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Cyanidophenyltris(trimethylphosphine)cobalt(II)

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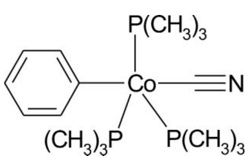
Key indicators: single-crystal X-ray study; *T* = 373 K; mean σ(C–C) = 0.003 Å; *R* factor = 0.029; *wR* factor = 0.077; data-to-parameter ratio = 20.3.

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*α 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*.

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

References

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supporting information

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Cyanidophenyltris(trimethylphosphine)cobalt(II)

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S1. 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).

S2. 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.

S3. 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 $U_{eq}(C)$.

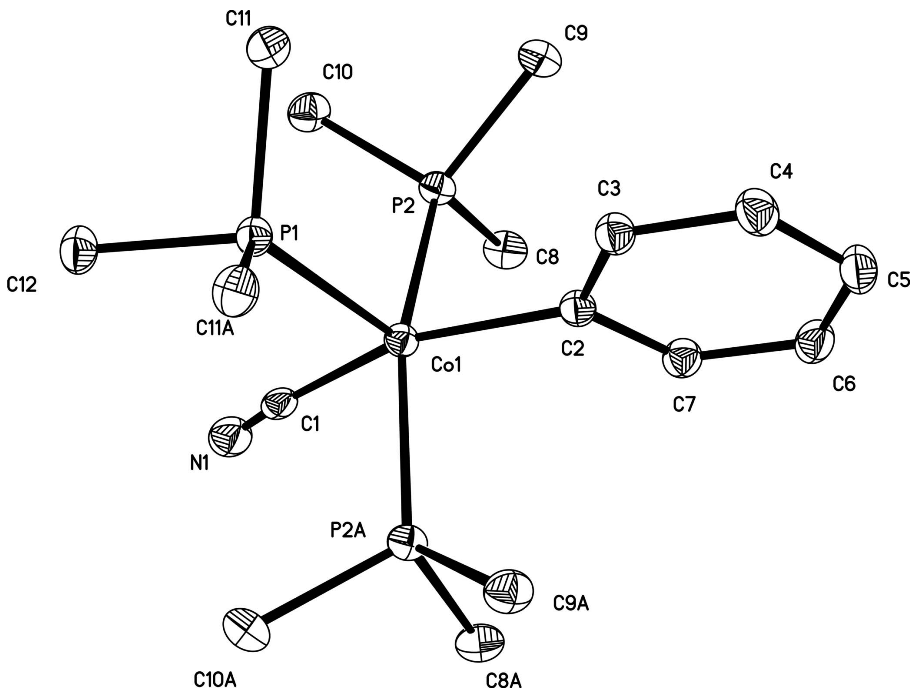

Figure 1

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

$[Co(C_6H_5)(CN)(C_3H_9P)_3]$
M_r = 390.27
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
a = 12.456 (3) Å
b = 11.420 (2) Å
c = 14.495 (3) Å
V = 2061.9 (7) Å^3
Z = 4
F(000) = 828
D_x = 1.257 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 11258 reflections
θ = 2.1–22.5°
μ = 1.06 mm^{-1}
T = 373 K
Block, dark red
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
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
θ_{max} = 27.1°, θ_{min} = 2.2°
h = −15→15
k = −14→14
l = −18→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.077$
$S = 1.04$
2373 reflections
117 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.7567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.019$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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.

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, º)

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 code: (i) *x*, −*y*+1/2, *z*.