Table 4. *Geometrical features around* $Na^+$ *ions* (Å)

| | | | |
|---|---|---|---|
| Na(*A*)–O(1*B*) | 2·275 (3) | Na(*B*)–O(1*B*) | 2·330 (3) |
| –O(2*B*) | 2·403 (3) | –O(2*B*) | 2·306 (3) |
| –O(1*A*) | 2·318 (3) | –O(1*A*) | 2·362 (3) |
| –O(2*A*) | 2·362 (3) | –O(2*A*) | 2·301 (3) |
| –O(4*B*) | 2·666 (3) | –O(4*B*) | 2·612 (3) |

molecules *A* and *B*. Both independent $Na^+$ ions are five-coordinated. Four short Na–O bonds are formed (Table 4) with the O atoms of the phosphate groups and build distorted tetrahedral $(NaO_2)_n$ chains. The fifth Na–O bond is ~13% elongated with respect to the other bonds and involves the O(4) atom of the epoxy group of molecule *B* (Fig. 1). Thus, the oxygen polyhedra around the $Na^+$ ions are actually forming infinite hybrid chains of the type $(NaO_2–NaO_3)_n$ along the *c* axis. This type of infinite chain has not been reported up to now and only a dimer of the type $O_3NaO_2NaO_3$ has been described (Bright, Milburn & Truter, 1971).

Disregarding O(4), the structure has a pseudocentre at $(0,0{\cdot}4,\frac{1}{4})$. This makes the space-group symmetry pseudo $P2_1/c$.

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*Acta Cryst.* (1984). C**40**, 359–362

# [2,9-Bis(*N*-methylhydrazino)-1,10-phenanthroline]dichlororhodium(III) Tetrafluoroborate Sesquihydrate, $[RhCl_2(C_{14}H_{16}N_6)]BF_4.1{\cdot}5H_2O$

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**Abstract.** $M_r = 555{\cdot}98$, triclinic, $P\bar{1}$, $a = 12{\cdot}200\,(2)$, $b = 13{\cdot}171\,(3)$, $c = 14{\cdot}259\,(3)$ Å, $\alpha = 110{\cdot}31\,(2)$, $\beta = 93{\cdot}90\,(1)$, $\gamma = 102{\cdot}60\,(2)°$, $U = 2071{\cdot}0\,(7)$ Å$^3$, $Z = 4$, $D_x = 1{\cdot}783$ Mg m$^{-3}$, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu(\text{Mo } K\alpha) = 1{\cdot}08$ mm$^{-1}$, $F(000) = 1112$, $T = 288$ K, final $R = 0{\cdot}058$ for 4925 unique observed reflections. The asymmetric unit contains two structurally similar mononuclear $Rh^{3+}$ cations and the associated $BF_4^-$ anions; three water molecules are involved in hydrogen bonding with both the cations and the anions. In each cation the Rh atom adopts a distorted octahedral geometry with the two Cl atoms in *trans* axial positions while the four equatorial positions are occupied by four N atoms of the planar hydrazino-phenanthroline ligand.

**Introduction.** Complexes of the 2,9-bis(*N*-methylhydrazino)-1,10-phenanthroline ligand have been reported previously for the first-row transition metals and for $Zn^{II}$, $Cd^{II}$ and $Hg^{II}$ (Lewis & O'Donoghue, 1980). In every case the ligand is assumed to be tetradentate *via* the phenanthroline N donors and the terminal $-NH_2$ groups, although there are no crystallographic data available. In an extension of this work a study of the complexes of this ligand with second- and third-row transition metals has been undertaken. The $Rh^{III}$ complex has been obtained in a highly crystalline form, and it was decided to carry out a single-crystal X-ray analysis in order to confirm the molecular geometry and because, to our knowledge, there have been no

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previous structural reports on $Rh^{III}$–phenanthroline systems. The results of this investigation are reported here.

