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(μ-Naphthalene-1,5-disulfonato-$\kappa^2O^1:O^5$)bis[triaqua(glycinato-κ^2N,O)-copper(II)]

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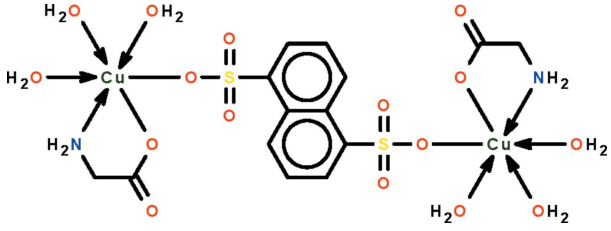
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.073; data-to-parameter ratio = 15.8.

In the title compound, $[Cu_2(C_2H_4NO_2)_2(C_{10}H_6O_6S_2)(H_2O)_6]$, the naphthalenedisulfonate group lies on a center of inversion and bridges two glycinate-chelated Cu^{II} atoms. The Cu^{II} atom exists in a $CuNO_4$ square-pyramidal geometry that is distorted towards an octahedron owing to a long Cu—$O_{sulfonate}$ bond [2.636 (2) Å]. In the crystal, extensive N—H···O and O—H···O hydrogen bonds link adjacent molecules into a three-dimensional network

Related literature

For a review of metal arenesulfonates, see: Cai (2004).



Experimental

Crystal data

$[Cu_2(C_2H_4NO_2)_2(C_{10}H_6O_6S_2)(H_2O)_6]$
M_r = 669.57
Monoclinic, $P2_1/c$
a = 5.802 (3) Å
b = 11.341 (6) Å
c = 17.613 (8) Å
β = 99.793 (18)°
V = 1142.1 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.13 mm^{-1}
T = 293 K
0.38 × 0.26 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.498, T_{max} = 0.688
10939 measured reflections
2615 independent reflections
2482 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.073
S = 1.07
2615 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2^{i}	0.84	2.02	2.741 (2)	143
O1w—H12···O5^{ii}	0.84	2.10	2.785 (2)	139
O2w—H21···O4^{iii}	0.84	2.00	2.773 (2)	152
O2w—H22···O4^{iv}	0.84	2.02	2.823 (2)	158
O3w—H31···O2^{ii}	0.84	1.91	2.676 (2)	151
O3w—H32···O3^{iv}	0.84	1.93	2.691 (2)	150
N1—H1···O5	0.88	2.53	3.079 (3)	121
N1—H2···O2^{ii}	0.88	2.50	3.194 (3)	137

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5523).

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Acta Cryst. (2012). E**68**, m730 [doi:10.1107/S1600536812019332]

(*μ*-Naphthalene-1,5-disulfonato-κ^2O^1:O^5)bis[triaqua(glycinato-κ^2N,O)copper(II)]

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S1. Comment

Metal arenesulfonates are generally crystalline compounds; in some, the metal is connected to the arenesulfonate by a covalent bond whereas in others, the arenesulfonate interacts indirectly with the metal center in an outer-sphere type of coordination (Cai, 2004). In the title compound (Scheme I), the Cu^{II} atom exists in a $CuNO_4$ square-pyramidal geometry that is distorted towards an octahedron owing to the long $Cu–O_{sulfonate}$ bond (2.636 (2) Å). The atom lies above the square plane (r.m.s. deviation 0.082 Å) and the apical water molecule lies 2.371 (2) Å above the plane (Fig.1). Extensive N–H···O and O–H···O hydrogen bonds link adjacent molecules into a three-dimensional network (Table 1).

S2. Experimental

Dicopper carbonate dihydroxide (1 mmol, 221 mg), glycine (2 mmol, 150 mg) 1,5-naphthalenedisulfonic acid tetrahydrate (2 mmol, 720 mg) were dissolved in water (10 ml). The solution was heated for 5 h and then filtered. Blue crystals separated from the solution after several days.

S3. Refinement

H-atoms were placed in calculated positions (C–H 0.93–0.97, N–H 0.88, O–H 0.84 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(*C*,*N*,*O*).

The (2 2 3) reflection was omitted owing to bad disagreement.

