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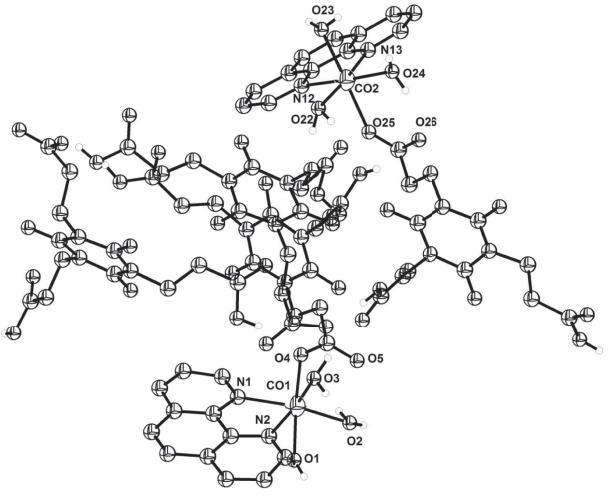
Crystal structure of triaqua-(1,10-phenanthroline)-(dihydrogen-3,3′,3″-(2,4,6-trioxo-1,3,5-triazinane-1,3,5-triyl)tripropanoato) cobalt(II) dihydrogen-3,3′,3″-(2,4,6-trioxo-1,3,5-triazinane-1,3,5-triyl)tripropanoate, $C_{72}H_{82}Co_2N_{16}O_{42}$



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Abstract

$C_{72}H_{82}Co_2N_{16}O_{42}$, triclinic, $P\bar{1}$, $a = 15.7653(19)$ Å, $b = 16.955(2)$ Å, $c = 18.838(2)$ Å, $\alpha = 70.35(2)°$, $\beta = 87.78(2)°$, $\gamma = 63.73(2)°$, $V = 4216.5(8)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0735$, $wR_{ref}(F^2) = 0.1405$, $T = 296(2)$ K.

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The crystal structure is shown in the figure, Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Red, Block, size 0.10×0.20×0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	5.02 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	50.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	22224, 1472
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 7580
$N(param)_{refined}$:	1202
Programs:	Bruker data collection and reduction software [7–9], SHELX [10]

Source of material

A mixture of $Co(NO_3)_2 \cdot 6H_2O$ (0.030 g, 0.1 mmol) 3,3′,3″-(2,4,6-trioxo-1,3,5-triazinane-1,3,5-triyl)tripropanoic acid (TTA) (0.036 g 0.1 mmol), 1,10-phenanthroline (phen) (0.020 g, 0.1 mmol), NaOH (0.2 M, 1.5 mL) and H_2O (10 mL) was stirred for about 30 min. The resulting solution was sealed in a Teflon-lined stainless autoclave and heated to 373 K for 3 days. The bottle was cooled to ambient temperature spontaneously. Red single crystals (about 66%, based on Co input) were recovered by vacuum filtration, drying in air.

Experimental details

The C-bound H atoms were geometrically placed (C—H = 0.93, 0.97 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

The O-bound H atoms were geometrically placed (O—H = 0.82 Å) and refined as riding with $U_{iso}(H) = 1.5U_{eq}(O)$.

Results and discussion

In recent years, extensive efforts have been focused on the rational design and controlled synthesis of coordination polymers, owing to their intriguing topological structures

