Table 2. *Bond lengths* (Å), *selected bond angles* (°) *and torsion angles* (°)

Mo—Mo′	3·2239 (11)	Mo—*Y*	2·234 (19)
Mo—C(0)	1·943 (21)	C(0)—O(0)	1·12 (3)
Mo—C(1)	1·955 (16)	C(1)—O(1)	1·135 (22)
Mo—C(2)	1·971 (14)	C(2)—O(2)	1·163 (19)
Mo—C(3)	2·345 (22)	C(3)—C(4)	1·35 (3)
Mo—C(4)	2·271 (21)	C(3)—C(7)	1·45 (3)
Mo—C(5)	2·316 (21)	C(4)—C(5)	1·44 (3)
Mo—C(6)	2·382 (19)	C(5)—C(6)	1·44 (3)
Mo—C(7)	2·395 (21)	C(6)—C(7)	1·37 (3)
Mo—*X*	2·011 (19)		

Mo′—Mo—C(0)	131·6 (6)	C(1)—Mo—*X*	128·6 (7)
Mo′—Mo—C(1)	73·1 (5)	C(1)—Mo—*Y*	153·4 (7)
Mo′—Mo—C(2)	70·8 (4)	C(2)—Mo—C(3)	163·6 (7)
Mo′—Mo—C(3)	105·5 (5)	C(2)—Mo—*X*	135·6 (7)
Mo′—Mo—*X*	115·3 (5)	C(2)—Mo—*Y*	110·6 (6)
Mo′—Mo—*Y*	118·4 (5)	C(3)—Mo—*Y*	56·3 (7)
C(0)—Mo—C(1)	78·5 (8)	Mo—C(0)—O(0)	177·5 (19)
C(0)—Mo—C(2)	74·1 (8)	Mo—C(1)—O(1)	171·7 (15)
C(0)—Mo—C(3)	116·9 (8)	Mo—C(2)—O(2)	173·1 (13)
C(0)—Mo—*X*	113·1 (8)		
C(0)—Mo—*Y*	104·5 (8)		
C(1)—Mo—C(2)	95·7 (6)		
C(1)—Mo—C(3)	98·4 (7)		

C(0)—Mo—Mo′—C(0′)	73·9 (12)	C(1)—Mo—Mo′—*Y*′	166·5 (7)
C(0)—Mo—Mo′—C(1′)	17·2 (10)	C(2)—Mo—Mo′—C(2′)	165·5 (6)
C(0)—Mo—Mo′—C(2′)	119·7 (10)	C(2)—Mo—Mo′—C(3′)	−31·3 (7)
C(0)—Mo—Mo′—C(3′)	−77·0 (10)	C(2)—Mo—Mo′—*X*′	−62·3 (7)
C(0)—Mo—Mo′—*X*′	−108·1 (10)	C(2)—Mo—Mo′—*Y*′	−91·0 (7)
C(0)—Mo—Mo′—*Y*′	−136·8 (10)	C(3)—Mo—Mo′—C(3′)	132·0 (8)
C(1)—Mo—Mo′—C(1′)	−39·6 (7)	C(3)—Mo—Mo′—*Y*′	72·3 (8)
C(1)—Mo—Mo′—C(2′)	62·9 (7)	*X*—Mo—Mo′—*X*′	69·9 (8)
C(1)—Mo—Mo′—C(3′)	−133·8 (8)	*Y*—Mo—Mo′—*Y*′	12·6 (8)
C(1)—Mo—Mo′—*X*′	−164·8 (8)		

The reaction of (3) with (4) could result in the attack of the nitrogen at a carbonyl to form $SiMe_3Cl$ and a reactive (16-electron) intermediate which will dimerize to (5) or (6). These are two stereoisomers, in which the entering nitrogen is *trans* or *cis* respectively to the other carbamoyl ligand, the *cis*-form being statistically twice as likely. Subsequent cleavage of the carbamoyl groups with the formation of a Mo—Mo bond would give (1) or (2) and organonitrogen material (not identified). Restricted rotation about the Mo—Mo bond, as noted above, will prevent conversion of (2) to (1).