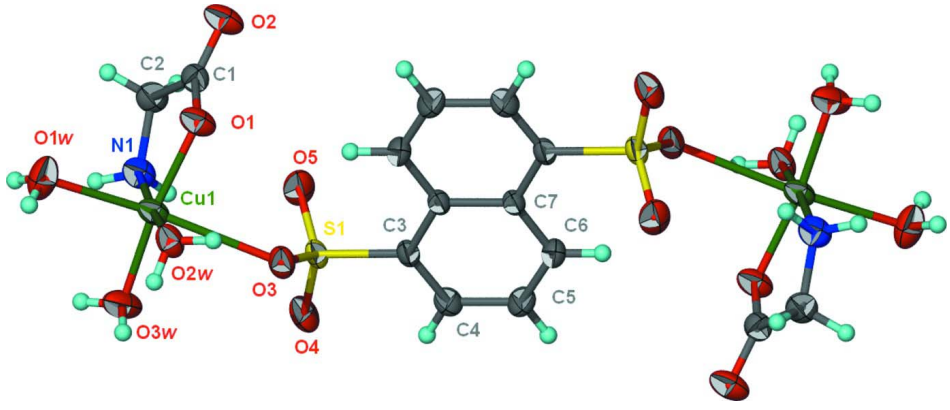

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. Symmetry-related atoms are not labeled.

(μ-Naphthalene-1,5-disulfonato-κ²O¹:O⁵)bis[triaqua(glycinato-κ²N,O)copper(II)]

Crystal data

$[Cu_2(C_2H_4NO_2)_2(C_{10}H_6O_6S_2)(H_2O)_6]$
$M_r = 669.57$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.802$ (3) Å
$b = 11.341$ (6) Å
$c = 17.613$ (8) Å
$\beta = 99.793$ (18)°
$V = 1142.1$ (9) Å^3
$Z = 2$
$F(000) = 684$
$D_x = 1.947$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10177 reflections
$\theta = 3.6$–27.5°
$\mu = 2.13$ mm^{-1}
$T = 293$ K
Prism, blue
0.38 × 0.26 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.498$, $T_{max} = 0.688$
10939 measured reflections
2615 independent reflections
2482 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.6°$
$h = -7 \rightarrow 6$
$k = -14 \rightarrow 14$
$l = -21 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.073$
$S = 1.07$
2615 reflections
166 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.6921P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.35965 (4)	0.51409 (2)	0.341914 (12)	0.02354 (9)
S1	0.70836 (8)	0.73372 (4)	0.44741 (2)	0.02159 (11)
O1	0.1995 (2)	0.64747 (12)	0.28644 (8)	0.0287 (3)
O2	0.2226 (3)	0.77425 (13)	0.19250 (8)	0.0343 (3)
O1w	0.1638 (3)	0.37202 (15)	0.26192 (9)	0.0397 (4)
H11	0.0956	0.3256	0.2879	0.060*
H12	0.2599	0.3342	0.2407	0.060*
O2w	0.1040 (3)	0.50030 (11)	0.40277 (8)	0.0265 (3)
H21	0.0939	0.5633	0.4271	0.040*
H22	0.1325	0.4441	0.4340	0.040*
O3w	0.5629 (3)	0.39956 (14)	0.40378 (8)	0.0369 (3)
H31	0.5917	0.3436	0.3756	0.055*
H32	0.4956	0.3734	0.4389	0.055*