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1)	2*i*	0.9032	−0.0372	0.1503	0.051
H(2)	2*i*	0.9997	0.0368	0.1219	0.058
H(3)	2*i*	0.9827	0.1392	0.0022	0.057
H(5)	2*i*	0.8960	0.2214	−0.1356	0.062
H(6)	2*i*	0.7822	0.2452	−0.2202	0.073
H(8)	2*i*	0.6444	0.2155	−0.2492	0.092
H(9A)	2*i*	0.5500	0.1430	−0.2045	0.091
H(10)	2*i*	0.5685	0.0569	−0.0772	0.072
H(14A)	2*i*	0.5390	0.1828	0.1887	0.050
H(14B)	2*i*	0.4402	0.1845	0.1759	0.050
H(15A)	2*i*	0.5210	0.2725	0.0574	0.061
H(15B)	2*i*	0.4210	0.2764	0.0466	0.061
H(17A)	2*i*	0.4732	0.5157	0.2154	0.091
H(17B)	2*i*	0.5609	0.4537	0.1833	0.091
H(18A)	2*i*	0.4292	0.6377	0.0982	0.087
H(18B)	2*i*	0.5215	0.5757	0.0700	0.087
H(21A)	2*i*	0.1571	0.4672	0.1588	0.097
H(21B)	2*i*	0.1767	0.5315	0.1936	0.097
H(26A)	2*i*	0.8415	0.1942	0.2263	0.070
H(26B)	2*i*	0.7434	0.2814	0.2185	0.070
H(27A)	2*i*	0.8280	0.2419	0.0920	0.055
H(27B)	2*i*	0.7343	0.3327	0.0872	0.055
H(29A)	2*i*	1.1302	0.3007	0.1911	0.059
H(29B)	2*i*	1.1149	0.2102	0.2187	0.059
H(30A)	2*i*	1.1530	0.2899	0.0725	0.064
H(30B)	2*i*	1.1316	0.2032	0.0964	0.064
H(33A)	2*i*	0.7617	0.6045	0.0631	0.060
H(33B)	2*i*	0.8635	0.5985	0.0707	0.060
H(34A)	2*i*	0.7608	0.5630	0.1949	0.063
H(34B)	2*i*	0.8661	0.5470	0.2062	0.063
H(38A)	2*i*	0.5847	−0.0807	0.4354	0.051
H(38B)	2*i*	0.5555	−0.1453	0.4097	0.051
H(39A)	2*i*	0.5152	0.0411	0.3188	0.049
H(39B)	2*i*	0.4915	−0.0235	0.2887	0.049
H(41A)	2*i*	0.2855	0.2283	0.4365	0.046
H(41B)	2*i*	0.1851	0.2302	0.4385	0.046
H(42A)	2*i*	0.2498	0.3143	0.3058	0.048
H(42B)	2*i*	0.1512	0.3124	0.3049	0.048
H(45A)	2*i*	0.1551	−0.0186	0.4157	0.050
H(45B)	2*i*	0.2470	−0.1037	0.4090	0.050
H(46A)	2*i*	0.1058	0.0412	0.2883	0.053
H(46B)	2*i*	0.2063	−0.0234	0.2714	0.053
H(49)	2*i*	0.3401	0.5863	0.3079	0.075
H(50)	2*i*	0.5047	0.5283	0.3285	0.097
H(51)	2*i*	0.5892	0.4131	0.4419	0.097
H(53)	2*i*	0.5871	0.3065	0.5738	0.101
H(54)	2*i*	0.5016	0.2674	0.6657	0.102
H(56)	2*i*	0.3371	0.2908	0.7103	0.097
H(57)	2*i*	0.1760	0.3626	0.6789	0.099
H(58)	2*i*	0.1091	0.4692	0.5581	0.075
H(62A)	2*i*	0.8355	0.3018	0.3370	0.064
H(62B)	2*i*	0.9359	0.2312	0.3251	0.064
H(63A)	2*i*	0.9683	0.1370	0.4502	0.057
H(63B)	2*i*	0.8786	0.2121	0.4705	0.057
H(65A)	2*i*	0.5730	0.1328	0.4461	0.074
H(65B)	2*i*	0.5825	0.2123	0.4646	0.074
H(66A)	2*i*	0.5466	0.2155	0.3188	0.094
H(66B)	2*i*	0.5723	0.2902	0.3316	0.094
H(3A)	2*i*	0.7526	−0.1124	0.2175	0.209
H(2A)	2*i*	0.6633	−0.0815	0.0958	0.209
H(1A)	2*i*	0.8546	−0.1824	0.0410	0.209
H(24A)	2*i*	−0.0062	0.6306	0.4063	0.209
H(22A)	2*i*	0.0910	0.6506	0.2641	0.209
H(23A)	2*i*	0.2001	0.6509	0.4596	0.209
H(22B)	2*i*	0.1417	0.6417	0.2484	0.209
H(69A)	2*i*	0.8567	−0.1250	0.4390	0.057
H(69B)	2*i*	0.9513	−0.1158	0.4256	0.057
H(70A)	2*i*	0.8052	−0.0562	0.3087	0.046
H(70B)	2*i*	0.8943	−0.0374	0.2931	0.046
H(1B)	2*i*	0.7690	−0.1304	−0.0107	0.074
H(2B)	2*i*	0.6355	−0.1233	0.0932	0.065
H(3B)	2*i*	0.7990	−0.1703	0.1798	0.058
H(7)	2*i*	0.5909	0.7092	0.1188	0.110
H(9)	2*i*	−0.0459	0.6434	0.1775	0.108
H(13)	2*i*	0.6931	0.1380	0.1343	0.083
H(17)	2*i*	1.3674	0.1151	0.1033	0.098
H(23B)	2*i*	0.0944	0.6840	0.4529	0.080
H(24B)	2*i*	0.0253	0.5423	0.3943	0.079
H(28)	2*i*	0.0532	−0.1135	0.2635	0.085
H(31)	2*i*	0.7886	−0.2084	0.3882	0.070
H(35)	2*i*	0.3794	0.3131	0.2764	0.272
H(38)	2*i*	0.9918	0.3931	0.3295	0.087