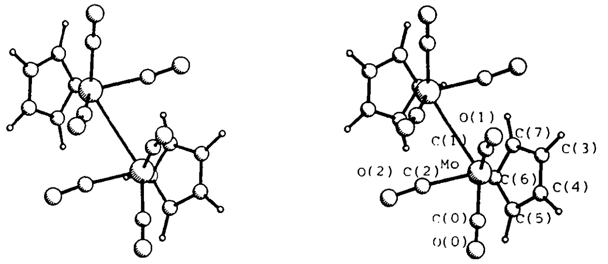

Fig. 1. View of (2) along the molecular twofold axis.

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Structure of *cis*-Bis(2,2′-bipyridine-*N*,*N*′)dichloromanganese(II)

By Paavo O. Lumme* and Eva Lindell

Department of Inorganic Chemistry, University of Helsinki, Vuorikatu 20, *SF*-00100 *Helsinki, Finland*

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Abstract. $[Mn(C_{10}H_8N_2)_2Cl_2]$, $M_r = 438{\cdot}22$, monoclinic, $P2_1/c$, $a = 8{\cdot}590\ (2)$, $b = 14{\cdot}415\ (5)$, $c = 15{\cdot}735\ (5)$ Å, $\beta = 98{\cdot}09\ (2)°$, $V = 1929\ (1)$ Å^3, $Z = 4$, $D_m = 1{\cdot}51$, $D_x = 1{\cdot}51$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 10{\cdot}1$ cm^{-1}, $F(000) = 892$, $T = 295$ K, $R = 0{\cdot}041$ for 2173 observed reflections. The Mn atom is distorted octahedral, being coordinated to four N and two Cl atoms. The basal plane is formed by the two Cl and two N atoms [N(2), N(4)] of the different bpy molecules and the apical positions are occupied by the two remaining N atoms [N(1), N(3)]. The *M*—N bond lengths vary from 2·264 (3) to 2·353 (3) Å; the

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* To whom correspondence should be addressed.

metal–chlorine bonds are 2·436 (2) and 2·449 (1) Å. The dihedral angle between the two bpy best planes is 90·7 (1)°.

Introduction. During recent years we have considered the possibility of using the anisotropic temperature factors or the equivalent values of the isotropic temperature factors (Hamilton, 1959) derived from them as indicators of thermal decomposition processes (Lumme, Mutikainen & Lindell, 1983; Lumme, 1985; Lumme & Lindell, 1987, and references cited therein). The question is important from the viewpoint of elucidation of the thermal decomposition processes, because there does not seem to be any other method to identify the order of escape of similar ligands from a structure during the thermal decomposition of a compound.

In this paper we describe the structure of *cis*-bis(2,2′-bipyridine-*N*,*N*′)dichloromanganese(II). The comparison of the thermal and structural relations will be published elsewhere.

Experimental. Yellow prismatic crystals 0·20 × 0·23 × 0·32 mm; Nicolet *P*3*F* diffractometer, graphite-monochromated Mo *K*α radiation, $\omega/2\theta$ scan; $3 \leq 2\theta \leq 55°$; lattice parameters from 21 reflections (2θ range: 5–19°); absorption corrections applied by φ-scan technique, min., max. transmission coefficients 0·84, 1·00; h 0→12, k 0→19, l −21→21; 2 intensity monitors varied ≤ 2%; 4905 total reflections, 4424 unique, 2173 with $I \geq 3\sigma(I)$; structure solved by Patterson and Fourier methods; H atoms were placed with $U = 0{\cdot}05$ Å^2 and the coordinates refined; full-matrix anisotropic refinement on F (of non-H atoms) yielded $R = 0{\cdot}041$, $wR = 0{\cdot}032$, $S = 1{\cdot}4$; $w = (\sigma_F)^{-1}$; max. $\Delta/\sigma = 0{\cdot}00455$, av. $\Delta/\sigma = 0{\cdot}000356$ in final cycle; final ΔF map showed ±0·3 e Å^{-3} near Mn atom; no correction for secondary extinction; scattering factors were from Cromer & Mann (1968) and corrections for anomalous dispersion from *International Tables for X-ray Crystallography* (1974); calculations performed with *XTAL*83 crystallographic programs (Stewart *et al.*, 1983) and *MPLN* (Truter & Vickery, 1973) for planes; calculations performed on a VAX 8600 computer.