**Experimental.** The free 2,9-bis(*N*-methylhydrazino)-1,10-phenanthroline ligand was prepared by literature methods (Lewis & O'Donoghue, 1980). 0·32 g ($10^{-3}$ mol) of this species, in aqueous ethanol (40 $cm^3$), was heated for 1 h, under reflux, with rhodium trichloride trihydrate (0·21 g, $10^{-3}$ mol). The volume of the solution was reduced under pressure, and concentrated aqueous sodium tetrafluoroborate solution (5 $cm^3$) added. After standing for 12 h at 277 K the orange product was filtered, washed with ice-cold ethanol and dried over $P_2O_5$ *in vacuo*; yield 80%. Microanalysis results: calculated C 29·7, H 3·5, N 14·9 wt%; found C 29·7, H 3·2, N 15·1 wt%. Room-temperature $^1H$ NMR (400 MHz) displayed resonances (p.p.m.), downfield of tetramethylsilane, as shown in Fig. 1.

Single crystals obtained as orange platelets from water. A preliminary photographic investigation (Weissenberg) established the space group and approximate cell dimensions. Crystal 0·42 × 0·27 × 0·05 mm. Syntex $P2_1$ diffractometer. Accurate unit-cell parameters derived from the $2\theta$ angles of 15 reflections, $20 < 2\theta < 30°$. 6334 reflections measured, $2\theta < 55°$ ($+h$, $\pm k$, $\pm l$), graphite-monochromated Mo $K\alpha$ radiation, 96-step $\omega/2\theta$ scan technique. Two standard reflections monitored throughout the course of data collection: no significant variation. Data corrected for absorption using an empirical pseudo-ellipsoid model and 490 azimuthal-scan data ($R_{int} = 0{\cdot}014$). Data averaged to give 4925 unique reflections with $F > 2\sigma(F)$. Patterson and Fourier techniques determined the positions of the two complex ions and one $BF_4^-$ group. After the first refinement cycle, three water molecules located from a difference map which also showed two somewhat distorted $BF_4^-$ ions close to inversion centres. Subsequently, their geometries were constrained and they were given an occupancy factor of 0·5, but the position of one F atom [F(31*)] later proved to be fully occupied. Refinement (on $F$) then continued with Rh, Cl and O atoms and the ordered $BF_4^-$ anisotropic. Successive difference maps yielded the locations of all H atoms attached to the organic ligands, but their positional parameters were refined only in the last cycle. The refinement (unit weights throughout) converged at $R = 0{\cdot}058$. Apart from some peaks around the disordered anions (up to 1·3 e Å$^{-3}$) the final difference map was featureless. No correction for secondary extinction.

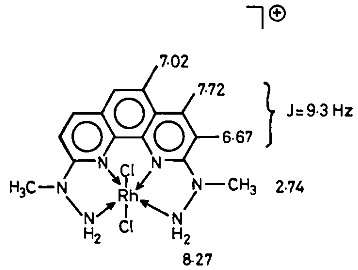

Fig. 1. A diagramatic representation of the cation showing the $^1H$ NMR assignments (shifts in p.p.m. relative to tetramethylsilane).

Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic temperature factors* (Å$^2$ $\times 10^3$), *with e.s.d.'s in parentheses*

