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A Dehydromolybdenocene Dimer: Di-μ-(σ:η-cyclopentadienyl)-bis(η-cyclopentadienyl)dimolybdenum(*Mo–Mo*)

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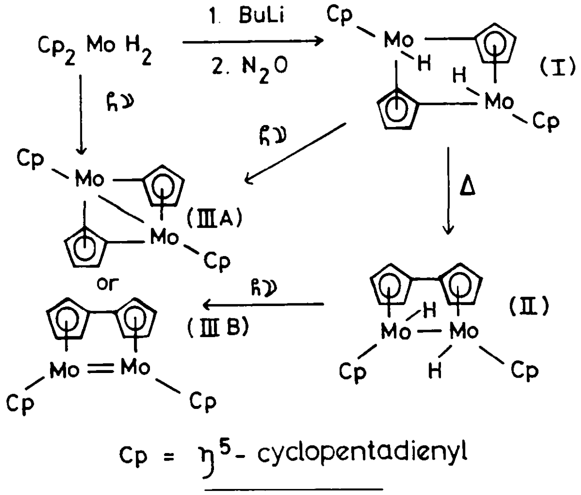
Abstract

$[Mo_2(C_5H_4)_2(C_5H_5)_2]$, $C_{20}H_{18}Mo_2$, $M_r = 450{\cdot}0$, orthorhombic, $a = 19{\cdot}061\,(3)$, $b = 12{\cdot}739\,(5)$, $c = 24{\cdot}850\,(7)$ Å, $U = 6034$ Å^3. Space group *Pbca*, $Z = 16$, $D_c = 1{\cdot}98$ Mg m^{-3}, Mo $K\alpha$ ($\lambda = 0{\cdot}71069$ Å), $\mu = 1{\cdot}59$ mm^{-1}. The asymmetric unit contains two crystallographically independent dimeric molecules $C_{20}H_{18}Mo_2$ with the Mo atoms bridged by two σ:η^5-cyclopentadienyl ligands. The Mo–Mo distance is 2·885 Å (mean value).

Introduction

Two dimeric forms of molybdenocene, (I) and (II), have been isolated (Green & Simpson, 1978; Cooper, Green, Couldwell & Prout, 1977). The photochemical activation by UV light of each of these complexes leads to the same product (III) of formula $C_{20}H_{18}Mo_2$. This is called dehydromolybdenocene and may be prepared directly by irradiation of $(\eta\text{-}C_5H_5)_2MoH_2$ in benzene (Berry, Davies & Green, 1978).



Because (III) can also be prepared by irradiation of (II) (this reaction involves a C—C bond breaking), it is not possible to choose between (III*A*) and (III*B*) from spectroscopic data alone. The structure analysis by X-ray diffraction reveals that (III*A*) is the correct structure.

Experimental

The crystals were supplied by M. L. H. Green and S. Simpson. A small dark-red needle 0·10 × 0·15 × 0·70 mm was sealed under nitrogen in a glass capillary and mounted on a Nonius CAD-4 diffractometer. With Mo $K\alpha$ radiation from a graphite monochromator, the cell dimensions and orientation matrix were obtained by least squares from the setting angles of 25 reflexions. The intensities of reflexions with $\theta < 26°$ were measured by an $\omega/2\theta$ scan, with a variable scan rate and an ω-scan angle of $1{\cdot}00 + 0{\cdot}35\tan\theta$. 2315 reflexions with $I > 3\sigma(I)$ were corrected for Lorentz and polarization effects but not for absorption and used in subsequent calculations. The structure was solved with *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1977) from 205 reflexions with $1{\cdot}50 < E < 2{\cdot}90$. The E map corresponding to the solution with the best figure of merit revealed the positions of the Mo atoms. All the C atoms were located by Fourier synthesis. The structure was refined by least squares

