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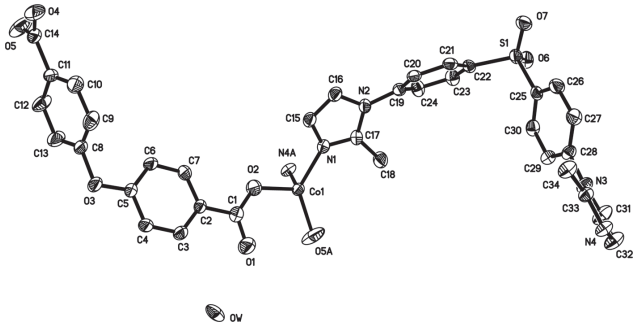
Crystal structure of poly{[μ_2-1,1′-(sulfonylbis(4,1-phenylene))bis(2-methyl-1*H*-imidazole)-κ^2N:N'][μ_2-4,4′-oxydibenzoato-κ^2O:O']cobalt(II)} hemihydrate, $C_{34}H_{27}N_4O_{7.5}SCo$



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Abstract

$C_{34}H_{27}N_4O_{7.5}SCo$, monoclinic, *Cc* (no. 9), $a = 23.7684(16)$ Å, $b = 13.5683(10)$ Å, $c = 10.0223(7)$ Å, $\beta = 94.405(2)°$ $V = 3222.6(4)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0427$, $wR_{ref}(F^2) = 0.0815$, $T = 293(2)$ K.

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A part of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of 4,4′-oxydibenzoic acid (0.2 mmol, 0.052 g), 1,1′-(sulfonylbis(4,1-phenylene))-bis(2-methyl-1*H*-imidazole) (0.2 mmol, 0.074 g), $CoCl_2{\cdot}6(H_2O)$ (0.2 mmol, 0.046 g), and H_2O (20 mL) was stirred for ten minutes. The mixture was transferred in a 25 mL stainless steel reactor with a Teflon liner and heated from 298 to 453 K in 5 h and a constant temperature was maintained at 453 K for 72 h. After cooling to room temperature, pink block crystals were collected in 56.6% yield based on the amounts of Co.

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Table 1: Data collection and handling.

Crystal:	Pink block
Size:	0.24 × 0.20 × 0.17 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.65 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	27.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11094, 5051, 0.045
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3695
$N(param)_{refined}$:	443
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5308(2)	0.7864(3)	0.2261(5)	0.0484(12)
C2	0.48309(16)	0.8393(3)	0.2843(4)	0.0400(10)
C3	0.48486(18)	0.8622(3)	0.4193(5)	0.0509(11)
H3	0.5159	0.8431	0.4754	0.061*
C4	0.44147(19)	0.9128(4)	0.4717(4)	0.0588(13)
H4	0.4433	0.9282	0.5623	0.071*
C5	0.39535(18)	0.9404(4)	0.3888(5)	0.0543(12)
C6	0.3921(2)	0.9173(4)	0.2542(5)	0.0638(15)
H6	0.3607	0.9351	0.1984	0.077*
C7	0.43619(19)	0.8674(4)	0.2041(4)	0.0604(13)
H7	0.4343	0.8522	0.1134	0.073*
C8	0.30971(19)	1.0321(4)	0.3658(5)	0.0524(11)
C9	0.31774(19)	1.1179(4)	0.3033(6)	0.0660(14)
H9	0.3529	1.1483	0.3114	0.079*
C10	0.2739(2)	1.1601(4)	0.2278(5)	0.0623(13)
H10	0.2789	1.2210	0.1879	0.075*
C11	0.22253(19)	1.1143(3)	0.2098(4)	0.0470(11)
C12	0.21585(19)	1.0260(4)	0.2744(6)	0.0713(16)
H12	0.1813	0.9935	0.2642	0.086*
C13	0.2594(2)	0.9854(4)	0.3538(6)	0.0737(16)
H13	0.2544	0.9264	0.3986	0.088*
C14	0.1751(3)	1.1610(6)	0.1254(5)	0.0751(18)
C15	0.56181(17)	0.9080(3)	−0.1749(5)	0.0483(11)
H15	0.5327	0.9292	−0.1251	0.058*
C16	0.57984(17)	0.9550(3)	−0.2827(5)	0.0497(11)
H16	0.5658	1.0135	−0.3202	0.060*
C17	0.63023(17)	0.8203(3)	−0.2427(4)	0.0438(11)
C18	0.6747(2)	0.7434(4)	−0.2466(6)	0.0668(15)
H18A	0.7094	0.7734	−0.2683	0.100*
H18B	0.6633	0.6951	−0.3133	0.100*
H18C	0.6801	0.7121	−0.1607	0.100*