Table 1. *Fractional atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^4) *of the non-*H *atoms with e.s.d.'s in parentheses*

$U_{\rm eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$ (Hamilton, 1959).

	x	y	z	$U_{\rm eq}$
Mn	2006·1 (7)	2660·2 (4)	383·8 (4)	340 (1)
Cl(1)	1215 (2)	3800 (1)	1383 (1)	648 (3)
Cl(2)	−283 (1)	2684 (1)	−737 (1)	581 (3)
N(1)	1416 (4)	1389 (2)	1136 (2)	392 (9)
N(2)	2851 (4)	1310 (2)	−257 (2)	400 (9)
N(3)	3655 (4)	3507 (2)	−310 (2)	362 (8)
N(4)	4488 (4)	2712 (2)	1201 (2)	370 (8)
C(1)	671 (5)	1455 (3)	1825 (3)	487 (12)
C(2)	109 (6)	711 (4)	2236 (3)	551 (14)
C(3)	340 (6)	−150 (4)	1912 (3)	632 (15)
C(4)	1113 (6)	−250 (3)	1218 (3)	551 (14)
C(5)	1648 (5)	532 (3)	832 (3)	381 (10)
C(6)	2480 (5)	492 (3)	64 (3)	383 (10)
C(7)	2827 (6)	−341 (3)	−310 (3)	557 (13)
C(8)	3566 (7)	−325 (4)	−1020 (4)	695 (16)
C(9)	3907 (7)	506 (4)	−1369 (3)	646 (16)
C(10)	3543 (6)	1305 (3)	−966 (3)	531 (13)
C(11)	3163 (6)	3957 (3)	−1045 (3)	457 (12)
C(12)	4137 (6)	4469 (3)	−1490 (3)	513 (14)
C(13)	5691 (6)	4516 (3)	−1167 (3)	530 (13)
C(14)	6250 (5)	4063 (3)	−413 (3)	448 (11)
C(15)	5198 (5)	3572 (3)	10 (2)	342 (9)
C(16)	5648 (4)	3129 (3)	866 (2)	326 (9)
C(17)	7148 (5)	3198 (3)	1318 (3)	514 (13)
C(18)	7430 (6)	2864 (3)	2150 (3)	538 (13)
C(19)	6251 (5)	2472 (3)	2499 (3)	513 (12)
C(20)	4795 (5)	2405 (3)	2006 (2)	464 (11)

Discussion. The atomic coordinates are given in Table 1,* and bond lengths and angles in *cis*-[Mn$^{\rm II}$(bpy)$_2$(Cl)$_2$] are shown in Table 2. Fig. 1 illustrates the geometry and labelling of the molecule. The crystal packing is shown in Fig. 2. The bond lengths and angles within both bipyridines are normal. The ligands form a distorted octahedral coordination sphere about the Mn atom, with the bipyridine groups exhibiting their usual acute N···N bite distances [N(1)···N(2) = 2·663 (4) and N(3)···N(4) = 2·646 (4) Å] and N—*M*—N angles [N(1)—Mn—N(2) = 70·2 (1) and N(3)—Mn—N(4) = 70·3 (1)°]. The values are very close to those found in *cis*-[Mn$^{\rm II}$(bpy)$_2$(NCS)$_2$] (Veidis, Dockum, Charron, Reiff & Brennan, 1981). The bipyridines are nearly planar {average r.m.s.d. from the calculated plane = 0·029 (6) [N(1)···plane] and 0·088 (6) Å [N(3)···plane]}, but show a boat form in the longitudinal direction of the ligand with respect to the best calculated ligand plane. The inter-ring distances C(5)—C(6) = 1·489 (6) and C(15)—C(16) = 1·492 (5) Å in bpy's are close to the distance in the free ligand (1·50 Å; Merritt & Schroeder, 1956). The dihedral angle between the two bpy best planes is 90·7 (1)°. The dihedral angle between the pyridyl rings containing N(1) and N(2) is 3·5 (18)° and N(3) and N(4) 11·0 (5)°.