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Table 1. *Fractional coordinates*

	x	*y*	*z*
Mo(1)	0·13152 (5)	0·04176 (7)	0·26730 (3)
Mo(2)	−0·01453 (4)	0·04581 (7)	0·23821 (4)
C(1)	0·0640 (6)	0·1729 (8)	0·2467 (5)
C(2)	0·0976 (6)	0·2032 (8)	0·2976 (5)
C(3)	0·1707 (7)	0·2098 (9)	0·2893 (5)
C(4)	0·1830 (6)	0·1932 (9)	0·2334 (5)
C(5)	0·1199 (6)	0·1710 (9)	0·2075 (4)
C(6)	0·1606 (7)	−0·130 (1)	0·2961 (6)
C(7)	0·2174 (6)	−0·062 (1)	0·3037 (5)
C(8)	0·2371 (6)	−0·029 (1)	0·2503 (5)
C(9)	0·1923 (7)	−0·071 (1)	0·2139 (6)
C(10)	0·1448 (7)	−0·1344 (9)	0·2418 (6)
C(11)	0·0353 (6)	0·0059 (8)	0·3136 (4)
C(12)	−0·0031 (6)	−0·0857 (9)	0·2953 (5)
C(13)	−0·0762 (6)	−0·062 (1)	0·2961 (5)
C(14)	−0·0850 (6)	0·041 (1)	0·3156 (5)
C(15)	−0·0186 (6)	0·0810 (9)	0·3276 (4)
C(16)	−0·0266 (8)	0·122 (1)	0·1521 (5)
C(17)	−0·0945 (8)	0·096 (1)	0·1725 (6)
C(18)	−0·0951 (6)	−0·015 (1)	0·1777 (5)
C(19)	−0·0285 (7)	−0·0551 (9)	0·1630 (4)
C(20)	0·0119 (6)	0·0317 (9)	0·1466 (5)
Mo(3)	0·22910 (5)	0·24657 (6)	0·00848 (4)
Mo(4)	0·37775 (5)	0·22495 (6)	−0·01253 (4)
C(21)	0·2862 (5)	0·2249 (9)	−0·0662 (4)
C(22)	0·2416 (6)	0·3121 (8)	−0·0759 (4)
C(23)	0·1700 (6)	0·283 (1)	−0·0720 (4)
C(24)	0·1677 (6)	0·174 (1)	−0·0623 (5)
C(25)	0·2383 (6)	0·1367 (8)	−0·0602 (4)
C(26)	0·1485 (7)	0·294 (1)	0·0733 (5)
C(27)	0·2140 (6)	0·290 (1)	0·0987 (4)
C(28)	0·2401 (7)	0·187 (1)	0·0966 (5)
C(29)	0·1900 (7)	0·124 (1)	0·0682 (5)
C(30)	0·1325 (6)	0·191 (1)	0·0551 (5)
C(31)	0·3185 (6)	0·3552 (7)	0·0175 (4)
C(32)	0·3590 (6)	0·4010 (7)	−0·0252 (5)
C(33)	0·4319 (6)	0·3908 (9)	−0·0125 (6)
C(34)	0·4373 (6)	0·345 (1)	0·0400 (5)
C(35)	0·3682 (6)	0·3273 (9)	0·0598 (4)
C(36)	0·3755 (6)	0·0420 (7)	−0·0055 (4)
C(37)	0·4268 (7)	0·0832 (9)	0·0309 (5)
C(38)	0·4770 (6)	0·1318 (8)	−0·0021 (5)
C(39)	0·4595 (6)	0·1230 (9)	−0·0575 (5)
C(40)	0·3944 (6)	0·0649 (8)	−0·0584 (4)
H(102)	0·0731	0·2170	0·3325
H(103)	0·2073	0·2240	0·3172
H(104)	0·2300	0·1965	0·2155
H(105)	0·1143	0·1564	0·1682
H(106)	0·1353	−0·1687	0·3250
H(107)	0·2396	−0·0417	0·3386
H(108)	0·2778	0·0178	0·2416
H(109)	0·1930	−0·0584	0·1741
H(110)	0·1060	−0·1759	0·2252
H(112)	0·0177	0·1539	0·2837
H(113)	−0·1154	−0·1098	0·2850
H(114)	−0·1305	0·0782	0·3201
H(115)	−0·0098	0·1519	0·3436
H(116)	−0·0097	0·1947	0·1433
H(117)	−0·1336	0·1455	0·1811
H(118)	−0·1357	−0·0580	0·1900
H(119)	−0·0131	−0·1303	0·1639
H(120)	0·0613	0·0280	0·1329
H(122)	0·2583	0·3846	−0·0847
H(123)	0·1289	0·3313	−0·0753
H(124)	0·1241	0·1302	−0·0577
H(125)	0·2522	0·0618	−0·0552
H(126)	0·1179	0·3571	0·0689
H(127)	0·2383	0·3508	0·1157
H(128)	0·2854	0·1617	0·1120
H(129)	0·1941	0·0482	0·0591
H(130)	0·0881	0·1700	0·0361
H(132)	0·3391	0·4343	−0·0584
H(133)	0·4719	0·4119	−0·0362
H(134)	0·4819	0·3283	0·0594
H(135)	0·3561	0·3001	0·0964
H(136)	0·3325	0·0027	0·0052
H(137)	0·4270	0·0779	0·0710
H(138)	0·5197	0·1684	0·0119
H(139)	0·4864	0·1513	−0·0889
H(140)	0·3677	0·0444	−0·0914