and potential applications [1–3]. Aromatic multicarboxylates, especially benzene multi-carboxylates, including 1,3-benzenedicarboxylate, 1,3,5-benzenetricarboxylate and 1,2,4,5- benzenetetracarboxylate have been widely utilized to create novel CPs [1–3]. Compared to these rigid ligands, 3,3′,3″-(2,4,6-trioxo-1,3,5-triazinane-1,3,5-triyl)tripropanoic acid (TTA) is semi-flexible and longer ligand, and may be good candidates for construction of CPs. In particular, coordination polymers with flexible ligands exhibit more complex and unusual structures, as functional groups on the ligands offer variable configurations. Some studies of metal-organic networks based on TTA ligands were reported. The results show that the ligand exhibits a special ability to formulate the compounds, and can adopt different coordination modes in different chemical environments [4–6]. Most of these compounds have a 2D or 3D structure. In this paper, we select TTA as spacer to obtain a cobalt complex.

There are two crystallographically independent cobalt(II) ions in the structure. Both the Col and Co2 ions are six-coordinated by three oxygen atoms from three aqua ligands, two nitrogen atoms from bidentate chelating phen ligand, and one oxygen atom from one TTA ligand. Their coordination

Table 3: Atomic displacement parameters (Å²).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	2*i*	0.72001(5)	−0.02489(5)	0.06879(4)	0.0311(4)	0.0329(5)	0.0414(5)	−0.0160(4)	0.0063(4)	−0.0176(4)
Co(2)	2*i*	0.17706(6)	0.55117(5)	0.40345(5)	0.0387(5)	0.0298(5)	0.0429(5)	−0.0168(4)	0.0057(4)	−0.0147(4)
C(1)	2*i*	0.8933(4)	0.0070(4)	0.1019(4)	0.038(4)	0.043(4)	0.056(4)	−0.021(3)	0.010(3)	−0.025(3)
C(2)	2*i*	0.9532(5)	0.0501(5)	0.0848(4)	0.050(4)	0.058(4)	0.053(5)	−0.030(4)	0.006(3)	−0.030(4)
C(3)	2*i*	0.9426(4)	0.1109(5)	0.0141(4)	0.037(4)	0.063(5)	0.066(5)	−0.032(4)	0.019(3)	−0.040(4)
C(4)	2*i*	0.8714(4)	0.1322(4)	−0.0420(4)	0.039(4)	0.031(3)	0.058(4)	−0.018(3)	0.014(3)	−0.021(3)