| | $x$ | $y$ | $z$ | $U$ |
|---|---|---|---|---|
| Rh | 1858 (1) | 2996 (1) | 306 (1) | 28 (1)† |
| Cl(1) | 1700 (2) | 3045 (2) | −1324 (2) | 41 (1)† |
| Cl(2) | 1941 (2) | 2888 (2) | 1892 (2) | 49 (1)† |
| N(1) | 3478 (6) | 3647 (6) | 564 (5) | 35 (2) |
| C(2) | 4232 (7) | 3057 (7) | 390 (6) | 31 (2) |
| C(3) | 5416 (7) | 3634 (7) | 686 (6) | 36 (2) |
| C(4) | 5701 (7) | 4771 (7) | 1135 (6) | 38 (2) |
| C(5) | 5065 (8) | 6605 (8) | 1840 (7) | 43 (2) |
| C(6) | 4176 (8) | 7061 (8) | 2029 (7) | 46 (2) |
| C(7) | 1997 (8) | 6759 (8) | 1949 (7) | 44 (2) |
| C(8) | 951 (7) | 6020 (8) | 1643 (6) | 40 (2) |
| C(9) | 842 (7) | 4832 (7) | 1088 (6) | 33 (2) |
| N(10) | 1799 (6) | 4549 (6) | 918 (5) | 35 (2) |
| C(11) | 2862 (7) | 5277 (7) | 1241 (6) | 32 (2) |
| C(12) | 3775 (7) | 4794 (7) | 1049 (6) | 31 (2) |
| C(13) | 4891 (7) | 5419 (7) | 1347 (6) | 32 (2) |
| C(14) | 3005 (7) | 6424 (7) | 1759 (6) | 37 (2) |
| N(15) | 3771 (6) | 1957 (7) | −44 (5) | 43 (2) |
| C(16) | 4397 (10) | 1123 (10) | −336 (8) | 65 (3) |
| N(17) | 2543 (6) | 1557 (6) | −217 (5) | 35 (2) |
| N(18) | −109 (6) | 3981 (6) | 734 (5) | 41 (2) |
| C(19) | −1233 (8) | 4040 (8) | 925 (7) | 43 (2) |
| N(20) | 67 (6) | 2856 (6) | 283 (5) | 39 (2) |
| Rh′ | 3117 (1) | 7366 (1) | 6247 (1) | 33 (1)† |
| Cl(1′) | 2840 (2) | 6654 (2) | 4481 (2) | 49 (1)† |
| Cl(2′) | 3436 (2) | 8113 (2) | 8009 (2) | 53 (1)† |
| N(1′) | 1821 (6) | 6220 (6) | 6255 (5) | 40 (2) |
| C(2′) | 790 (8) | 6342 (8) | 6255 (7) | 41 (2) |
| C(3′) | −84 (8) | 5442 (8) | 6285 (7) | 45 (2) |
| C(4′) | 167 (8) | 4500 (8) | 6293 (7) | 44 (2) |
| C(5′) | 1745 (8) | 3454 (8) | 6321 (7) | 46 (2) |
| C(6′) | 2831 (8) | 3469 (8) | 6312 (7) | 50 (2) |
| C(7′) | 4865 (8) | 4586 (8) | 6292 (7) | 44 (2) |
| C(8′) | 5526 (8) | 5550 (8) | 6281 (7) | 42 (2) |
| C(9′) | 5040 (7) | 6446 (7) | 6272 (6) | 34 (2) |
| N(10′) | 3939 (6) | 6279 (6) | 6262 (5) | 38 (2) |
| C(11′) | 3255 (7) | 5309 (7) | 6280 (6) | 36 (2) |
| C(12′) | 2103 (7) | 5285 (7) | 6283 (6) | 38 (2) |
| C(13′) | 1305 (8) | 4351 (8) | 6298 (7) | 42 (2) |
| C(14′) | 3684 (7) | 4412 (7) | 6286 (6) | 39 (2) |
| N(15′) | 678 (7) | 7324 (7) | 6197 (6) | 47 (2) |
| C(16′) | −347 (9) | 7717 (9) | 6264 (8) | 54 (3) |
| N(17′) | 1737 (6) | 8108 (7) | 6203 (5) | 45 (2) |
| N(18′) | 5542 (7) | 7443 (7) | 6237 (6) | 46 (2) |
| C(19′) | 6759 (8) | 7865 (8) | 6273 (7) | 47 (2) |
| N(20′) | 4832 (6) | 8207 (6) | 6280 (5) | 43 (2) |
| B(1) | 2719 (12) | −663 (13) | 1292 (11) | 63 (6)† |
| F(11) | 2821 (7) | −1583 (7) | 558 (6) | 115 (4)† |
| F(12) | 3606 (9) | −286 (8) | 2034 (7) | 144 (6)† |
| F(13) | 2574 (11) | 150 (9) | 994 (9) | 161 (8)† |
| F(14) | 1751 (8) | −987 (9) | 1642 (8) | 138 (7)† |
| B(2) | 6007 (26) | −350 (23) | 4541 (21) | 102 (11) |
| F(21) | 5490 (15) | −1404 (15) | 4461 (13) | 115 (6) |
| F(22) | 6081 (17) | −271 (16) | 3655 (14) | 129 (7) |
| F(23) | 7020 (27) | 67 (31) | 5175 (26) | 307 (19) |
| F(24) | 5422 (28) | 480 (24) | 5141 (27) | 265 (17) |
| B(3) | 525 (33) | −531 (29) | 4362 (30) | 360 (69) |
| F(31*) | 976 (10) | −1444 (10) | 4360 (8) | 155 (4) |
| F(32) | −220 (44) | −166 (49) | 5027 (40) | 352 (22) |
| F(33) | 1450 (26) | 409 (25) | 4535 (24) | 243 (14) |
| F(34) | −22 (27) | −694 (27) | 3408 (23) | 249 (15) |
| O(1*w*) | 1046 (7) | −1553 (9) | −1347 (8) | 99 (6)† |
| O(2*w*) | 2168 (9) | 505 (8) | −2492 (6) | 101 (5)† |
| O(3*w*) | −40 (11) | −157 (11) | 1149 (16) | 238 (12)† |

