3)	2.3569(4)
S-Si	2.1134(5)
P(1)-C(7)	1.8108(14)
P(1)-C(13)	1.8639(15)
P(1)-C(10)	1.8690(15)
P(2)-C(8)	1.8187(14)
P(2)-C(16)	1.8593(14)
P(2)-C(19)	1.8670(15)
P(3)-C(9)	1.8339(15)
P(3)-C(22)	1.8748(15)
P(3)-C(25)	1.8849(14)
Si-C(28)	1.8821(15)
Si-C(34)	1.8853(15)
Si-C(40)	1.8938(15)
B-C(1)	1.638(2)
B-C(9)	1.651(2)
B-C(7)	1.662(2)
B-C(8)	1.672(2)
C(1)-C(6)	1.401(2)
C(1)-C(2)	1.405(2)
C(2)-C(3)	1.388(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.387(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.387(2)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.535(2)
C(10)-C(12)	1.538(2)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.534(2)
C(13)-C(15)	1.536(2)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9800

C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(18)	1.534(2)
C(16)-C(17)	1.538(2)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(21)	1.533(2)
C(19)-C(20)	1.538(2)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(24)	1.530(2)
C(22)-C(23)	1.537(2)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(27)	1.529(2)
C(25)-C(26)	1.531(2)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(29)	1.397(2)
C(28)-C(33)	1.409(2)
C(29)-C(30)	1.388(2)
C(29)-H(29)	0.9500
C(30)-C(31)	1.390(2)
C(30)-H(30)	0.9500
C(31)-C(32)	1.383(2)
C(31)-H(31)	0.9500
C(32)-C(33)	1.392(2)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.400(2)
C(34)-C(35)	1.408(2)

C(35)-C(36)	1.392(2)
C(35)-H(35)	0.9500
C(36)-C(37)	1.387(2)
C(36)-H(36)	0.9500
C(37)-C(38)	1.374(2)
C(37)-H(37)	0.9500
C(38)-C(39)	1.389(2)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(45)	1.399(2)
C(40)-C(41)	1.405(2)
C(41)-C(42)	1.382(2)
C(41)-H(41)	0.9500
C(42)-C(43)	1.392(2)
C(42)-H(42)	0.9500
C(43)-C(44)	1.381(2)
C(43)-H(43)	0.9500
C(44)-C(45)	1.397(2)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500

S-Co-P(1)	136.692(17)
S-Co-P(2)	126.303(17)
P(1)-Co-P(2)	90.303(16)
S-Co-P(3)	105.643(16)
P(1)-Co-P(3)	92.753(16)
P(2)-Co-P(3)	93.267(15)
Si-S-Co	131.53(2)
C(7)-P(1)-C(13)	104.83(7)
C(7)-P(1)-C(10)	107.23(7)
C(13)-P(1)-C(10)	108.68(7)
C(7)-P(1)-Co	114.91(5)
C(13)-P(1)-Co	116.77(5)
C(10)-P(1)-Co	104.01(5)
C(8)-P(2)-C(16)	103.96(7)
C(8)-P(2)-C(19)	109.94(7)
C(16)-P(2)-C(19)	108.54(7)
C(8)-P(2)-Co	112.69(5)
C(16)-P(2)-Co	118.81(5)
C(19)-P(2)-Co	102.80(5)
C(9)-P(3)-C(22)	105.74(7)
C(9)-P(3)-C(25)	106.54(7)
C(22)-P(3)-C(25)	99.84(6)
C(9)-P(3)-Co	109.88(5)
C(22)-P(3)-Co	111.49(5)
C(25)-P(3)-Co	121.93(5)
C(28)-Si-C(34)	106.45(7)
C(28)-Si-C(40)	107.24(7)
C(34)-Si-C(40)	109.12(6)
C(28)-Si-S	119.82(5)
C(34)-Si-S	108.09(5)
C(40)-Si-S	105.82(5)
C(1)-B-C(9)	107.91(11)
C(1)-B-C(7)	110.14(11)

C(9)-B-C(7)	110.48(12)
C(1)-B-C(8)	107.92(11)
C(9)-B-C(8)	110.99(12)
C(7)-B-C(8)	109.36(12)
C(6)-C(1)-C(2)	114.74(13)
C(6)-C(1)-B	123.89(13)
C(2)-C(1)-B	121.34(13)
C(3)-C(2)-C(1)	122.95(15)
C(3)-C(2)-H(2)	118.5
C(1)-C(2)-H(2)	118.5
C(4)-C(3)-C(2)	120.09(14)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	118.91(14)
C(5)-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	119.98(15)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	123.26(14)
C(5)-C(6)-H(6)	118.4
C(1)-C(6)-H(6)	118.4
B-C(7)-P(1)	114.97(10)
B-C(7)-H(7A)	108.5
P(1)-C(7)-H(7A)	108.5
B-C(7)-H(7B)	108.5
P(1)-C(7)-H(7B)	108.5
H(7A)-C(7)-H(7B)	107.5
B-C(8)-P(2)	115.63(9)
B-C(8)-H(8A)	108.4
P(2)-C(8)-H(8A)	108.4
B-C(8)-H(8B)	108.4
P(2)-C(8)-H(8B)	108.4
H(8A)-C(8)-H(8B)	107.4
B-C(9)-P(3)	115.66(10)
B-C(9)-H(9A)	108.4
P(3)-C(9)-H(9A)	108.4
B-C(9)-H(9B)	108.4
P(3)-C(9)-H(9B)	108.4
H(9A)-C(9)-H(9B)	107.4
C(11)-C(10)-C(12)	111.42(13)
C(11)-C(10)-P(1)	116.44(11)
C(12)-C(10)-P(1)	112.65(11)
C(11)-C(10)-H(10)	105.0
C(12)-C(10)-H(10)	105.0
P(1)-C(10)-H(10)	105.0
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5

H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(15)	111.60(13)
C(14)-C(13)-P(1)	113.44(11)
C(15)-C(13)-P(1)	114.65(11)
C(14)-C(13)-H(13)	105.4
C(15)-C(13)-H(13)	105.4
P(1)-C(13)-H(13)	105.4
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(18)-C(16)-C(17)	110.28(13)
C(18)-C(16)-P(2)	114.07(11)
C(17)-C(16)-P(2)	115.34(11)
C(18)-C(16)-H(16)	105.4
C(17)-C(16)-H(16)	105.4
P(2)-C(16)-H(16)	105.4
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(21)-C(19)-C(20)	111.29(13)
C(21)-C(19)-P(2)	113.37(10)
C(20)-C(19)-P(2)	114.58(11)
C(21)-C(19)-H(19)	105.6
C(20)-C(19)-H(19)	105.6
P(2)-C(19)-H(19)	105.6
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5

H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(24)-C(22)-C(23)	111.00(12)
C(24)-C(22)-P(3)	110.61(10)
C(23)-C(22)-P(3)	114.93(11)
C(24)-C(22)-H(22)	106.6
C(23)-C(22)-H(22)	106.6
P(3)-C(22)-H(22)	106.6
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(27)-C(25)-C(26)	110.52(12)
C(27)-C(25)-P(3)	113.33(10)
C(26)-C(25)-P(3)	115.78(10)
C(27)-C(25)-H(25)	105.4
C(26)-C(25)-H(25)	105.4
P(3)-C(25)-H(25)	105.4
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(29)-C(28)-C(33)	117.25(13)
C(29)-C(28)-Si	121.89(11)
C(33)-C(28)-Si	120.81(11)
C(30)-C(29)-C(28)	121.73(14)
C(30)-C(29)-H(29)	119.1
C(28)-C(29)-H(29)	119.1
C(29)-C(30)-C(31)	119.90(15)
C(29)-C(30)-H(30)	120.0
C(31)-C(30)-H(30)	120.0
C(32)-C(31)-C(30)	119.78(15)
C(32)-C(31)-H(31)	120.1
C(30)-C(31)-H(31)	120.1
C(31)-C(32)-C(33)	120.19(14)
C(31)-C(32)-H(32)	119.9

C(33)-C(32)-H(32)	119.9
C(32)-C(33)-C(28)	121.14(14)
C(32)-C(33)-H(33)	119.4
C(28)-C(33)-H(33)	119.4
C(39)-C(34)-C(35)	116.90(14)
C(39)-C(34)-Si	122.16(12)
C(35)-C(34)-Si	120.91(11)
C(36)-C(35)-C(34)	121.61(15)
C(36)-C(35)-H(35)	119.2
C(34)-C(35)-H(35)	119.2
C(37)-C(36)-C(35)	119.86(16)
C(37)-C(36)-H(36)	120.1
C(35)-C(36)-H(36)	120.1
C(38)-C(37)-C(36)	119.51(15)
C(38)-C(37)-H(37)	120.2
C(36)-C(37)-H(37)	120.2
C(37)-C(38)-C(39)	120.94(15)
C(37)-C(38)-H(38)	119.5
C(39)-C(38)-H(38)	119.5
C(38)-C(39)-C(34)	121.18(15)
C(38)-C(39)-H(39)	119.4
C(34)-C(39)-H(39)	119.4
C(45)-C(40)-C(41)	117.48(14)
C(45)-C(40)-Si	122.11(11)
C(41)-C(40)-Si	120.41(11)
C(42)-C(41)-C(40)	121.63(14)
C(42)-C(41)-H(41)	119.2
C(40)-C(41)-H(41)	119.2
C(41)-C(42)-C(43)	120.05(15)
C(41)-C(42)-H(42)	120.0
C(43)-C(42)-H(42)	120.0
C(44)-C(43)-C(42)	119.45(15)
C(44)-C(43)-H(43)	120.3
C(42)-C(43)-H(43)	120.3
C(43)-C(44)-C(45)	120.59(15)
C(43)-C(44)-H(44)	119.7
C(45)-C(44)-H(44)	119.7
C(44)-C(45)-C(40)	120.79(15)
C(44)-C(45)-H(45)	119.6
C(40)-C(45)-H(45)	119.6

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Symmetry transformations used to generate equivalent atoms:

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj52. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co	129(1)	116(1)	94(1)	8(1)	11(1)	5(1)
S	211(2)	151(2)	112(2)	1(1)	43(2)	17(2)
P(1)	114(2)	136(2)	115(2)	15(2)	8(2)	16(1)
P(2)	141(2)	106(2)	97(2)	-1(1)	-8(2)	-2(1)
P(3)	130(2)	102(2)	100(2)	5(1)	6(2)	-4(1)
Si	144(2)	120(2)	103(2)	-2(2)	1(2)	6(2)
B	125(7)	145(8)	88(7)	13(6)	10(6)	-16(6)
C(1)	136(7)	103(6)	102(7)	-16(5)	9(6)	-28(5)
C(2)	181(8)	169(7)	135(8)	1(6)	-16(6)	1(6)
C(3)	144(7)	208(8)	208(9)	-51(7)	29(6)	-19(6)
C(4)	219(7)	171(7)	143(7)	-43(6)	80(7)	-48(6)
C(5)	258(8)	137(7)	119(7)	10(6)	7(6)	-17(6)
C(6)	166(7)	121(7)	132(7)	-10(6)	5(6)	2(5)
C(7)	128(7)	157(7)	101(7)	13(6)	8(5)	-7(5)
C(8)	118(6)	136(7)	106(7)	11(5)	0(6)	-8(5)
C(9)	143(7)	144(7)	97(7)	-5(6)	3(6)	4(5)
C(10)	121(7)	182(7)	173(8)	15(6)	-4(6)	-8(5)
C(11)	255(9)	294(9)	205(9)	3(7)	-67(7)	-63(7)
C(12)	146(8)	264(8)	306(10)	40(7)	38(7)	-28(6)
C(13)	160(7)	163(7)	184(8)	34(6)	33(7)	46(6)
C(14)	208(8)	235(8)	282(10)	90(7)	3(7)	74(7)
C(15)	250(9)	237(8)	279(10)	-9(7)	87(8)	70(7)
C(16)	233(8)	116(6)	148(8)	9(6)	-18(7)	5(6)
C(17)	308(9)	146(7)	228(9)	17(7)	-19(7)	-70(6)
C(18)	307(9)	168(7)	225(9)	-26(7)	-19(8)	48(7)
C(19)	187(7)	126(7)	119(7)	-10(6)	-19(6)	-2(6)
C(20)	163(7)	293(8)	178(8)	-11(7)	-59(7)	-28(7)
C(21)	295(9)	200(8)	121(8)	-25(6)	-34(7)	2(6)
C(22)	139(7)	129(6)	150(7)	6(6)	-13(6)	-2(5)
C(23)	198(8)	207(8)	245(9)	-24(7)	-14(7)	59(6)
C(24)	228(8)	198(8)	156(8)	40(6)	-26(7)	-3(6)
C(25)	152(7)	106(6)	158(7)	11(6)	-10(6)	-10(5)
C(26)	219(8)	128(7)	184(8)	-21(6)	-24(7)	-23(6)
C(27)	246(8)	167(7)	228(9)	10(7)	81(7)	-53(6)
C(28)	190(8)	137(7)	87(7)	-11(6)	18(6)	5(5)
C(29)	202(8)	164(7)	171(8)	4(6)	-13(7)	-22(6)
C(30)	229(8)	186(8)	206(9)	28(7)	-23(7)	57(6)
C(31)	334(9)	131(7)	213(9)	24(7)	87(8)	34(7)
C(32)	251(9)	149(7)	261(9)	-15(7)	58(7)	-52(6)
C(33)	170(7)	174(7)	209(8)	-21(7)	15(6)	-4(6)
C(34)	149(7)	154(7)	132(7)	15(6)	8(6)	-30(6)
C(35)	190(8)	232(8)	171(8)	-7(7)	-6(6)	-5(6)
C(36)	268(9)	328(10)	136(8)	-49(7)	11(6)	-75(7)
C(37)	225(8)	328(9)	140(8)	62(7)	-73(7)	-95(7)
C(38)	182(8)	257(9)	233(9)	76(7)	-40(7)	-1(6)
C(39)	184(8)	183(8)	166(8)	25(6)	10(6)	7(6)

C(40)	155(7)	146(7)	102(7)	18(6)	-32(6)	8(5)
C(41)	180(7)	176(7)	108(7)	-4(6)	-12(6)	4(6)
C(42)	178(7)	266(9)	159(8)	14(7)	6(6)	14(6)
C(43)	172(8)	246(8)	255(9)	62(7)	-17(7)	-55(7)
C(44)	218(8)	153(7)	322(10)	-21(7)	-61(8)	-9(6)
C(45)	193(8)	135(7)	227(9)	-16(6)	-22(7)	27(6)

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**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj52.**

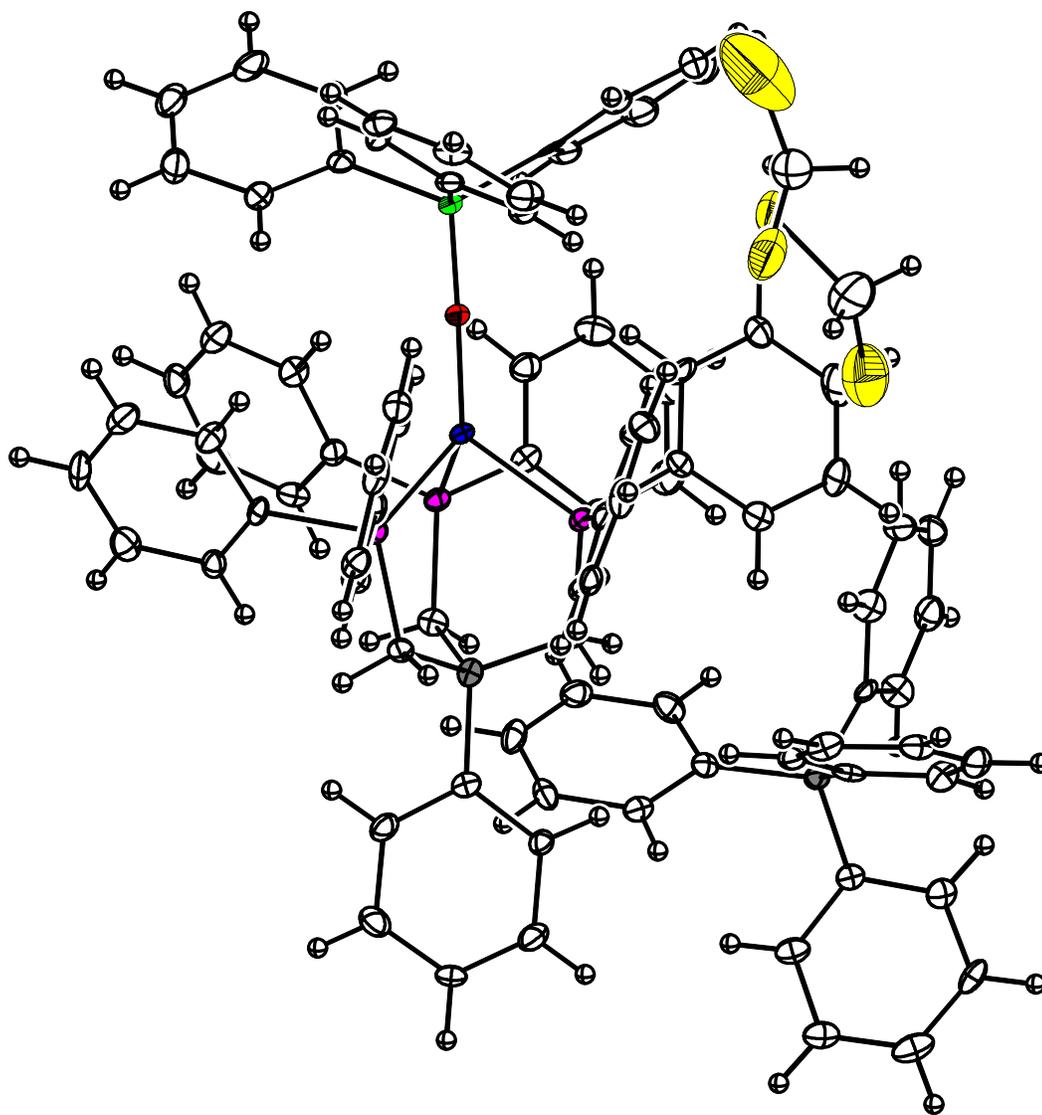
	x	y	z	$U_{\text{iso}}$
H(2)	1251	871	743	19
H(3)	1378	869	679	22
H(4)	1300	932	612	21
H(5)	1087	987	610	21
H(6)	960	986	673	17
H(7A)	831	980	727	15
H(7B)	901	1065	751	15
H(8A)	1146	1035	788	14
H(8B)	1162	937	812	14
H(9A)	1038	788	770	15
H(9B)	892	809	757	15
H(10)	678	844	795	19
H(11A)	545	839	731	38
H(11B)	690	871	720	38
H(11C)	576	946	722	38
H(12A)	456	959	799	36
H(12B)	531	924	843	36
H(12C)	463	851	810	36
H(13)	742	1156	800	20
H(14A)	526	1089	751	36
H(14B)	661	1114	729	36
H(14C)	577	1193	752	36
H(15A)	570	1195	841	38
H(15B)	624	1105	865	38
H(15C)	500	1097	834	38
H(16)	968	1161	811	20
H(17A)	1124	1266	828	34
H(17B)	1197	1169	822	34
H(17C)	1169	1208	871	34
H(18A)	952	1216	901	35
H(18B)	832	1165	877	35
H(18C)	883	1262	859	35
H(19)	1087	940	912	17
H(20A)	1287	1064	885	32
H(20B)	1279	957	871	32
H(20C)	1301	986	922	32
H(21A)	1113	1043	969	31
H(21B)	979	1068	945	31
H(21C)	1106	1130	936	31
H(22)	1122	830	868	17
H(23A)	1218	681	859	32
H(23B)	1180	726	812	32
H(23C)	1091	647	833	32
H(24A)	980	686	911	29
H(24B)	983	791	927	29
H(24C)	1113	730	928	29
H(25)	879	654	849	17

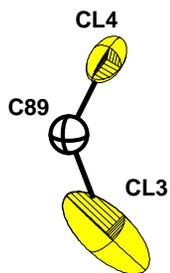
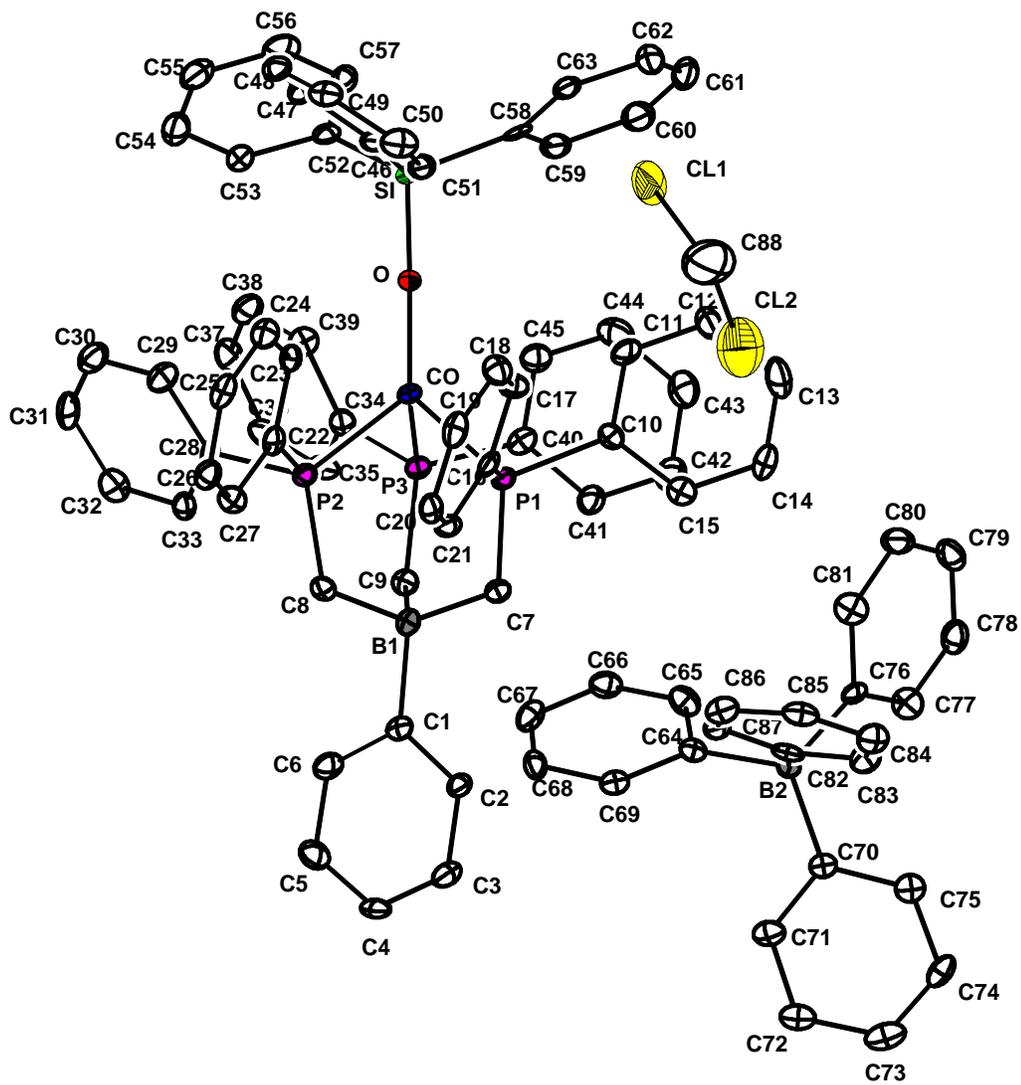
H(26A)	739	601	795	27
H(26B)	854	657	772	27
H(26C)	715	704	777	27
H(27A)	639	749	856	32
H(27B)	732	726	897	32
H(27C)	664	643	870	32
H(29)	440	1108	944	21
H(30)	396	1264	933	25
H(31)	553	1375	950	27
H(32)	757	1330	975	26
H(33)	802	1173	986	22
H(35)	650	1084	1067	24
H(36)	767	1076	1133	29
H(37)	949	980	1138	28
H(38)	1014	895	1076	27
H(39)	900	904	1010	21
H(41)	426	1037	1030	19
H(42)	228	967	1044	24
H(43)	177	826	1010	27
H(44)	328	754	964	28
H(45)	529	823	950	22