C(5)	2*i*	0.8571(5)	0.1922(4)	−0.1197(4)	0.054(4)	0.035(4)	0.069(5)	−0.025(3)	0.015(4)	−0.016(4)
C(6)	2*i*	0.7885(5)	0.2072(5)	−0.1698(4)	0.068(5)	0.043(4)	0.055(5)	−0.023(4)	0.006(4)	0.000(4)
C(7)	2*i*	0.7251(5)	0.1664(4)	−0.1478(4)	0.052(4)	0.043(4)	0.041(4)	−0.017(4)	0.001(3)	−0.002(3)
C(8)	2*i*	0.6533(6)	0.1787(6)	−0.1981(4)	0.078(6)	0.080(6)	0.051(5)	−0.033(5)	−0.015(4)	−0.002(4)
C(9)	2*i*	0.5970(6)	0.1364(6)	−0.1714(5)	0.075(6)	0.084(6)	0.056(5)	−0.038(5)	−0.023(4)	−0.005(5)
C(10)	2*i*	0.6094(5)	0.0832(5)	−0.0948(4)	0.050(4)	0.062(5)	0.066(5)	−0.029(4)	−0.014(4)	−0.015(4)
C(11)	2*i*	0.7352(4)	0.1089(4)	−0.0726(4)	0.033(3)	0.033(4)	0.045(4)	−0.008(3)	0.001(3)	−0.014(3)
C(12)	2*i*	0.8120(4)	0.0888(4)	−0.0187(3)	0.028(3)	0.029(3)	0.043(4)	−0.008(3)	0.004(3)	−0.015(3)
C(13)	2*i*	0.5443(4)	0.1009(4)	0.1275(4)	0.028(3)	0.033(4)	0.057(4)	−0.010(3)	0.003(3)	−0.019(3)
C(14)	2*i*	0.4956(4)	0.1851(4)	0.1521(3)	0.036(4)	0.038(4)	0.058(4)	−0.017(3)	0.005(3)	−0.025(3)
C(15)	2*i*	0.4654(5)	0.2744(4)	0.0822(4)	0.047(4)	0.041(4)	0.066(5)	−0.012(3)	0.012(3)	−0.032(4)
C(16)	2*i*	0.4784(5)	0.3947(5)	0.1172(5)	0.038(4)	0.043(4)	0.110(7)	−0.018(4)	0.011(4)	−0.036(4)
C(17)	2*i*	0.4958(5)	0.5036(5)	0.1697(5)	0.068(5)	0.071(6)	0.111(7)	−0.045(5)	0.004(5)	−0.039(5)
C(18)	2*i*	0.4944(5)	0.5886(5)	0.1143(5)	0.067(5)	0.065(5)	0.104(7)	−0.041(5)	0.007(5)	−0.035(5)
C(19)	2*i*	0.5518(5)	0.6212(6)	0.1497(5)	0.065(5)	0.064(5)	0.080(6)	−0.044(5)	0.015(5)	−0.035(5)
C(20)	2*i*	0.3407(6)	0.5096(6)	0.1494(7)	0.048(5)	0.071(6)	0.24(1)	−0.020(5)	0.031(6)	−0.107(8)
C(21)	2*i*	0.1815(6)	0.5127(6)	0.1497(5)	0.095(7)	0.102(7)	0.084(7)	−0.070(6)	0.018(5)	−0.044(6)
C(22)	2*i*	0.1341(6)	0.5910(6)	0.0823(5)	0.073(6)	0.078(6)	0.082(6)	−0.035(5)	−0.025(5)	0.012(5)
C(23)	2*i*	0.0261(6)	0.6457(6)	0.1030(6)	0.053(5)	0.069(6)	0.094(7)	−0.032(5)	0.011(5)	−0.050(6)
C(24)	2*i*	0.3238(5)	0.3963(5)	0.1069(5)	0.040(4)	0.047(4)	0.119(7)	−0.015(4)	0.005(4)	−0.050(5)
