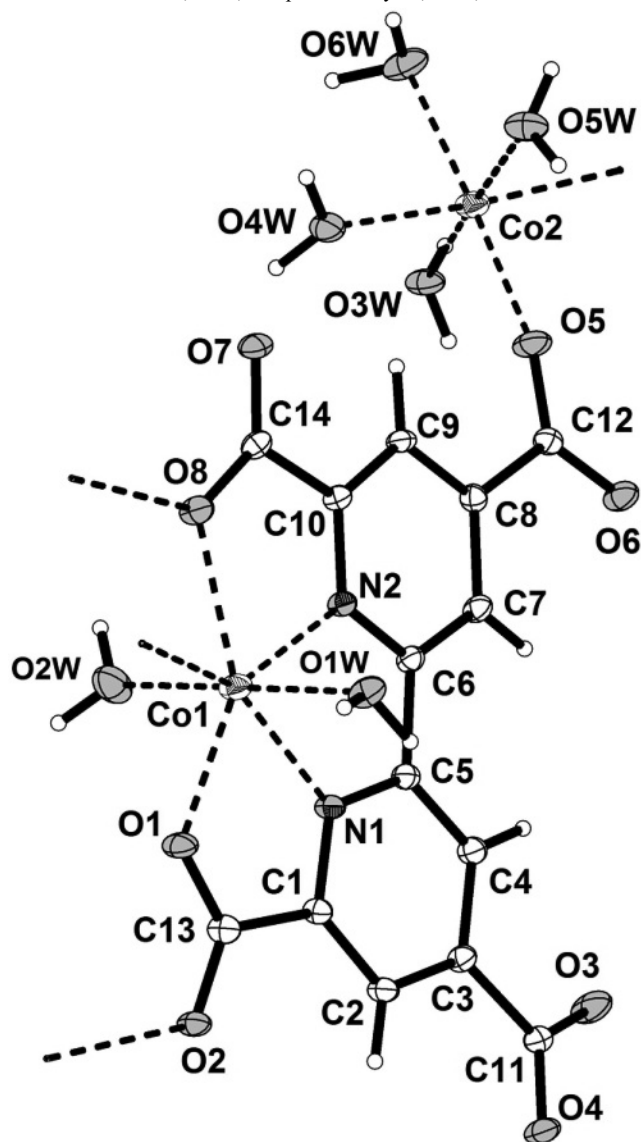


Crystal structure of poly[(μ -2,2'-bipyridine-3,3',5,5'-tetracarboxylato)-hexaaqua-dicobalt(II)], $C_{14}H_{16}Co_2N_2O_{14}$

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Abstract

$C_{14}H_{16}Co_2N_2O_{14}$, monoclinic, $C2/c$ (no. 15), $a = 26.257(3)$ Å, $b = 6.7342(7)$ Å, $c = 21.401(2)$ Å, $\beta = 108.856(1)^\circ$, $V = 3581.0$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0254$, $wR_{\text{ref}}(F^2) = 0.0669$, $T = 296$ K.

Source of material

Tris(2-aminoethyl)amine (0.74 g, 5.1 mmol) and 3-ethoxysalicylaldehyde (2.53 g, 15.2 mmol) in EtOH (30 ml) were stirred for 3 h at room temperature. After removal of the undissolved by filtration, the solvent of the filtrate was evaporated and the residue was recrystallized from a mixture of acetone/pentane at -85°C , to give a yellow solid (2.67 g). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from an ether solution.

Table 1. Data collection and handling.

Crystal:	red blocks, size 0.21×0.32×0.46 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	19.40 cm ⁻¹
Diffractometer, scan mode:	Rigaku R-Axis RAPID, ω
$2\theta_{\text{max}}$:	55.06°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	15038, 4119
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 3506
$N(\text{param})_{\text{refined}}$:	289
Programs:	SHELX [15]

Discussion

Aromatic carboxylic acids have been widely used in the field of coordination chemistry [1–4]. Some of the reasons are that aromatic carboxylic acids have good coordination ability with transition metals, and for their capability of acting as bridging and chelating ligands in various coordination modes [5]. The structural design or modification of coordination polymer frameworks has become a very active field. Because of their intriguing network architecture and packing motifs, and their potential applications in the catalyst, magnetic or molecular sensors [6–9], give rise to a strong interest in the design and synthesis of complexes [10–13]. The 2,2'-bipyridine-3,3',5,5'-tetracarboxylate has already been used as a bridging ligand to prepare the polymeric complex [14]. The asymmetric unit of the structure is shown in Fig. 1. In the title complex two Co atoms are in different environment: Co1 is seven-coordinated by two N atoms, two O atoms from water ligands and three atoms from carboxylate moieties; Co2 is coordinated only by six O atoms: four water ligands and two carboxylate moieties. There are extensive hydrogen bonds in the crystal, which stabilize crystal.

