Crystal structure of bis(aniline)dichlorocobalt, $[(C_6H_5NH_2)_2CoCl_2]$

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$C_{12}H_{14}Cl_2CoN_2$, monoclinic, $C12/c1$ (No. 15), $a = 26.142(6)$ Å, $b = 4.801(1)$ Å, $c = 11.607(2)$ Å, $\beta = 108.82(3)^\circ$, $V = 1378.9$ Å³, $Z = 4$, $R(F) = 0.061$, $R_w(F) = 0.136$.

Table 1. Parameters used for the X-ray data collection

Crystal:	red-brown plate, size 0.05 x 0.15 x 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	16.11 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	1205
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	88
Program:	SHELXTL-plus

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
Hn(A)	8f	-0.061(3)	-0.36(2)	0.248(7)	0.05(3)
Hn(B)	8f	-0.048(4)	-0.24(2)	0.376(8)	0.07(3)
H(2A)	8f	-0.1434(4)	-0.233(2)	0.0982(9)	0.13(2)
H(3A)	8f	-0.2246(5)	0.006(3)	0.049(1)	0.13(2)
H(4A)	8f	-0.2394(5)	0.327(3)	0.187(1)	0.13(2)
H(5A)	8f	-0.1715(5)	0.431(3)	0.362(1)	0.13(2)
H(6A)	8f	-0.0898(5)	0.195(2)	0.4125(9)	0.13(2)

Source of material: The compound is prepared by the reaction of disodium 1,3-bis(phenyltriazene)benzene (see ref. 1) with $CoCl_2 \cdot 6H_2O$ in tetrahydrofuran upon addition of ethanol and standing in air several days.

The molecule has the symmetry 2. The aniline and chloride ligands form a near tetrahedral arrangement about the Co center as predicted from powder X-ray data (see ref. 2) and is similar to the structure of the related complex dichloro-di(*p*-toluidine)cobalt (see refs. 3, 4).

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co	4e	0	0.0555(4)	1/4	0.031(1)	0.0336(9)	0.0345(9)	0	0.0123(7)	0
Cl	8f	0.0415(1)	0.3261(5)	0.4108(2)	0.068(2)	0.056(2)	0.047(1)	-0.000(1)	0.016(1)	-0.004(1)
N	8f	-0.0571(3)	-0.184(2)	0.2896(8)	0.051(6)	0.046(5)	0.053(5)	0.003(4)	0.017(4)	-0.002(4)
C(1)	8f	-0.1087(4)	-0.045(2)	0.2610(8)	0.040(6)	0.049(5)	0.064(6)	0.003(5)	0.017(5)	0.010(5)
C(2)	8f	-0.1490(4)	-0.101(2)	0.1516(9)	0.054(7)	0.066(8)	0.061(6)	-0.001(6)	0.002(5)	-0.001(6)
C(3)	8f	-0.1976(5)	0.041(3)	0.123(1)	0.053(8)	0.10(1)	0.090(8)	0.007(8)	0.003(6)	0.014(8)
C(4)	8f	-0.2062(5)	0.238(3)	0.205(1)	0.060(9)	0.09(1)	0.10(1)	0.019(8)	0.039(8)	0.022(9)

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Table 3. (Continued)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(5)	8f	−0.1661(5)	0.296(3)	0.310(1)	0.069(9)	0.069(8)	0.087(8)	0.020(7)	0.037(7)	0.011(7)
C(6)	8f	−0.1170(5)	0.155(2)	0.3400(9)	0.080(8)	0.063(7)	0.053(6)	0.017(6)	0.037(6)	0.013(5)

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