† The equivalent isotropic thermal parameter (defined as one third of the trace of the orthogonalized $U_{ij}$ tensor) is given for these atoms which were refined anisotropically.

Neutral-atom scattering factors employed (*International Tables for X-ray Crystallography*, 1974). All computations performed with *SHELX*76 (Sheldrick, 1976).

**Discussion.** Atomic parameters are given in Table 1.* There are no major structural differences between the two Rh-containing complex cations within the asymmetric unit; a least-squares fit results in an r.m.s. deviation of 0·078 (2) Å, the largest displacements being 0·18 (1) Å for C(19) and 0·13 (1) Å for Cl(1). The Rh atom exhibits a distorted octahedral coordination geometry with the central ion situated in the $N_4$ donor plane [$\Delta$ = 0·03 (1) and 0·00 (2) Å] of the hydrazino-phenanthroline ligand while the two $Cl^-$ ions occupy two *trans* axial sites. The donor N—Rh distances range from 1·923 (9) to 2·154 (8) Å; the shorter lengths are associated with the phenanthroline N atoms. A similar trend in these distances has been observed in an $Ni^{II}$ macrocycle complex incorporating the phenanthroline unit (Ansell, Lewis, Raithby, Ramsden & Schröder, 1982).

The geometry of the quadridentate ligand (Table 2) is similar to that observed in complexes where it forms part of a quinquedentate macrocycle (Haque, Liles, McPartlin & Tasker, 1977; Lewis, O'Donoghue & Raithby, 1980; Bishop, Lewis, O'Donoghue, Raithby & Ramsden, 1980; Hanton & Raithby, 1980). The main differences occur within the substituents which, as a result of the interrupted conjugation, show typical N—N single-bond distances. The trisubstituted N atoms are planar (angle sums 358·8–360·0°) whereas the amino groups are pyramidal. The complexation of the latter induces a considerable bend of the substituent chains towards the central ion, as reflected by the angular distortions at C(2), C(9), N(15) and N(18). This leads to N(17)—*M*—N(20) angles about 20° smaller than in the corresponding macrocyclic complexes. In contrast to the 'primed' phenanthroline ring system, which is planar within experimental error [$\sigma$ = 0·01 (1) Å], the 'unprimed' one [$\sigma$ = 0·06 (1) Å] has the shape of a shallow dome extending through the substituents with the methyl groups displaced by 0·15 (1) and 0·28 (1) Å away from the Rh (see Fig. 2*a*).

