Crystal structure of bis(tetrafluorophthlato-κO)(2,2′-bipyridine-$\kappa^2 N,N'$)copper(II), $Cu(C_8HF_4O_4)_2(C_{10}H_8N_2)$

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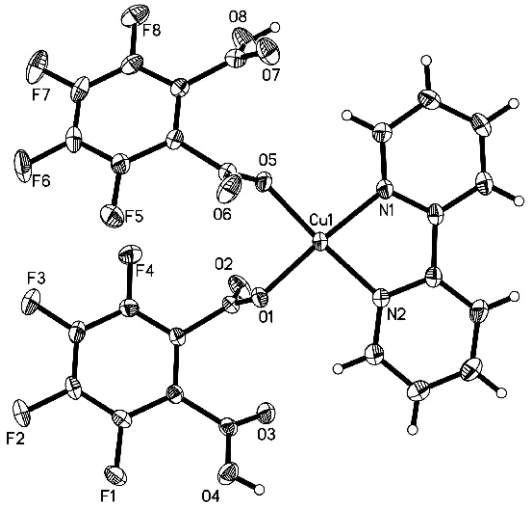

Abstract

$C_{26}H_{10}CuF_8N_2O_8$, triclinic, $P\bar{1}$ (no. 2), a = 9.720(1) Å, b = 11.608(1) Å, c = 12.719(2) Å, α = 68.273(1)°, β = 72.623(1)°, γ = 81.361(1)°, V = 1271.0 Å^3, Z = 2, $R_{gt}(F)$ = 0.031, $wR_{ref}(F^2)$ = 0.083, T = 296 K.

Source of material

The mixture of $Cu(OAc)_2 \cdot H_2O$ (20.0 mg, 0.1 mmol) and tetrafluorophthlic acid (23.6 mg, 0.1 mmol), 2,2′-bipyridine (31.2 mg, 0.2 mmol) were added to a H_2O solution (15 ml) in a Teflon lined stainless steel reactor. The mixture was heated at 433 K for 3 days, and then slowly cooled down to room temperature for crystallization of the blue crystals of the title compound.

Discussion

In recent years, the rational design of coordination polymers based on multitopic or flexible bridging ligands as linkers and metal centers as connectors, represents one of the most rapidly developing fields owing to their potential as functional materials with electronic, magnetic, optical and catalytic applications [1-9]. It is well known that organic ligands play a crucial role in the design and construction of desirable frameworks. The changes in symmetry flexibility and length of organic ligands can result in a remarkable class of material bearing diverse architectures and functions [10-14]. Phthalic acid and its derivatives present versatile coordination modes that may yield predetermined networks.

In the crystal structure of the title compound, the asymmetric unit consists of one Cu(II) ion, two tetrafluorophthlate and one 2,2′-bipyridine (bipy) ligand. The copper(II) ion is four-coordinated by two N atoms from a chelating bipy and two O atoms from the deprotonated 1-carboxyl groups of two tetrafluorophthlate ligands, forming a slightly distorted parallelogram. The bond angles around central Cu(II) ion are 89.32(7)°, 94.55(7)°, 94.70(7)°, 81.47(8)°, adding up to 360.04°. The bond lengths are d(Cu—N) = 1.983(2) Å and 1.974(2) Å, d(Cu—O) = 1.946(2) Å and 1.949(2) Å. In the complex, there exist inter-molecular hydrogen bonds: d(O4–H4···O6) = 2.542(2) Å and d(O8–H8···O2) = 2.558(3) Å between two carboxyl of tetrafluorophthlate. An extended two-dimensional network of hydrogen bonds contributes to the stability of the structure.

Table 1. Data collection and handling.

Crystal:	blue block, size 0.17 × 0.25 × 0.28 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	9.75 cm^{-1}
Diffractometer, scan mode:	Bruker SMART Apex II, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9702, 4682
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3895
$N(param)_{refined}$:	408
Programs:	SHELXS-97, SHELXL-97, SHELXTL [15]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(4)	2*i*	0.2787	–0.1312	0.7461	0.071
H(8)	2*i*	0.6446	0.1562	–0.2322	0.104
H(18)	2*i*	0.9663	–0.3557	0.1752	0.062
H(19)	2*i*	1.0545	–0.2615	–0.0260	0.072
H(20)	2*i*	0.9445	–0.0778	–0.1220	0.069
H(21)	2*i*	0.7564	0.0118	–0.0145	0.059
H(23)	2*i*	0.8579	–0.4372	0.3704	0.064
H(24)	2*i*	0.7400	–0.4981	0.5693	0.076
H(25)	2*i*	0.5596	–0.3693	0.6376	0.067
H(26)	2*i*	0.4967	–0.1861	0.5065	0.056