with a large-block approximation. H atoms were positioned geometrically and included in the calculation, their location being adjusted after each cycle. Each reflexion was assigned a weight $w = 1/\sum_{r=1}^{n} A_r T_r(X)$ where n is the number of coefficients, A_r, for a Chebyshev series, T_r is the polynomial function and X is $|F_o|/|F_o(\mathrm{max})|$. Three coefficients, A_r, were used with values 185·5, 256·6 and 78·2 (Rollett, 1965). The refinement converged at $R = 0{\cdot}038$ ($R_w = 0{\cdot}045$). Calculations were performed with the Oxford University ICL 1906A and the London University CDC 7600 computers with the Oxford *CRYSTALS* package (Carruthers, 1975). The final positional parameters are given in Table 1.[*] Table 2 lists some interatomic distances and interbond angles with their e.s.d.'s calculated from the variance–covariance matrix.

Discussion

The crystal structure consists of two crystallographically independent but chemically identical dimeric units $C_{20}H_{18}Mo_2$ in general positions in the cell. One dimer is shown in Fig. 1. The dimer closely resembles the niobiocene dimer (Guggenberger, 1973). The Mo atoms are bridged by two $\sigma:\eta^5$-C_5H_4 groups. The ^{1}H NMR spectrum indicates that the dimer is diamagnetic so that the 2·885 Å Mo—Mo contact is considered to be a direct bonding interaction. The coordination is completed by an η^5-C_5H_5 group to give each Mo atom an 18e configuration.

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[*] Lists of structure factors and anisotropic thermal parameters for the non-hydrogen atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34556 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Selected interatomic distances* (Å) *and bond angles* (°)

Mo(1)–Mo(2)	2·877 (1)		
Mo(1)–C(11)	2·213 (10)	Mo(2)–C(1)	2·214 (11)
Mo(1)–C(1)	2·170 (10)	Mo(2)–C(11)	2·161 (10)
Mo(1)–C(2)	2·284 (10)	Mo(2)–C(12)	2·206 (12)
Mo(1)–C(3)	2·333 (11)	Mo(2)–C(13)	2·310 (12)
Mo(1)–C(4)	2·322 (11)	Mo(2)–C(14)	2·347 (12)
Mo(1)–C(5)	2·229 (11)	Mo(2)–C(15)	2·267 (11)
Mo(1)–C(6)	2·368 (12)	Mo(2)–C(16)	2·363 (12)
Mo(1)–C(7)	2·290 (11)	Mo(2)–C(17)	2·323 (13)
Mo(1)–C(8)	2·244 (11)	Mo(2)–C(18)	2·284 (11)
Mo(1)–C(9)	2·272 (12)	Mo(2)–C(19)	2·284 (10)
Mo(1)–C(10)	2·346 (11)	Mo(2)–C(20)	2·339 (12)
C(11)–Mo(1)–Mo(2)	48·1 (3)	C(1)–Mo(2)–Mo(1)	48·3 (3)
Mo(3)–Mo(4)	2·894 (1)		
Mo(3)–C(31)	2·207 (10)	Mo(4)–C(21)	2·196 (10)
Mo(3)–C(21)	2·168 (10)	Mo(4)–C(31)	2·141 (9)
Mo(3)–C(22)	2·269 (11)	Mo(4)–C(32)	2·293 (10)
Mo(3)–C(23)	2·342 (11)	Mo(4)–C(33)	2·352 (11)
Mo(3)–C(24)	2·309 (11)	Mo(4)–C(34)	2·309 (11)
Mo(3)–C(25)	2·214 (10)	Mo(4)–C(35)	2·228 (11)
Mo(3)–C(26)	2·304 (12)	Mo(4)–C(36)	2·338 (9)
Mo(3)–C(27)	2·327 (11)	Mo(4)–C(37)	2·302 (11)
Mo(3)–C(28)	2·327 (11)	Mo(4) C(38)	2·248 (10)
Mo(3)–C(29)	2·276 (11)	Mo(4)–C(39)	2·315 (11)
Mo(3)–C(30)	2·287 (11)	Mo(4)–C(40)	2·358 (10)
C(31)–Mo(3)–Mo(4)	47·3 (2)	C(21)–Mo(4)–Mo(3)	48·1 (4)

