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$Co(dmgH)_2(NO_2)[C_6H_3(CH_3)_2NH_2]$–$Co(dmgH)_2(NO_2)(C_6H_3Cl_2NH_2)$ cocrystal

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The structure of the (3,4-dimethylaniline)bis(dimethylglyoximato)nitrocobalt(III)–(3,4-dichloroaniline)bis(dimethylglyoximato)nitrocobalt(III) (1/1) cocrystal, $[Co(NO_2)(C_4H_7N_2O_2)_2(C_8H_{11}N)]\cdot[Co(NO_2)(C_4H_7N_2O_2)_2(C_6H_5Cl_2N)]$, is reported. The complex crystallizes in space group $P\overline{1}$ with statistical disorder between the chloro and methyl substituents.

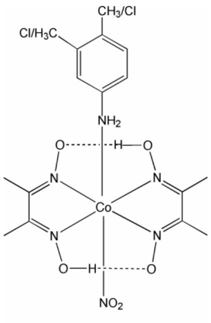
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.062
wR factor = 0.167
Data-to-parameter ratio = 18.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In an attempt to cocrystallize molecular compounds, we tried to exploit charge–transfer interactions between electronically different arene rings in neighbouring molecules. The cocrystal presented here does not show short aryl–aryl contacts, however. In order to develop a reasonable model for the refinement of the chloro *versus* methyl disorder, a database search in the CSD (*X-Blackboard*, Version 2.3.8, April 2002; Allen & Kennard, 1993) was performed. A total of 233 218 entries contained 108 1,2-dimethylaryl fragments with H atoms in the 3- and 6-positions (no disorder, coordinates available, error-free, $R < 0.1$). Carbon–methyl distances in our model were constrained to the resulting mean distance of 1.509 Å. The chloro substituents were allowed to refine freely; the components of the anisotropic displacement parameters for the related Cl and methyl substituents were constrained to be equal. In agreement with tentative refinements of the occupancies, the model is based on an equal distribution of the chloro and methyl substituents. Intermolecular hydrogen bonds (*cf* Table 2) link two neighbouring molecules related by inversion (Fig. 2).



(I)

Experimental

$Co(dmgH)_2(NO_2)(OH_2)$ (Shkurpelo *et al.*, 1979; Englert *et al.*, 1999) was reacted separately with 3,4-dimethylaniline (L1) and 3,4-dichloroaniline (L2) to give complexes $Co(dmgH)_2(NO_2)(L1)$ and $Co(dmgH)_2(NO_2)(L2)$, respectively. The binary crystals formed from an equimolar solution of both complexes in acetone.

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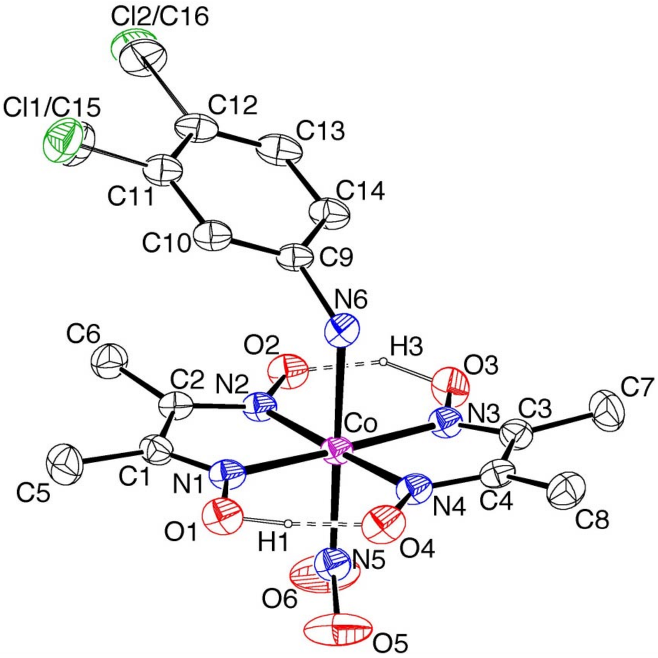

Figure 1
Displacement ellipsoid plot (30% probability) of (I).

