

largest peak on the final difference map was $1.5 \text{ e } \text{\AA}^{-3}$ near Co, while the most negative excursion was $-0.5 \text{ e } \text{\AA}^{-3}$. Extinction corrections were made. Atomic scattering factors from the *SHELXTL* program package. Atomic coordinates are listed in Table 1 and bond distances and angles are given in Table 2. A view of the structure is shown in Fig. 1.*

Related literature. This structure is isomorphous with the room-temperature phase of $[(\text{C}_2\text{H}_5)_2\text{NH}_2]_2\text{ZnCl}_4 \cdot \text{H}_2\text{O}$ (Bloomquist & Willett, 1981). The latter undergoes a phase transition to a $P2_1nm$ phase at 330 K and melts at 362 K. Differential scanning calorimetry (DSC) measurements on the cobalt analog reported here also indicate a phase transition at 330 K, with melting at 360 K (Van Oort, Neshvad & White, 1987).

The $[(\text{C}_2\text{H}_5)_2\text{NH}_2]_2\text{CuCl}_4$ system shows interesting behavior (Willett, Haugen, Lebsach & Morrey, 1974; Harlow & Simonsen, 1977; Bloomquist, Pressprich & Willett, 1988). At room temperature, a superstructure is apparent with a tripling of the length of one unit-cell axis. At 323 K, the structure undergoes a phase transition to a new phase with two crystallographically independent CuCl_4^{2-} anions.

* Tables of data collection parameters, anisotropic thermal parameters, H-atom parameters and structure factors as well as a stereoview of the unit cell have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53727 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

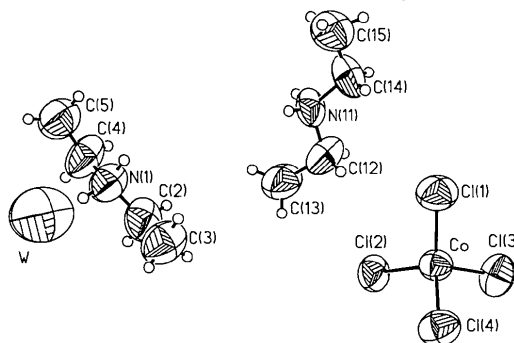


Fig. 1. Illustration of the structure of $[(\text{C}_2\text{H}_5)_2\text{NH}_2]_2\text{CoCl}_4 \cdot \text{H}_2\text{O}$.

Acknowledgement is made to the Boeing Company and to NSF, through grant CHE-8408407, for the establishment of the X-ray diffraction facility.

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Acta Cryst. (1991). **C47**, 1084–1087

1,4-Dimethyl-1,4-diazoniabicyclo[2.2.2]octane Octachlorotricuprate(II)

BY MARCUS R. BOND AND ROGER D. WILLETT

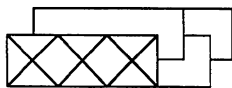
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Abstract. $\text{C}_8\text{H}_{18}\text{N}_2^{2+} \cdot [\text{Cu}_3\text{Cl}_8]^{2-}$, $M_r = 616.5$, monoclinic, $P2_1/n$, $a = 7.335(2)$, $b = 19.499(8)$, $c = 13.532(6)$ Å, $\beta = 100.79(3)^\circ$, $V = 1901(1)$ Å³, $Z = 4$, $D_x = 2.15 \text{ Mg m}^{-3}$, $\lambda(\text{Mo K}\alpha) = 0.71069$ Å, $\mu = 4.45 \text{ mm}^{-1}$, $F(000) = 1212$, $T = 295 \text{ K}$, $R = 0.0569$ for 1436 unique observed [$F \geq 3\sigma(F)$] reflections and 196 parameters. The structure consists of discrete organic cations and stacks of quasiplanar symmetrically bridged $\text{Cu}_3\text{Cl}_8^{2-}$ dimers. A pronounced alternation of Cu—Cl distances occurs within the

trimeric units: 2.243(4) Å for terminal Cu—Cl, 2.369(4) Å for first Cu—Cl bridge and 2.269(4) Å for inner Cu—Cl bridge distances. The primary coordination geometry is nearly planar for the central Cu(2) atom, while a pronounced folding is exhibited for terminal Cu atoms. Formation of semi-coordinate bonds between oligomeric units leads to the formation of stacks of trimers parallel to the a axis and yields a very elongated octahedral coordination sphere for each Cu^{II} ion. When each trimer is

represented by an envelope, the semicoordinate bond formation leads to the generation of a stacking pattern illustrated in (I). The Geiser notation for the stacking is $3\left(\frac{1}{2}, \frac{1}{2}\right)\left(\frac{1}{2}, -\frac{1}{2}\right)$.