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	2*i*	0.58853(3)	–0.04879(2)	0.24322(2)	0.0343(2)	0.0314(2)	0.0338(2)	0.0100(1)	–0.0079(1)	–0.0116(1)
N(1)	2*i*	0.7483(2)	–0.1166(2)	0.1400(2)	0.035(1)	0.033(1)	0.036(1)	0.0058(8)	–0.0092(9)	–0.0148(8)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(2)	2*i*	0.6353(2)	–0.2026(2)	0.3639(2)	0.033(1)	0.033(1)	0.035(1)	0.0037(8)	–0.0086(9)	–0.0112(8)
O(1)	2*i*	0.4262(2)	0.0028(2)	0.3523(1)	0.0315(9)	0.0428(9)	0.0398(9)	0.0099(7)	–0.0090(7)	–0.0180(8)
O(2)	2*i*	0.2498(2)	–0.0595(2)	0.3083(2)	0.047(1)	0.071(1)	0.064(1)	0.0002(9)	–0.0076(9)	–0.050(1)
O(3)	2*i*	0.2463(2)	–0.1626(2)	0.5884(2)	0.056(1)	0.037(1)	0.046(1)	0.0080(8)	–0.0160(9)	–0.0182(8)
O(4)	2*i*	0.2428(2)	–0.0649(2)	0.7108(2)	0.061(1)	0.042(1)	0.047(1)	0.0081(9)	–0.0315(9)	–0.0148(8)
O(5)	2*i*	0.5543(2)	0.1007(1)	0.1168(1)	0.050(1)	0.0305(9)	0.0369(9)	0.0117(7)	–0.0150(8)	–0.0135(7)
O(6)	2*i*	0.6292(2)	0.2453(2)	0.1619(2)	0.071(1)	0.042(1)	0.062(1)	0.0032(9)	–0.045(1)	–0.0115(9)
O(7)	2*i*	0.7369(2)	0.2374(2)	–0.1315(2)	0.041(1)	0.075(1)	0.063(1)	0.007(1)	–0.0170(9)	–0.039(1)
O(8)	2*i*	0.5757(2)	0.1934(2)	–0.2013(2)	0.046(1)	0.104(2)	0.092(2)	0.003(1)	–0.016(1)	–0.076(2)
F(1)	2*i*	0.0300(2)	0.1080(1)	0.7052(1)	0.0424(8)	0.0590(9)	0.0383(8)	0.0035(7)	–0.0045(6)	–0.0264(7)
F(2)	2*i*	–0.0853(2)	0.3099(2)	0.5699(2)	0.061(1)	0.0526(9)	0.072(1)	0.0238(8)	–0.0107(9)	–0.0366(8)
F(3)	2*i*	–0.0249(2)	0.3590(1)	0.3358(2)	0.073(1)	0.0438(9)	0.066(1)	0.0216(8)	–0.0302(9)	–0.0094(8)
F(4)	2*i*	0.1480(2)	0.2026(1)	0.2379(1)	0.070(1)	0.0575(9)	0.0349(8)	0.0042(8)	–0.0191(7)	–0.0131(7)
F(5)	2*i*	0.3509(2)	0.3734(2)	0.1920(1)	0.071(1)	0.062(1)	0.0447(9)	0.0101(8)	–0.0120(8)	–0.0297(8)
F(6)	2*i*	0.1767(2)	0.5261(2)	0.0691(2)	0.066(1)	0.064(1)	0.103(2)	0.0360(9)	–0.024(1)	–0.045(1)
F(7)	2*i*	0.2117(2)	0.5489(2)	–0.1578(2)	0.081(1)	0.051(1)	0.105(2)	0.0206(9)	–0.066(1)	–0.014(1)
F(8)	2*i*	0.4264(2)	0.4201(2)	–0.2605(1)	0.087(1)	0.061(1)	0.0411(9)	–0.0118(9)	–0.0336(9)	–0.0050(7)
C(1)	2*i*	0.1882(2)	0.0722(2)	0.4205(2)	0.028(1)	0.033(1)	0.035(1)	0.0020(9)	–0.008(1)	–0.016(1)
C(2)	2*i*	0.1585(2)	0.0463(2)	0.5424(2)	0.025(1)	0.034(1)	0.034(1)	0.0004(9)	–0.0087(9)	–0.014(1)
C(3)	2*i*	0.0655(2)	0.1284(2)	0.5897(2)	0.031(1)	0.043(1)	0.032(1)	–0.002(1)	–0.004(1)	–0.019(1)