The Mn atom lies practically in the best plane calculated through the N(2), N(4), Cl(1) and Cl(2) atoms [r.m.s.d. 0·007 (1) Å]. The crystal structure is formed by discrete molecular units which pack in columns in the **a** direction (Fig. 2). There are no hydrogen bonds, but the structure is stabilized through weak stacking of the bpy molecules in the **a** and **b** directions.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths and angles and planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44566 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å) *and angles* (°)

Mn coordination sphere			
Mn–Cl(1)	2·436 (2)	Mn–N(2)	2·353 (3)
Mn–Cl(2)	2·449 (1)	Mn–N(3)	2·264 (3)
Mn–N(1)	2·276 (3)	Mn–N(4)	2·331 (3)
Cl(1)–Mn–Cl(2)	100·75 (5)	N(1)–Mn–N(3)	152·2 (1)
Cl(1)–Mn–N(1)	96·01 (9)	N(1)–Mn–N(4)	89·6 (1)
Cl(1)–Mn–N(2)	164·86 (9)	N(2)–Mn–N(3)	89·3 (1)
Cl(1)–Mn–N(3)	101·41 (9)	N(2)–Mn–N(4)	87·1 (1)
Cl(1)–Mn–N(4)	86·50 (9)	N(3)–Mn–N(4)	70·3 (1)
Cl(2)–Mn–N(1)	99·83 (9)	Mn–N(1)–C(1)	122·1 (3)
Cl(2)–Mn–N(2)	88·16 (8)	Mn–N(2)–C(10)	124·2 (3)
Cl(2)–Mn–N(3)	97·96 (8)	Mn–N(3)–C(11)	122·3 (3)
Cl(2)–Mn–N(4)	167·38 (8)	Mn–N(4)–C(20)	123·9 (3)
N(1)–Mn–N(2)	70·2 (1)		
2,2′-Bipyridines			
N(1)–C(1)	1·339 (6)	C(6)–C(7)	1·388 (6)
C(1)–C(2)	1·373 (7)	C(7)–C(8)	1·360 (9)
C(2)–C(3)	1·366 (8)	C(8)–C(9)	1·367 (9)
C(3)–C(4)	1·364 (8)	C(9)–C(10)	1·372 (8)
C(4)–C(5)	1·390 (7)	C(10)–N(2)	1·336 (6)
C(5)–N(1)	1·350 (5)	N(2)–C(6)	1·339 (5)
C(5)–C(6)	1·489 (6)		
N(1)–C(1)–C(2)	124·9 (4)	C(5)–C(6)–C(7)	122·3 (4)
C(1)–C(2)–C(3)	117·0 (5)	C(6)–C(7)–C(8)	119·1 (5)
C(2)–C(3)–C(4)	120·5 (5)	C(7)–C(8)–C(9)	119·7 (5)
C(3)–C(4)–C(5)	119·5 (5)	C(8)–C(9)–C(10)	118·3 (5)
C(4)–C(5)–N(1)	121·0 (4)	C(9)–C(10)–N(2)	123·2 (5)
C(4)–C(5)–C(6)	123·3 (4)	C(10)–N(2)–C(6)	117·9 (4)
C(5)–N(1)–C(1)	117·5 (4)	N(2)–C(6)–C(7)	121·7 (4)
N(3)–C(11)	1·341 (5)	C(16)–C(17)	1·385 (6)
C(11)–C(12)	1·378 (7)	C(17)–C(18)	1·383 (7)
C(12)–C(13)	1·361 (7)	C(18)–C(19)	1·343 (7)
C(13)–C(14)	1·380 (6)	C(19)–C(20)	1·379 (6)
C(14)–C(15)	1·389 (6)	C(20)–N(4)	1·333 (5)
C(15)–N(3)	1·354 (5)	N(4)–C(16)	1·334 (5)
C(15)–C(16)	1·429 (5)		
N(3)–C(11)–C(12)	123·8 (4)	C(15)–C(16)–C(17)	122·5 (4)
C(11)–C(12)–C(13)	118·1 (4)	C(16)–C(17)–C(18)	119·2 (4)
C(12)–C(13)–C(14)	120·0 (5)	C(17)–C(18)–C(19)	119·5 (4)
C(13)–C(14)–C(15)	118·8 (4)	C(18)–C(19)–C(20)	118·4 (4)
C(14)–C(15)–N(3)	121·7 (3)	C(19)–C(20)–N(4)	123·6 (4)
C(14)–C(15)–C(16)	123·2 (3)	C(20)–N(4)–C(16)	117·8 (3)
C(15)–N(3)–C(11)	117·4 (4)	N(4)–C(16)–C(17)	121·4 (4)