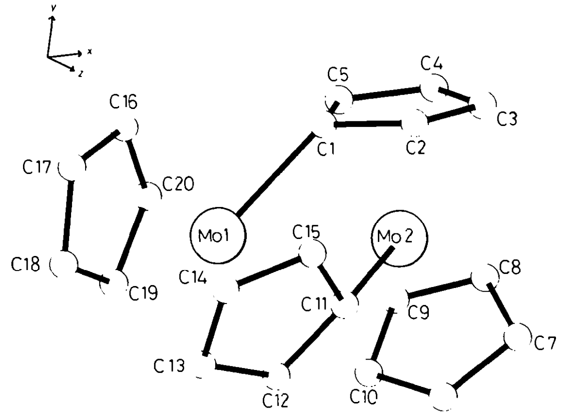

Fig. 1. A generalized projection of one of the two dehydromolybdenocene molecules in the unit cell.

Although each half of the dimer can be considered to be analogous to a $(\eta^5\text{-}C_5H_5)_2MoX_2$ system, the Mo stereochemistry is significantly different from that commonly found (Prout, Cameron, Forder, Critchley, Denton & Rees, 1974). In the monomeric $(\eta^5\text{-}C_5H_5)_2$-MoX_2 complexes the ligands X lie near to a plane *Xp* perpendicular to the plane *Np* containing the normals to the cyclopentadienyl rings at the Mo atoms (Fig. 2) and the line of intersection of *Xp* and *Np* bisects the X–Mo–X angle. In contrast, in dehydromolybdenocene the Mo–C σ-bond lies close to the line of intersection of *Xp* and *Np* and the Mo–Mo bond makes an angle of 50·8° (mean) to this line of intersection and is 1·204 Å (mean) out of the *Xp* plane. This arrangement of the metal–metal bond and the metal–carbon bond closely resembles that in Guggenberger's (1973) niobiocene and it is reasonable to assume that the distribution of non-bonding electron pairs in dehydromolybdenocene parallels the disposition of the Nb–H bonds in niobiocene. Therefore, it is concluded that three possible dispositions of the non-bonding electrons in 18 electron $(\eta^5\text{-}C_5H_5)_2MX_2$ must be considered, the Ballhausen & Dahl (1961) location, *i.e.* within the X–M–X angle, the Alcock (1967) location, outside the X–M–X angle, and the new asymmetric arrangement in the dehydromolybdenocene (Fig. 3). This latter is in no way inconsistent with the Green, Green & Prout (1972) interpretation of the electronic structures of bent metallocenes or with its extension by Lauher & Hoffman (1976).

Further details of the dehydromolybdenocene coordination are described by the parameters defined in Fig. 2 and listed in Table 3. The φ angle, 145·0–145·8° is larger than is usual in bent metallocenes other than hydrides, and the metal–ring distances are significantly shorter for the $\sigma:\eta^5$ rings (1·90 Å mean) than for the η^5 rings (1·97 Å mean). The stereochemistry is not quite the same around each of the Mo atoms in the dimer. In particular Mo–Mo′ and Mo–C are on opposite sides of the *Np* plane for Mo(1) and Mo(4) but on the same side for Mo(2) and Mo(3). Nevertheless, dehydromolybdenocene like niobiocene has a near exact non-crystallographic twofold axis and the ^{1}H NMR spectrum (Green & Simpson, 1978) shows that the minor deviations from twofold symmetry disappear in solution. The deviations are therefore attributed to crystal-packing effects.

The twofold symmetry confirms an essentially *trans* character for the dehydromolybdenocene and niobiocene complexes with the non-bonding electron pairs

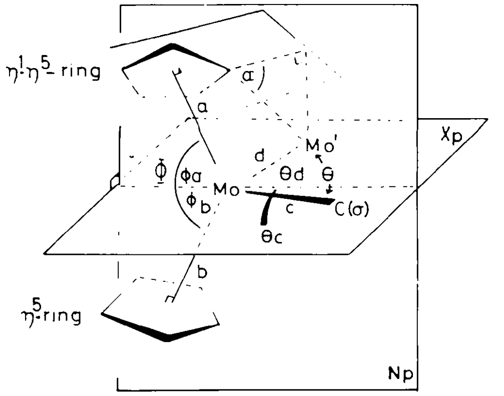

Fig. 2. The definition of the molecular parameters used in the text and in Table 3.

