Table 1. *Selected geometric parameters (Å, °)*

Cu—N1	1.957 (4)	C1—O1	1.266 (5)
Cu—O2	1.957 (3)	C1—N1	1.290 (6)
Cu—O1^{i}	2.028 (3)	C1—C1^{i}	1.528 (9)
Cu—N2	2.062 (4)	O2—C9	1.279 (5)
Cu—O3^{ii}	2.302 (4)	O3—C9	1.236 (5)
Cu···O3	2.818 (4)		
N1—Cu—O1^{i}	82.47 (15)	N2—Cu—O3	88.24 (13)
O2—Cu—O1^{i}	86.61 (13)	O3^{ii}—Cu—O3	144.72 (12)
N1—Cu—N2	92.44 (15)	O1—C1—N1	129.1 (4)
O2—Cu—N2	96.86 (15)	O1—C1—C1^{i}	117.2 (5)
N1—Cu—O3^{ii}	97.28 (16)	C1—N1—C2	119.5 (4)
O2—Cu—O3^{ii}	93.75 (13)	C1—N1—Cu	115.0 (3)
O1^{i}—Cu—O3^{ii}	98.27 (14)	C2—N1—Cu	125.6 (3)
N2—Cu—O3^{ii}	90.73 (14)	C4—N2—C8	118.0 (4)
N1—Cu—O3	118.01 (15)	C4—N2—Cu	123.1 (3)
O2—Cu—O3	51.48 (12)	C8—N2—Cu	118.8 (3)
O1^{i}—Cu—O3	86.72 (13)		

Symmetry codes: (i) $-x, -y, -z$; (ii) $x, \frac{1}{2} - y, z - \frac{1}{2}$.

The maximum and minimum electron-density peaks are at 0.83 and 0.81 Å, respectively, from the Cu^{II} atom.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *SDP* (Frenz, 1978). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997). Molecular graphics: *ORTEP*III (Burnett & Johnson, 1996). Software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1463). Services for accessing these data are described at the back of the journal.

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Dichlorobis(pyrimidine-*N*)cobalt(II) and its bromo derivative

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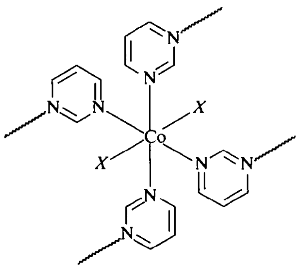
Abstract

The title compounds, [$CoCl_2(C_4H_4N_2)_2$] and [$CoBr_2(C_4H_4N_2)_2$], show weak ferromagnetism below 5 K. The relationship between the magnetic properties and the structure is discussed. The crystals of the Cl and Br derivatives are isomorphous. The Co atom is coordinated with two halogen atoms and four N atoms of pyrimidine molecules at axial and equatorial positions, respectively, to form the octahedral geometry. The nearest neighbouring Co atoms are bridged by the pyrimidine molecules to form a three-dimensional network. As the pyrimidine molecules are considered to conduct antiferromagnetic interactions, the weak ferromagnetism may result from the chiral structure of the crystals.

Comment

Pyrimidine-bridged transition metal complexes have been studied as molecular magnets (Mitsubori, Ishida, Nogami & Iwamura, 1994; Mitsubori, Ishida, Nogami, Iwamura *et al.*, 1994; Ishida *et al.*, 1995; Oshio & Ichida, 1995; Francesconi *et al.*, 1979; Lloret *et al.*, 1998). Some Cu^{II}–pyrimidine complexes were analysed by X-rays to clarify the origin of the magnetic properties. In most of the complexes, the Cu atoms are linked together through the pyrimidine molecules to form one-dimensional chains and the magnetic properties are related to the coordination positions of the pyrimidine molecules to the Cu atoms (Ishida & Nogami, 1997; Ishida *et al.*, 1997). Recently, it was found that dichlorobis(pyrimidine-*N*)cobalt(II), (I), and its bromo derivative, (II), show weak ferromagnetism below 5 K (Nakayama *et al.*, 1998). In this paper, we report the structures of (I) and (II), and discuss the relationship between the structures and the magnetic properties.



(I) X = Cl
(II) X = Br

The crystals of (I) and (II) are chiral and their crystal structures are essentially the same, but are mirror images to each other. The enantiomorphic crystals were resolved spontaneously and an enantiomorphic crystal was chosen at random for measurement.