O3	0.4994 (2)	0.66501 (11)	0.45410 (7)	0.0270 (3)
O4	0.9218 (3)	0.67519 (12)	0.48533 (8)	0.0327 (3)
O5	0.7143 (3)	0.76531 (13)	0.36808 (8)	0.0345 (3)
N1	0.5974 (3)	0.53828 (15)	0.27352 (9)	0.0280 (3)
H1	0.7251	0.5697	0.2999	0.034*
H2	0.6344	0.4702	0.2548	0.034*
C1	0.2931 (3)	0.68561 (16)	0.23169 (10)	0.0236 (3)
C2	0.4970 (3)	0.61731 (17)	0.21047 (11)	0.0279 (4)
H2A	0.4444	0.5714	0.1643	0.033*
H2B	0.6160	0.6719	0.1996	0.033*
C3	0.6918 (3)	0.86710 (14)	0.49908 (9)	0.0200 (3)
C4	0.8728 (3)	0.89338 (16)	0.55662 (10)	0.0258 (4)
H4	0.9958	0.8404	0.5691	0.031*
C5	0.8744 (4)	1.00050 (17)	0.59723 (12)	0.0275 (4)
H5	0.9982	1.0174	0.6366	0.033*
C6	0.6966 (3)	1.07958 (16)	0.57946 (10)	0.0239 (3)
H6	0.7024	1.1507	0.6060	0.029*
C7	0.5021 (3)	1.05448 (14)	0.52074 (9)	0.0186 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02546 (13)	0.02263 (14)	0.02478 (14)	0.00560 (8)	0.01067 (9)	0.00671 (8)
S1	0.0305 (2)	0.01428 (19)	0.0221 (2)	0.00179 (15)	0.01062 (16)	−0.00129 (14)
O1	0.0311 (6)	0.0273 (7)	0.0307 (7)	0.0076 (5)	0.0134 (5)	0.0098 (5)
O2	0.0379 (7)	0.0294 (7)	0.0378 (8)	0.0054 (6)	0.0131 (6)	0.0152 (6)
O1w	0.0462 (9)	0.0409 (9)	0.0350 (8)	−0.0102 (7)	0.0153 (7)	−0.0150 (7)
O2w	0.0324 (7)	0.0199 (6)	0.0310 (7)	0.0022 (5)	0.0162 (6)	0.0001 (5)
O3w	0.0491 (8)	0.0386 (8)	0.0266 (7)	0.0221 (7)	0.0162 (6)	0.0093 (6)
O3	0.0362 (7)	0.0196 (6)	0.0270 (6)	−0.0049 (5)	0.0107 (5)	−0.0012 (5)
O4	0.0352 (7)	0.0224 (6)	0.0420 (8)	0.0107 (6)	0.0106 (6)	−0.0027 (6)
O5	0.0529 (9)	0.0306 (7)	0.0241 (6)	−0.0039 (6)	0.0187 (6)	−0.0018 (5)
N1	0.0273 (8)	0.0283 (8)	0.0302 (8)	0.0054 (6)	0.0103 (6)	0.0031 (6)
C1	0.0254 (8)	0.0210 (8)	0.0246 (8)	−0.0019 (7)	0.0046 (7)	0.0005 (6)
C2	0.0325 (9)	0.0286 (9)	0.0247 (8)	0.0019 (7)	0.0113 (7)	0.0021 (7)
C3	0.0266 (8)	0.0145 (7)	0.0202 (7)	0.0013 (6)	0.0076 (6)	−0.0006 (6)
C4	0.0259 (8)	0.0224 (8)	0.0282 (9)	0.0057 (7)	0.0021 (7)	0.0003 (7)
C5	0.0274 (9)	0.0269 (9)	0.0255 (9)	−0.0008 (7)	−0.0033 (7)	−0.0042 (7)
C6	0.0288 (8)	0.0194 (8)	0.0226 (8)	−0.0018 (7)	0.0023 (7)	−0.0037 (6)
C7	0.0239 (8)	0.0142 (7)	0.0183 (7)	0.0001 (6)	0.0051 (6)	0.0000 (6)

Geometric parameters (Å, º)

Cu1—O1	1.9485 (15)	O3w—H32	0.8400
Cu1—O3w	1.9566 (15)	N1—C2	1.468 (2)
Cu1—O2w	1.9783 (16)	N1—H1	0.8800
Cu1—N1	1.9988 (18)	N1—H2	0.8800
Cu1—O1w	2.3081 (17)	C1—C2	1.513 (3)

Cu1—O3	2.636 (2)	C2—H2A	0.9700
S1—O5	1.4486 (15)	C2—H2B	0.9700
S1—O4	1.4626 (15)	C3—C4	1.363 (3)
S1—O3	1.4629 (15)	C3—C7^{i}	1.430 (2)
S1—C3	1.7763 (18)	C4—C5	1.409 (3)
O1—C1	1.261 (2)	C4—H4	0.9300
O2—C1	1.248 (2)	C5—C6	1.362 (3)
O1w—H11	0.8400	C5—H5	0.9300
O1w—H12	0.8400	C6—C7	1.424 (2)
O2w—H21	0.8400	C6—H6	0.9300
O2w—H22	0.8400	C7—C3^{i}	1.430 (2)
O3w—H31	0.8400	C7—C7^{i}	1.434 (3)

