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Bis[*N*-(2-aminoethyl)morpholine]copper(II) bis(tetrafluoroborate)

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Key indicators

Single-crystal X-ray study
T = 170 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.092
Data-to-parameter ratio = 17.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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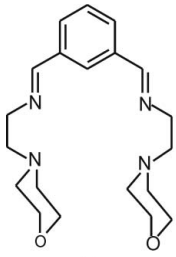
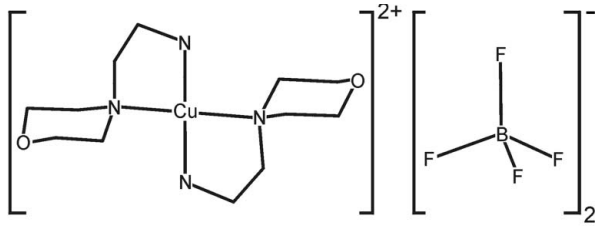
In the crystal structure of the title compound, $[Cu(C_6H_{14}N_2O)_2](BF_4)_2$, the Cu atom is coordinated by four N atoms of two symmetry-related *N*-(2-aminoethyl)morpholine ligands in a slightly distorted square-planar geometry. Including two longer contacts to two F atoms of two symmetry-related tetrafluoroborate anions, the coordination polyhedron can be described as a tetragonal bipyramid. The Cu atom is located on a centre of inversion, whereas the *N*-(2-aminoethyl)-morpholine ligand and the tetrafluoroborate anion are located in general positions. The crystal packing is stabilized by N—H···F and N—H···O hydrogen bonds.

Comment

The structure determination of the title compound, (II), was undertaken as part of a project on the synthesis of binuclear copper(II) complexes. Crystals of (II) were obtained by accident in the reaction of copper(II) bis(tetrafluoroborate) with [2-(morpholin-4-yl)ethyl][1-(3-{[(*E*)-2-(morpholin-4-yl)-ethylimino]methyl}phenyl)-(*E*)-methylidene]amine, (I), in methanol.



(I)



(II)

The asymmetric unit of (II) consists of one Cu atom located on a centre of inversion, one crystallographically independent *N*-(2-aminoethyl)morpholine ligand and one crystallographically independent tetrafluoroborate anion, the ligand and anion lying in general positions. Each Cu atom is surrounded by four N atoms of two symmetry-related *N*-(2-aminoethyl)morpholine ligands in a slightly distorted square-planar geometry. The Cu—N bond lengths are 1.9904 (15) and 2.1270 (14) Å and the *cis*-N—Cu—N angles are 94.56 (6) and 85.44 (6)° (Table 1 and Fig. 1). There are two additional long contacts between the Cu atom and two F atoms of two symmetry-related tetrafluoroborate anions of 2.5019 (12) Å. If these two contacts are included in the copper coordination, the coordination polyhedron can be described as a slightly distorted tetragonal bipyramid (Fig. 2). The crystal packing is stabilized by N—H···F and N—H···O hydrogen bonds (Table 2).

Experimental

A solution of $Cu(BF_4)_2$ (0.8 g) in methanol (10 ml) was added to a solution of [2-(morpholin-4-yl)ethyl][1-(3-{[(*E*)-2-(morpholin-4-yl)-ethylimino]methyl}phenyl)-(*E*)-methylidene]amine [(I), 0.4 g] in methanol (10 ml). The colour of the solution rapidly changed to dark blue and after 30 min a violet solid precipitated. This solid was washed with diethyl ether and dried under vacuum. Afterwards, it was dissolved in acetonitrile to give a dark-blue solution. After 3 d, violet crystals were obtained by diffusion of diethyl ether into the former solution.