(I)

Experimental. The title compound, (DMDABCO)- Cu_3Cl_8 , was prepared in an attempt to synthesize analogs of $[(\text{CH}_3)_4\text{N}][\text{CuCl}_3]$ (Weenk & Spek, 1976) which contains chains of face-shared octahedra with an unusual sequence of ordering of the Jahn–Teller elongated axes and undergoes phase transitions involving dynamic rearrangements of these axes (Willett, Bond, Haije, Soonieus & Maaskant, 1988). The 1,4-dimethyl-1,4-diazoniabicyclo[2.2.2]octane dication was one of the cations chosen, since it can be viewed as a dimer consisting of two $(\text{CH}_3)_4\text{N}^+$ cations.

Red needle-shaped crystals were grown by slow evaporation of a stoichiometric solution of 1,4-dimethyl-1,4-diazoniabicyclo[2.2.2]octane chloride and $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ in concentrated hydrochloric acid. A rod-shaped crystal (maximum dimension 0.2 mm) was coated with a thin layer of an epoxy-type glue and mounted on a thin glass fiber. A Syntex P_2 diffractometer, upgraded to Nicolet P_3F specifications and equipped with a graphite monochromator, was utilized for the diffraction experiments (Campana, Shepard & Litchman, 1981). The lattice constants were determined from 24 accurately centered reflections in the range $26 \leq 2\theta \leq 37^\circ$. Intensity data were collected with ω scans (scan range = 0.9° and scan speeds of $6\text{--}60^\circ \text{min}^{-1}$) with two check reflections (020 and 211) measured every 96 reflections. Empirical absorption corrections, assuming an ellipsoidally shaped crystal, were applied (transmission range: 0.50–0.97). A total of 2806 reflections were measured out to $2\theta = 45^\circ$, with h, k, l ranges of $0 \leq h \leq 7, 0 \leq k \leq 21$ and $-13 \leq l \leq 14$, to yield 2492 unique reflections (merging $R_{\text{int}} = 0.040$). The data reduction, structure solution and refinement on F were carried out with the *SHELXTL* program package (Sheldrick, 1985) on a Data General Eclipse computer system. The Cu and Cl atoms were obtained *via* the direct-method routine *SOLV* and the remaining non-H atoms were located on the subsequent difference map. Anisotropic refinement of non-H atoms. H atoms were constrained to calculated positions ($\text{C—H} = 0.96 \text{ \AA}$) and were assigned isotropic thermal parameters 1.2 times the associated C atoms. The final refinement resulted in $R = 0.0569$ and $wR = 0.0523$ for the 3σ data set

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters ($\text{\AA}^2 \times 10^3$) for (DMDABCO) Cu_3Cl_8

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Cu(1)	1042 (2)	1123 (1)	1610 (1)	43 (1)
Cu(2)	2500 (2)	375 (1)	-376 (1)	44 (1)
Cu(3)	3730 (2)	-398 (1)	-2414 (1)	42 (1)
Cl(1)	-30 (4)	669 (2)	2914 (3)	44 (1)
Cl(2)	1840 (5)	33 (2)	1129 (2)	44 (1)
Cl(3)	3526 (5)	-676 (2)	-731 (3)	45 (1)
Cl(4)	5317 (5)	-1368 (2)	-2599 (3)	46 (1)
Cl(5)	3761 (5)	-43 (2)	-3965 (3)	47 (1)
Cl(6)	3188 (5)	744 (2)	-1852 (2)	46 (1)
Cl(7)	1341 (5)	1410 (2)	-51 (3)	44 (1)
Cl(8)	213 (4)	2212 (2)	1871 (3)	47 (1)
N(1)	-1345 (13)	1448 (5)	5977 (8)	44 (4)
C(2)	-366 (18)	2010 (7)	6626 (10)	49 (6)
C(3)	440 (18)	2529 (7)	5948 (9)	47 (5)
N(4)	687 (14)	2162 (5)	4997 (8)	44 (4)
C(5)	1553 (17)	1475 (7)	5272 (10)	54 (6)
C(6)	151 (17)	1017 (7)	5634 (10)	51 (6)
C(7)	-2516 (16)	1758 (7)	5045 (10)	52 (6)
C(8)	-1265 (16)	2062 (7)	4382 (9)	45 (5)
Cl(1)	-2505 (20)	1023 (7)	6541 (12)	65 (7)
C(4)	1819 (20)	2593 (7)	4428 (10)	60 (7)