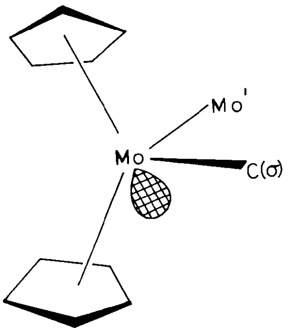

Fig. 3. A sketch of the environment of one molybdenum atom with the possible location of the non-bonding electrons shown by cross hatching.

Table 3. *Structural parameters referring to Fig.* 2.

All e.s.d.'s for distances are in the range 10–20 × 10^{-3} Å, except for the *d* values (1 × 10^{-3} Å). The e.s.d.'s for angles are in the range 0·3–0·6°.

	Mo(1)	Mo(2)	Mo(3)	Mo(4)
a	1·908Å	1·897Å	1·900Å	1·899Å
b	1·971	1·983	1·964	1·970
c	2·170	2·214	2·207	2·196
d	2·877	2·877	2·894	2·894
α	38·2°	38·5°	37·6°	37·7°
Φ	145·0	145·2	145·2	145·8
φ_a	74·3	75·2	74·5	75·8
φ_b	70·7	70·0	70·7	70·0
θ*	48·1	48·3	47·3	48·1
θ_c	7·7	6·8†	6·5†	6·3
θ_d	49·0	53·0†	51·3†	49·9

* $\theta \neq \theta_c + \theta_d$. θ_c and θ_d are not coplanar.
† The ligands C and Mo′ are on the same side of the plane *Np*.

Table 4. *Distances* (Å) *in the cyclopentadienyl rings*

$\sigma:\eta^5$ rings		η^5 rings	
C(1)–C(2)	1·470 (16)	C(6)–C(7)	1·397 (18)
C(2)–C(3)	1·411 (17)	C(7)–C(8)	1·443 (17)
C(3)–C(4)	1·423 (17)	C(8)–C(9)	1·354 (19)
C(4)–C(5)	1·395 (16)	C(9)–C(10)	1·399 (20)
C(5)–C(1)	1·445 (15)	C(10)–C(6)	1·382 (20)
C(11)–C(12)	1·451 (15)	C(16)–C(17)	1·431 (20)
C(13)–C(13)	1·426 (16)	C(17)–C(18)	1·419 (17)
C(13)–C(14)	1·409 (17)	C(18)–C(19)	1·418 (17)
C(14)–C(15)	1·397 (15)	C(19)–C(20)	1·407 (15)
C(15)–C(11)	1·448 (15)	C(20)–C(16)	1·371 (17)
C(21)–C(22)	1·420 (15)	C(26)–C(27)	1·401 (18)
C(22)–C(23)	1·417 (17)	C(27)–C(28)	1·403 (17)
C(23)–C(24)	1·410 (17)	C(28)–C(29)	1·433 (18)
C(24)–C(25)	1·426 (16)	C(29)–C(30)	1·427 (18)
C(25)–C(21)	1·456 (15)	C(30)–C(26)	1·421 (17)
C(31)–C(32)	1·435 (15)	C(36)–C(37)	1·431 (16)
C(32)–C(33)	1·432 (15)	C(37)–C(38)	1·404 (17)
C(33)–C(34)	1·433 (18)	C(38)–C(39)	1·419 (17)
C(34)–C(35)	1·424 (16)	C(39)–C(40)	1·445 (16)
C(35)–C(31)	1·460 (15)	C(40)–C(36)	1·393 (14)

