Crystal structure of pyridinium trichloropyridine cobalt(II), $C_5H_6N[CoCl_3(C_5H_5N)]$

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Source of material: The compound was obtained as a byproduct from the reaction of anhydrous cobalt(II)chloride with an isocyanide in the presence of pyridine. The title compound crystallized from acetonitrile as deep blue prisms. All reactions were carried out under an argon atmosphere. The anion $[CoCl_3(C_5H_5N)]^-$ has been described in the literature (see refs. 1-3).

$C_{10}H_{11}Cl_3CoN_2$, monoclinic, $P12_1/n1$ (No. 14), $a = 7.797(4)$ Å, $b = 21.375(4)$ Å, $c = 8.871(3)$ Å, $\beta = 111.44(3)^\circ$, $V = 1376.1$ Å³, $Z = 4$, $R(F) = 0.033$, $R_w(F^2) = 0.085$.

References

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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	0.21299(5)	0.11399(2)	0.33181(5)	0.0394(2)	0.0556(3)	0.0496(2)	0.0008(2)	0.0195(2)	-0.0017(2)
Cl(1)	4e	0.5208(1)	0.10137(4)	0.4148(1)	0.0378(4)	0.0812(5)	0.0698(5)	0.0029(4)	0.0171(4)	-0.0048(4)
Cl(2)	4e	0.0808(1)	0.01923(4)	0.3027(1)	0.0665(6)	0.0649(5)	0.1222(8)	-0.0159(4)	0.0489(6)	-0.0227(5)
Cl(3)	4e	0.1036(1)	0.17471(5)	0.1134(1)	0.0643(6)	0.1036(7)	0.0636(5)	0.0232(5)	0.0312(4)	0.0244(5)
N(1)	4e	0.1572(3)	0.1589(1)	0.5104(3)	0.048(1)	0.052(1)	0.047(1)	0.000(1)	0.021(1)	0.004(1)
N(2)	4e	0.5567(6)	0.0370(2)	0.7804(4)	0.116(3)	0.067(2)	0.067(2)	0.022(2)	0.049(2)	0.001(2)
C(1)	4e	0.2703(5)	0.2039(2)	0.5952(4)	0.067(2)	0.059(2)	0.062(2)	-0.014(2)	0.029(2)	-0.004(2)
C(2)	4e	0.2308(7)	0.2394(2)	0.7059(5)	0.103(3)	0.062(2)	0.066(2)	-0.016(2)	0.036(2)	-0.017(2)
C(3)	4e	0.0701(7)	0.2298(2)	0.7308(5)	0.112(4)	0.066(2)	0.058(2)	0.017(2)	0.045(2)	0.003(2)
C(4)	4e	-0.0468(6)	0.1839(2)	0.6444(5)	0.068(2)	0.085(3)	0.068(2)	0.009(2)	0.041(2)	0.002(2)
C(5)	4e	0.0016(5)	0.1488(2)	0.5373(4)	0.046(2)	0.066(2)	0.053(2)	-0.001(2)	0.020(2)	-0.001(2)
C(6)	4e	0.6825(6)	0.0734(2)	0.8805(6)	0.072(3)	0.082(3)	0.112(3)	0.008(2)	0.055(3)	0.003(3)
C(7)	4e	0.6369(6)	0.1102(2)	0.9814(6)	0.061(3)	0.096(3)	0.097(3)	-0.012(2)	0.018(2)	-0.030(3)
C(8)	4e	0.4616(6)	0.1103(2)	0.9784(5)	0.071(3)	0.086(3)	0.068(2)	0.008(2)	0.032(2)	-0.012(2)
C(9)	4e	0.3349(5)	0.0720(2)	0.8749(5)	0.054(2)	0.073(2)	0.089(3)	0.005(2)	0.028(2)	0.016(2)
C(10)	4e	0.3840(7)	0.0354(2)	0.7742(5)	0.075(3)	0.068(2)	0.069(2)	-0.002(2)	0.003(2)	0.001(2)

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

Crystal:	blue prism, size 0.2 x 0.2 x 0.4 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ :	18.04 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	2409
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	189
Programs:	SHELXS-86, SHELXL-93

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

Atom	Site	x	y	z	U _{iso}
H(11)	4e	0.392(5)	0.207(2)	0.576(4)	0.07(1)
H(21)	4e	0.309(6)	0.269(2)	0.763(5)	0.10(1)
H(31)	4e	0.036(6)	0.252(2)	0.799(5)	0.09(1)
H(41)	4e	-0.159(5)	0.175(2)	0.651(4)	0.07(1)
H(51)	4e	-0.076(4)	0.117(1)	0.472(4)	0.047(8)
H(61)	4e	0.825(9)	0.070(3)	0.884(7)	0.18(2)
H(71)	4e	0.709(7)	0.133(2)	1.039(5)	0.10(2)
H(81)	4e	0.442(6)	0.135(2)	1.052(5)	0.10(1)
H(91)	4e	0.214(6)	0.068(2)	0.870(4)	0.08(1)
H(101)	4e	0.279(7)	0.008(2)	0.697(6)	0.13(2)
H(N2)	4e	0.582(7)	0.014(2)	0.717(5)	0.10(2)