with $w = 1/[\sigma^2(F) + gF^2]$ and $g = 0.00015$. $R = 0.121$ and $wR = 0.0635$ for the full data set. The goodness of fit is 1.37 and the largest positive and negative peaks on the final difference electron density map were 0.6 [near Cu(2)] and -0.7 e \AA^{-3} . The parameter shift on the final least-squares cycle, $|\Delta/\sigma|$, was 0.032 (maximum). Atomic scattering factors were those supplied by the *SHELXTL* program package. Atomic coordinates are listed in Table 1 while Table 2 gives pertinent bond distances and angles.* A view of the structure is given in Fig. 1. The stacking is shown in Fig. 2.

Related literature. Quasi-planar $\text{Cu}_2\text{X}_{2n}\text{L}_2$ ($X = \text{Cl, Br; L} = \text{Cl, Br}$ or neutral ligand) species with values of n ranging from 1 to 7 (Bond, 1990; Willett & Rundle, 1964; Halvorson, Grigereit & Willett, 1987; Grigereit, Ramakrishna, Place, Willett, Pellacani, Manfredini, Menabue, Bonamartini-Corradi & Battaglia, 1987; Manfredini, Pellacani, Bonamartini-Corradi, Battaglia, Guarini, Giusti, Pon, Willett & West, 1990) have been reported. Systematic variations of bond distances and angles with the value of n have been analyzed (Willett, 1988). The wide variety of stacking patterns, assembled through the formation of semicoordinate bonds, has been

* Tables of data collection parameters, anisotropic thermal parameters, H-atom parameters and structure factors as well as a stereoview of the unit cell have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53731 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Bond lengths (Å) and angles (°) for (DMDABCO)Cu₃Cl₈

Cu(1)—Cl(1)	2.244 (4)	Cu(3)—Cl(6)	2.409 (4)
Cu(1)—Cl(2)	2.329 (4)	Cu(3)—Cl(1A)	2.723 (3)
Cu(1)—Cl(7)	2.366 (4)	Cu(3)—Cl(2B)	3.450 (4)
Cu(1)—Cl(8)	2.255 (4)	N(1)—C(2)	1.502 (16)
Cu(1)—Cl(4A)	2.795 (3)	N(1)—C(6)	1.521 (17)
Cu(1)—Cl(3B)	3.450 (4)	N(1)—C(7)	1.513 (15)
Cu(2)—Cl(2)	2.280 (4)	N(1)—C(1)	1.496 (19)
Cu(2)—Cl(3)	2.267 (4)	C(2)—C(3)	1.555 (19)
Cu(2)—Cl(6)	2.266 (4)	C(3)—N(4)	1.513 (17)
Cu(2)—Cl(7)	2.264 (4)	N(4)—C(5)	1.500 (16)
Cu(2)—Cl(3A)	3.074 (4)	N(4)—C(8)	1.527 (14)
Cu(2)—Cl(2B)	3.255 (4)	N(4)—C(4)	1.492 (19)
Cu(3)—Cl(3)	2.372 (4)	C(5)—C(6)	1.512 (19)
Cu(3)—Cl(4)	2.259 (4)	C(7)—C(8)	1.518 (19)
Cu(3)—Cl(5)	2.215 (4)		