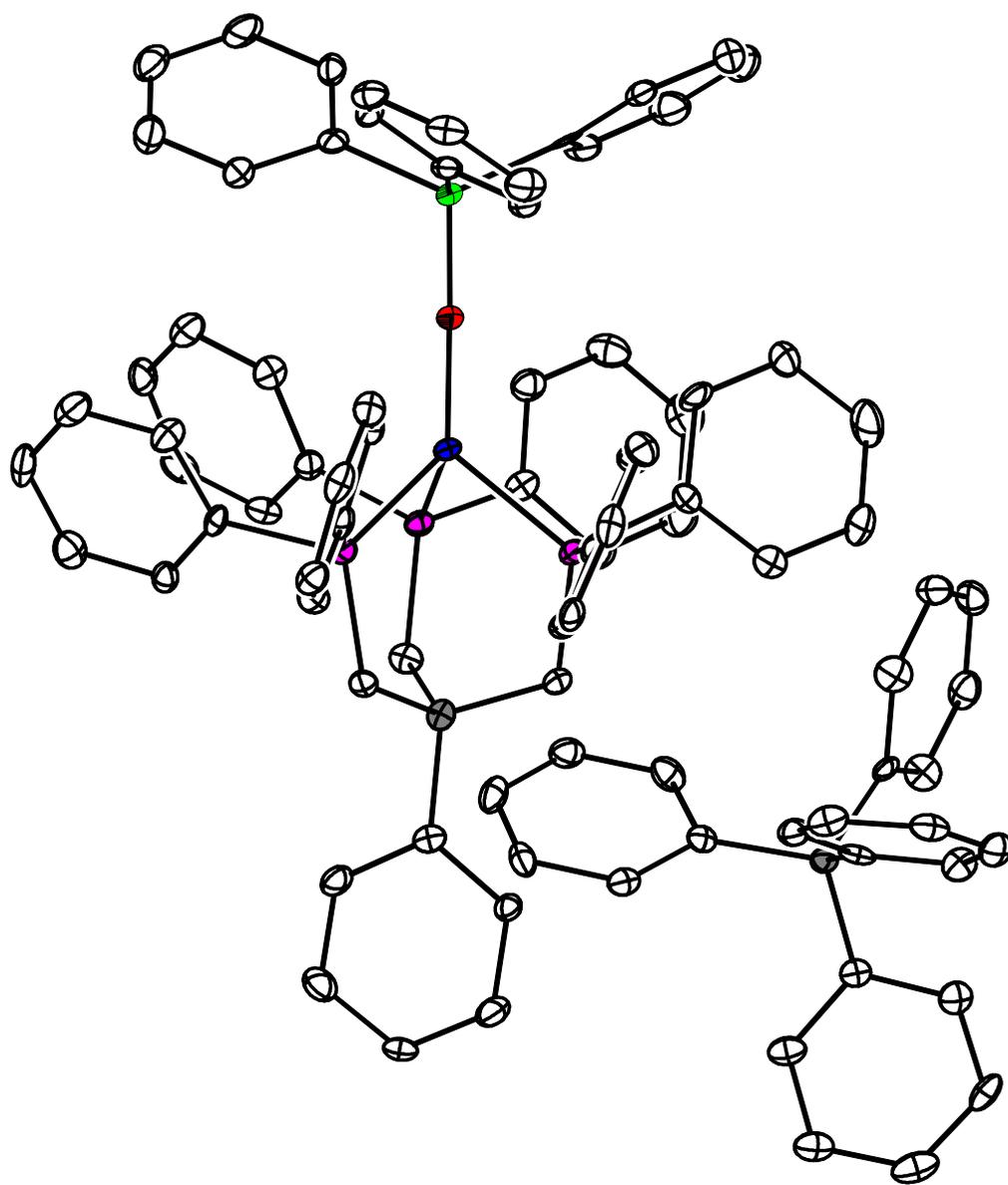
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L. X-ray report for  $\{[\text{PhBP}_3]\text{CoOSiPh}_3\} \{\text{BPh}_4\}$ , **16**  $\{\text{BPh}_4\}$ .

## Crystal Structure report for DMJ40, $\{[\text{PhBP}_3]\text{CoOSiPh}_3\} \{\text{BPh}_4\}$







**Table 1. Crystal Data and Structure Analysis Details for dmj40.**

Empirical formula	$C_{87}H_{76}B_2CoOP_3Si \cdot 1\frac{1}{2} CH_2Cl_2$
Formula weight	1466.50
Crystallization solvent	Methylene Chloride
Crystal shape	Rough block
Crystal color	Dark green
Crystal size	0.09 x 0.10 x 0.30 mm

**Data Collection**

Preliminary photograph(s)	rotation	
Type of diffractometer	SMART 1000 CCD	
Wavelength	0.71073 Å MoK $\alpha$	
Data collection temperature	100 K	
Theta range for 5929 reflections used in lattice determination	2.22 to 25.83°	
Unit cell dimensions	a = 13.592(2) Å b = 14.814(2) Å c = 19.251(3) Å	$\alpha = 72.567(3)^\circ$ $\beta = 87.945(3)^\circ$ $\gamma = 82.565(2)^\circ$
Volume	3667.0(9) Å <sup>3</sup>	
Z	2	
Crystal system	triclinic	
Space group	P $\bar{1}$ (# 2)	
Density (calculated)	1.328 g/cm <sup>3</sup>	
F(000)	1530	
Theta range for data collection	1.5 to 28.3°	
Completeness to theta = 28.26°	89.9%	
Index ranges	-17 ≤ h ≤ 18, -19 ≤ k ≤ 19, -24 ≤ l ≤ 24	
Reflections collected	42043	
Independent reflections	16319 [R <sub>int</sub> = 0.1300]	
Reflections > 2σ(I)	7907	
Average σ(I)/(net I)	0.1968	
Absorption coefficient	0.47 mm <sup>-1</sup>	
Reflections monitored for decay	1206	
Decay of standards	0%	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	16319 / 0 / 907
Treatment of hydrogen atoms	Calculated positions and U <sub>iso</sub>
Goodness-of-fit on F <sup>2</sup>	1.11
Final R indices [I>2σ(I), 7907 reflections]	R1 = 0.0643, wR2 = 0.1156
R indices (all data)	R1 = 0.1658, wR2 = 0.1381
Type of weighting scheme used	σ
Weighting scheme used	w=1/[σ <sup>2</sup> (Fo <sup>2</sup> )+(0.02) <sup>2</sup> ]
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	1.33 and -1.45 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART
Data collection	SMART and SAINT
Data reduction	SAINT v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

**References**

## Special Refinement Details

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

Two low angle reflections (1 0 1 and 0 1 1) were omitted from the refinement due to poor agreement with the structure. The carbon atom in the second solvent molecule was refined isotropically due to disorder in the solvent.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj40.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co	2994(1)	8599(1)	2557(1)	11(1)
P(1)	3084(1)	7242(1)	3425(1)	13(1)
P(2)	4595(1)	8398(1)	2396(1)	12(1)
P(3)	3191(1)	9342(1)	3355(1)	12(1)
O	2110(2)	8992(2)	1845(1)	14(1)
Si	1301(1)	9380(1)	1168(1)	13(1)
B(1)	4781(4)	7821(3)	3990(3)	13(1)
C(1)	5681(3)	7487(3)	4609(2)	12(1)
C(2)	5752(3)	6634(3)	5185(2)	14(1)
C(3)	6553(3)	6366(3)	5673(2)	20(1)
C(4)	7290(3)	6931(3)	5599(2)	21(1)
C(5)	7250(3)	7786(3)	5041(2)	21(1)
C(6)	6444(3)	8043(3)	4561(2)	18(1)
C(7)	3952(3)	7062(3)	4153(2)	15(1)
C(8)	5347(3)	7867(3)	3196(2)	12(1)
C(9)	4223(3)	8896(3)	3977(2)	15(1)
C(10)	1838(3)	7071(3)	3785(2)	15(1)
C(11)	975(3)	7562(3)	3406(2)	18(1)
C(12)	52(3)	7390(3)	3694(3)	25(1)
C(13)	-30(4)	6707(3)	4369(3)	29(1)
C(14)	822(4)	6198(3)	4752(2)	27(1)
C(15)	1748(3)	6385(3)	4461(2)	22(1)
C(16)	3401(3)	6327(3)	2971(2)	14(1)
C(17)	2682(3)	6171(3)	2525(2)	16(1)
C(18)	2913(3)	5548(3)	2127(2)	19(1)
C(19)	3861(3)	5066(3)	2155(2)	21(1)
C(20)	4581(3)	5190(3)	2598(2)	16(1)
C(21)	4350(3)	5822(3)	3009(2)	14(1)
C(22)	4859(3)	7716(3)	1758(2)	13(1)
C(23)	4147(3)	7686(3)	1258(2)	12(1)
C(24)	4379(3)	7170(3)	768(2)	17(1)
C(25)	5314(3)	6663(3)	772(2)	20(1)
C(26)	6023(3)	6674(3)	1278(2)	18(1)
C(27)	5804(3)	7196(3)	1762(2)	17(1)
C(28)	4988(3)	9554(3)	1923(2)	12(1)
C(29)	4810(3)	9949(3)	1170(2)	20(1)
C(30)	5067(3)	10841(3)	812(2)	22(1)
C(31)	5508(3)	11355(3)	1176(2)	23(1)
C(32)	5692(3)	10976(3)	1920(2)	21(1)
C(33)	5437(3)	10081(3)	2287(2)	14(1)
C(34)	3229(3)	10599(3)	2873(2)	14(1)
C(35)	3534(3)	11194(3)	3237(2)	17(1)
C(36)	3559(3)	12161(3)	2880(2)	21(1)
C(37)	3262(3)	12530(3)	2159(2)	21(1)
C(38)	2951(3)	11953(3)	1791(2)	21(1)
C(39)	2926(3)	10994(3)	2134(2)	16(1)