The Co atoms are coordinated with four N atoms of pyrimidine molecules and two halogen atoms at the equatorial and axial positions, respectively, to form an octahedral geometry (Figs. 1 and 2). In (I), two chains are generated by symmetry operations of 4_1 and 4_3 screw axes along the *c* axis. As a *trans* coordination of the pyrimidine molecule is generated by the 4_1 screw axis, the Co atoms are linked through *trans*-coordinated pyrimidine molecules to form a one-dimensional chain structure. On the other hand, a *cis* coordination of the pyrimidine molecule is generated by the 4_3 screw axis, therefore, the generated chain is made up of the Co atoms and *cis*-coordinated pyrimidine molecules. Two of these neighbouring chains are joined and a three-dimensional network is formed (Fig. 3). In (II), since the crystal is the mirror image of the crystal of (I), *cis* and *trans* coordinations of pyrimidine molecules are generated by the 4_1 and 4_3 screw axes, respectively, forming the enantiomeric structure to that of (I). The Co atoms are arranged tetrahedrally to form a distorted diamond structure, in which tetrahedrons are elongated along the *c* axis (Fig. 4). The interatomic distances between Co atoms, bridged by a pyrimidine molecule, are 6.2126 (9) and 6.2506 (5) Å for (I) and (II), respectively. The Co^{iv}—Co—Co^{v} and Co^{iv}—Co—Co^{vi} angles are 73.32 (2) and 130.05 (1)°, respectively, for (I) and 74.60 (1) and 129.25 (1)° for (II) [symmetry codes: for (I), (iv) $x, -y+\frac{1}{2}, -z+\frac{1}{4}$; (v) $x, -y-\frac{1}{2}, -z+\frac{1}{4}$; (vi) $x-\frac{1}{2}, -y, -z-\frac{1}{4}$; for (II), (iv) $x, -y-\frac{1}{2}, -z+\frac{1}{4}$; (v) $x, -y+\frac{1}{2}, -z+\frac{1}{4}$; (vi) $x-\frac{1}{2}, -y, -z-\frac{1}{4}$].

The interatomic distances between Co atoms are too great to make magnetic interactions directly, therefore the magnetic interactions are considered to be conducted through the coordinated pyrimidine molecules. In the Cu^{II}–pyrimidine complexes, the equatorial-bridging pyrimidine molecules are considered to be conductors of the antiferromagnetic interactions. Since the Co atoms are linked through equatorially coordinated pyrimidine molecules to form the three-dimensional network, the in-

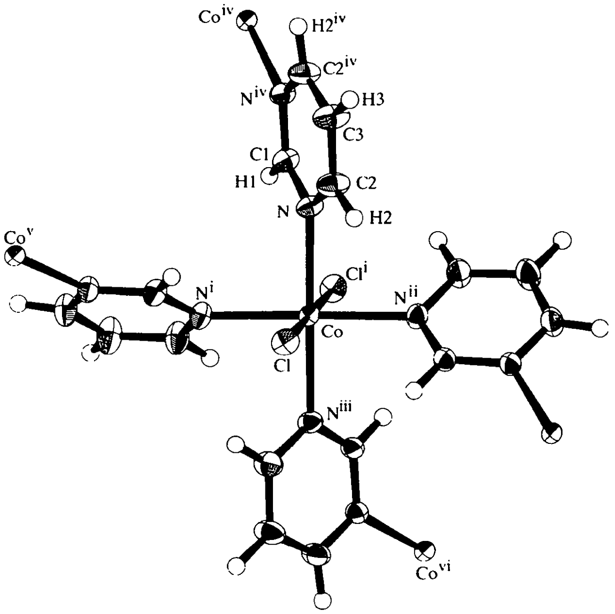


Fig. 1. *ORTEP*II (Johnson, 1976) drawing of the Cl derivative. Displacement ellipsoids are drawn at 50% probability for non-H atoms and H atoms are shown as small spheres. [Symmetry codes: (i) $-x, -y, z$; (ii) $y, x, -z$; (iii) $-y, -x, -z$; (iv) $x, -y+\frac{1}{2}, -z+\frac{1}{4}$; (v) $x, -y-\frac{1}{2}, -z+\frac{1}{4}$; (vi) $x-\frac{1}{2}, -y, -z-\frac{1}{4}$.]