Cl(1)—Cu(1)—Cl(2)	90.2 (1)	Cl(5)—Cu(3)—Cl(1A)	90.7 (1)
Cl(1)—Cu(1)—Cl(7)	161.6 (1)	Cl(6)—Cu(3)—Cl(1A)	92.4 (1)
Cl(2)—Cu(1)—Cl(7)	83.0 (1)	Cu(1)—Cl(1)—Cu(3A)	111.1 (1)
Cl(1)—Cu(1)—Cl(8)	95.9 (1)	Cu(1)—Cl(2)—Cu(2)	95.1 (1)
Cl(2)—Cu(1)—Cl(8)	172.9 (1)	Cu(2)—Cl(3)—Cu(3)	94.6 (1)
Cl(7)—Cu(1)—Cl(8)	90.1 (1)	Cu(2)—Cl(3)—Cu(2A)	92.6 (1)
Cl(1)—Cu(1)—Cl(4A)	97.8 (1)	Cu(3)—Cl(3)—Cu(2A)	101.5 (1)
Cl(2)—Cu(1)—Cl(4A)	91.3 (1)	Cu(3)—Cl(4)—Cu(1A)	105.7 (1)
Cl(7)—Cu(1)—Cl(4A)	99.4 (1)	Cu(2)—Cl(6)—Cu(3)	93.6 (1)
Cl(8)—Cu(1)—Cl(4A)	91.5 (1)	Cu(1)—Cl(7)—Cu(2)	94.5 (1)
Cl(2)—Cu(2)—Cl(3)	93.4 (1)	C(2)—N(1)—C(6)	106.8 (9)
Cl(2)—Cu(2)—Cl(6)	178.4 (1)	C(2)—N(1)—C(7)	109.2 (9)
Cl(3)—Cu(2)—Cl(6)	87.8 (1)	C(6)—N(1)—C(7)	107.2 (10)
Cl(2)—Cu(2)—Cl(7)	86.4 (1)	C(2)—N(1)—C(1)	111.2 (10)
Cl(3)—Cu(2)—Cl(7)	177.4 (1)	C(6)—N(1)—C(1)	111.2 (10)
Cl(6)—Cu(2)—Cl(7)	92.4 (1)	C(7)—N(1)—C(1)	111.0 (9)
Cl(2)—Cu(2)—Cl(3A)	87.8 (1)	N(1)—C(2)—C(3)	108.8 (10)
Cl(3)—Cu(2)—Cl(3A)	87.4 (1)	C(2)—C(3)—N(4)	108.3 (10)
Cl(6)—Cu(2)—Cl(3A)	91.3 (1)	C(3)—N(4)—C(5)	108.9 (9)
Cl(7)—Cu(2)—Cl(3A)	95.3 (1)	C(3)—N(4)—C(8)	105.9 (9)
Cl(3)—Cu(3)—Cl(4)	92.4 (1)	C(5)—N(4)—C(8)	109.4 (9)
Cl(3)—Cu(3)—Cl(5)	174.2 (1)	C(3)—N(4)—C(4)	109.8 (10)
Cl(4)—Cu(3)—Cl(5)	93.4 (1)	C(5)—N(4)—C(4)	112.4 (10)
Cl(3)—Cu(3)—Cl(6)	82.2 (1)	C(8)—N(4)—C(4)	110.3 (9)
Cl(4)—Cu(3)—Cl(6)	158.0 (1)	N(4)—C(5)—C(6)	109.0 (10)
Cl(5)—Cu(3)—Cl(6)	92.4 (1)	N(1)—C(6)—C(5)	110.3 (10)
Cl(3)—Cu(3)—Cl(1A)	87.4 (1)	N(1)—C(7)—C(8)	109.7 (9)
Cl(4)—Cu(3)—Cl(1A)	108.7 (1)	N(4)—C(8)—C(7)	109.7 (9)

A denotes atom transformed by $1-x$, \bar{y} , \bar{z} ; B denotes atom transformed by \bar{x} , \bar{y} , \bar{z} .

documented (Geiser, Willett, Lindbeck & Emerson, 1986; Bond & Willett, 1989). Recently a phenomenological model has been developed to predict possible stacking patterns (Willett, Bond & Pon, 1990), many of which have not currently been observed.

Previous quasi-planar trimeric species reported include Cu₃Cl₈²⁻ (Bond, Willett, Rubins, Zaspel, Hutton & Drumheller, 1990; Grigereit *et al.*, 1987), [Cu₃Cl₆(CH₃CN)₂] (Willett & Rundle, 1964), [Cu₃Cl₆(H₂O)₂] (Swank & Willett, 1974), [Cu₃Cl₆(dmf)₂] (Nifontova, Laventev, Ponomarev, Filipenko, Krasochka, Atovmyan & Khidekel, 1981) and Cu₃Br₈²⁻ (Grigereit *et al.*, 1987; Fletcher, Hansen, Livermore & Willett, 1983). Because of competing magnetic exchange within and between trimers, the magnetic behavior of these systems is characterized by pseudo-spin frustration behavior (Grigereit & Willett, 1987; Bond *et al.*, 1990).

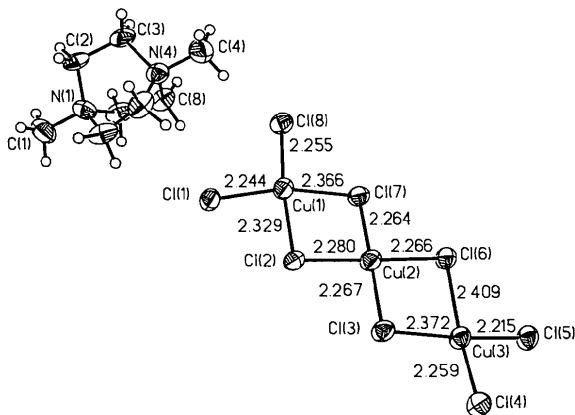


Fig. 1. Illustration of the asymmetric unit in (DMDABCO)-Cu₃Cl₈. Distances are in Å.