C(40)	2035(3)	9328(3)	3852(2)	16(1)
C(41)	1945(3)	8771(3)	4581(2)	20(1)
C(42)	1029(4)	8747(3)	4915(2)	25(1)
C(43)	177(4)	9270(3)	4529(2)	26(1)
C(44)	267(4)	9830(3)	3820(3)	24(1)
C(45)	1180(3)	9859(3)	3485(2)	19(1)
C(46)	1608(3)	8677(3)	513(2)	14(1)
C(47)	1836(3)	9093(3)	-224(2)	16(1)
C(48)	2067(3)	8544(3)	-696(2)	18(1)
C(49)	2068(3)	7574(3)	-455(2)	17(1)
C(50)	1834(3)	7137(3)	272(2)	23(1)
C(51)	1616(3)	7678(3)	742(2)	15(1)
C(52)	1408(3)	10665(3)	690(2)	13(1)
C(53)	2313(3)	10911(3)	363(2)	18(1)
C(54)	2441(4)	11844(3)	-17(2)	24(1)
C(55)	1658(4)	12566(3)	-76(2)	26(1)
C(56)	761(4)	12350(3)	245(2)	26(1)
C(57)	644(3)	11412(3)	619(2)	16(1)
C(58)	26(3)	9211(3)	1551(2)	15(1)
C(59)	-389(3)	9707(3)	2037(2)	20(1)
C(60)	-1331(3)	9583(3)	2336(2)	25(1)
C(61)	-1875(4)	8954(3)	2165(2)	25(1)
C(62)	-1493(3)	8461(3)	1694(2)	22(1)
C(63)	-554(3)	8587(3)	1384(2)	15(1)
B(2)	2525(4)	6619(3)	7228(3)	13(1)
C(64)	3033(3)	7573(3)	6737(2)	12(1)
C(65)	2502(3)	8504(3)	6583(2)	19(1)
C(66)	2894(3)	9313(3)	6165(2)	19(1)
C(67)	3837(3)	9238(3)	5869(2)	19(1)
C(68)	4389(3)	8347(3)	6011(2)	17(1)
C(69)	3997(3)	7547(3)	6446(2)	16(1)
C(70)	2981(3)	6247(3)	8070(2)	12(1)
C(71)	3884(3)	6461(3)	8259(2)	17(1)
C(72)	4279(3)	6130(3)	8965(2)	19(1)
C(73)	3754(4)	5549(3)	9523(2)	23(1)
C(74)	2859(3)	5315(3)	9358(2)	18(1)
C(75)	2488(3)	5667(3)	8649(2)	17(1)
C(76)	1315(3)	6938(3)	7218(2)	12(1)
C(77)	785(3)	7277(3)	7739(2)	21(1)
C(78)	-216(3)	7632(3)	7667(2)	22(1)
C(79)	-740(3)	7658(3)	7056(3)	23(1)
C(80)	-238(3)	7338(3)	6515(2)	22(1)
C(81)	765(3)	6979(3)	6599(2)	21(1)
C(82)	2712(3)	5714(3)	6869(2)	13(1)
C(83)	2270(3)	4881(3)	7200(2)	19(1)
C(84)	2288(3)	4137(3)	6899(2)	19(1)
C(85)	2792(3)	4167(3)	6251(2)	18(1)
C(86)	3270(3)	4952(3)	5921(2)	18(1)
C(87)	3211(3)	5704(3)	6219(2)	17(1)
C(88)	390(5)	4895(4)	2568(3)	73(2)
C(89)	9589(9)	5333(7)	9140(5)	52(4)
Cl(1)	91(1)	5977(1)	1897(1)	67(1)
Cl(2)	614(1)	5061(1)	3438(1)	68(1)
Cl(3)	10000	5000	10000	170(2)

Cl(4)

8623(3)

5688(2)

8940(2)

51(1)

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**Table 3.** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj40.

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Co-O	1.766(3)
Co-P(2)	2.1817(13)
Co-P(3)	2.1836(13)
Co-P(1)	2.1874(12)
O-Si	1.652(3)
O-Co-P(2)	124.43(10)
O-Co-P(3)	124.82(10)
P(2)-Co-P(3)	90.50(5)
O-Co-P(1)	125.59(10)
P(2)-Co-P(1)	90.67(5)
P(3)-Co-P(1)	90.18(5)
Si-O-Co	178.6(2)

---

Symmetry transformations used to generate equivalent atoms:

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj40.**

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Co-O	1.766(3)
Co-P(2)	2.1817(13)
Co-P(3)	2.1836(13)
Co-P(1)	2.1874(12)
P(1)-C(7)	1.800(4)
P(1)-C(16)	1.822(4)
P(1)-C(10)	1.827(5)
P(2)-C(8)	1.792(4)
P(2)-C(22)	1.811(4)
P(2)-C(28)	1.821(4)
P(3)-C(9)	1.801(4)
P(3)-C(40)	1.809(5)
P(3)-C(34)	1.822(4)
O-Si	1.652(3)
Si-C(46)	1.866(5)
Si-C(52)	1.871(4)
Si-C(58)	1.876(5)
B(1)-C(7)	1.650(6)
B(1)-C(1)	1.660(6)
B(1)-C(9)	1.667(6)
B(1)-C(8)	1.674(6)
C(1)-C(6)	1.389(6)
C(1)-C(2)	1.405(5)
C(2)-C(3)	1.402(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.364(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.389(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.398(6)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.401(5)
C(10)-C(15)	1.403(6)
C(11)-C(12)	1.376(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.398(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.399(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.386(6)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.398(6)
C(16)-C(17)	1.407(6)

C(17)-C(18)	1.367(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.384(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.386(6)
C(19)-H(19)	0.9500
C(20)-C(21)	1.396(6)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.403(5)
C(22)-C(27)	1.409(6)
C(23)-C(24)	1.386(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.390(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.399(6)
C(25)-H(25)	0.9500
C(26)-C(27)	1.380(6)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(33)	1.400(6)
C(28)-C(29)	1.407(5)
C(29)-C(30)	1.379(6)
C(29)-H(29)	0.9500
C(30)-C(31)	1.377(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.392(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.384(6)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(35)	1.387(6)
C(34)-C(39)	1.420(5)
C(35)-C(36)	1.395(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.383(6)
C(36)-H(36)	0.9500
C(37)-C(38)	1.375(6)
C(37)-H(37)	0.9500
C(38)-C(39)	1.379(6)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(45)	1.399(5)
C(40)-C(41)	1.409(6)
C(41)-C(42)	1.380(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.407(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.379(6)
C(43)-H(43)	0.9500
C(44)-C(45)	1.377(6)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(47)	1.408(6)

C(46)-C(51)	1.411(6)
C(47)-C(48)	1.393(6)
C(47)-H(47)	0.9500
C(48)-C(49)	1.371(6)
C(48)-H(48)	0.9500
C(49)-C(50)	1.400(6)
C(49)-H(49)	0.9500
C(50)-C(51)	1.379(6)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-C(57)	1.393(6)
C(52)-C(53)	1.403(6)
C(53)-C(54)	1.386(6)
C(53)-H(53)	0.9500
C(54)-C(55)	1.390(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.379(7)
C(55)-H(55)	0.9500
C(56)-C(57)	1.387(6)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(63)	1.402(6)
C(58)-C(59)	1.415(6)
C(59)-C(60)	1.395(6)
C(59)-H(59)	0.9500
C(60)-C(61)	1.380(7)
C(60)-H(60)	0.9500
C(61)-C(62)	1.374(6)
C(61)-H(61)	0.9500
C(62)-C(63)	1.400(6)
C(62)-H(62)	0.9500
C(63)-H(63)	0.9500
B(2)-C(76)	1.650(6)
B(2)-C(70)	1.664(6)
B(2)-C(64)	1.665(6)
B(2)-C(82)	1.672(7)
C(64)-C(69)	1.407(6)
C(64)-C(65)	1.423(5)
C(65)-C(66)	1.388(6)
C(65)-H(65)	0.9500
C(66)-C(67)	1.389(6)
C(66)-H(66)	0.9500
C(67)-C(68)	1.386(6)
C(67)-H(67)	0.9500
C(68)-C(69)	1.387(6)
C(68)-H(68)	0.9500
C(69)-H(69)	0.9500
C(70)-C(71)	1.393(6)
C(70)-C(75)	1.397(6)
C(71)-C(72)	1.400(5)
C(71)-H(71)	0.9500
C(72)-C(73)	1.398(6)
C(72)-H(72)	0.9500
C(73)-C(74)	1.378(6)

C(73)-H(73)	0.9500
C(74)-C(75)	1.395(5)
C(74)-H(74)	0.9500
C(75)-H(75)	0.9500
C(76)-C(77)	1.390(6)
C(76)-C(81)	1.412(5)
C(77)-C(78)	1.389(6)
C(77)-H(77)	0.9500
C(78)-C(79)	1.387(6)
C(78)-H(78)	0.9500
C(79)-C(80)	1.391(6)
C(79)-H(79)	0.9500
C(80)-C(81)	1.395(6)
C(80)-H(80)	0.9500
C(81)-H(81)	0.9500
C(82)-C(87)	1.404(6)
C(82)-C(83)	1.408(6)
C(83)-C(84)	1.389(6)
C(83)-H(83)	0.9500
C(84)-C(85)	1.394(6)
C(84)-H(84)	0.9500
C(85)-C(86)	1.379(6)
C(85)-H(85)	0.9500
C(86)-C(87)	1.391(6)
C(86)-H(86)	0.9500
C(87)-H(87)	0.9500
C(88)-Cl(1)	1.741(5)
C(88)-Cl(2)	1.807(7)
C(88)-H(88A)	0.9900
C(88)-H(88B)	0.9900
C(89)-Cl(4)	1.372(12)
C(89)-Cl(3)	1.675(10)
C(89)-H(89A)	0.9900
C(89)-H(89B)	0.9900
Cl(3)-C(89)#1	1.675(10)
O-Co-P(2)	124.43(10)
O-Co-P(3)	124.82(10)
P(2)-Co-P(3)	90.50(5)
O-Co-P(1)	125.59(10)
P(2)-Co-P(1)	90.67(5)
P(3)-Co-P(1)	90.18(5)
C(7)-P(1)-C(16)	109.46(19)
C(7)-P(1)-C(10)	110.6(2)
C(16)-P(1)-C(10)	105.0(2)
C(7)-P(1)-Co	117.37(15)
C(16)-P(1)-Co	105.33(13)
C(10)-P(1)-Co	108.31(14)
C(8)-P(2)-C(22)	109.87(19)
C(8)-P(2)-C(28)	108.4(2)
C(22)-P(2)-C(28)	103.98(19)
C(8)-P(2)-Co	116.84(15)
C(22)-P(2)-Co	108.70(14)
C(28)-P(2)-Co	108.23(14)

C(9)-P(3)-C(40)	110.3(2)
C(9)-P(3)-C(34)	110.1(2)
C(40)-P(3)-C(34)	103.9(2)
C(9)-P(3)-Co	118.01(15)
C(40)-P(3)-Co	105.12(15)
C(34)-P(3)-Co	108.37(14)
Si-O-Co	178.6(2)
O-Si-C(46)	108.60(17)
O-Si-C(52)	108.88(17)
C(46)-Si-C(52)	108.89(19)
O-Si-C(58)	108.50(16)
C(46)-Si-C(58)	110.4(2)
C(52)-Si-C(58)	111.53(19)
C(7)-B(1)-C(1)	112.3(3)
C(7)-B(1)-C(9)	109.4(4)
C(1)-B(1)-C(9)	109.1(3)
C(7)-B(1)-C(8)	110.1(4)
C(1)-B(1)-C(8)	105.4(3)
C(9)-B(1)-C(8)	110.5(3)
C(6)-C(1)-C(2)	116.0(4)
C(6)-C(1)-B(1)	120.2(4)
C(2)-C(1)-B(1)	123.8(4)
C(3)-C(2)-C(1)	121.3(4)
C(3)-C(2)-H(2)	119.3
C(1)-C(2)-H(2)	119.3
C(4)-C(3)-C(2)	120.6(4)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	120.2(4)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	118.5(4)
C(4)-C(5)-H(5)	120.8
C(6)-C(5)-H(5)	120.8
C(1)-C(6)-C(5)	123.4(4)
C(1)-C(6)-H(6)	118.3
C(5)-C(6)-H(6)	118.3
B(1)-C(7)-P(1)	115.2(3)
B(1)-C(7)-H(7A)	108.5
P(1)-C(7)-H(7A)	108.5
B(1)-C(7)-H(7B)	108.5
P(1)-C(7)-H(7B)	108.5
H(7A)-C(7)-H(7B)	107.5
B(1)-C(8)-P(2)	116.0(3)
B(1)-C(8)-H(8A)	108.3
P(2)-C(8)-H(8A)	108.3
B(1)-C(8)-H(8B)	108.3
P(2)-C(8)-H(8B)	108.3
H(8A)-C(8)-H(8B)	107.4
B(1)-C(9)-P(3)	114.6(3)
B(1)-C(9)-H(9A)	108.6
P(3)-C(9)-H(9A)	108.6
B(1)-C(9)-H(9B)	108.6
P(3)-C(9)-H(9B)	108.6