C(25)	2*i*	0.7293(4)	0.1776(4)	0.1976(4)	0.031(4)	0.040(4)	0.054(5)	−0.012(3)	0.003(3)	−0.019(4)
C(26)	2*i*	0.7799(5)	0.2353(5)	0.1954(4)	0.052(4)	0.065(5)	0.082(6)	−0.037(4)	0.007(4)	−0.041(4)
C(27)	2*i*	0.7955(4)	0.2865(4)	0.1173(4)	0.035(4)	0.042(4)	0.078(5)	−0.026(3)	0.008(3)	−0.030(4)
C(28)	2*i*	0.9496(4)	0.2784(5)	0.1446(4)	0.041(4)	0.039(4)	0.059(5)	−0.018(3)	0.012(3)	−0.024(3)
C(29)	2*i*	1.1056(4)	0.2652(5)	0.1750(4)	0.039(4)	0.056(4)	0.065(5)	−0.024(3)	0.007(3)	−0.032(4)
C(30)	2*i*	1.1593(4)	0.2348(5)	0.1148(4)	0.030(4)	0.073(5)	0.062(5)	−0.018(3)	0.006(3)	−0.037(4)
C(31)	2*i*	1.2630(4)	0.1699(4)	0.1424(4)	0.036(4)	0.045(4)	0.055(5)	−0.018(3)	0.007(3)	−0.025(4)
C(32)	2*i*	0.9650(4)	0.4201(4)	0.1263(4)	0.037(4)	0.044(4)	0.077(5)	−0.020(3)	0.009(3)	−0.036(4)
C(33)	2*i*	0.8222(5)	0.5718(4)	0.0955(4)	0.053(4)	0.027(3)	0.071(5)	−0.016(3)	0.002(4)	−0.021(3)
C(34)	2*i*	0.8065(5)	0.5846(4)	0.1722(4)	0.058(4)	0.034(4)	0.066(5)	−0.020(3)	0.005(4)	−0.018(3)
C(35)	2*i*	0.7696(5)	0.6876(5)	0.1623(4)	0.062(5)	0.037(4)	0.052(5)	−0.023(4)	0.011(4)	−0.016(3)
C(36)	2*i*	0.8078(5)	0.4299(5)	0.1060(4)	0.039(4)	0.048(4)	0.081(5)	−0.024(4)	0.007(4)	−0.037(4)
C(37)	2*i*	0.6659(4)	−0.1293(4)	0.3583(4)	0.032(4)	0.043(4)	0.053(4)	−0.018(3)	0.005(3)	−0.024(3)
C(38)	2*i*	0.5748(4)	−0.0957(4)	0.3920(3)	0.038(4)	0.044(4)	0.050(4)	−0.022(3)	0.008(3)	−0.018(3)
C(39)	2*i*	0.4971(4)	−0.0094(4)	0.3335(3)	0.028(3)	0.041(4)	0.054(4)	−0.013(3)	0.011(3)	−0.022(3)
C(40)	2*i*	0.3703(4)	0.1043(4)	0.3773(4)	0.034(4)	0.036(4)	0.058(4)	−0.015(3)	0.004(3)	−0.022(3)
C(41)	2*i*	0.2362(4)	0.2279(4)	0.4076(3)	0.039(4)	0.028(3)	0.055(4)	−0.016(3)	0.008(3)	−0.023(3)
C(42)	2*i*	0.1980(4)	0.3144(4)	0.3353(3)	0.039(4)	0.030(3)	0.053(4)	−0.013(3)	0.004(3)	−0.022(3)
C(43)	2*i*	0.1524(5)	0.4040(4)	0.3531(3)	0.047(4)	0.033(4)	0.047(4)	−0.021(3)	0.004(3)	−0.013(3)
C(44)	2*i*	0.2175(4)	0.0997(4)	0.3906(3)	0.034(4)	0.030(3)	0.048(4)	−0.017(3)	0.001(3)	−0.014(3)