C(4)	2*i*	0.0039(3)	0.2323(2)	0.5213(2)	0.035(1)	0.041(1)	0.052(2)	0.011(1)	–0.009(1)	–0.026(1)
C(5)	2*i*	0.0332(3)	0.2571(2)	0.4033(2)	0.041(1)	0.032(1)	0.050(2)	0.008(1)	–0.017(1)	–0.011(1)
C(6)	2*i*	0.1230(3)	0.1757(2)	0.3546(2)	0.038(1)	0.042(1)	0.033(1)	0.001(1)	–0.010(1)	–0.013(1)
C(7)	2*i*	0.2963(3)	–0.0042(2)	0.3555(2)	0.036(1)	0.036(1)	0.031(1)	0.004(1)	–0.005(1)	–0.014(1)
C(8)	2*i*	0.2212(2)	–0.0714(2)	0.6154(2)	0.024(1)	0.040(1)	0.033(1)	–0.001(1)	–0.0039(9)	–0.013(1)
C(9)	2*i*	0.4791(2)	0.3073(2)	0.0326(2)	0.035(1)	0.029(1)	0.036(1)	0.0026(9)	–0.014(1)	–0.010(1)
C(10)	2*i*	0.4973(2)	0.3184(2)	–0.0843(2)	0.036(1)	0.030(1)	0.034(1)	–0.003(1)	–0.011(1)	–0.009(1)
C(11)	2*i*	0.4078(3)	0.4022(2)	–0.1465(2)	0.052(2)	0.036(1)	0.037(1)	–0.008(1)	–0.021(1)	–0.005(1)
C(12)	2*i*	0.3000(3)	0.4718(2)	–0.0961(3)	0.053(2)	0.032(1)	0.064(2)	0.007(1)	–0.034(1)	–0.007(1)
C(13)	2*i*	0.2821(3)	0.4606(2)	0.0177(3)	0.044(2)	0.035(1)	0.067(2)	0.012(1)	–0.018(1)	–0.022(1)
C(14)	2*i*	0.3732(3)	0.3809(2)	0.0803(2)	0.048(2)	0.035(1)	0.040(1)	0.004(1)	–0.012(1)	–0.016(1)
C(15)	2*i*	0.5636(3)	0.2102(2)	0.1103(2)	0.038(1)	0.035(1)	0.032(1)	0.006(1)	–0.010(1)	–0.010(1)
C(16)	2*i*	0.6178(3)	0.2459(2)	–0.1418(2)	0.041(1)	0.042(1)	0.034(1)	–0.006(1)	–0.007(1)	–0.012(1)
C(17)	2*i*	0.8090(2)	–0.2253(2)	0.1957(2)	0.032(1)	0.032(1)	0.043(1)	0.006(1)	–0.014(1)	–0.019(1)
C(18)	2*i*	0.9242(3)	–0.2811(3)	0.1356(2)	0.049(2)	0.048(2)	0.054(2)	0.019(1)	–0.011(1)	–0.023(1)
C(19)	2*i*	0.9764(3)	–0.2252(3)	0.0158(3)	0.050(2)	0.062(2)	0.056(2)	0.017(1)	0.002(1)	–0.028(2)
C(20)	2*i*	0.9121(3)	–0.1158(3)	–0.0411(2)	0.064(2)	0.057(2)	0.039(2)	0.008(2)	0.002(1)	–0.019(1)
C(21)	2*i*	0.7991(3)	–0.0633(2)	0.0237(2)	0.057(2)	0.042(1)	0.038(1)	0.011(1)	–0.007(1)	–0.011(1)
C(22)	2*i*	0.7430(2)	–0.2764(2)	0.3241(2)	0.035(1)	0.030(1)	0.043(1)	0.005(1)	–0.013(1)	–0.015(1)
C(23)	2*i*	0.7839(3)	–0.3869(2)	0.3990(2)	0.063(2)	0.038(2)	0.054(2)	0.017(1)	–0.020(1)	–0.015(1)
C(24)	2*i*	0.7141(4)	–0.4229(3)	0.5176(3)	0.079(2)	0.042(2)	0.052(2)	0.012(2)	–0.020(2)	–0.001(1)
C(25)	2*i*	0.6068(3)	–0.3472(3)	0.5581(3)	0.062(2)	0.049(2)	0.041(2)	0.002(1)	–0.010(1)	–0.002(1)
C(26)	2*i*	0.5698(3)	–0.2378(2)	0.4791(2)	0.043(2)	0.044(2)	0.045(2)	0.006(1)	–0.007(1)	–0.012(1)