H(9A)-C(9)-H(9B)	107.6
C(11)-C(10)-C(15)	118.9(4)
C(11)-C(10)-P(1)	123.1(3)
C(15)-C(10)-P(1)	118.0(3)
C(12)-C(11)-C(10)	120.8(4)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	119.9(4)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(12)-C(13)-C(14)	120.2(5)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(15)-C(14)-C(13)	119.4(4)
C(15)-C(14)-H(14)	120.3
C(13)-C(14)-H(14)	120.3
C(14)-C(15)-C(10)	120.8(4)
C(14)-C(15)-H(15)	119.6
C(10)-C(15)-H(15)	119.6
C(21)-C(16)-C(17)	118.9(4)
C(21)-C(16)-P(1)	122.4(3)
C(17)-C(16)-P(1)	118.6(3)
C(18)-C(17)-C(16)	120.5(4)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(19)	120.3(4)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(18)-C(19)-C(20)	120.6(4)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(19)-C(20)-C(21)	119.5(4)
C(19)-C(20)-H(20)	120.3
C(21)-C(20)-H(20)	120.3
C(20)-C(21)-C(16)	120.2(4)
C(20)-C(21)-H(21)	119.9
C(16)-C(21)-H(21)	119.9
C(23)-C(22)-C(27)	118.7(4)
C(23)-C(22)-P(2)	121.9(3)
C(27)-C(22)-P(2)	119.4(3)
C(24)-C(23)-C(22)	120.5(4)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(23)-C(24)-C(25)	120.5(4)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	119.4(4)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(27)-C(26)-C(25)	120.5(4)
C(27)-C(26)-H(26)	119.7
C(25)-C(26)-H(26)	119.7
C(26)-C(27)-C(22)	120.4(4)
C(26)-C(27)-H(27)	119.8

C(22)-C(27)-H(27)	119.8
C(33)-C(28)-C(29)	118.5(4)
C(33)-C(28)-P(2)	122.1(3)
C(29)-C(28)-P(2)	119.4(3)
C(30)-C(29)-C(28)	119.9(4)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
C(31)-C(30)-C(29)	121.2(4)
C(31)-C(30)-H(30)	119.4
C(29)-C(30)-H(30)	119.4
C(30)-C(31)-C(32)	119.8(4)
C(30)-C(31)-H(31)	120.1
C(32)-C(31)-H(31)	120.1
C(33)-C(32)-C(31)	119.6(4)
C(33)-C(32)-H(32)	120.2
C(31)-C(32)-H(32)	120.2
C(32)-C(33)-C(28)	121.0(4)
C(32)-C(33)-H(33)	119.5
C(28)-C(33)-H(33)	119.5
C(35)-C(34)-C(39)	118.9(4)
C(35)-C(34)-P(3)	119.6(3)
C(39)-C(34)-P(3)	121.4(3)
C(34)-C(35)-C(36)	120.6(4)
C(34)-C(35)-H(35)	119.7
C(36)-C(35)-H(35)	119.7
C(37)-C(36)-C(35)	119.5(4)
C(37)-C(36)-H(36)	120.2
C(35)-C(36)-H(36)	120.2
C(38)-C(37)-C(36)	120.7(4)
C(38)-C(37)-H(37)	119.6
C(36)-C(37)-H(37)	119.6
C(37)-C(38)-C(39)	120.6(4)
C(37)-C(38)-H(38)	119.7
C(39)-C(38)-H(38)	119.7
C(38)-C(39)-C(34)	119.7(4)
C(38)-C(39)-H(39)	120.2
C(34)-C(39)-H(39)	120.2
C(45)-C(40)-C(41)	118.4(4)
C(45)-C(40)-P(3)	118.5(3)
C(41)-C(40)-P(3)	123.1(3)
C(42)-C(41)-C(40)	120.2(4)
C(42)-C(41)-H(41)	119.9
C(40)-C(41)-H(41)	119.9
C(41)-C(42)-C(43)	120.3(4)
C(41)-C(42)-H(42)	119.9
C(43)-C(42)-H(42)	119.9
C(44)-C(43)-C(42)	119.5(5)
C(44)-C(43)-H(43)	120.2
C(42)-C(43)-H(43)	120.2
C(45)-C(44)-C(43)	120.4(4)
C(45)-C(44)-H(44)	119.8
C(43)-C(44)-H(44)	119.8
C(44)-C(45)-C(40)	121.2(4)
C(44)-C(45)-H(45)	119.4

C(40)-C(45)-H(45)	119.4
C(47)-C(46)-C(51)	116.2(4)
C(47)-C(46)-Si	123.3(3)
C(51)-C(46)-Si	120.5(3)
C(48)-C(47)-C(46)	121.7(4)
C(48)-C(47)-H(47)	119.1
C(46)-C(47)-H(47)	119.1
C(49)-C(48)-C(47)	120.6(4)
C(49)-C(48)-H(48)	119.7
C(47)-C(48)-H(48)	119.7
C(48)-C(49)-C(50)	119.4(4)
C(48)-C(49)-H(49)	120.3
C(50)-C(49)-H(49)	120.3
C(51)-C(50)-C(49)	120.1(4)
C(51)-C(50)-H(50)	120.0
C(49)-C(50)-H(50)	120.0
C(50)-C(51)-C(46)	122.1(4)
C(50)-C(51)-H(51)	118.9
C(46)-C(51)-H(51)	118.9
C(57)-C(52)-C(53)	116.3(4)
C(57)-C(52)-Si	125.0(3)
C(53)-C(52)-Si	118.7(3)
C(54)-C(53)-C(52)	122.0(4)
C(54)-C(53)-H(53)	119.0
C(52)-C(53)-H(53)	119.0
C(53)-C(54)-C(55)	119.7(5)
C(53)-C(54)-H(54)	120.1
C(55)-C(54)-H(54)	120.1
C(56)-C(55)-C(54)	119.8(4)
C(56)-C(55)-H(55)	120.1
C(54)-C(55)-H(55)	120.1
C(55)-C(56)-C(57)	119.7(4)
C(55)-C(56)-H(56)	120.2
C(57)-C(56)-H(56)	120.2
C(56)-C(57)-C(52)	122.5(4)
C(56)-C(57)-H(57)	118.7
C(52)-C(57)-H(57)	118.7
C(63)-C(58)-C(59)	116.8(4)
C(63)-C(58)-Si	122.4(4)
C(59)-C(58)-Si	120.8(4)
C(60)-C(59)-C(58)	121.7(5)
C(60)-C(59)-H(59)	119.2
C(58)-C(59)-H(59)	119.2
C(61)-C(60)-C(59)	119.9(5)
C(61)-C(60)-H(60)	120.1
C(59)-C(60)-H(60)	120.1
C(62)-C(61)-C(60)	119.9(5)
C(62)-C(61)-H(61)	120.1
C(60)-C(61)-H(61)	120.1
C(61)-C(62)-C(63)	120.9(5)
C(61)-C(62)-H(62)	119.6
C(63)-C(62)-H(62)	119.6
C(62)-C(63)-C(58)	120.9(4)
C(62)-C(63)-H(63)	119.5

C(58)-C(63)-H(63)	119.5
C(76)-B(2)-C(70)	111.8(4)
C(76)-B(2)-C(64)	106.8(3)
C(70)-B(2)-C(64)	110.2(3)
C(76)-B(2)-C(82)	106.7(3)
C(70)-B(2)-C(82)	108.6(3)
C(64)-B(2)-C(82)	112.8(4)
C(69)-C(64)-C(65)	114.3(4)
C(69)-C(64)-B(2)	124.7(4)
C(65)-C(64)-B(2)	121.1(4)
C(66)-C(65)-C(64)	122.7(4)
C(66)-C(65)-H(65)	118.7
C(64)-C(65)-H(65)	118.7
C(65)-C(66)-C(67)	120.3(4)
C(65)-C(66)-H(66)	119.8
C(67)-C(66)-H(66)	119.8
C(68)-C(67)-C(66)	119.1(4)
C(68)-C(67)-H(67)	120.4
C(66)-C(67)-H(67)	120.4
C(67)-C(68)-C(69)	119.9(4)
C(67)-C(68)-H(68)	120.1
C(69)-C(68)-H(68)	120.1
C(68)-C(69)-C(64)	123.6(4)
C(68)-C(69)-H(69)	118.2
C(64)-C(69)-H(69)	118.2
C(71)-C(70)-C(75)	114.3(4)
C(71)-C(70)-B(2)	123.8(4)
C(75)-C(70)-B(2)	121.9(4)
C(70)-C(71)-C(72)	123.8(4)
C(70)-C(71)-H(71)	118.1
C(72)-C(71)-H(71)	118.1
C(73)-C(72)-C(71)	119.4(4)
C(73)-C(72)-H(72)	120.3
C(71)-C(72)-H(72)	120.3
C(74)-C(73)-C(72)	118.7(4)
C(74)-C(73)-H(73)	120.7
C(72)-C(73)-H(73)	120.7
C(73)-C(74)-C(75)	120.1(4)
C(73)-C(74)-H(74)	120.0
C(75)-C(74)-H(74)	120.0
C(74)-C(75)-C(70)	123.7(4)
C(74)-C(75)-H(75)	118.1
C(70)-C(75)-H(75)	118.1
C(77)-C(76)-C(81)	115.2(4)
C(77)-C(76)-B(2)	125.6(4)
C(81)-C(76)-B(2)	118.8(4)
C(78)-C(77)-C(76)	123.3(4)
C(78)-C(77)-H(77)	118.3
C(76)-C(77)-H(77)	118.3
C(79)-C(78)-C(77)	120.3(4)
C(79)-C(78)-H(78)	119.9
C(77)-C(78)-H(78)	119.9
C(78)-C(79)-C(80)	118.5(4)
C(78)-C(79)-H(79)	120.8

C(80)-C(79)-H(79)	120.8
C(79)-C(80)-C(81)	120.4(4)
C(79)-C(80)-H(80)	119.8
C(81)-C(80)-H(80)	119.8
C(80)-C(81)-C(76)	122.3(4)
C(80)-C(81)-H(81)	118.8
C(76)-C(81)-H(81)	118.8
C(87)-C(82)-C(83)	113.6(4)
C(87)-C(82)-B(2)	127.1(4)
C(83)-C(82)-B(2)	119.1(4)
C(84)-C(83)-C(82)	123.3(4)
C(84)-C(83)-H(83)	118.3
C(82)-C(83)-H(83)	118.3
C(83)-C(84)-C(85)	120.5(4)
C(83)-C(84)-H(84)	119.8
C(85)-C(84)-H(84)	119.8
C(86)-C(85)-C(84)	118.3(4)
C(86)-C(85)-H(85)	120.9
C(84)-C(85)-H(85)	120.9
C(85)-C(86)-C(87)	120.1(4)
C(85)-C(86)-H(86)	119.9
C(87)-C(86)-H(86)	119.9
C(86)-C(87)-C(82)	124.1(4)
C(86)-C(87)-H(87)	118.0
C(82)-C(87)-H(87)	118.0
Cl(1)-C(88)-Cl(2)	111.9(4)
Cl(1)-C(88)-H(88A)	109.2
Cl(2)-C(88)-H(88A)	109.2
Cl(1)-C(88)-H(88B)	109.2
Cl(2)-C(88)-H(88B)	109.2
H(88A)-C(88)-H(88B)	107.9
Cl(4)-C(89)-Cl(3)	123.7(6)
Cl(4)-C(89)-H(89A)	106.4
Cl(3)-C(89)-H(89A)	106.4
Cl(4)-C(89)-H(89B)	106.4
Cl(3)-C(89)-H(89B)	106.4
H(89A)-C(89)-H(89B)	106.5
C(89)#1-Cl(3)-C(89)	180.000(4)

