differences in the coordination polyhedra (the Cu complexes of this type usually have square-pyramidal geometry). An additional factor could be the higher degree of hydration generally found in Ni complexes as compared with their Cu analogues; the presence of H_2O allows the O atoms of the uncoordinated COO groups to satisfy their affinity for bonding by formation of hydrogen bonds.

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Structure of Bis(ethylenediamine)isothiocyanatocopper(II) Tetrafluoroborate, Violet Isomer

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Abstract. $[Cu(NCS)(C_2H_8N_2)_2]BF_4$, $M_r = 328{\cdot}67$, orthorhombic, *Pnam*, $a = 15{\cdot}379\ (4)$, $b = 10{\cdot}788\ (2)$, $c = 7{\cdot}610\ (2)$ Å, $V = 1262{\cdot}5\ (1)$ Å^3, $Z = 4$, $D_m = 1{\cdot}73$, $D_x = 1{\cdot}73$ g cm^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1{\cdot}5418$ Å, $\mu = 43{\cdot}7$ cm^{-1}, $F(000) = 668$, $T = 293$ K, $R = 0{\cdot}042$ for 593 observed reflections. The Cu atom is in a tetragonally distorted octahedral environment with the four ethylenediamine N atoms in an approximately square-planar configuration [Cu—N1 2·018 (4) and Cu—N2 2·009 (4) Å] and two N(isothiocyanate) atoms in axial positions [Cu—N 2·720 (2) Å]. The isothiocyanate group thus forms a bridging unit between two $[Cu(en)_2]^{2+}$ cations, giving an infinite chain structure.

Introduction. The complexes of $[Cu(NCS)(en)_2]X$ where $X = Cl^-$, Br^-, NO_3^-, BF_4^- and ClO_4^- were investigated as models for the study of the isomerism of Cu^{II} complexes, as well as for the study of the influence of anion X exchange on the bonding mode of the NCS groups (Macašková, Otrubová, Ondrejovič & Gažo, 1987). For $X = BF_4^-$ two isomers of $[Cu(NCS)(en)_2]BF_4$ were prepared: blue and violet; these isomers differ in electronic and infrared spectra. The present paper reports the crystal structure of the violet isomer.

Experimental. Dark-violet prismatic crystals, 0·30 × 0·40 × 0·25 mm; D_m measured by flotation; Weissenberg photographs indicated space group *Pnam*, Syntex $P2_1$ computer-controlled four-circle diffractometer with graphite-monochromated Cu $K\alpha$ radiation; cell parameters by least squares from the 15 selected reflections with $3{\cdot}95 \leq 2\theta \leq 23{\cdot}28°$; intensity

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measurements carried out within $0 \leq 2\theta \leq 100°$, range of *hkl*: $h\,0\rightarrow 14$, $k\,0\rightarrow 10$, $l\,0\rightarrow 7$. Two standard reflections after every 98, no significant intensity variation; no correction for absorption; 593 independent reflections with $I \geq 1{\cdot}96\sigma(I)$; Cu position from Patterson map, other non-H atoms from Fourier map. Anisotropic full-matrix refinement (except H atoms) based on *F*. $R = 0{\cdot}0419$, $wR = 0{\cdot}0428$, $w = K[\sigma^2(F_o) + g(F_o^2)]$, $K = 1{\cdot}00$, $g = 0{\cdot}04525$; $(\Delta/\sigma)_{\max}$ in final least-squares cycle 0·3; max. and min. values of residual $\Delta\rho = 0{\cdot}38$ and $-0{\cdot}60\,\mathrm{e\,Å^{-3}}$. Calculations performed with *SHELX*76 program system (Sheldrick, 1976); scattering factors from *International Tables for X-ray Crystallography* (1974).

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters for non-*H *atoms, with e.s.d.'s in parentheses*

$$U_{\mathrm{eq}} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33}).$$

	x	y	z	U_{eq}(Å^2)
Cu	0·0	0·0	0·0	0·035 (1)
N1	−0·1284 (4)	0·0171 (6)	−0·0492 (10)	0·039 (4)
N2	−0·0379 (4)	−0·0281 (6)	0·2496 (7)	0·037 (4)
C1	−0·1743 (6)	0·0327 (9)	0·1201 (11)	0·047 (6)
C2	−0·1323 (5)	−0·0535 (8)	0·2499 (12)	0·047 (5)
S	0·0984 (2)	0·25	0·3557 (4)	0·065 (2)
C	0·0426 (7)	0·25	0·1731 (18)	0·047 (6)
N	0·0040 (6)	0·25	0·0454 (16)	0·052 (7)
B	0·3357 (7)	0·25	−0·0823 (15)	0·043 (7)
F1	0·3042 (4)	0·25	−0·2560 (8)	0·062 (4)
F2	0·2657 (5)	0·25	0·0278 (9)	0·076 (5)
F3	0·3817 (3)	0·3553 (4)	−0·0617 (8)	0·075 (3)