The crystal packing (Fig. 3) is characterized by a clear separation of hydrophilic and hydrophobic regions. Centrosymmetric pairs of the two complex ions, which are nearly perpendicular to **c** and **c***, respectively, and thus inclined at 29 (1)°, alternate along **c** with shortest inter-pair contacts C(13)···C(7′) 3·36 (2) and C(4)···C(14′) 3·43 (2) Å. Translation along **a** generates double layers composed of one kind of phenanthroline ligand separated by 3·37 (6) and 3·38 (1) Å, respectively. Since the aromatic ring systems show a staggered arrangement, each overlaps partially with two others. The orientation of the complex cations is such that the polar amino groups point towards the hydrophilic layer in the *ac* plane which contains the counter ions and water molecules.

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

The right-hand columns contain respective values for the 'primed' cation.
B—F distances 1·31 (4)–1·49 (5) Å; F—B—F angles 97 (2)–121 (5)°.

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Rh–Cl(1) | 2·343 (3) | 2·332 (2) | C(3)–C(4) | 1·360 (12) | 1·345 (16) | C(9)–N(18) | 1·348 (10) | 1·342 (13) |
| Rh–Cl(2) | 2·312 (3) | 2·328 (2) | C(4)–C(13) | 1·423 (14) | 1·444 (14) | N(10)–C(11) | 1·373 (9) | 1·375 (12) |
| Rh–N(1) | 1·928 (6) | 1·937 (7) | C(5)–C(6) | 1·349 (15) | 1·322 (15) | C(11)–C(12) | 1·397 (13) | 1·399 (13) |
| Rh–N(10) | 1·945 (7) | 1·923 (9) | C(5)–C(13) | 1·433 (12) | 1·409 (16) | C(11)–C(14) | 1·396 (12) | 1·394 (15) |
| Rh–N(17) | 2·154 (8) | 2·131 (9) | C(6)–C(14) | 1·439 (12) | 1·449 (14) | C(12)–C(13) | 1·378 (10) | 1·400 (13) |
| Rh–N(20) | 2·150 (7) | 2·132 (7) | C(7)–C(8) | 1·361 (12) | 1·354 (14) | N(15)–C(16) | 1·434 (16) | 1·450 (15) |
| N(1)–C(2) | 1·312 (12) | 1·302 (13) | C(7)–C(14) | 1·407 (14) | 1·408 (13) | N(15)–N(17) | 1·449 (10) | 1·465 (11) |
| N(1)–C(12) | 1·375 (10) | 1·362 (14) | C(8)–C(9) | 1·459 (12) | 1·436 (15) | N(18)–C(19) | 1·429 (13) | 1·458 (12) |
| C(2)–C(3) | 1·435 (11) | 1·426 (13) | C(9)–N(10) | 1·314 (12) | 1·311 (11) | N(18)–N(20) | 1·467 (11) | 1·452 (13) |
| Cl(1)–Rh–Cl(2) | 177·6 (1) | 178·4 (1) | N(1)–C(2)–C(3) | 118·7 (7) | 117·7 (10) | C(12)–C(11)–C(14) | 122·9 (7) | 122·7 (8) |
| Cl(1)–Rh–N(1) | 92·2 (2) | 91·3 (2) | N(1)–C(2)–N(15) | 113·4 (7) | 114·6 (8) | N(1)–C(12)–C(11) | 115·0 (7) | 115·3 (8) |
