Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cyanidophenyltris(trimethylphosphine)cobalt(II)

Fengli Yu,[a,b] Qibao Wang[a] and Xiaoyan Li[a]*

[a]School of Chemistry and Chemical Engineering, Shandong University, Shanda Nanlu 27, Jinan 250100, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Zhengzhou Road 58, Qingdao 266042, People's Republic of China
Correspondence e-mail: xli63@sdu.edu.cn

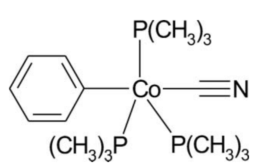
Received 12 November 2007; accepted 30 November 2007

Key indicators: single-crystal X-ray study; T = 373 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.077; data-to-parameter ratio = 20.3.

The title molecule, $[Co(C_6H_5)(CN)(C_3H_9P)_3]$, lies on a crystallographic mirror plane with the Co^{II} ion coordinated in a distorted square-pyramidal environment with one of the P atoms in the apical position. In the basal plane, the phenyl substituent is *trans* to the cyanide group with a C—Co—C angle which is significantly distorted from linearity.

Related literature

For related structures, see: Li *et al.* (2006).



Experimental

Crystal data

$[Co(C_6H_5)(CN)(C_3H_9P)_3]$
M_r = 390.27
Orthorhombic, *Pnma*
a = 12.456 (3) Å
b = 11.420 (2) Å
c = 14.495 (3) Å
V = 2061.9 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 373 (2) K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.742, T_{max} = 0.816
12996 measured reflections
2373 independent reflections
2185 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.077
S = 1.04
2373 reflections
117 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—C2	1.970 (2)	Co1—P2	2.2034 (6)
Co1—C1	2.011 (3)	Co1—P1	2.2745 (7)
C2—Co1—C1	157.00 (9)	C2—Co1—P1	104.05 (6)
C2—Co1—P2	88.168 (17)	C1—Co1—P1	98.96 (6)
C1—Co1—P2	87.783 (16)	P2—Co1—P1	100.188 (13)
P2—Co1—P2^i	159.58 (3)		

Symmetry code: (i) $x, -y+\frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

This work was supported by the NSFC (grant Nos. 20572062 and 20372042).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2572).

References

Bruker (2001). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, X. Y., Sun, H. J., Yu, F. L., Florke, U. & Klein, H.-F. (2006). *Organometallics*, **25**, 4695–4697.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2008). E**64**, m112 [doi:10.1107/S1600536807064781]

Cyanidophenyltris(trimethylphosphine)cobalt(II)

F. Yu, Q. Wang and X. Li

Comment

In the molecular structure of the title compound the Co^{II} ion is in a distorted square-pyramidal coordination environment with atom P1 in the apical position. In the equatorial plane, the phenyl ring substituent and cyano group are *trans* to each other. The distortion from ideal geometry of the angles around Co1 is most likely due to the steric effects of the bulky $P(Me)_3$ groups. The Co1—C2 bond is relatively short, while the Co—C1 bond is relatively long compared to related distances in a complex reported by Li *et al.* (2006).

Experimental

All air-sensitive and volatile materials were handled *in vacuo* or under argon atmosphere using standard Schlenk techniques. A solution of benzonitrile (0.63 g, 1.74 mmol) in 10 ml of pentane was combined with a solution of tetra(trimethylphosphine)cobalt(0) (0.18 g, 1.75 mmol) in 50 ml of pentane at 193 K. The reaction mixture was allowed to warm to ambient temperature and stirred for 16 h to form a red-brown, turbid solution, which was filtered. Red-brown crystals of the title compound were obtained from the filtrate at 251 K.

Refinement

H atoms were included in calculated positions and refined as riding atoms with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

Figures

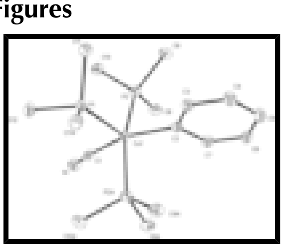


Fig. 1. The molecular structure with atom labels and 30% probability displacement ellipsoids for non-H atoms [symmetry code: (A) $x - y + 1/2, z$].