Crystal data

$[Co(NO_2)(C_4H_7N_2O_2)_2(C_8H_{11}N)]\cdot[Co(NO_2)(C_4H_7N_2O_2)_2(C_6H_5Cl_2N)]$
$M_r = 953.54$
Triclinic, $P\overline{1}$
$a = 7.0400$ (14) Å
$b = 11.890$ (2) Å
$c = 13.104$ (3) Å
$\alpha = 116.95$ (3)°
$\beta = 91.45$ (3)°
$\gamma = 96.00$ (3)°
$V = 969.1$ (3) Å^3
$Z = 1$
$D_x = 1.634$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10332 reflections
$\theta = 2.3$–28.6°
$\mu = 1.07$ mm^{-1}
$T = 293$ (2) K
Rod, brown
0.60 × 0.12 × 0.03 mm

Data collection

Bruker CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.566$, $T_{max} = 0.969$
10330 measured reflections
4855 independent reflections
3246 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 28.6°$
$h = -9 \rightarrow 9$
$k = -15 \rightarrow 15$
$l = -17 \rightarrow 17$

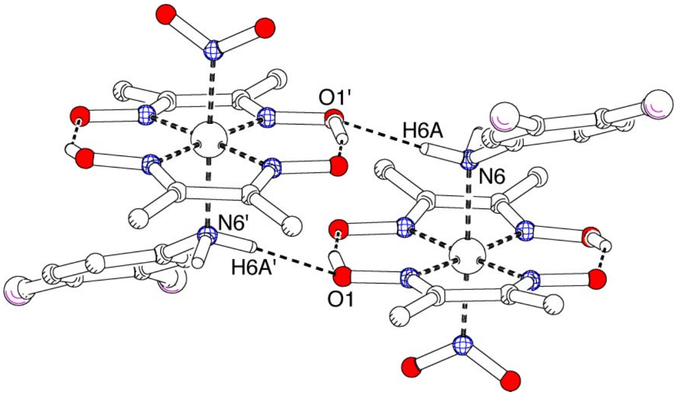

Figure 2
PLATON (Spek, 1990) representation of two neighboring molecules, showing intra- and intermolecular hydrogen bonds.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.167$
$S = 1.01$
4855 reflections
268 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.084P)^2 + 0.4P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.014$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—N2	1.884 (3)	Co—N6	2.044 (3)
Co—N4	1.886 (3)	C11—C15	1.509
Co—N3	1.895 (3)	C11—Cl1	1.717 (6)
Co—N1	1.904 (3)	C12—C16	1.509
Co—N5	1.907 (4)	C12—Cl2	1.737 (5)
N1—Co1—N5	89.35 (15)	N2—Co1—N6	91.63 (14)
N2—Co1—N5	90.16 (15)	N3—Co1—N6	88.00 (14)
N3—Co1—N5	92.64 (15)	N4—Co1—N6	85.88 (14)
N4—Co1—N5	92.32 (15)	N6—Co1—N5	177.98 (13)
N1—Co1—N6	90.01 (14)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O4	1.05	1.45	2.483 (5)	167
O3—H3···O2	1.13	1.45	2.507 (4)	151
N6—H6A···O1^i	0.95	2.17	3.108 (4)	171

Symmetry code: (i) $1-x, -y, -z$.

All H atoms on C atoms were introduced in idealized positions (C—H 0.98 Å) and included as riding, with $U_{iso}(H) = 1.3U_{eq}$(non-H). H atoms in the intramolecular hydrogen bonds were located from difference Fourier syntheses and were treated as riding on the closest O atom, with refined isotropic displacement parameters. Atoms C15 and C16 were treated as riding on C11 and C12, respectively. The methyl groups C5, C6, C7 and C8 were allowed to rotate but not to tip.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART;* data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXL*97.

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