| Cl(2)–Rh–N(1) | 90·1 (2) | 90·3 (2) | C(3)–C(2)–N(15) | 127·9 (9) | 127·7 (9) | N(1)–C(12)–C(13) | 122·7 (8) | 123·0 (9) |
| Cl(1)–Rh–N(10) | 92·1 (2) | 90·3 (2) | C(2)–C(3)–C(4) | 118·1 (9) | 120·0 (9) | C(11)–C(12)–C(13) | 122·3 (7) | 121·7 (10) |
| Cl(2)–Rh–N(10) | 89·1 (2) | 89·9 (2) | C(3)–C(4)–C(13) | 123·7 (8) | 123·1 (9) | C(4)–C(13)–C(5) | 129·7 (7) | 131·9 (9) |
| N(1)–Rh–N(10) | 83·4 (3) | 83·4 (3) | C(6)–C(5)–C(13) | 120·9 (8) | 123·2 (10) | C(4)–C(13)–C(12) | 114·1 (7) | 112·6 (10) |
| Cl(1)–Rh–N(17) | 90·4 (2) | 89·1 (2) | C(5)–C(6)–C(14) | 124·1 (9) | 123·2 (11) | C(5)–C(13)–C(12) | 116·1 (8) | 115·4 (9) |
| Cl(2)–Rh–N(17) | 89·3 (2) | 91·3 (2) | C(8)–C(7)–C(14) | 122·5 (9) | 122·0 (10) | C(6)–C(14)–C(7) | 130·9 (8) | 131·1 (10) |
| N(1)–Rh–N(17) | 76·7 (3) | 77·0 (3) | C(7)–C(8)–C(9) | 120·1 (9) | 120·6 (9) | C(6)–C(14)–C(11) | 113·6 (8) | 113·8 (8) |
| N(10)–Rh–N(17) | 160·1 (3) | 160·4 (3) | C(8)–C(9)–N(10) | 115·8 (7) | 117·1 (8) | C(7)–C(14)–C(11) | 115·5 (7) | 115·1 (9) |
| Cl(1)–Rh–N(20) | 89·9 (2) | 90·1 (2) | C(8)–C(9)–N(18) | 128·6 (8) | 129·4 (8) | C(2)–N(15)–C(16) | 125·1 (8) | 126·2 (9) |
| Cl(2)–Rh–N(20) | 88·3 (2) | 88·4 (2) | N(10)–C(9)–N(18) | 115·5 (8) | 113·4 (9) | C(2)–N(15)–N(17) | 118·2 (8) | 115·5 (8) |
| N(1)–Rh–N(20) | 160·5 (3) | 160·1 (4) | Rh–N(10)–C(9) | 122·4 (5) | 123·9 (7) | C(16)–N(15)–N(17) | 116·7 (7) | 117·7 (9) |
| N(10)–Rh–N(20) | 77·1 (3) | 76·8 (3) | Rh–N(10)–C(11) | 112·4 (6) | 113·0 (6) | Rh–N(17)–N(15) | 107·8 (5) | 109·4 (6) |
| N(17)–Rh–N(20) | 122·7 (3) | 122·8 (3) | C(9)–N(10)–C(11) | 124·9 (7) | 123·1 (9) | C(9)–N(18)–C(19) | 126·5 (7) | 125·2 (9) |
| Rh–N(1)–C(2) | 123·8 (5) | 123·4 (7) | N(10)–C(11)–C(12) | 115·9 (7) | 115·2 (9) | C(9)–N(18)–N(20) | 115·7 (7) | 117·0 (7) |
| Rh–N(1)–C(12) | 113·3 (6) | 113·0 (6) | N(10)–C(11)–C(14) | 121·2 (8) | 122·1 (8) | C(19)–N(18)–N(20) | 116·6 (7) | 117·5 (8) |
| C(2)–N(1)–C(12) | 122·6 (7) | 123·6 (8) | | | | Rh–N(20)–N(18) | 109·0 (4) | 108·7 (5) |

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* Tables of structure factors, anisotropic thermal parameters, H-atom parameters and $BF_4^-$ distances and angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38971 (43 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