(C–C) mean in η^5 rings = 1·409
(C–C) mean in $\sigma:\eta^5$ rings = 1·429

or H atoms on opposite sides of the Mo–Mo vector. Dehydromolybdenocene is related to the known tungstenocenes (Couldwell & Prout, 1979) by a shortening of the *M*–*M*′ contact together with a twist about the *M*–*M*′ vector. However, the *M*–C lengths and the angles φ are virtually unchanged and the metal atoms remain almost directly over the centroids of the η^5 rings. The shortening of the *M*–*M*′ contact is accommodated by changes in the directions of *M*–*M*′ and *M*–C(σ) with respect to the *Np* and *Xp* planes and by bending *M*–C(σ) out of the plane of the $\sigma:\eta^5$ ring by some 40°, which appears to be a feature common to all $\sigma:\eta^5$ bridging cyclopentadienyl groups in compounds that have a direct metal–metal bond {*e.g.* niobiocene, Nb–Nb 3·105 Å, Nb–C(σ) 31·6° out of plane (Guggenberger, 1973); $(C_5H_5)(CO)Mo(C_5H_4)$-$Mn(CO)_4$, Mo–Mn 2·96 Å, Mn–C(σ) 40° out of plane (Hoxmeier, Deubzer & Kaesz, 1971); $[(C_5H_5)$-$Ti(C_5H_4)Al(C_2H_5)_2]_2$, Ti–Ti 3·110 Å, Ti–C($\sigma$) 35° out of plane (Corradini & Sirigu, 1967), but contrast tungstenocene, W–W 3·811 Å, W–C(σ) coplanar with ring (Couldwell & Prout, 1979) and dehydrothoriocene, Th–Th 4·305 Å, Th–C(σ) coplanar with ring (Baker, Raymond, Marks & Wachter, 1974)}. No particular pattern of bond distances has been found for the $\sigma:\eta^5$ rings as in the niobiocene dimer (for a discussion on the C–C bond distances, see Guggenberger, 1973). The only rational difference between the two types of ring is the C–C mean bond distance (1·409 Å for the η^5 rings and 1·429 Å for the $\sigma:\eta^5$ rings) (Table 4). The $\sigma:\eta^5$ rings are σ-bonded to the Mo atoms (Mo–C 2·207 Å mean). These bonds are out of the $\sigma:\eta^5$ ring plane. The mean value for the angle α (Fig. 2) is 38·0°.

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Crystal and Molecular Structure of Bis(1,8-naphthyridine)copper(II) Chloride

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Abstract

The structure of $[Cu(C_8H_6N_2)_2]Cl_2, C_{16}H_{12}CuN_4^{2+}.2Cl^-$, has been determined and refined by least squares. The space group is $C2/c$ and the unit-cell parameters are a = 13·786 (1), b = 8·192 (1), c = 16·396 (1) Å, and β = 122·5 (1)°. The number of formula units in the unit cell is four and the density is 1·68 Mg m^{-3}. The structure is composed of isolated molecules, with approximately square-planar coordination about the Cu ion, and with *cis* geometry of the ligands. The 1,8-naphthyridine molecule is monodentate.

The ligand 1,8-naphthyridine (hereafter NN) has attracted wide attention in the last ten years as an example of a strong base ligand with a very small 'bite'. It has been found coordinated in a variety of configurations and the chemistry is complex. In many complexes with first-row transition metals, four NN molecules coordinate bidentately but very unsymmetrically to a central metal ion to give trigonal dodecahedral geometry (Clearfield, Singh & Bernal, 1970; Singh, Clearfield & Bernal, 1971); similar coordination but different geometries have been found for some mercury complexes (Dewan, Kepert & White, 1975; Epstein, Dewan, Kepert & White, 1974). Sacconi and co-workers have reported two complexes in which the NN ligand coordinates in a *syn-syn* bidentate manner to two metal atoms (Gatteschi, Mealli & Sacconi, 1977; Sacconi, Mealli & Gatteschi, 1974), and Dixon and co-workers have described structures in which the NN is primarily coordinated through only one of its two N atoms (Dixon, 1977; Bushnell, Dixon & Khan, 1978). The title compound of this paper is another member of this last class.

Experimental

1,8-Naphthyridine was prepared by the method of Paudler & Kress (1967). Starting materials were practical grade and were used without further purification. The crude product was purified by vacuum sublimation. Bis(1,8-naphthyridine)copper(II) chloride was prepared by mixing solutions of stoichiometric quantities of $CuCl_2$ and NN in water, and allowing excess solvent to evaporate. The product separated as green prismatic crystals on slow evaporation. Analyses: calc. Cu 16·10, C 48·68, H 3·06, Cl 17·96%; found: Cu 15·90, C 48·69, H 2·77, Cl 18·13%.

Crystal data

$C_{16}H_{12}Cl_2CuN_4$, FW 394·74, monoclinic, a = 13·786 (1), b = 8·192 (1), c = 16·396 (1) Å, β = 122·5 (1)°, V = 1561·71 Å^3, Z = 4, $F(000)$ = 796, D_c = 1·68, D_m = 1·68 Mg m^{-3}; λ(Mo $K\alpha$) = 0·7107 Å, μ = 1·73 mm^{-1}.

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