Cyanidophenyltris(trimethylphosphine)cobalt(II)

Crystal data

$[Co(C_6H_5)(CN)(C_3H_9P)_3]$	F_{000} = 828
M_r = 390.27	D_x = 1.257 Mg m^{-3}
Orthorhombic, *Pnma*	Mo *K*α radiation λ = 0.71073 Å

Hall symbol: -P 2ac 2n	Cell parameters from 11258 reflections
a = 12.456 (3) Å	θ = 2.1–22.5°
b = 11.420 (2) Å	μ = 1.06 mm^{-1}
c = 14.495 (3) Å	T = 373 (2) K
V = 2061.9 (7) Å^3	Block, dark red
Z = 4	0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer	2373 independent reflections
Radiation source: fine-focus sealed tube	2185 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
T = 193(2) K	θ_{max} = 27.1°
ω scans	θ_{min} = 2.2°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 15$
T_{min} = 0.742, T_{max} = 0.816	$k = -14 \rightarrow 14$
12996 measured reflections	$l = -18 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H-atom parameters constrained
$wR(F^2)$ = 0.077	$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.7567P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.019
2373 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
117 parameters	$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. 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 > 2sigma(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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.75567 (2)	0.2500	0.524811 (19)	0.02152 (10)	
P1	0.66451 (4)	0.2500	0.66077 (4)	0.02425 (13)	
P2	0.77302 (3)	0.06011 (3)	0.50237 (3)	0.02474 (11)	
C1	0.9064 (2)	0.2500	0.57450 (15)	0.0281 (4)	
C2	0.64192 (16)	0.2500	0.43042 (14)	0.0243 (4)	
C3	0.53100 (17)	0.2500	0.44650 (15)	0.0272 (4)	
H3	0.5067	0.2500	0.5072	0.033*	
C4	0.45567 (18)	0.2500	0.37551 (17)	0.0328 (5)	
H4	0.3828	0.2500	0.3895	0.039*	
C5	0.4886 (2)	0.2500	0.28431 (17)	0.0358 (5)	
H5	0.4384	0.2500	0.2368	0.043*	
C6	0.5977 (2)	0.2500	0.26512 (16)	0.0341 (5)	
H6	0.6213	0.2500	0.2043	0.041*	
C7	0.67166 (18)	0.2500	0.33676 (15)	0.0290 (4)	
H7	0.7444	0.2500	0.3222	0.035*	
C8	0.87110 (13)	0.03228 (14)	0.41206 (12)	0.0352 (4)	
H8A	0.8863	−0.0500	0.4094	0.053*	
H8B	0.9359	0.0745	0.4253	0.053*	
H8C	0.8428	0.0577	0.3538	0.053*	
C9	0.65951 (13)	−0.02741 (14)	0.46370 (12)	0.0324 (3)	
H9A	0.6314	0.0049	0.4076	0.049*	
H9B	0.6047	−0.0269	0.5102	0.049*	
H9C	0.6826	−0.1064	0.4529	0.049*	
C10	0.82540 (13)	−0.02849 (15)	0.59702 (12)	0.0347 (4)	
H10A	0.8433	−0.1051	0.5745	0.052*	
H10B	0.7719	−0.0350	0.6444	0.052*	
H10C	0.8885	0.0081	0.6218	0.052*	
C11	0.57347 (13)	0.12794 (15)	0.68682 (11)	0.0323 (3)	
H11A	0.6130	0.0558	0.6862	0.048*	
H11B	0.5177	0.1248	0.6412	0.048*	
H11C	0.5421	0.1394	0.7467	0.048*	
C12	0.74842 (18)	0.2500	0.76408 (16)	0.0333 (5)	
H12A	0.7893	0.3212	0.7665	0.050*	0.50
H12B	0.7964	0.1842	0.7622	0.050*	0.50
H12C	0.7037	0.2446	0.8178	0.050*	0.50
N1	0.9851 (2)	0.2500	0.59240 (15)	0.0423 (5)	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01951 (15)	0.02179 (16)	0.02326 (17)	0.000	−0.00048 (10)	0.000
P1	0.0231 (3)	0.0276 (3)	0.0220 (2)	0.000	−0.00096 (19)	0.000
P2	0.0226 (2)	0.0224 (2)	0.0292 (2)	0.00031 (14)	0.00004 (14)	−0.00009 (14)
C1	0.0460 (14)	0.0156 (9)	0.0227 (9)	0.000	0.0052 (9)	0.000