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Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+2

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj40. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co	128(3)	102(3)	95(3)	-16(2)	-22(3)	4(3)
P(1)	145(6)	116(6)	105(6)	-6(5)	-19(5)	-24(5)
P(2)	132(6)	107(6)	115(6)	-14(5)	-12(5)	-10(5)
P(3)	136(6)	99(6)	122(6)	-31(5)	-17(5)	6(5)
O	115(16)	145(16)	138(15)	-11(13)	-17(13)	-2(13)
Si	131(7)	127(7)	107(6)	-14(5)	-22(5)	-3(5)
B(1)	160(30)	130(30)	110(30)	-60(20)	20(20)	-10(20)
C(1)	150(20)	140(20)	90(20)	-71(19)	6(18)	19(19)
C(2)	170(20)	140(20)	100(20)	-25(19)	-13(19)	-43(19)
C(3)	240(30)	190(30)	130(20)	0(20)	-30(20)	-20(20)
C(4)	180(30)	260(30)	170(20)	-20(20)	-90(20)	-50(20)
C(5)	190(30)	240(30)	240(30)	-90(20)	-30(20)	-70(20)
C(6)	220(30)	100(20)	180(20)	-6(19)	-30(20)	0(20)
C(7)	140(20)	120(20)	140(20)	4(19)	-19(19)	-2(19)
C(8)	100(20)	90(20)	170(20)	-35(19)	-5(19)	22(18)
C(9)	150(20)	200(30)	120(20)	-80(20)	12(19)	0(20)
C(10)	140(20)	160(30)	170(20)	-50(20)	-11(19)	-40(20)
C(11)	200(30)	110(20)	170(20)	30(20)	-30(20)	30(20)
C(12)	140(30)	260(30)	300(30)	10(20)	10(20)	-40(20)
C(13)	190(30)	290(30)	380(30)	-80(30)	130(20)	-50(20)
C(14)	290(30)	310(30)	180(30)	10(20)	70(20)	-110(20)
C(15)	190(30)	250(30)	200(30)	-40(20)	-20(20)	-50(20)
C(16)	200(30)	120(20)	80(20)	13(18)	11(19)	-60(20)
C(17)	160(20)	150(20)	170(20)	-50(20)	-30(20)	-10(20)
C(18)	180(30)	210(30)	200(30)	-90(20)	10(20)	-40(20)
C(19)	290(30)	160(30)	180(30)	-50(20)	80(20)	-100(20)
C(20)	140(20)	80(20)	210(30)	10(20)	30(20)	-2(19)
C(21)	170(20)	120(20)	130(20)	-10(19)	-41(19)	-28(19)
C(22)	160(20)	40(20)	160(20)	-4(18)	35(19)	-15(19)
C(23)	140(20)	90(20)	130(20)	-32(19)	28(19)	-29(18)
C(24)	220(30)	180(30)	150(20)	-80(20)	20(20)	-50(20)
C(25)	280(30)	140(30)	150(20)	-30(20)	80(20)	-40(20)
C(26)	190(30)	160(30)	150(20)	-30(20)	30(20)	10(20)
C(27)	160(20)	140(20)	200(30)	-60(20)	-10(20)	-10(20)
C(28)	130(20)	110(20)	100(20)	-13(19)	55(18)	-7(19)
C(29)	260(30)	150(30)	170(20)	-20(20)	-10(20)	-20(20)
C(30)	240(30)	200(30)	170(30)	0(20)	20(20)	30(20)
C(31)	230(30)	140(30)	270(30)	-10(20)	90(20)	-70(20)
C(32)	200(30)	160(30)	280(30)	-80(20)	10(20)	-30(20)
C(33)	130(20)	130(20)	160(20)	-30(20)	28(19)	-14(19)
C(34)	120(20)	100(20)	180(20)	-22(19)	7(19)	14(19)
C(35)	150(20)	190(30)	190(20)	-70(20)	-50(20)	0(20)
C(36)	190(30)	160(30)	310(30)	-120(20)	-70(20)	-20(20)
C(37)	200(30)	110(20)	310(30)	-30(20)	0(20)	-50(20)
C(38)	240(30)	160(30)	180(30)	-10(20)	0(20)	0(20)
C(39)	200(30)	110(20)	180(20)	-75(19)	0(20)	-10(20)

C(40)	200(30)	130(20)	130(20)	-46(19)	0(20)	10(20)
C(41)	180(30)	240(30)	150(20)	-30(20)	20(20)	-10(20)
C(42)	260(30)	280(30)	190(30)	-70(20)	40(20)	-30(20)
C(43)	230(30)	310(30)	260(30)	-140(20)	90(20)	-40(20)
C(44)	190(30)	300(30)	260(30)	-120(20)	-30(20)	30(20)
C(45)	200(30)	150(30)	200(30)	-40(20)	-20(20)	10(20)
C(46)	110(20)	160(30)	130(20)	-30(19)	-38(19)	6(19)
C(47)	150(20)	140(20)	160(20)	20(20)	0(20)	-10(20)
C(48)	150(20)	240(30)	120(20)	-50(20)	1(19)	30(20)
C(49)	160(30)	250(30)	140(20)	-140(20)	-10(20)	60(20)
C(50)	260(30)	150(30)	280(30)	-80(20)	-80(20)	10(20)
C(51)	150(20)	170(30)	130(20)	-40(20)	-13(19)	-10(20)
C(52)	180(20)	150(20)	90(20)	-42(19)	-47(19)	-30(20)
C(53)	180(30)	210(30)	140(20)	-20(20)	-10(20)	-40(20)
C(54)	270(30)	260(30)	200(30)	-20(20)	20(20)	-110(20)
C(55)	380(30)	230(30)	160(30)	-10(20)	-60(20)	-110(20)
C(56)	300(30)	120(30)	290(30)	20(20)	-80(20)	30(20)
C(57)	190(30)	160(30)	140(20)	-40(20)	0(20)	-70(20)
C(58)	170(20)	130(20)	90(20)	63(19)	-62(19)	40(20)
C(59)	160(30)	260(30)	140(20)	-40(20)	-20(20)	30(20)
C(60)	220(30)	320(30)	180(30)	-50(20)	-10(20)	20(20)
C(61)	190(30)	290(30)	200(30)	20(20)	60(20)	10(20)
C(62)	180(30)	230(30)	230(30)	-10(20)	0(20)	-50(20)
C(63)	170(30)	150(20)	110(20)	2(19)	-27(19)	0(20)
B(2)	110(30)	130(30)	130(30)	-20(20)	0(20)	0(20)
C(64)	140(20)	110(20)	150(20)	-66(19)	-23(19)	-14(19)
C(65)	170(30)	190(30)	250(30)	-110(20)	-10(20)	-40(20)
C(66)	200(30)	140(30)	220(30)	-40(20)	-50(20)	10(20)
C(67)	310(30)	150(30)	140(20)	-30(20)	0(20)	-110(20)
C(68)	160(30)	240(30)	150(20)	-80(20)	30(20)	-100(20)
C(69)	170(30)	150(20)	150(20)	-40(20)	-30(20)	0(20)
C(70)	160(20)	80(20)	130(20)	-73(19)	-10(19)	14(19)
C(71)	180(30)	150(20)	170(20)	-70(20)	-20(20)	60(20)
C(72)	210(30)	140(20)	220(30)	-90(20)	-70(20)	40(20)
C(73)	320(30)	150(30)	190(30)	-80(20)	-70(20)	100(20)
C(74)	280(30)	80(20)	150(20)	3(19)	40(20)	20(20)
C(75)	200(30)	120(20)	200(30)	-70(20)	-10(20)	0(20)
C(76)	170(20)	60(20)	110(20)	12(18)	-32(19)	-6(19)
C(77)	210(30)	210(30)	220(30)	-100(20)	10(20)	-10(20)
C(78)	200(30)	180(30)	220(30)	-30(20)	60(20)	0(20)
C(79)	140(30)	180(30)	330(30)	-10(20)	0(20)	0(20)
C(80)	210(30)	200(30)	230(30)	-20(20)	-70(20)	-20(20)
C(81)	220(30)	150(30)	270(30)	-90(20)	-10(20)	20(20)
C(82)	100(20)	150(20)	170(20)	-100(20)	-78(19)	42(19)
C(83)	240(30)	180(30)	160(20)	-70(20)	0(20)	-20(20)
C(84)	240(30)	100(20)	230(30)	-30(20)	-30(20)	-10(20)
C(85)	190(30)	140(30)	230(30)	-100(20)	-90(20)	30(20)
C(86)	200(30)	180(30)	150(20)	-80(20)	-10(20)	60(20)
C(87)	150(20)	210(30)	130(20)	-30(20)	-10(20)	-10(20)
C(88)	720(50)	500(40)	770(50)	180(40)	-270(40)	-210(40)
C(89)	850(100)	250(60)	60(50)	290(40)	400(60)	430(60)
Cl(1)	349(9)	472(10)	854(13)	373(9)	-68(9)	-141(8)
Cl(2)	734(13)	523(11)	812(13)	-202(9)	137(10)	-193(9)
Cl(3)	700(20)	408(19)	3800(70)	-320(30)	-520(30)	8(16)

Cl(4)    750(20)    435(19)    329(17)    -40(14)    28(16)    -242(18)

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**Table 6. Hydrogen coordinates ( $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj40.**

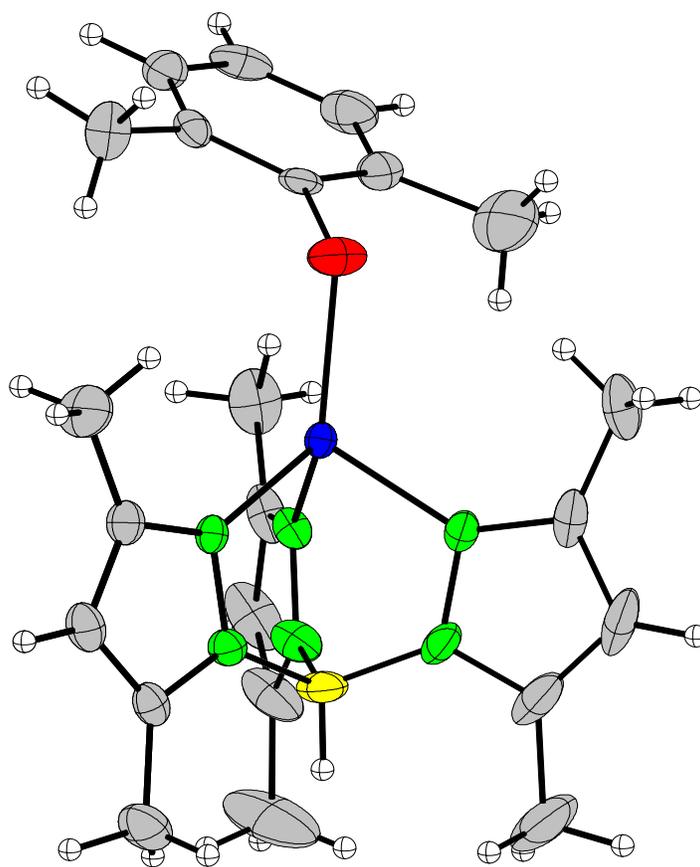
	x	y	z	$U_{\text{iso}}$
H(2)	525	623	525	16
H(3)	658	579	606	23
H(4)	783	674	593	25
H(5)	776	818	499	25
H(6)	642	863	418	21
H(7A)	358	710	459	18
H(7B)	431	641	426	18
H(8A)	561	721	320	15
H(8B)	592	823	316	15
H(9A)	472	935	385	18
H(9B)	398	887	447	18
H(11)	103	802	294	22
H(12)	-53	774	344	30
H(13)	-67	659	457	35
H(14)	77	573	521	32
H(15)	233	604	472	26
H(17)	203	650	250	19
H(18)	242	544	183	23
H(19)	402	465	187	25
H(20)	523	485	262	19
H(21)	484	591	332	17
H(23)	350	802	125	15
H(24)	389	716	43	21
H(25)	547	631	43	23
H(26)	666	632	129	21
H(27)	629	720	210	20
H(29)	451	960	91	24
H(30)	494	1111	31	27
H(31)	569	1197	92	27
H(32)	599	1133	218	25
H(33)	557	982	279	17
H(35)	373	1094	373	21
H(36)	378	1256	313	25
H(37)	327	1319	192	25
H(38)	275	1222	130	25
H(39)	271	1060	188	19
H(41)	252	841	484	24
H(42)	97	838	541	29
H(43)	-46	924	475	31
H(44)	-30	1020	356	29
H(45)	123	1025	300	23
H(47)	183	976	-40	20
H(48)	223	885	-119	21
H(49)	223	720	-78	20
H(50)	182	647	44	27
H(51)	147	737	124	18
H(53)	286	1042	40	22