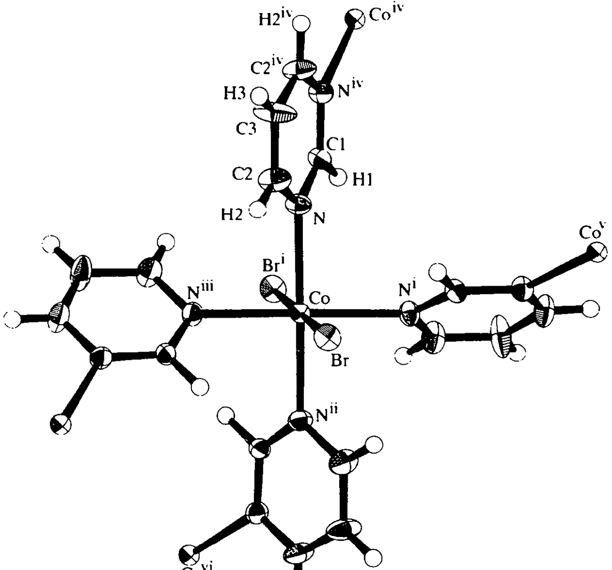


Fig. 2. *ORTEP*II (Johnson, 1976) drawing of the Br derivative. Displacement ellipsoids are drawn at 50% probability for non-H atoms and H atoms are shown as small spheres. [Symmetry codes: (i) $-x, -y, z$; (ii) $y, x, -z$; (iii) $-y, -x, -z$; (iv) $x, -y-\frac{1}{2}, -z+\frac{1}{4}$; (v) $x, -y+\frac{1}{2}, -z+\frac{1}{4}$; (vi) $x-\frac{1}{2}, -y, -z-\frac{1}{4}$.]

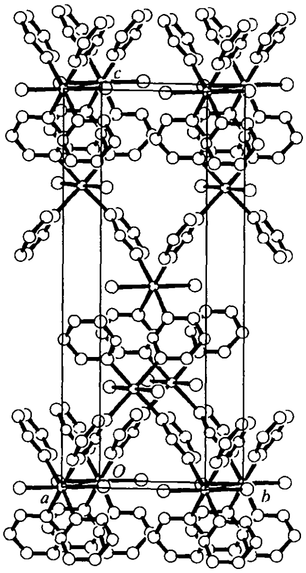


Fig. 3. The crystal structure of the Cl derivative.

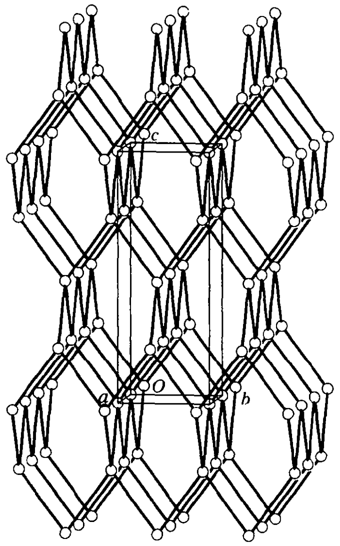


Fig. 4. The crystal structure of the Cl derivative. Only the Co atoms are shown in the figure. The three-dimensional network forms an elongated diamond structure.

teractions in the network are considered to be antiferromagnetic, if the mechanism of conducting the magnetic interaction is the same as those of the Cu^{II} complexes (Ishida & Nogami, 1997; Ishida *et al.*, 1997). The remaining weak ferromagnetism may be due to the chirality of the crystals (Dzyaloshinsky, 1958; Kzialoshinskii, 1958; Moriya, 1960*a*,*b*).

To elucidate the conduction of magnetism through the pyrimidine molecules, the electron-density distribution analysis is indispensable, as well as consideration of the coordination geometries of the pyrimidine molecules. The electron-density distribution analysis of (I) by the multipole expansion method is now in progress.

Experimental

The crystal of (I) was obtained from a methanol solution of a 1:2 mixture of dichlorocobalt(II) hexahydrate and pyrimidine. The crystal of (II) was obtained by the same procedure using dibromocobalt(II) hexahydrate instead of dichlorocobalt(II) hexahydrate.

Compound (I)

Crystal data

$[CoCl_2(C_4H_4N_2)_2]$
$M_r = 290.01$
Tetragonal
$I4_122$
$a = 7.419\ (2)$ Å
$c = 19.935\ (4)$ Å
$V = 1097.1\ (3)$ Å^3
$Z = 4$
$D_x = 1.756$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–$15°$
$\mu = 2.020$ mm^{-1}
$T = 293$ K
Rhombohedron
0.36 × 0.15 × 0.08 mm
Violet

Data collection

Rigaku AFC-7*R* diffractometer
$\omega/2\theta$ scans
Absorption correction: analytical
$T_{min} = 0.689$, $T_{max} = 0.847$
1016 measured reflections
509 independent reflections (plus 298 Friedel-related reflections)