The intermolecular Cl(1)···Cl(2) distance is 3·763 (2) Å. The shortest intermolecular Cl···H distances are Cl(1)···H(9) = 2·86 (4) and Cl(2)···H(8) = 2·76 (4) Å with Cl(1)···C(11) = 3·573 (5) and Cl(2)···C(10) = 3·496 (5) Å, respectively; the shortest intramolecular Cl···H distances are Cl(1)···H(5^{i}) = 2·88 (4) and Cl(2)···H(6^{ii}) = 2·78 (4) Å with Cl(1)···C(7^{i}) = 3·639 (5) and Cl(2)···C(8^{ii}) = 3·505 (6) Å, respectively [(i): $-x, -y, -z$ and (ii): $-x, y + \frac{1}{2}, -z + \frac{1}{2}$].

The Mn—N bond lengths in this complex occur in two distinct sets. The Mn—N(bpy) *trans* to N(bpy) and *trans* to Cl atoms average 2·270 (3) and 2·342 (3) Å, respectively, and are in the range of values for two other Mn^{II} complexes: 2·286 (8) and 2·312 (8) Å for *cis*-[Mn^{II}(bpy)$_2$(NCS)$_2$] (Veidis *et al.*, 1981) and 2·311 (4) Å for *catena*-[Mn^{II}(phosphinato)$_2$(bpy)] (Weakley, 1978); but differ from 2·04 and 2·06 Å for *cis*-[Mn^{II}(bpy)$_2$(NCO)$_2$] (Cincadze, Civcivadze & Orbeladze, 1975). The longer Mn—N(bpy) bonds occur when N(bpy) are *trans* to the Cl atoms.

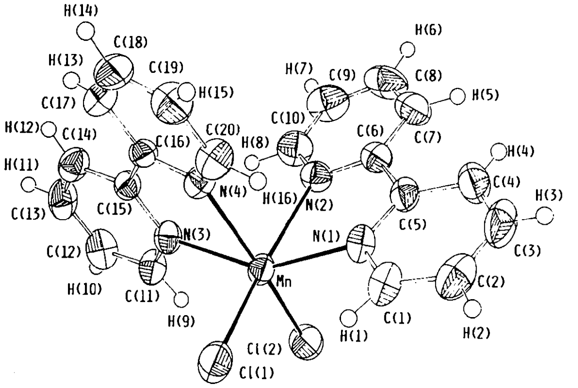

Fig. 1. *ORTEP* (Johnson, 1965) drawing with the numbering scheme of the [Mn(C$_{10}$N$_2$H$_8$)$_2$(Cl)$_2$] complex (50% probability ellipsoids are shown for the non-H atoms).

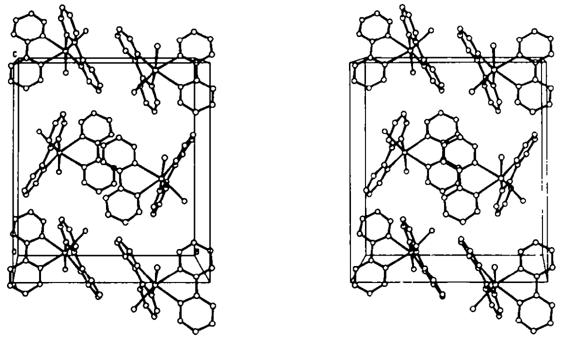

Fig. 2. Stereoview of the molecular packing as viewed down **a**.

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