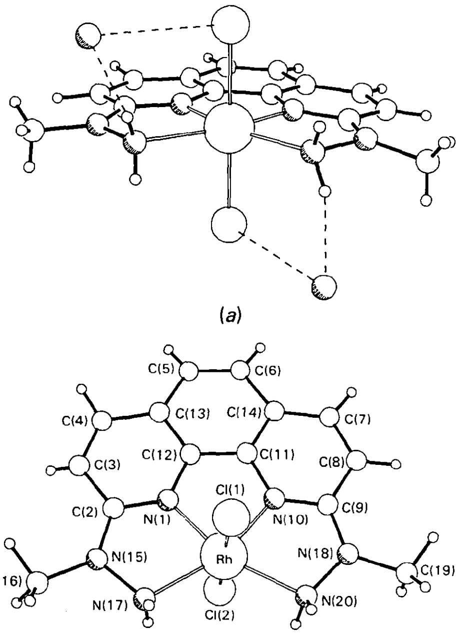

Fig. 2. The structures of the two complex ions with the atom-numbering scheme. The two water molecules bridging the 'unprimed' cation are also shown. N and O atoms are shaded and hydrogen bonds indicated by broken lines.

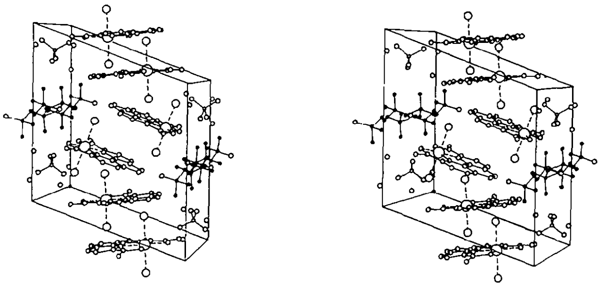

Fig. 3. Stereoscopic packing diagram viewed along **a** with **c** vertical. Disordered atoms are drawn as black dots. H atoms are omitted.

Table 3. *Hydrogen-bond distances* (Å) *with e.s.d.'s in parentheses*

| | | | |
|---|---|---|---|
| N(17)–H···O(2*w*) | 3·01 (2) | N(17′)–H···F(31*) | 3·02 (3) |
| N(17)–H′···F(13) | 2·94 (3) | N(17′)–H′···O(2*w*) | 2·96 (2) |
| N(20)–H···O(1*w*) | 2·86 (2) | N(20′)–H··· F(21) | 2·94 (3) |
| | | F(24) | 3·13 (5) |
| N(20)–H′···F(14) | 3·26 (3) | N(20′)–H′···F(12) | 3·07 (3) |
| O(1*w*)–H···Cl(2) | 3·58 (1) | O(1*w*)–H′···Cl(2′) | 3·19 (1) |
| O(2*w*)–H···Cl(1) | 3·37 (1) | O(2*w*)–H′··· F(22) | 2·80 (4) |
| | | F(34) | 2·94 (5) |
| O(3*w*)–H···F(14) | 2·80 (4) | O(3*w*)–H′···O(1*w*) | 2·73 (4) |

While one $BF_4^-$ ion is ordered, the other is distributed over two positions so close to inversion centres that only half occupancy is possible.

There is a circular arrangement of hydrogen bonds connecting the hydrophilic layers with the complex ions. All polar H atoms participate in H bonding (Table 3). In the 'unprimed' complex ion, amino groups and Cl atoms are bridged by water molecules O(1*w*) and O(2*w*) (see Fig. 2*a*), which also interact with the 'primed' cation. Not only the ordered $BF_4^-$, which accepts four H bonds (three from $NH_2$ groups), but also the disordered one take part in H bonding. In one of its positions, two symmetry-related $BF_4^-$ ions which are mutually exclusive interact with N(20′) so that always one of the two possible H bonds is present. In the alternative position, connected with the first one by two H bonds from O(2*w*), there is only an interaction between N(17′) and F(31*). This is just the atom whose position surprisingly turned out to be fully occupied, but otherwise one polar amino H atom would be without an H-bond acceptor in half its positions. The best explanation for this seems to be that the respective centrosymmetric position of F(31*) is always occupied by a water molecule, which would then also interact with F(32) across the inversion centre.

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