C(45)	2*i*	0.2050(4)	−0.0370(4)	0.3842(3)	0.050(4)	0.030(3)	0.053(4)	−0.025(3)	0.004(3)	−0.013(3)
C(46)	2*i*	0.1603(4)	−0.0207(4)	0.3074(4)	0.040(4)	0.033(4)	0.062(5)	−0.021(3)	0.001(3)	−0.013(3)
C(47)	2*i*	0.1290(4)	−0.0946(5)	0.3152(4)	0.040(4)	0.043(4)	0.055(5)	−0.024(3)	0.001(3)	−0.019(4)
C(48)	2*i*	0.3502(4)	−0.0222(4)	0.3590(3)	0.031(3)	0.029(3)	0.048(4)	−0.014(3)	0.003(3)	−0.014(3)
C(49)	2*i*	0.3732(6)	0.5416(5)	0.3549(4)	0.080(6)	0.066(5)	0.063(5)	−0.048(5)	0.018(4)	−0.031(4)
C(50)	2*i*	0.4732(6)	0.5058(7)	0.3667(6)	0.071(6)	0.102(7)	0.128(9)	−0.065(6)	0.043(6)	−0.079(7)
C(51)	2*i*	0.5231(6)	0.4385(6)	0.4340(6)	0.044(5)	0.087(7)	0.141(9)	−0.025(5)	0.016(6)	−0.084(7)
C(52)	2*i*	0.4735(5)	0.4077(5)	0.4920(5)	0.046(5)	0.060(5)	0.094(6)	−0.018(4)	0.002(5)	−0.055(5)
C(53)	2*i*	0.5209(6)	0.3365(6)	0.5643(6)	0.065(6)	0.066(6)	0.115(9)	−0.006(5)	−0.028(6)	−0.053(6)
C(54)	2*i*	0.4695(7)	0.3129(5)	0.6187(6)	0.095(8)	0.042(5)	0.089(7)	−0.011(5)	−0.046(6)	−0.013(5)
C(55)	2*i*	0.3683(6)	0.3548(5)	0.6073(4)	0.079(6)	0.048(5)	0.057(5)	−0.024(4)	−0.021(5)	−0.019(4)
C(56)	2*i*	0.3096(8)	0.3340(6)	0.6615(5)	0.129(8)	0.064(6)	0.044(5)	−0.050(6)	0.001(6)	−0.003(4)
C(57)	2*i*	0.2147(7)	0.3760(6)	0.6432(5)	0.114(8)	0.090(7)	0.055(6)	−0.067(6)	0.009(5)	−0.010(5)
C(58)	2*i*	0.1751(6)	0.4401(5)	0.5700(4)	0.078(5)	0.072(5)	0.053(5)	−0.050(5)	0.019(4)	−0.020(4)
C(59)	2*i*	0.3203(5)	0.4212(4)	0.5347(4)	0.063(5)	0.035(4)	0.047(4)	−0.023(4)	−0.005(4)	−0.017(3)
C(60)	2*i*	0.3750(5)	0.4484(4)	0.4769(4)	0.048(4)	0.035(4)	0.063(5)	−0.017(3)	−0.005(4)	−0.027(4)
C(61)	2*i*	0.9453(4)	0.3154(4)	0.3786(4)	0.041(4)	0.041(4)	0.066(5)	−0.021(3)	0.012(4)	−0.023(4)
C(62)	2*i*	0.9009(5)	0.2597(5)	0.3606(4)	0.052(4)	0.058(5)	0.064(5)	−0.036(4)	0.005(4)	−0.024(4)
C(63)	2*i*	0.9027(4)	0.1847(4)	0.4319(4)	0.043(4)	0.048(4)	0.065(5)	−0.027(3)	0.000(3)	−0.026(4)
C(64)	2*i*	0.7497(5)	0.1824(5)	0.4268(4)	0.043(4)	0.051(4)	0.069(5)	−0.028(4)	0.013(3)	−0.036(4)

