Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Cyanidophenyltris(trimethylphosphine)cobalt(II)

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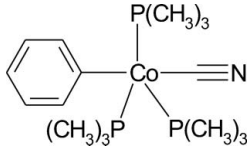
Received 12 November 2007; accepted 30 November 2007

Key indicators: single-crystal X-ray study; $T$ = 373 K; mean $\sigma$(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
$\mu$ = 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.
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# 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

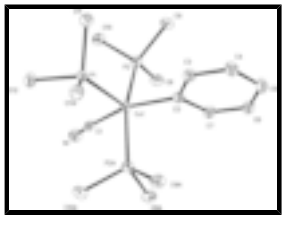


Fig. 1. The molecular structure with atom labels and 30% probability displacement ellipsoids for non-H atoms [symmetry code: (A) $x - y + 1/2, z$].

## 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<br>λ = 0.71073 Å |

| | |
|---|---|
| Hall symbol: -P 2ac 2n | Cell parameters from 11258 reflections |
| $a$ = 12.456 (3) Å | θ = 2.1–22.5º |
| $b$ = 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 | $\theta_{max}$ = 27.1º |
| ω scans | $\theta_{min}$ = 2.2º |
| 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 $F^2 > 2$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 |

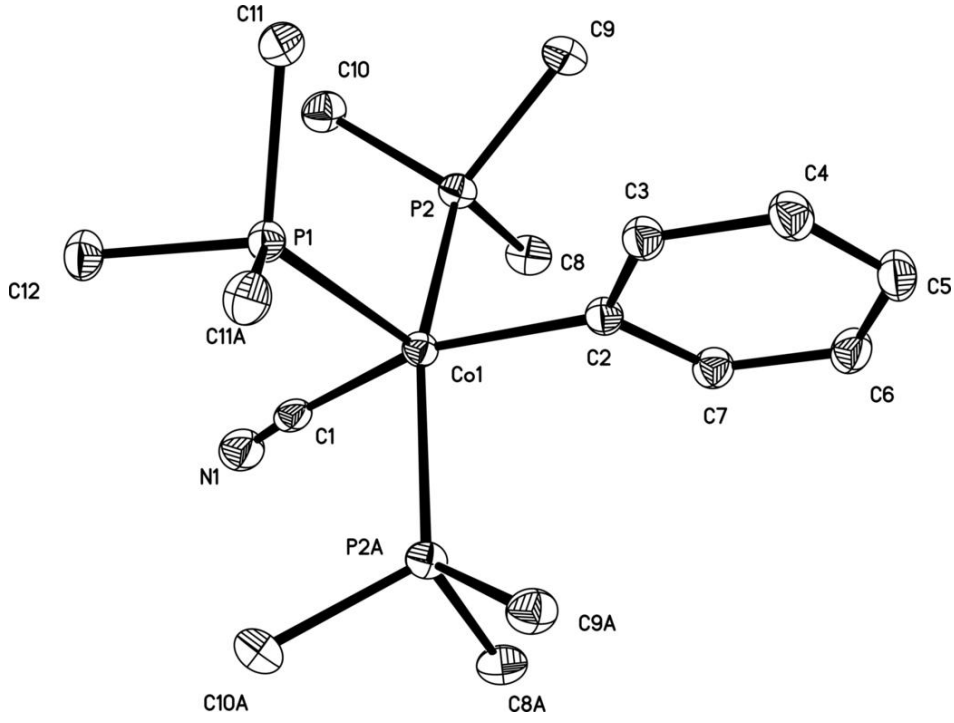
*Geometric parameters (Å, °)*

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