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C19	0.65858(17)	0.9252(3)	−0.4292(4)	0.0417(10)
C20	0.67745(17)	1.0214(3)	−0.4360(4)	0.0430(10)
H20	0.6632	1.0696	−0.3819	0.052*
C21	0.71748(17)	1.0457(3)	−0.5236(4)	0.0444(10)
H21	0.7304	1.1102	−0.5294	0.053*
C22	0.73796(17)	0.9722(3)	−0.6026(4)	0.0427(10)
C23	0.71624(19)	0.8779(4)	−0.6016(4)	0.0530(12)
H23	0.7291	0.8300	−0.6583	0.064*
C24	0.67539(18)	0.8552(4)	−0.5159(5)	0.0532(12)
H24	0.6594	0.7926	−0.5171	0.064*
C25	0.85302(17)	1.0144(3)	−0.5788(4)	0.0423(10)
C26	0.87869(18)	1.1056(4)	−0.5658(5)	0.0550(12)
H26	0.8660	1.1583	−0.6192	0.066*
C27	0.92382(19)	1.1163(3)	−0.4710(5)	0.0547(12)
H27	0.9428	1.1762	−0.4631	0.066*
C28	0.94078(17)	1.0399(3)	−0.3892(4)	0.0431(10)
C29	0.91475(18)	0.9487(3)	−0.4026(5)	0.0474(11)
H29	0.9268	0.8968	−0.3469	0.057*
C30	0.87102(18)	0.9356(4)	−0.4988(4)	0.0502(11)
H30	0.8537	0.8744	−0.5102	0.060*
C31	1.0277(2)	0.9871(4)	−0.2526(6)	0.0673(15)
H31	1.0331	0.9262	−0.2922	0.081*
C32	1.0599(2)	1.0281(4)	−0.1529(6)	0.0651(14)
H32	1.0922	0.9995	−0.1113	0.078*
C33	0.99369(17)	1.1308(3)	−0.2014(4)	0.0431(10)
C34	0.95531(18)	1.2184(3)	−0.1991(5)	0.0568(12)
H34A	0.9169	1.1976	−0.2180	0.085*
H34B	0.9650	1.2651	−0.2654	0.085*
H34C	0.9594	1.2486	−0.1122	0.085*
N1	0.59324(13)	0.8238(2)	−0.1503(3)	0.0415(8)
N2	0.62316(13)	0.8990(3)	−0.3259(3)	0.0431(8)
N3	0.98475(14)	1.0533(3)	−0.2854(4)	0.0494(9)
N4	1.03869(15)	1.1182(3)	−0.1200(4)	0.0495(10)
O1	0.56746(16)	0.7450(3)	0.3015(4)	0.0848(12)
O2	0.53050(14)	0.7865(3)	0.1005(3)	0.0741(10)
O3	0.35362(13)	0.9896(3)	0.4491(3)	0.0808(12)
O4	0.1773(2)	1.2488(4)	0.0959(5)	0.127(2)
O5	0.1342(2)	1.1101(4)	0.0864(5)	0.1077(18)
O6	0.80625(12)	0.9112(2)	−0.7751(3)	0.0576(8)
O7	0.78568(13)	1.0914(3)	−0.7658(3)	0.0618(9)
Co1	0.58385(2)	0.71971(4)	−0.00574(4)	0.04081(15)
S1	0.79523(5)	0.99825(9)	−0.69968(11)	0.0498(3)
H1[a]	0.567(2)	0.695(3)	0.477(3)	0.011(18)*
H2[a]	0.552(2)	0.616(3)	0.570(5)	0.03(2)*
OW[a]	0.5741(3)	0.6682(6)	0.5580(6)	0.075(2)

[a]Occupancy: 0.50.

Experimental details

The U_{iso} values of the hydrogen atoms of parts of carbon group were set to $1.2U_{eq}$(C). Hydrogen atoms of water molecules were located from electron density map. A Flack parameter of 0.012(15) was obtained [2].

Discussion

The research of metal-organic frameworks (MOFs) are significant and unparalleled for their diversified, designable and tailorable structures as well as unique chemical and physical properties. Over the past three decades, MOFs have been paid much attention for their great potential applications in many areas [3–8].

In the title complex, there is one crystallographically independent cobalt(II) ion, one 4,4′-oxydibenzoate, one 1,1′-(sulfonylbis(4,1-phenylene))bis(2-methyl-1*H*-imidazole) and one half of a water molecule. The cobalt(II) is four-coordinated by two O atoms from two 4,4′-oxydibenzoate ligands, and two N atoms from two 1,1′-(sulfonylbis(4,1-phenylene))bis(2-methyl-1H-imidazole) ligands to form a distorted tetrahedron. The distances between Co and the coordinated atoms are: d(Co1—N1) = 2.048(3) Å, d(Co1—N4) = 2.042(4) Å, d(Co1—O2) = 1.942(3) Å, and d(Co1—O5) = 2.080(4) Å, respectively. The Co(II) coordination angles are in the normal range from 91.50(16)° to 135.82(19)°. The Co(II) ions are bridged by 4,4′-oxydibenzoato and 1,1′-(sulfonylbis(4,1-phenylene))bis(2-methyl-1*H*-imidazole) ligands into a 2D-network. The crystal structure is also stabilized by hydrogen bonds.

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