Table 3: (continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(65)	2*i*	0.5958(4)	0.1798(5)	0.4288(5)	0.036(4)	0.077(5)	0.110(7)	−0.036(4)	0.041(4)	−0.066(5)
C(66)	2*i*	0.5448(5)	0.2476(5)	0.3533(5)	0.035(4)	0.059(5)	0.141(8)	−0.020(4)	0.003(5)	−0.037(6)
C(67)	2*i*	0.4360(9)	0.3040(8)	0.370(1)	0.07(1)	0.055(7)	0.37(3)	−0.044(7)	−0.08(1)	−0.01(1)
C(68)	2*i*	0.7409(4)	0.0444(4)	0.4216(3)	0.048(4)	0.042(4)	0.046(4)	−0.026(3)	0.008(3)	−0.021(3)
C(69)	2*i*	0.8839(5)	−0.0861(4)	0.4072(3)	0.056(4)	0.032(4)	0.058(5)	−0.020(3)	0.000(3)	−0.018(3)
C(70)	2*i*	0.8722(4)	−0.0805(4)	0.3258(3)	0.038(4)	0.029(3)	0.042(4)	−0.011(3)	0.000(3)	−0.012(3)
C(71)	2*i*	0.9281(4)	−0.1764(4)	0.3193(4)	0.038(4)	0.028(3)	0.049(4)	−0.011(3)	−0.005(3)	−0.018(3)
C(72)	2*i*	0.8922(5)	0.0534(4)	0.4106(3)	0.040(4)	0.045(4)	0.045(4)	−0.022(3)	0.006(3)	−0.022(3)
N(1)	2*i*	0.8228(3)	0.0264(3)	0.0523(3)	0.026(3)	0.036(3)	0.043(3)	−0.014(2)	0.002(2)	−0.018(3)
N(2)	2*i*	0.6777(3)	0.0686(3)	−0.0458(3)	0.033(3)	0.041(3)	0.047(3)	−0.017(3)	0.000(2)	−0.016(3)
N(3)	2*i*	0.4203(4)	0.3604(3)	0.1007(3)	0.031(3)	0.036(3)	0.104(5)	−0.011(3)	0.008(3)	−0.038(3)
N(4)	2*i*	0.4344(4)	0.4716(4)	0.1394(4)	0.046(4)	0.057(4)	0.159(7)	−0.026(3)	0.014(4)	−0.067(4)
N(5)	2*i*	0.2872(4)	0.4731(5)	0.1296(5)	0.035(4)	0.081(5)	0.25(1)	−0.024(4)	0.024(5)	−0.114(6)
N(6)	2*i*	0.8528(3)	0.3340(3)	0.1220(3)	0.032(3)	0.034(3)	0.084(4)	−0.015(3)	0.005(3)	−0.034(3)
N(7)	2*i*	1.0022(3)	0.3243(3)	0.1474(3)	0.031(3)	0.040(3)	0.071(4)	−0.017(3)	0.008(3)	−0.031(3)
N(8)	2*i*	0.8665(3)	0.4701(3)	0.1072(3)	0.034(3)	0.033(3)	0.075(4)	−0.016(2)	0.010(3)	−0.031(3)
N(9)	2*i*	0.2593(3)	0.0154(3)	0.3785(3)	0.033(3)	0.033(3)	0.053(3)	−0.021(2)	0.007(2)	−0.023(3)
N(10)	2*i*	0.2758(3)	0.1401(3)	0.3914(3)	0.035(3)	0.027(3)	0.046(3)	−0.015(2)	0.005(2)	−0.017(2)
N(11)	2*i*	0.4035(3)	0.0228(3)	0.3618(3)	0.027(3)	0.031(3)	0.052(3)	−0.014(2)	0.006(2)	−0.017(2)
