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Key indicators

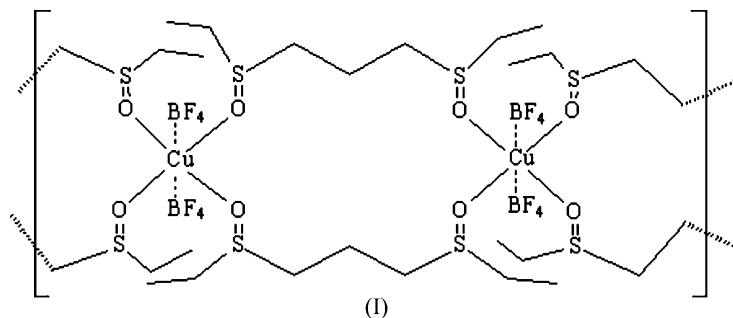
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.042
 wR factor = 0.117
Data-to-parameter ratio = 15.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[bis(tetrafluoroborato)copper(II)]-
bis[μ -1,3-bis(ethylsulfinyl)propane- $\kappa^2\text{O}:\text{O}'$]]**

The title complex, $[\text{Cu}(\text{BF}_4)_2(\text{C}_7\text{H}_{16}\text{O}_2\text{S}_2)_2]_n$, is isostructural with the perchlorate analog [Li *et al.* (2005). *Cryst. Growth Des.* **5**, 1919–1932], both having a double-bridging one-dimensional chain structure containing sixteen-membered macrocyclic units. Each Cu atom lies on a crystallographic inversion center

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Comment

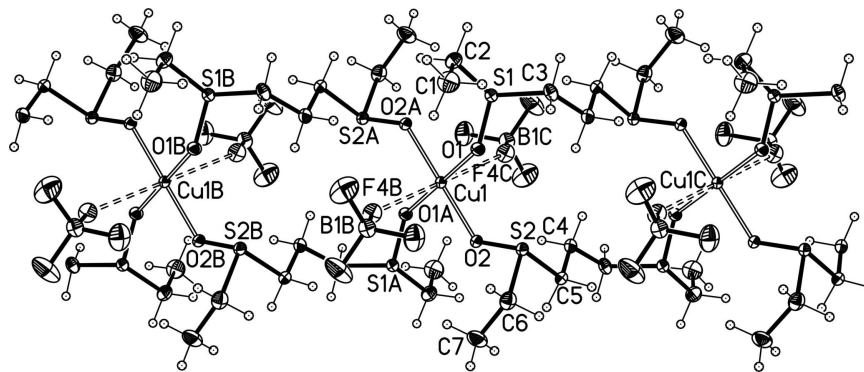
In recent years, we have been focusing on the investigation of flexible disulfoxide metal complexes (Li *et al.*, 2004, 2005). As part of these efforts, we report here the crystal structure of a copper(II) complex $[\text{Cu}(L)_2(\text{BF}_4)_2]_n$, (I), where L is 1,3-bis(ethylsulfinyl)propane, which is isostructural with the perchlorate analog reported by us (Li *et al.*, 2005), having a double-bridging one-dimensional chain structure containing sixteen-membered macrocyclic units (Fig. 1). Selected geometric parameters are listed in Table 1.



Each copper(II) center, located on a crystallographic inversion center, is in a tetragonally elongated octahedral coordination environment formed by four O atoms of distinct L ligands in the equatorial plane and two F atoms of BF_4^- in the axial positions. The Cu–F distance is 2.575 (2) Å, which should be considered as a weak coordination. In (I), the intramolecular Cu...Cu distance is 7.767 (2) Å. In the crystal structure of (I), all the chains are arranged parallel to the crystallographic a -axis direction.

Experimental

The ligand 1,3-bis(ethylsulfinyl)propane (L) was synthesized according to the method reported by Zhang *et al.* (1995). Single crystals of (I) suitable for X-ray analysis were obtained by diffusing an acetone solution (4 ml) of $\text{Cu}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$ (35 mg, 0.1 mmol) into a chloroform solution (4 ml) of L (39 mg, 0.2 mmol) using diethoxyethane (3 ml) as interlayer and dehydrating reagent at room


Figure 1

Part of the polymeric chain of (I), showing 20% probability displacement ellipsoids and the atomic numbering. Atoms labeled with the suffixes A, B and C are generated by the symmetry operations $(-x, 1 - y, -z)$, $(x - 1, y, z)$ and $(1 - x, 1 - y, -z)$, respectively.

temperature. After 14 d, blue crystals were collected. Yield: 48%. Analysis calculated for $C_{14}H_{32}CuB_2F_8O_4S_4$: C 26.71, H 5.13%; found: C 26.56, H 5.21%. IR (cm^{-1}): 3430 (*m*), 2934(*m*), 1635 (*w*), 1449 (*m*), 1411 (*w*), 1382 (*w*), 1060 (*s*), 982 (*s*), 952 (*s*), 522 (*m*). In the IR spectrum, the strong S=O stretching vibration at 982 cm^{-1} is lower than that of the free ligand (1019 cm^{-1}) (Li *et al.*, 2005), indicating that O atoms of *L* coordinate to metal ions.

Crystal data

$[Cu(BF_4)_2(C_7H_{16}O_2S_2)_2]$
 $M_r = 629.80$
 Monoclinic, $P2_1/n$
 $a = 7.767\text{ (3) \AA}$
 $b = 11.091\text{ (5) \AA}$
 $c = 15.094\text{ (7) \AA}$
 $\beta = 96.074\text{ (8)^\circ}$
 $V = 1293.0\text{ (10) \AA}^3$
 $Z = 2$

$D_x = 1.617\text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 1640 reflections
 $\theta = 2.9\text{--}26.5^\circ$
 $\mu = 1.24\text{ mm}^{-1}$
 $T = 293\text{ (2) K}$
 Block, blue
 $0.22 \times 0.18 \times 0.18\text{ mm}$

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{\min} = 0.762$, $T_{\max} = 0.835$
 6471 measured reflections

2408 independent reflections
 2109 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$
 $\theta_{\text{max}} = 25.5^\circ$
 $h = -6 \rightarrow 9$
 $k = -13 \rightarrow 12$
 $l = -18 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.117$
 $S = 1.03$
 2408 reflections
 151 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0799P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.59\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.65\text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu1—O1	1.931 (2)	S1—O1	1.5284 (19)
Cu1—O2	1.9411 (17)	S2—O2	1.5331 (18)
O1—Cu1—O1 ⁱ	180	O1—S1—C2	105.67 (14)
O1—Cu1—O2 ⁱ	87.50 (8)	O2—S2—C5	103.52 (12)
O1—Cu1—O2	92.50 (8)	O2—S2—C6	104.61 (13)
O2 ⁱ —Cu1—O2	180	C5—S2—C6	99.74 (14)
O1—S1—C3	101.33 (13)		

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

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.96 or 0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.5$ or 1.2 times $U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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References

- Bruker (1998). SMART (Version 5.051), SAINT (Version 5.01), SADABS (Version 2.03) and SHELXTL (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
- Li, J.-R., Bu, X.-H. & Zhang, R.-H. (2004). *Inorg. Chem.* **43**, 237–244.
- Li, J.-R., Bu, X.-H., Zhang, R.-H. & Ribas, J. (2005). *Cryst. Growth Des.* **5**, 1919–1932.
- Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.
- Zhang, R.-H., Zhan, Y.-L. & Chen, J.-T. (1995). *Synth. React. Inorg. Met.-Org. Chem.* **25**, 283–292.