696 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 30°$
$h = -10 \rightarrow 0$
$k = -3 \rightarrow 10$
$l = -14 \rightarrow 26$
3 standard reflections every 100 reflections intensity decay: 0.85%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.074$
$S = 1.025$
807 reflections
45 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2 + 0.9736P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.283$ e Å^{-3}
$\Delta\rho_{min} = -0.253$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = −0.03 (4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (I)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Co	0	0	0	0.01896
Cl	0.22958 (9)	−0.22958 (9)	0	0.0276
N	0.1448 (3)	0.1585 (4)	0.0762 (1)	0.0240
C1	0.0626 (6)	1/4	1/8	0.0246
C2	0.3251 (4)	0.1613 (5)	0.0760 (2)	0.0315
C3	0.4226 (6)	1/4	1/8	0.0375

Table 2. *Selected geometric parameters (Å, °) for (I)*

Co—N	2.200 (2)	N—C2	1.338 (4)
Co—Cl	2.409 (1)	C2—C3	1.382 (4)
N—C1	1.334 (3)		

N^i—Co—N	92.7 (1)	C1—N—C2	116.8 (3)
N^{ii}—Co—N	87.4 (1)	C1—N—Co	123.5 (2)
N^{iii}—Co—N	176.3 (1)	C2—N—Co	119.7 (2)
N—Co—Cl	91.87 (7)	N—C1—N^{iv}	125.6 (4)
N—Co—Cl^i	88.13 (7)	N—C2—C3	121.9 (3)
Cl—Co—Cl^i	180	C2—C3—$C2^{iv}$	116.9 (4)

Symmetry codes: (i) $-x, -y, z$; (ii) $y, x, -z$; (iii) $-y, -x, -z$; (iv) $x, \frac{1}{2} - y, \frac{1}{4} - z$.

Compound (II)

Crystal data

$[CoBr_2(C_4H_4N_2)_2]$
$M_r = 378.93$
Tetragonal
$I4_122$
$a = 7.576$ (1) Å
$c = 19.889$ (2) Å
$V = 1141.4$ (3) Å^3
$Z = 4$
$D_x = 2.205$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–15°
$\mu = 8.475$ mm^{-1}
$T = 293$ K
Rhombohedron
0.30 × 0.30 × 0.15 mm
Violet

Data collection

Rigaku AFC-7*R* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.172$, $T_{max} = 0.280$
769 measured reflections
420 independent reflections (plus 242 Friedel-related reflections)

557 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 27.5°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 25$
3 standard reflections every 100 reflections intensity decay: 0.16%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.140$
$S = 1.037$
662 reflections
40 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1028P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.721$ e Å^{-3}
$\Delta\rho_{min} = -1.214$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0106 (16)
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = 0.02 (6)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (II)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Co	0	0	0	0.0173
Br	0.24064 (9)	0.24064 (9)	0	0.0268
N	0.1410 (8)	−0.1569 (9)	0.0768 (2)	0.0218
C1	0.0627 (13)	−1/4	1/8	0.0207
C2	0.3182 (9)	−0.1615 (10)	0.0769 (4)	0.0299
C3	0.4126 (16)	−1/4	1/8	0.042

Table 4. *Selected geometric parameters (Å, °) for (II)*

Co—N	2.212 (6)	N—C2	1.343 (9)
Co—Br	2.578 (1)	C2—C3	1.370 (9)
N—C1	1.329 (7)		
N—Co—N^i	92.6 (3)	C1—N—C2	115.6 (6)
N—Co—N^{ii}	175.6 (3)	C1—N—Co	124.6 (5)
N—Co—N^{iii}	87.6 (3)	C2—N—Co	119.8 (5)
N—Co—Br^i	87.8 (2)	N^{iv}—C1—N	127.0 (9)
N—Co—Br	92.2 (2)	N—C2—C3	122.3 (7)
Br^i—Co—Br	180	$C2^{iv}$—C3—C2	117 (1)

Symmetry codes: (i) $-x, -y, z$; (ii) $y, x, -z$; (iii) $-y, -x, -z$; (iv) $x, -\frac{1}{2} - y, \frac{1}{4} - z$.

In the Br derivative, the isotropic displacement parameters of the H atoms were constrained to be $1.2U_{eq}$(C). Atom H2 was refined as a riding model. The C2—H2 distance was constrained to be 0.93 Å. The positions of other H atoms were refined. In the Cl derivative, the refined C—H distances were in the range 0.96 (3)–1.09 (5) Å.

For both compounds, data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1993). Program(s) used to solve structures: *SIR*92 (Altomare *et al.*, 1994) for (I); the structure of the Cl derivative was used as an initial model for (II). For both compounds, program(s) used to refine structures: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SV* (Nemoto & Ohashi, 1993) and *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: OA1090). Services for accessing these data are described at the back of the journal.