C2	0.0265 (9)	0.0215 (9)	0.0247 (9)	0.000	−0.0022 (8)	0.000
C3	0.0265 (10)	0.0286 (10)	0.0266 (10)	0.000	−0.0016 (8)	0.000
C4	0.0275 (10)	0.0345 (11)	0.0364 (11)	0.000	−0.0065 (9)	0.000
C5	0.0409 (12)	0.0341 (11)	0.0325 (11)	0.000	−0.0139 (10)	0.000
C6	0.0470 (13)	0.0310 (11)	0.0244 (10)	0.000	−0.0019 (9)	0.000
C7	0.0306 (11)	0.0290 (10)	0.0275 (10)	0.000	0.0013 (8)	0.000
C8	0.0325 (8)	0.0308 (8)	0.0421 (9)	0.0023 (7)	0.0067 (7)	−0.0037 (7)
C9	0.0302 (8)	0.0272 (7)	0.0398 (8)	−0.0031 (6)	−0.0006 (6)	−0.0024 (7)
C10	0.0327 (8)	0.0307 (8)	0.0407 (9)	0.0046 (6)	−0.0022 (7)	0.0065 (7)
C11	0.0321 (7)	0.0359 (8)	0.0289 (7)	−0.0044 (7)	0.0023 (6)	0.0010 (6)
C12	0.0315 (11)	0.0434 (13)	0.0251 (11)	0.000	−0.0037 (8)	0.000
N1	0.0585 (15)	0.0298 (10)	0.0386 (11)	0.000	0.0021 (11)	0.000

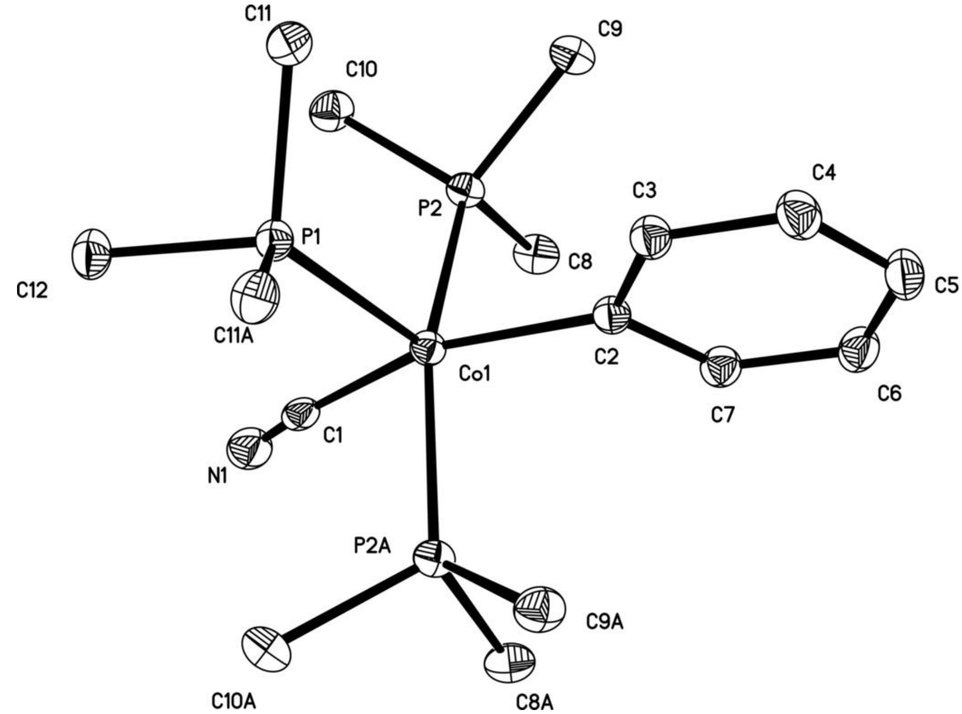
Geometric parameters (Å, °)