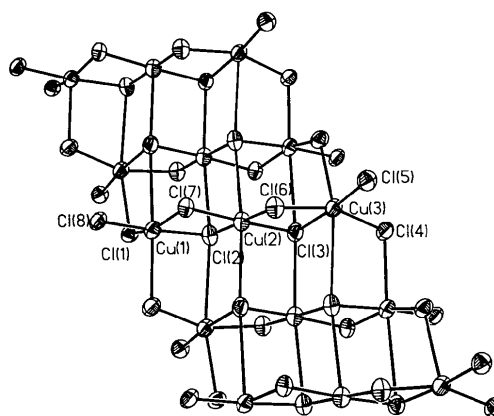


Fig. 2. Thermal ellipsoid plot of (Cu₃Cl₈²⁻)_n stacks in (DMDABCO)Cu₃Cl₈.

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Tetracarbonyl(norbornadiene)chromium(0) at 178 K

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Abstract. $\{(2,3-\eta,5,6-\eta)\text{-Bicyclo}[2.2.1]\text{hepta-}2,5\text{-diene}\}$ tetracarbonylchromium(0), $[\text{Cr}(\text{C}_7\text{H}_8)(\text{CO})_4]$, $M_r = 256.2$, monoclinic, $P2_1/c$, $a = 9.570$ (4), $b = 9.799$ (3), $c = 10.996$ (5) Å, $\beta = 91.08$ (3)°, $V = 1031.1$ (7) Å³, $Z = 4$, $D_x = 1.65$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 1.1$ mm⁻¹, $F(000) = 520$, $T = 178$ K. The structure was refined to $R = 0.029$ for 2073 unique observed reflections. The coordination of the Cr atom is pseudo-octahedral, counting each coordinated double bond as one ligand site. The Cr—C(olefin) bond lengths are 2.283–2.310 (2) Å, with Cr—(C=C midpoint) 2.181, 2.201 Å. The Cr—C(carbonyl) bonds *trans* to the olefin are shorter than those *cis* [1.861, 1.866 *cf.* 1.889, 1.904 (2) Å]. The olefinic H atoms (refined freely) each lie *ca* 0.2 Å out of the respective C=C=C planes.

Experimental. Crystals were obtained from petroleum ether (313–333 K). A yellow tablet 0.6 × 0.6 × 0.16 mm was mounted in inert oil on a glass fibre, which was transferred to the cold gas stream of the diffractometer (Siemens *R3m/V* with LT-2 low-temperature attachment). ω scan. 3611 intensities were measured to $2\theta_{\text{max}} 50^\circ$ with monochromated Mo $K\alpha$ radiation (quadrant $-h + k \pm l$ and some $+h$ equivalents, index ranges $h - 12 \rightarrow 4$, $k 0 \rightarrow 12$, $l - 14 \rightarrow 14$). The orientation matrix was refined from setting angles of 50 reflections in the range $2\theta 20\text{--}23^\circ$. 3 standard reflections monitored every 147 reflections showed no intensity variation. An absorption correction based on ψ scans was applied, with transmissions 0.68–0.95. Averaging equivalent

reflections gave 2368 unique reflections ($R_{\text{int}} 0.020$), of which 2073 with $F > 4\sigma(F)$ were used for all calculations performed with the program system Siemens *SHELXTL Plus* (Sheldrick, 1987).

The structure was solved by direct methods and submitted to full-matrix anisotropic least-squares refinement on F . Olefinic H atoms were refined freely, other H atoms using a riding model. The final $R = 0.029$, with $wR 0.038$. The weighting scheme was $w^{-1} = \sigma^2(F) + 0.0003F^2$. 161 parameters; $S 1.45$; max. $\Delta/\sigma 0.002$, max. and min. $\Delta\rho + 0.29$, -0.55 e Å⁻³, respectively. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Final atomic coordinates are given in Table 1, with derived bond lengths and angles in Table 2.* The molecule of the title compound is shown in Fig. 1.

Related literature. Structural aspects of tetracarbonyl(diene)chromium(0) complexes have been discussed by Pavkovic & Zaluzec (1989).

We thank the Fonds der Chemischen Industrie for financial support. The sample was provided by Mr Thomas Kaukorat.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53701 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.