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(11A)	8f	1.0816	−0.0090	0.3911	0.023
H(11B)	8f	1.0808	−0.0017	0.3325	0.023
H(9B)	8f	0.6509	0.3980	0.3037	0.031
H(12A)	8f	0.9736	0.6512	0.3158	0.031
H(12B)	8f	1.0225	0.7307	0.3277	0.031
H(6A)	8f	0.7530	0.4399	0.4671	0.022

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Table 2. continued.

Atom	Site	x	y	z	U _{iso}
H(6B)	8f	0.7004	0.4430	0.4441	0.022
H(7B)	8f	0.7667	0.4253	0.3083	0.025
H(7C)	8f	0.7353	0.2904	0.2720	0.025
H(8A)	8f	0.7454	−0.1536	0.3376	0.025
H(8B)	8f	0.6924	−0.1455	0.3129	0.025

Table 2. continued.

Atom	Site	x	y	z	U _{iso}
H(9C)	8f	0.6351	0.2248	0.2867	0.029
H(2)	8f	1.1828	0.4144	0.5612	0.017
H(4)	8f	1.0405	0.2600	0.5812	0.016
H(7)	8f	0.9527	0.1971	0.5237	0.016
H(9)	8f	0.8453	0.1402	0.3411	0.015

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Co(1)	8f	1.034035(9)	0.32387(4)	0.33885(1)	0.0101(1)	0.0186(1)	0.0085(1)	−0.00202(9)	0.00225(9)	−0.00072(9)
Co(2)	8f	0.724131(9)	0.17856(4)	0.37715(1)	0.0097(1)	0.0223(2)	0.0088(1)	−0.00281(9)	0.00277(9)	−0.0000(1)
N(1)	8f	1.06830(6)	0.3462(2)	0.44787(7)	0.0095(7)	0.0170(8)	0.0105(7)	−0.0018(6)	0.0029(6)	−0.0016(6)
N(2)	8f	0.97160(6)	0.2482(2)	0.38285(7)	0.0103(7)	0.0148(8)	0.0102(7)	−0.0003(6)	0.0025(6)	−0.0006(6)
O(1)	8f	1.11470(5)	0.4409(2)	0.36500(6)	0.0140(6)	0.0280(8)	0.0099(6)	−0.0064(5)	0.0026(5)	−0.0021(5)
O(2)	8f	1.19160(5)	0.5308(2)	0.44297(6)	0.0107(6)	0.0257(7)	0.0110(6)	−0.0044(5)	0.0034(5)	−0.0010(5)
O(3)	8f	1.10956(5)	0.3107(2)	0.69117(7)	0.0157(7)	0.049(1)	0.0120(7)	−0.0023(6)	0.0039(6)	0.0057(6)
O(4)	8f	1.19199(5)	0.3165(2)	0.68114(6)	0.0120(6)	0.0267(8)	0.0118(6)	−0.0008(5)	0.0001(5)	0.0001(5)
O(5)	8f	0.80138(5)	0.0957(2)	0.43124(7)	0.0093(6)	0.0365(8)	0.0157(7)	−0.0023(6)	0.0019(5)	0.0029(6)
O(6)	8f	0.86428(5)	0.0741(2)	0.52973(6)	0.0132(6)	0.0304(8)	0.0118(6)	−0.0006(6)	0.0040(5)	0.0024(6)
O(7)	8f	0.87016(5)	0.1669(2)	0.23148(6)	0.0164(6)	0.0269(8)	0.0114(6)	−0.0070(6)	−0.0008(5)	0.0002(5)
O(8)	8f	0.95461(5)	0.2862(2)	0.25696(6)	0.0121(6)	0.0256(8)	0.0115(6)	−0.0004(5)	0.0047(5)	0.0002(5)