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Bis-adduct of trimethylamine with aluminium trichloride

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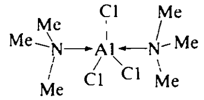
Abstract

In the molecule of trichlorobis(trimethylamine)aluminium(III), $[AlCl_3(C_3H_9N)_2]$, the metal centre is five-coordinate and the two N atoms occupy the axial positions of the trigonal bipyramid. The arrangement of the substituents bonded to Al and N is staggered.

Comment

The reaction of $AlMe_{3-n}Cl_n$ with one mole equivalent of Me_3N results in the corresponding Lewis acid–base complexes $Me_3N \rightarrow AlMe_{3-n}Cl_n$ ($n \leq 3$; Gelbrich *et al.*, 1999). The analogous reaction carried out with the basic materials in a 1:2 molar ratio may lead to the appropriate bis-adducts, such as the title compound $(Me_3N)_2AlCl_3$, (I).



$$Me_3N \rightarrow AlCl_3 \leftarrow NMe_3$$

(I)

Adduct (I) crystallizes in space group *Pnma* with four formula units per unit cell. The Al and N atoms, one Cl ligand and two methyl substituents occupy special positions on a mirror plane. As observed for the $Me_3N \rightarrow AlMe_{3-n}Cl_n$ series of mono-adducts, the arrangement of the halogen and methyl substituents with respect to the donor–acceptor bond is staggered (Gelbrich *et al.*, 1999). Analysing the coordination of the metal atom, the state of transition along the Berry pseudo-rotational pathway from trigonal bipyramidal to square pyramidal was found to be 3.8%, with a small difference of 5.4° from true Berry pseudo-rotational geometry (Holmes, 1984). Therefore, the polyhedron around aluminium is a slightly distorted trigonal bipyramid with axial N atoms. Within the equatorial $AlCl_3$ moiety, the sum of the Cl—Al1—Cl angles is 360.00 (4)°. The axial–axial N1—Al1—N2 angle is 178.76 (5)°. The increased coordination number of the metal atom results in a lengthening of Al—Cl by approximately 0.05 Å compared with the corresponding distance in the mono-adduct. The N→Al donor–acceptor bonds are nearly equal and, resulting from the higher coordination number of aluminium, are longer by 0.211 (5) Å than in $Me_3N \rightarrow AlCl_3$. As expected, the geometries around the N1 and N2 atoms and the N—C distances correspond closely in both complexes. Comparison of the N—Al distance with the values reported for $(Me_3N)_2AlH_3$ [2.18 (1) Å; Heitsch *et al.*, 1963] and for $[\{(C_5H_5)(C_5H_4CH_2NMe_2)\}Fe]_2AlH_3$ [2.168 (2) and 2.178 (2) Å; Nlate *et al.*, 1997] indicate that $AlCl_3$ is a slightly better acceptor than AlH_3. Somewhat surprisingly, the mean N→Al distances of 2.058 (3) and 2.037 (4) Å reported for the bis-adducts of $AlCl_3$ with Me_2HN (Ahmed *et al.*, 1977) and $^iPrH_2N$ (Chang *et al.*, 1997), respectively, are considerably shorter than those in (I). In connection with this, it is worth noting that, on the basis of the dissociation enthalpies of their mono-adducts with $AlMe_3$ (30 and 31 kcal mol^{-1}), the abilities of Me_3N and NMe_2H to act as electron donors have been considered to be equal (Hendrickson *et al.*, 1968).

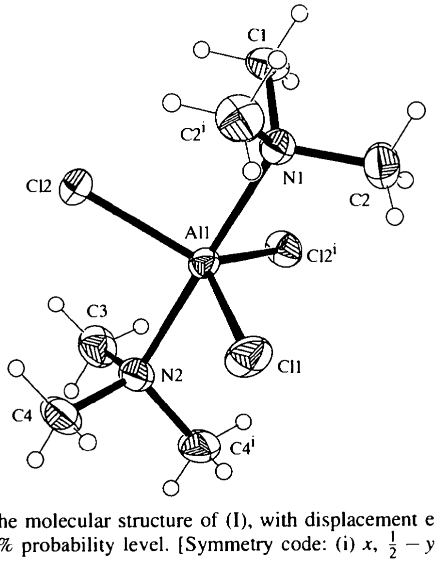


Fig. 1. The molecular structure of (I), with displacement ellipsoids at the 50% probability level. [Symmetry code: (i) $x, \frac{1}{2} - y, z$.]