Crystal data

$[Cu(C_6H_{14}N_2O)_2](BF_4)_2$	$Z = 1$
$M_r = 497.54$	$D_x = 1.663$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.6461$ (6) Å	Cell parameters from 6907 reflections
$b = 8.4018$ (7) Å	$\theta = 1.5$–28°
$c = 8.4258$ (7) Å	$\mu = 1.19$ mm^{-1}
$\alpha = 85.89$ (1)°	$T = 170$ (2) K
$\beta = 78.08$ (1)°	Block, violet
$\gamma = 69.757$ (9)°	0.11 × 0.10 × 0.09 mm
$V = 496.90$ (7) Å^3	

Data collection

Stoe IPDS diffractometer	$R_{int} = 0.032$
φ scans	$\theta_{max} = 28.0°$
Absorption correction: none	$h = -9 \rightarrow 10$
4509 measured reflections	$k = -10 \rightarrow 11$
2317 independent reflections	$l = -11 \rightarrow 11$
2158 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.1224P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.034$	
$wR(F^2) = 0.092$	
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
2317 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
134 parameters	$\Delta\rho_{min} = -0.93$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.051 (8)

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.9904 (15)	Cu1—N1	2.1270 (14)
N2—Cu1—N2^{i}	180	N2—Cu1—N1	85.44 (6)
N2—Cu1—N1^{i}	94.56 (6)	N1^{i}—Cu1—N1	180

Symmetry code: (i) $1-x, 1-y, 1-z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2C···F1^{ii}	0.92	2.20	3.006 (2)	146
N2—H2D···O1^{iii}	0.92	2.24	3.0376 (19)	145
N2—H2D···F3^{i}	0.92	2.40	3.0781 (19)	130

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $2-x, 1-y, 1-z$; (iii) $x, y, 1+z$.

All H atoms were located in a difference map and were positioned with idealized geometry, with C—H = 0.99 Å and N—H = 0.92 Å, and refined using a riding model [U_{iso}(H) = 1.2U_{eq}(C,N)].

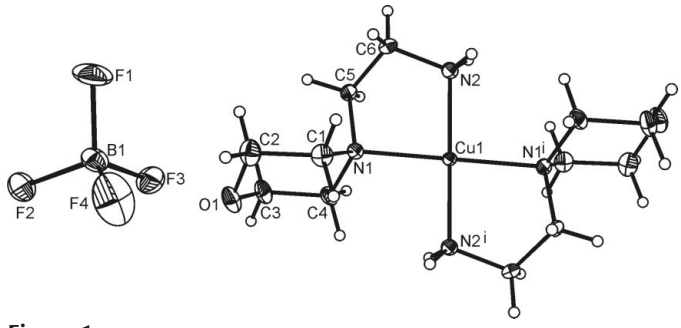


Figure 1
The component ions of the title compound, showing the copper coordination, with the atom labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

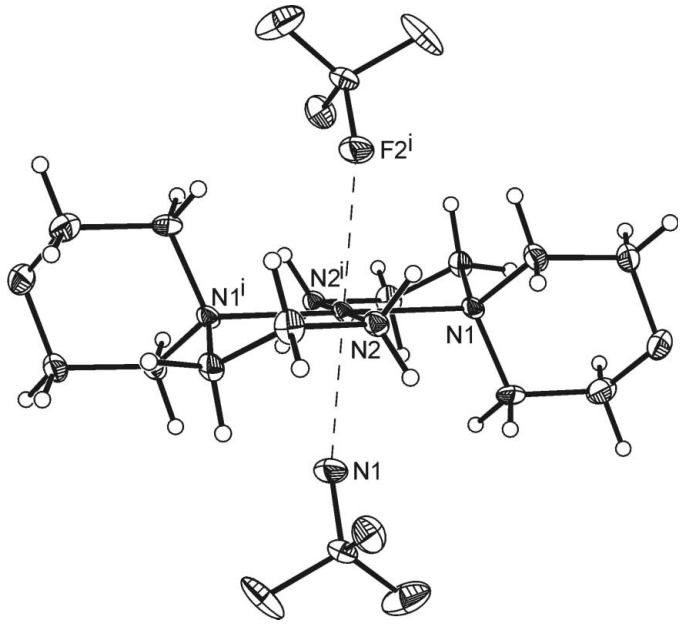


Figure 2
The structure of the title compound, viewed side-on, showing the labelling of selected atoms. The long Cu···F contacts to the tetrafluoroborate anions are shown as dashed lines.

Data collection: *IPDS Program Package* (Stoe & Cie, 1998); cell refinement: *IPDS Program Package*; data reduction: *IPDS Program Package*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXTL*.

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