Table 2. *Interatomic distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

Cu—N1	2·018 (4)	N—C	1·138 (9)
Cu—N2	2·009 (4)	C—S	1·633 (10)
Cu—N	2·720 (2)	B—F1	1·408 (8)
N1—C1	1·479 (7)	B—F2	1·364 (9)
C1—C2	1·503 (8)	B—F3	1·365 (5)
N2—C2	1·479 (7)		
N1—Cu—N2	84·6 (2)	N1—C1—C2	107·3 (5)
N1—Cu—N1′	180·0 (3)	N2—C2—C1	107·8 (4)
N1—Cu—N2′	95·1 (3)	N—C—S	179·8 (3)
N1—Cu—N	91·5 (5)	F1—B—F3	107·1 (4)
N2—Cu—N	87·9 (4)	F2—B—F3	110·9 (4)
Cu—N1—C1	108·4 (4)	F1—B—F2	107·7 (7)
Cu—N2—C2	108·3 (3)	Cu—N—C	96·0 (5)

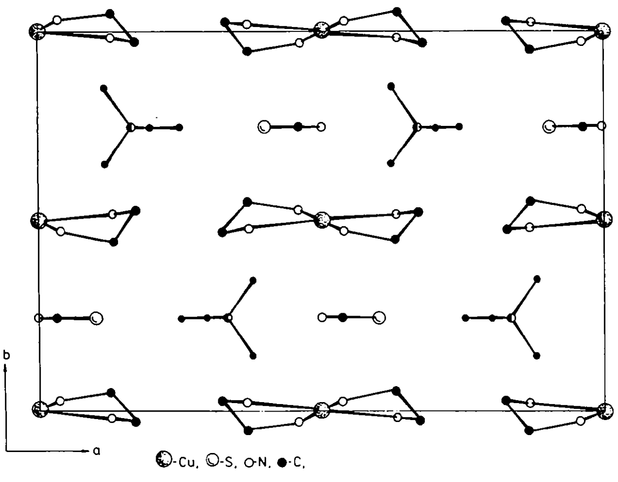

Fig. 1. Packing of the molecules projected along **c**.

Discussion. Atomic coordinates are listed in Table 1.* Table 2 gives the bond distances and angles. The crystal structure (Fig. 1) consists of $[\mathrm{Cu(en)_2}]^{2+}$ cations with four N atoms from ethylenediamine ligands in an approximately square-planar configuration, the isothiocyanate groups axial to the $\mathrm{CuN_4}$ plane, and $\mathrm{BF_4^-}$ anions. The isothiocyanate thus forms a bridging unit between the $[\mathrm{Cu(en)_2}]^{2+}$ cations and gives rise to an infinite chain structure of tetragonally distorted $\mathrm{CuN_4N_2}$ octahedral units. The $[\mathrm{Cu(en)_2}]^{2+}$ units have crystallographic symmetry $\bar{1}$, while the isothiocyanate groups and tetrafluoroborate ion lie on mirror planes at $y = 0{\cdot}25$ and $0{\cdot}75$.

The Cu—N1(en) and Cu—N2(en) interatomic distances are 2·018 (4) and 2·009 (4) Å, respectively. These values are comparable with those found for $[\mathrm{Cu(NCS)_2(en)_2}]$ (Brown & Lingafelter, 1964), $[\mathrm{Cu(NCS)(en)_2}]\mathrm{ClO_4}$ (Cannas, Carta & Marongiu, 1973) and $[\mathrm{Cu(NCS)(en)_2}]\mathrm{Br}$ (Pervuchina, Podberezskaja & Kiričenko, 1982), where the average Cu—N(en) distances range from 1·99 to 2·03 Å. The Cu—N(NCS) distance in $[\mathrm{Cu(NCS)(en)_2}]\mathrm{BF_4}$ is 2·720 (2) Å and the Cu—N—C(NCS) angle is 96·0 (5)°, in agreement with corresponding values found in $[\mathrm{Cu(NCS)(en)_2}]\mathrm{ClO_4}$ and $[\mathrm{Cu(NCS)(en)_2}]\mathrm{Br}$ cited above. The crystal structure of the title compound demonstrates that the exchange of one NCS group in $[\mathrm{Cu(NCS)_2(en)_2}]$ (Brown & Lingafelter, 1964) by anions X ($X = \mathrm{Cl^-}$, $\mathrm{Br^-}$, $\mathrm{ClO_4^-}$, $\mathrm{BF_4^-}$, $\mathrm{NO_3^-}$) leads to a different orientation of the remaining isothiocyanate in the coordination polyhedron of the Cu atom.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44472 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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