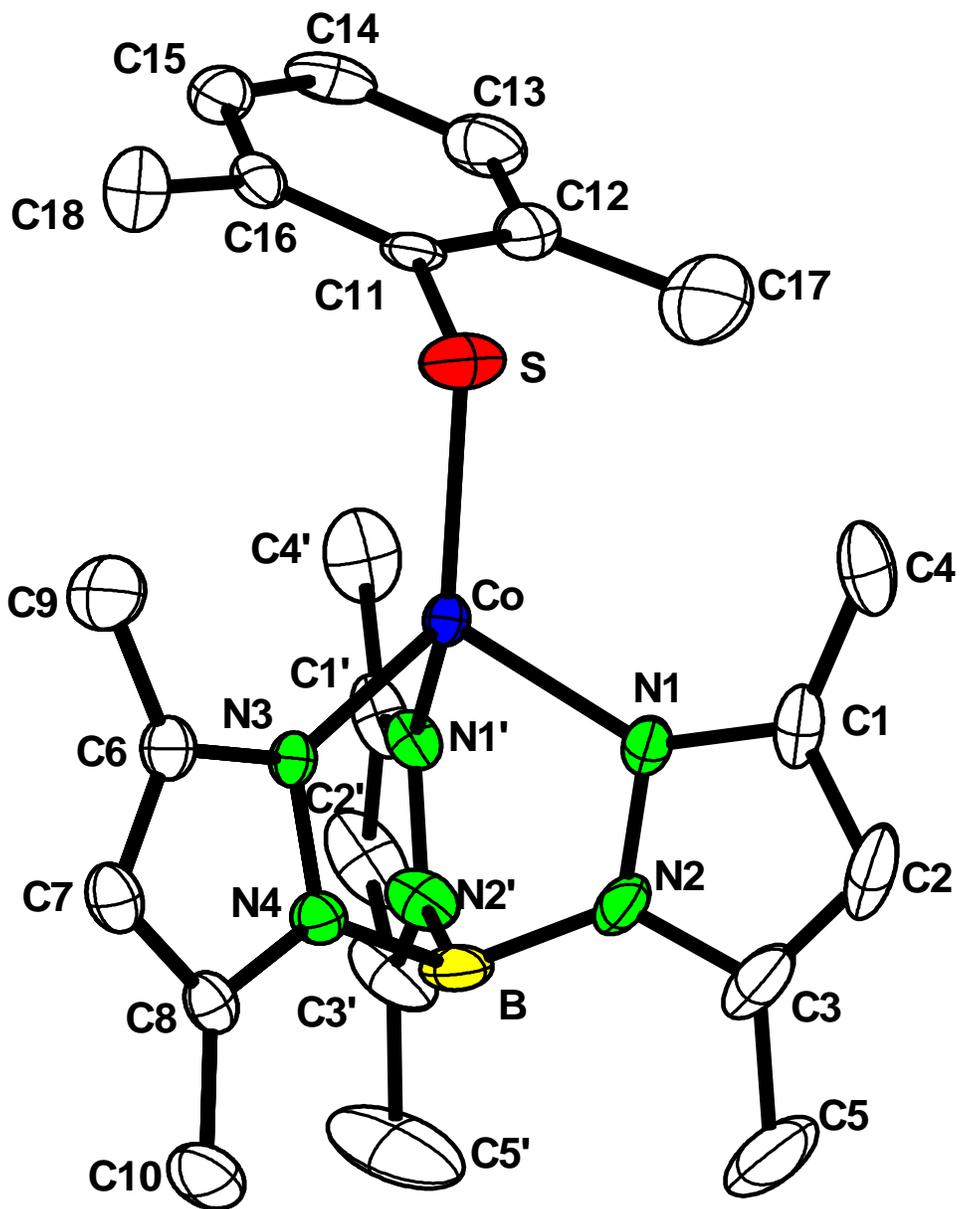
H(54)	306	1199	-24	29
H(55)	174	1321	-34	31
H(56)	22	1284	21	31
H(57)	2	1127	83	20
H(59)	-2	1014	216	23
H(60)	-160	993	266	30
H(61)	-251	886	237	30
H(62)	-187	803	158	27
H(63)	-31	825	105	19
H(65)	185	858	678	23
H(66)	252	992	608	23
H(67)	410	979	557	23
H(68)	503	828	581	21
H(69)	440	695	655	19
H(71)	425	685	789	20
H(72)	490	630	906	22
H(73)	401	532	1001	27
H(74)	250	492	973	22
H(75)	186	550	855	20
H(77)	112	727	816	25
H(78)	-54	786	804	26
H(79)	-143	789	701	28
H(80)	-58	736	609	26
H(81)	109	675	623	25
H(83)	194	483	765	22
H(84)	195	360	714	23
H(85)	281	366	604	21
H(86)	364	498	549	22
H(87)	353	624	597	20
H(88A)	99	454	242	87
H(88B)	-16	450	262	87
H(89A)	1000	582	886	62
H(89B)	975	477	896	62

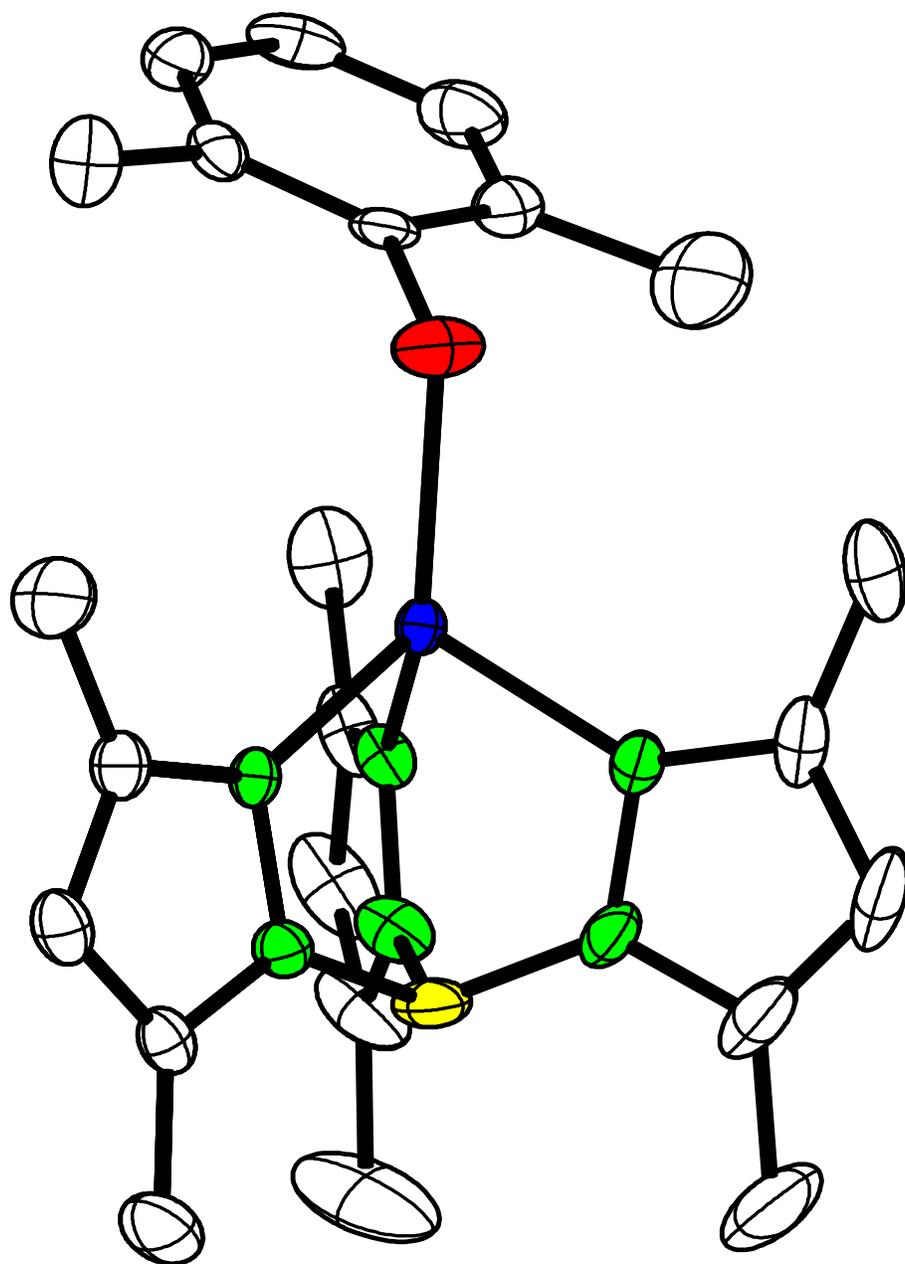
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M. X-ray report for  $[\text{Tp}^{3,5\text{-Me}_2}]\text{CoS}(2,6\text{-Me}_2\text{-Ph})$ , (17).