References

1. Ma, L. F.; Wang, L. Y.; Wang, Y. Y.; Du, M.; Wang, J. G.: Synthesis, Structure and Properties of Mn(II) Coordination Frameworks based on *R*-isophthalate (*R*= -CH_3 or -$C(CH_3)_3$) and Various Dipyridyl-type Co-ligands. Cryst. Eng. Comm. **11** (2009) 109-117.
2. Furukawa, H.; Yaghi, O. M.: Storage of Hydrogen, Methane, and Carbon Dioxide in Highly Porous Covalent Organic Frameworks for Clean Energy Applications. J. Am. Chem. Soc. **131** (2009) 8875-8883.
3. Braverman, M. A.; Staples, R. J.; Supkowski, R. M.; LaDuca, R. L.: Effect of Pendant Arm Position and Length on the Structure and Properties of Nichel Aromatic Dicarboxylate Coordination Polymers Incorporating a Kinked Organodiimine. Polyhedron **27** (2008) 2291-2300.
4. Han, M. L.; Ling, X. L.; Wang, J. G.; Mi, L. W.: Crystal Structure of *cis*-diaquabis(1,10-phenanthroline)zinc(II) bis(3-amino-4-chlorobenzenesulphonate) dihydrate, $[(Zn(H_2O)_2(C_{12}H_8N_2)_2](H_2NC_6H_3ClSO_3)_2 \cdot 2H_2O$. Z. Kristallogr. NCS **225** (2010) 410-412.
5. Ma, L. F.; Wang, L. Y.; Wang, J. G.; Wang, Y. F.; Feng, X.: Two Novel Three-Dimensional Lead(II) Coordination Polymers Involving 16-Membered Rings: $[Pb_2(Bs\text{-}glu)_2(bipy)_2]$ and $[Pb_2(Bs\text{-}glu)_2(phen)_2]$. Z. Anorg. Allg. Chem. **632** (2006) 487-490.
6. Mi, L. W.; Han, M. L.; Li, D. P.; Chen, W. H.; Zheng, Z.: A Novel Two-Dimensional Cadmium Polymeric Aminonaphthalene Sulfonate and its Application in the Synthesis of CdS Materials. Z. Anorg. Allg. Chem. **634** (2008) 373-376.
7. Furukawa, H.; Yaghi, O. M.: Storage of Hydrogen, Methane, and Carbon Dioxide in Highly Porous Covalent Organic Frameworks for Clean Energy Applications. J. Am. Chem. Soc. **131** (2009) 8875-8883.
8. Du, Z. Y.; Li, X. L.; Liu, Q. Y.; Mao, J. G.: Novel Cadmium(II) Phosphonatophenylsulfonate Cluster Compounds: Syntheses, Structures, and Luminescent Properties. Cryst. Growth Des. **7** (2007) 1501-1507.
9. Liu, G. X.; Huang, Y. Q.; Chu, Q.; Okamura, T.; Sun, W. Y.: Effect of N-Donor Ancillary Ligands on Supramolecular Architectures of a Series of Zinc(II) and Cadmium(II) Complexes with Flexible Tricarboxylate. Cryst. Growth Des. **8** (2008) 3233-3245.
10. Braverman, M. A.; LaDuca, R. L.: Luminescent Two- and Three-Dimensional Zinc Coordination Polymers Containing Isomers of Phenylenediacetate and a Kinked Tethering Organodiimine. Cryst. Growth Des. **7** (2007) 2343-2351.
11. Mi, L. W.; Han, M. L.; Li, D. P.; Chen, W. H.; Zheng, Z.: A Novel Two-Dimensional Cadmium Polymeric Aminonaphthalene Sulfonate and its Application in the Synthesis of CdS Materials. Z. Anorg. Allg. Chem. **634** (2008) 373-376.
12. Ma, L. F.; Wang, L. Y.; Wang, Y. Y.; Batten, S. R.; Wang, J. G.: Self-Assembly of a Series of Cobalt(II) Coordination Polymers Constructed from H_2tbip and Dipyridyl-Based Ligands. Inorg. Chem. **48** (2009) 915-924.
13. Yang, F.; Ren, Y. X.; Li, D. S.; Fu, F.; Qi, G. C.; Wang, Y. Y.: 1D Zigzag Chain and 0D Monomer Cd(II)/Zn(II) Compounds Based on Flexible Phenylenediacetic Ligand: Synthesis, Crystal Structure and Fluorescent Properties. J. Mol. Struct. **892** (2008) 283-288.
14. Dalrymple, S. A.; Shimizu, G. K. H.: Selective guest inclusion in a non-porous H-bonded host. Chem. Comm. (2006) 956-958.
15. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.