O1—Cu1—O3w	170.20 (7)	Cu1—N1—H1	110.0
O1—Cu1—O2w	89.75 (6)	C2—N1—H2	110.0
O3w—Cu1—O2w	94.72 (7)	Cu1—N1—H2	110.0
O1—Cu1—N1	84.86 (6)	H1—N1—H2	108.4
O3w—Cu1—N1	90.81 (7)	O2—C1—O1	123.76 (17)
O2w—Cu1—N1	174.45 (6)	O2—C1—C2	118.17 (16)
O1—Cu1—O1w	95.31 (7)	O1—C1—C2	118.03 (16)
O3w—Cu1—O1w	93.67 (8)	N1—C2—C1	110.61 (15)
O2w—Cu1—O1w	86.50 (6)	N1—C2—H2A	109.5
N1—Cu1—O1w	92.67 (7)	C1—C2—H2A	109.5
O5—S1—O4	113.29 (9)	N1—C2—H2B	109.5
O5—S1—O3	111.43 (9)	C1—C2—H2B	109.5
O4—S1—O3	111.76 (9)	H2A—C2—H2B	108.1
O5—S1—C3	107.21 (9)	C4—C3—C7^{i}	121.37 (15)
O4—S1—C3	105.54 (8)	C4—C3—S1	117.72 (13)
O3—S1—C3	107.12 (8)	C7^{i}—C3—S1	120.89 (13)
C1—O1—Cu1	114.77 (12)	C3—C4—C5	120.24 (16)
Cu1—O1w—H11	109.5	C3—C4—H4	119.9
Cu1—O1w—H12	109.5	C5—C4—H4	119.9
H11—O1w—H12	109.5	C6—C5—C4	120.77 (17)
Cu1—O2w—H21	109.5	C6—C5—H5	119.6
Cu1—O2w—H22	109.5	C4—C5—H5	119.6
H21—O2w—H22	109.5	C5—C6—C7	120.72 (17)
Cu1—O3w—H31	109.5	C5—C6—H6	119.6
Cu1—O3w—H32	109.5	C7—C6—H6	119.6
H31—O3w—H32	109.5	C6—C7—C3^{i}	123.13 (15)
C2—N1—Cu1	108.28 (12)	C6—C7—C7^{i}	119.03 (19)
C2—N1—H1	110.0	C3^{i}—C7—C7^{i}	117.83 (18)

O2w—Cu1—O1—C1	−174.25 (13)	O4—S1—C3—C4	4.06 (16)
N1—Cu1—O1—C1	4.42 (13)	O3—S1—C3—C4	123.29 (15)
O1w—Cu1—O1—C1	−87.80 (14)	O5—S1—C3—C7^{i}	61.24 (16)
O1—Cu1—N1—C2	−13.65 (13)	O4—S1—C3—C7^{i}	−177.71 (14)
O3w—Cu1—N1—C2	175.17 (13)	O3—S1—C3—C7^{i}	−58.48 (16)
O1w—Cu1—N1—C2	81.45 (13)	C7^{i}—C3—C4—C5	−1.1 (3)

Cu1—O1—C1—O2	−175.95 (15)	S1—C3—C4—C5	177.09 (15)
Cu1—O1—C1—C2	6.4 (2)	C3—C4—C5—C6	−0.4 (3)
Cu1—N1—C2—C1	19.48 (19)	C4—C5—C6—C7	1.6 (3)
O2—C1—C2—N1	164.25 (17)	C5—C6—C7—C3^{i}	178.49 (18)
O1—C1—C2—N1	−18.0 (2)	C5—C6—C7—C7^{i}	−1.3 (3)
O5—S1—C3—C4	−116.99 (15)		

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H11···O2^{ii}	0.84	2.02	2.741 (2)	143
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O3*w*—H31···O2^{iii}	0.84	1.91	2.676 (2)	151
O3*w*—H32···O3^{v}	0.84	1.93	2.691 (2)	150
N1—H1···O5	0.88	2.53	3.079 (3)	121
N1—H2···O2^{iii}	0.88	2.50	3.194 (3)	137

Symmetry codes: (ii) −*x*, *y*−1/2, −*z*+1/2; (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*−1, *y*, *z*; (v) −*x*+1, −*y*+1, −*z*+1.