## Crystal Structure Report for DMJ 53, $[\text{Tp}^*]\text{CoS}(2,6\text{-Me}_2\text{-Ph})$







**Table 1. Crystal Data and Structure Analysis Details for dmj53.**

Empirical formula	C <sub>23</sub> H <sub>31</sub> BCoN <sub>6</sub> S
Formula weight	493.34
Crystallization solvent	Toluene/Petroleum Ether
Crystal shape	Plate
Crystal color	Green
Crystal size	0.04 x 0.33 x 0.37 mm

**Data Collection**

Preliminary photograph(s)	rotation	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å MoK $\alpha$	
Data collection temperature	100 K	
Theta range for 5428 reflections used in lattice determination	2.31 to 31.87°	
Unit cell dimensions	a = 23.0774(18) Å b = 13.6982(10) Å c = 7.9439(6) Å	$\alpha = 90^\circ$ $\beta = 90^\circ$ $\gamma = 90^\circ$
Volume	2511.2(3) Å <sup>3</sup>	
Z	4	
Crystal system	orthorhombic	
Space group	Pnma (# 62)	
Density (calculated)	1.305 g/cm <sup>3</sup>	
F(000)	1036	
Theta range for data collection	1.8 to 32.8°	
Completeness to theta = 32.79°	87.3%	
Index ranges	-29 ≤ h ≤ 33, -20 ≤ k ≤ 19, -10 ≤ l ≤ 10	
Data collection scan type	phi and omega scans	
Reflections collected	39060	
Independent reflections	4206 [R <sub>int</sub> = 0.0753]	
Reflections > 2σ(I)	3059	
Average σ(I)/(net I)	0.0452	
Absorption coefficient	0.79 mm <sup>-1</sup>	
Absorption correction	none	
Reflections monitored for decay	204	
Decay of standards	0	

**Table 1 (cont.)****Structure Solution and Refinement**

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4206 / 0 / 202
Treatment of hydrogen atoms	calculated positions and Uiso
Goodness-of-fit on F <sup>2</sup>	2.11
Final R indices [I>2σ(I), 3059 reflections]	R1 = 0.0468, wR2 = 0.0722
R indices (all data)	R1 = 0.0700, wR2 = 0.0737
Type of weighting scheme used	Sigma
Weighting scheme used	1/[σ <sup>2</sup> (Fo <sup>2</sup> )]
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.34 and -0.49 e·Å <sup>-3</sup>

**Programs Used**

Cell refinement	SMART v5.054
Data collection	SMART and SAINT
Data reduction	SAINTE v6.22
Structure solution	SHELXS-97
Structure refinement	SHELXL-97
Graphics	Diamond v2.1

## Special Refinement Details

Refinement of  $F^2$  against ALL reflections. The weighted R-factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ , conventional R-factors ( $R$ ) are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

A mirror plane creates one third of the Tp ligand and also causes the thiolate to be disordered into two halves over two positions. One position is shown in the diagram.

**Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj53.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.**

	x	y	z	$U_{\text{eq}}$
Co	8082(1)	2500	3909(1)	17(1)
S	9029(1)	2835(1)	3367(1)	35(1)
N(1)	7660(1)	1423(1)	5156(2)	22(1)
N(2)	7071(1)	1581(1)	5213(2)	30(1)
N(3)	7509(1)	2500	1985(2)	17(1)
N(4)	6937(1)	2500	2496(2)	21(1)
B	6804(1)	2500	4399(3)	32(1)
C(1)	7762(1)	570(1)	5928(2)	31(1)
C(2)	7243(1)	177(2)	6478(2)	47(1)
C(3)	6817(1)	817(2)	6010(2)	46(1)
C(4)	8359(1)	174(1)	6104(2)	42(1)
C(5)	6177(1)	771(2)	6295(3)	86(1)
C(6)	7503(1)	2500	305(3)	24(1)
C(7)	6933(1)	2500	-264(3)	27(1)
C(8)	6584(1)	2500	1138(3)	22(1)
C(9)	8051(1)	2500	-682(3)	44(1)
C(10)	5943(1)	2500	1254(3)	39(1)
C(11)	9445(1)	1819(2)	4073(4)	23(1)
C(12)	9567(2)	1693(3)	5774(4)	31(1)
C(13)	9891(2)	891(3)	6291(5)	39(1)
C(14)	10102(2)	212(3)	5139(7)	36(1)
C(15)	9995(2)	371(2)	3451(5)	30(1)
C(16)	9672(1)	1161(2)	2887(4)	23(1)
C(17)	9359(2)	2500	7068(4)	62(1)
C(18)	9586(2)	1317(3)	1034(5)	40(1)

**Table 3. Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj53.**

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Co-N(3)	2.0213(18)
Co-N(1)	2.0265(13)
Co-S	2.2725(10)

N(3)-Co-N(1)	93.16(5)
N(1)-Co-N(1)#1	93.39(8)
N(3)-Co-S	119.04(6)
N(1)-Co-S	134.57(5)
N(1)#1-Co-S	114.07(5)

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Symmetry transformations used to generate equivalent atoms:

#1  $x, -y+1/2, z$

**Table 4. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for dmj53.**

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Co-N(3)	2.0213(18)
Co-N(1)	2.0265(13)
Co-N(1)#1	2.0265(13)
Co-S	2.2725(10)
Co-S#1	2.2725(10)
S-C(11)	1.782(3)
N(1)-C(1)	1.341(2)
N(1)-N(2)	1.3769(19)
N(2)-C(3)	1.357(2)
N(2)-B	1.543(2)
N(3)-C(6)	1.335(3)
N(3)-N(4)	1.383(3)
N(4)-C(8)	1.350(3)
N(4)-B	1.543(3)
B-N(2)#1	1.543(2)
B-H(1)	1.0000
C(1)-C(2)	1.384(3)
C(1)-C(4)	1.488(3)
C(2)-C(3)	1.369(3)
C(2)-H(2)	0.9500
C(3)-C(5)	1.496(3)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.393(3)
C(6)-C(9)	1.488(4)
C(7)-C(8)	1.374(3)
C(7)-H(7)	0.9500
C(8)-C(10)	1.482(3)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.391(5)
C(11)-C(16)	1.404(4)
C(12)-C(13)	1.392(5)
C(12)-C(17)	1.584(4)
C(13)-C(14)	1.393(7)
C(13)-H(13)	0.9500
C(14)-C(15)	1.381(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.390(5)
C(15)-H(15)	0.9500
C(16)-C(18)	1.500(5)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800

C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
N(3)-Co-N(1)	93.16(5)
N(3)-Co-N(1)#1	93.16(5)
N(1)-Co-N(1)#1	93.39(8)
N(3)-Co-S	119.04(6)
N(1)-Co-S	134.57(5)
N(1)#1-Co-S	114.07(5)
N(3)-Co-S#1	119.04(6)
N(1)-Co-S#1	114.07(5)
N(1)#1-Co-S#1	134.57(5)
S-Co-S#1	23.30(4)
C(11)-S-Co	107.54(11)
C(1)-N(1)-N(2)	107.18(14)
C(1)-N(1)-Co	140.67(13)
N(2)-N(1)-Co	112.12(10)
C(3)-N(2)-N(1)	108.74(15)
C(3)-N(2)-B	130.68(18)
N(1)-N(2)-B	120.56(15)
C(6)-N(3)-N(4)	106.48(18)
C(6)-N(3)-Co	139.73(17)
N(4)-N(3)-Co	113.79(13)
C(8)-N(4)-N(3)	109.94(17)
C(8)-N(4)-B	131.6(2)
N(3)-N(4)-B	118.51(18)
N(4)-B-N(2)#1	109.36(14)
N(4)-B-N(2)	109.36(14)
N(2)#1-B-N(2)	109.3(2)
N(4)-B-H(1)	109.6
N(2)#1-B-H(1)	109.6
N(2)-B-H(1)	109.6
N(1)-C(1)-C(2)	109.36(18)
N(1)-C(1)-C(4)	121.57(16)
C(2)-C(1)-C(4)	129.08(16)
C(3)-C(2)-C(1)	106.70(16)
C(3)-C(2)-H(2)	126.6
C(1)-C(2)-H(2)	126.6
N(2)-C(3)-C(2)	108.02(17)
N(2)-C(3)-C(5)	122.0(2)
C(2)-C(3)-C(5)	129.9(2)
C(1)-C(4)-H(4A)	109.5
C(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5

H(5B)-C(5)-H(5C)	109.5
N(3)-C(6)-C(7)	109.5(2)
N(3)-C(6)-C(9)	121.2(2)
C(7)-C(6)-C(9)	129.3(2)
C(8)-C(7)-C(6)	106.9(2)
C(8)-C(7)-H(7)	126.6
C(6)-C(7)-H(7)	126.6
N(4)-C(8)-C(7)	107.2(2)
N(4)-C(8)-C(10)	123.5(2)
C(7)-C(8)-C(10)	129.3(2)
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(16)	119.8(3)
C(12)-C(11)-S	120.8(3)
C(16)-C(11)-S	119.4(3)
C(11)-C(12)-C(13)	119.5(3)
C(11)-C(12)-C(17)	118.9(3)
C(13)-C(12)-C(17)	121.5(3)
C(12)-C(13)-C(14)	121.5(4)
C(12)-C(13)-H(13)	119.3
C(14)-C(13)-H(13)	119.3
C(15)-C(14)-C(13)	118.0(4)
C(15)-C(14)-H(14)	121.0
C(13)-C(14)-H(14)	121.0
C(14)-C(15)-C(16)	122.2(4)
C(14)-C(15)-H(15)	118.9
C(16)-C(15)-H(15)	118.9
C(15)-C(16)-C(11)	118.9(3)
C(15)-C(16)-C(18)	119.8(3)
C(11)-C(16)-C(18)	121.2(3)
C(12)-C(17)-H(17A)	109.5
C(12)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

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Symmetry transformations used to generate equivalent atoms:

#1  $x, -y+1/2, z$

**Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^4$ ) for dmj53. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$**

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Co	204(2)	146(1)	149(2)	0	5(2)	0
S	234(5)	214(4)	597(6)	69(4)	57(4)	7(3)
N(1)	257(8)	213(7)	177(7)	30(5)	-18(6)	-56(6)
N(2)	275(9)	448(9)	182(7)	92(7)	9(6)	-126(7)
N(3)	224(11)	151(9)	143(10)	0	3(8)	0
N(4)	202(11)	248(10)	188(10)	0	-12(9)	0
B	155(17)	560(20)	234(15)	0	33(11)	0
C(1)	510(12)	217(8)	189(9)	45(7)	-77(9)	-117(8)
C(2)	686(16)	445(12)	273(11)	180(9)	-103(10)	-314(12)
C(3)	425(13)	742(15)	223(9)	123(10)	-27(10)	-340(11)
C(4)	642(15)	209(9)	405(11)	85(9)	-110(11)	47(9)
C(5)	494(16)	1520(30)	551(17)	413(17)	-25(13)	-525(18)
C(6)	297(16)	234(12)	184(12)	0	-10(10)	0
C(7)	345(15)	257(12)	212(12)	0	-87(12)	0
C(8)	270(14)	160(10)	236(12)	0	-67(11)	0
C(9)	421(18)	730(20)	176(13)	0	27(12)	0
C(10)	300(16)	489(16)	372(16)	0	-119(13)	0
C(11)	97(17)	246(16)	344(19)	-14(15)	-26(15)	-3(13)
C(12)	230(20)	420(20)	280(20)	-44(16)	22(15)	-21(17)
C(13)	280(20)	620(30)	290(20)	51(19)	-66(17)	-20(20)
C(14)	170(30)	420(30)	500(30)	110(30)	-90(20)	5(19)
C(15)	240(20)	241(18)	400(20)	-45(15)	-1(16)	13(15)
C(16)	216(19)	197(16)	270(19)	-26(14)	-19(14)	-55(14)
C(17)	600(20)	920(30)	335(18)	0	90(16)	0
C(18)	530(30)	340(20)	320(20)	-41(18)	-10(20)	18(18)

**Table 6. Hydrogen coordinates (  $\times 10^3$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for dmj53.**

	x	y	z	$U_{\text{iso}}$
H(1)	638	250	458	38
H(2)	719	-42	706	56
H(4A)	864	63	559	63
H(4B)	838	-46	554	63
H(4C)	845	10	730	63
H(5A)	605	137	686	128
H(5B)	608	20	700	128
H(5C)	598	71	521	128
H(7)	681	250	-140	33
H(9A)	836	282	-3	66
H(9B)	799	285	-174	66
H(9C)	817	183	-93	66
H(10A)	578	271	18	58
H(10B)	582	295	214	58
H(10C)	581	184	152	58
H(13)	997	80	746	47
H(14)	1031	-34	550	43
H(15)	1015	-7	265	35
H(17A)	894	260	695	93
H(17B)	956	311	684	93
H(17C)	945	228	822	93
H(18A)	975	195	71	60
H(18B)	917	130	77	60
H(18C)	978	80	41	60