O(1W)	8f	1.06222(5)	0.0130(2)	0.35188(6)	0.0169(6)	0.0251(8)	0.0135(6)	0.0021(6)	0.0027(5)	−0.0012(6)
O(2W)	8f	1.00589(6)	0.6298(2)	0.33158(8)	0.0181(7)	0.0204(8)	0.0395(9)	−0.0003(6)	0.0094(6)	0.0024(6)
O(3W)	8f	0.72805(5)	0.4355(2)	0.43395(6)	0.0128(6)	0.0313(8)	0.0112(6)	−0.0050(6)	0.0036(5)	−0.0038(6)
O(4W)	8f	0.75198(5)	0.3138(2)	0.30677(6)	0.0193(7)	0.0317(8)	0.0111(6)	−0.0089(6)	0.0034(5)	0.0001(6)
O(5W)	8f	0.71899(5)	−0.0849(2)	0.32393(7)	0.0131(6)	0.0290(8)	0.0207(7)	−0.0020(6)	0.0047(5)	−0.0058(6)
O(6W)	8f	0.64647(5)	0.2710(2)	0.32009(7)	0.0158(7)	0.0437(9)	0.0117(7)	0.0021(6)	0.0025(5)	−0.0013(6)
C(1)	8f	1.12019(7)	0.3942(3)	0.47552(9)	0.0112(8)	0.0140(9)	0.0118(8)	−0.0012(7)	0.0038(7)	−0.0017(7)
C(2)	8f	1.14629(7)	0.3862(3)	0.54336(9)	0.0104(8)	0.0170(9)	0.0132(9)	−0.0020(7)	0.0025(7)	−0.0016(7)
C(3)	8f	1.11598(7)	0.3345(3)	0.58386(9)	0.0134(8)	0.0147(9)	0.0105(8)	−0.0002(7)	0.0021(7)	−0.0002(7)
C(4)	8f	1.06165(7)	0.2911(3)	0.55510(9)	0.0117(8)	0.0165(9)	0.0118(8)	−0.0005(7)	0.0043(7)	0.0001(7)
C(5)	8f	1.03928(7)	0.2950(3)	0.48662(9)	0.0106(8)	0.0138(9)	0.0122(8)	−0.0007(7)	0.0030(7)	−0.0001(7)
C(6)	8f	0.98280(7)	0.2448(3)	0.44907(9)	0.0105(8)	0.0143(9)	0.0113(8)	0.0009(7)	0.0029(7)	0.0010(7)
C(7)	8f	0.94393(7)	0.2000(3)	0.47802(9)	0.0130(8)	0.0170(9)	0.0090(8)	0.0005(7)	0.0030(7)	0.0002(7)
C(8)	8f	0.89154(7)	0.1592(3)	0.43771(9)	0.0111(8)	0.0124(9)	0.0134(9)	0.0005(7)	0.0049(7)	0.0006(7)
C(9)	8f	0.87995(7)	0.1657(3)	0.36927(9)	0.0087(7)	0.0162(9)	0.0116(8)	−0.0010(7)	0.0007(6)	0.0000(7)
C(10)	8f	0.92133(7)	0.2110(3)	0.34415(9)	0.0112(8)	0.0137(9)	0.0101(8)	0.0000(7)	0.0020(7)	−0.0006(7)
C(11)	8f	1.14147(7)	0.3196(3)	0.65846(9)	0.0131(8)	0.0165(9)	0.0121(9)	−0.0019(7)	0.0021(7)	0.0008(7)
C(12)	8f	0.84869(7)	0.1061(3)	0.46887(9)	0.0106(8)	0.0155(9)	0.0144(9)	−0.0005(7)	0.0041(7)	0.0006(7)
C(13)	8f	1.14482(7)	0.4585(3)	0.42412(9)	0.0133(8)	0.018(1)	0.0120(8)	−0.0008(7)	0.0057(7)	−0.0029(7)
C(14)	8f	0.91358(7)	0.2220(3)	0.27084(9)	0.0138(8)	0.0153(9)	0.0099(8)	0.0021(7)	0.0026(7)	−0.0008(7)

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