Co1—C2	1.970 (2)	C5—H5	0.9300
Co1—C1	2.011 (3)	C6—C7	1.388 (3)
Co1—P2	2.2034 (6)	C6—H6	0.9300
Co1—P2^{i}	2.2034 (6)	C7—H7	0.9300
Co1—P1	2.2745 (7)	C8—H8A	0.9600
P1—C12	1.826 (2)	C8—H8B	0.9600
P1—C11	1.8362 (16)	C8—H8C	0.9600
P1—C11^{i}	1.8362 (16)	C9—H9A	0.9600
P2—C9	1.8200 (16)	C9—H9B	0.9600
P2—C8	1.8186 (16)	C9—H9C	0.9600
P2—C10	1.8252 (16)	C10—H10A	0.9600
C1—N1	1.014 (3)	C10—H10B	0.9600
C2—C3	1.401 (3)	C10—H10C	0.9600
C2—C7	1.407 (3)	C11—H11A	0.9600
C3—C4	1.393 (3)	C11—H11B	0.9600
C3—H3	0.9300	C11—H11C	0.9600
C4—C5	1.384 (4)	C12—H12A	0.9602
C4—H4	0.9300	C12—H12B	0.9602
C5—C6	1.388 (4)	C12—H12C	0.9602
C2—Co1—C1	157.00 (9)	C5—C6—H6	120.0
C2—Co1—P2	88.168 (17)	C7—C6—H6	120.0
C1—Co1—P2	87.783 (16)	C6—C7—C2	123.2 (2)
C2—Co1—P2^{i}	88.168 (17)	C6—C7—H7	118.4
C1—Co1—P2^{i}	87.783 (16)	C2—C7—H7	118.4
P2—Co1—P2^{i}	159.58 (3)	P2—C8—H8A	109.5
C2—Co1—P1	104.05 (6)	P2—C8—H8B	109.5
C1—Co1—P1	98.96 (6)	H8A—C8—H8B	109.5
P2—Co1—P1	100.188 (13)	P2—C8—H8C	109.5
P2^{i}—Co1—P1	100.188 (13)	H8A—C8—H8C	109.5
C12—P1—C11	100.65 (7)	H8B—C8—H8C	109.5
C12—P1—C11^{i}	100.65 (7)	P2—C9—H9A	109.5
C11—P1—C11^{i}	98.78 (11)	P2—C9—H9B	109.5

C12—P1—Co1	115.14 (8)	H9A—C9—H9B	109.5
C11—P1—Co1	119.11 (5)	P2—C9—H9C	109.5
C11^{i}—P1—Co1	119.11 (5)	H9A—C9—H9C	109.5
C9—P2—C8	101.78 (8)	H9B—C9—H9C	109.5
C9—P2—C10	101.81 (8)	P2—C10—H10A	109.5
C8—P2—C10	101.78 (8)	P2—C10—H10B	109.5
C9—P2—Co1	120.65 (6)	H10A—C10—H10B	109.5
C8—P2—Co1	110.13 (6)	P2—C10—H10C	109.5
C10—P2—Co1	118.01 (6)	H10A—C10—H10C	109.5
N1—C1—Co1	173.8 (2)	H10B—C10—H10C	109.5
C3—C2—C7	114.84 (19)	P1—C11—H11A	109.5
C3—C2—Co1	126.43 (16)	P1—C11—H11B	109.5
C7—C2—Co1	118.73 (16)	H11A—C11—H11B	109.5
C4—C3—C2	122.8 (2)	P1—C11—H11C	109.5
C4—C3—H3	118.6	H11A—C11—H11C	109.5
C2—C3—H3	118.6	H11B—C11—H11C	109.5
C5—C4—C3	120.4 (2)	P1—C12—H12A	109.5
C5—C4—H4	119.8	P1—C12—H12B	109.5
C3—C4—H4	119.8	H12A—C12—H12B	109.5
C4—C5—C6	118.8 (2)	P1—C12—H12C	109.5
C4—C5—H5	120.6	H12A—C12—H12C	109.5
C6—C5—H5	120.6	H12B—C12—H12C	109.5
C5—C6—C7	120.0 (2)		

Symmetry codes: (i) x, $-y+1/2$, z.

Fig. 1


C11
C10
C9
P2
C3
C4
P1
C12
C11A
C8
C5
C2
Co1
C6
C7
C1
N1
P2A
C9A
C10A
C8A