N(12)	2*i*	0.3249(4)	0.5143(3)	0.4079(3)	0.052(3)	0.039(3)	0.048(3)	−0.027(3)	0.016(3)	−0.023(3)
N(13)	2*i*	0.2259(4)	0.4620(3)	0.5161(3)	0.047(3)	0.040(3)	0.050(4)	−0.023(3)	0.008(3)	−0.016(3)
N(14)	2*i*	0.8453(3)	0.1393(3)	0.4207(3)	0.038(3)	0.040(3)	0.060(4)	−0.022(3)	0.004(3)	−0.026(3)
N(15)	2*i*	0.6997(3)	0.1330(3)	0.4269(3)	0.039(3)	0.047(3)	0.062(4)	−0.027(3)	0.015(3)	−0.034(3)
N(16)	2*i*	0.8370(3)	0.0077(3)	0.4138(3)	0.042(3)	0.033(3)	0.050(3)	−0.020(3)	0.004(2)	−0.019(3)
O(1)	2*i*	0.8035(3)	−0.1310(3)	0.0212(2)	0.047(3)	0.049(3)	0.059(3)	−0.017(2)	0.006(2)	−0.033(2)
O(2)	2*i*	0.6153(3)	−0.0679(3)	0.0658(3)	0.035(2)	0.034(2)	0.065(3)	−0.016(2)	0.001(2)	−0.022(2)
O(3)	2*i*	0.7808(3)	−0.1160(3)	0.1776(2)	0.041(2)	0.030(2)	0.042(3)	−0.013(2)	0.006(2)	−0.015(2)
O(4)	2*i*	0.6297(3)	0.0772(3)	0.1147(2)	0.032(2)	0.036(2)	0.066(3)	−0.017(2)	0.011(2)	−0.032(2)
O(5)	2*i*	0.4982(3)	0.0601(3)	0.1184(3)	0.026(2)	0.049(3)	0.112(4)	−0.019(2)	0.014(2)	−0.049(3)
O(6)	2*i*	0.5792(4)	0.5930(4)	0.2155(3)	0.127(5)	0.118(5)	0.076(4)	−0.097(4)	0.012(4)	−0.030(4)
O(7)	2*i*	0.5637(4)	0.6897(4)	0.0980(3)	0.082(4)	0.070(4)	0.089(4)	−0.046(3)	0.003(3)	−0.034(3)
O(8)	2*i*	−0.0320(4)	0.7000(4)	0.0516(4)	0.059(4)	0.099(5)	0.091(5)	−0.015(3)	0.015(3)	−0.033(4)
O(9)	2*i*	0.0110(3)	0.6274(4)	0.1749(3)	0.040(3)	0.056(3)	0.107(5)	−0.004(3)	−0.020(3)	−0.037(3)
O(10)	2*i*	0.5621(3)	0.3597(3)	0.1136(3)	0.033(3)	0.065(3)	0.157(6)	−0.020(3)	0.010(3)	−0.044(4)
O(11)	2*i*	0.3057(4)	0.5732(4)	0.1762(5)	0.071(4)	0.101(5)	0.257(9)	−0.027(4)	0.019(5)	−0.129(6)
O(12)	2*i*	0.2758(3)	0.3628(3)	0.0938(3)	0.044(3)	0.067(3)	0.163(6)	−0.026(3)	0.010(3)	−0.073(4)
O(13)	2*i*	0.7236(3)	0.1672(3)	0.1320(3)	0.051(3)	0.065(3)	0.082(4)	−0.039(3)	0.025(2)	−0.047(3)
O(14)	2*i*	0.7006(4)	0.1446(4)	0.2531(3)	0.080(4)	0.079(4)	0.060(4)	−0.050(3)	0.012(3)	−0.020(3)
O(15)	2*i*	0.9859(3)	0.1940(3)	0.1612(3)	0.042(3)	0.042(3)	0.121(5)	−0.017(2)	0.007(3)	−0.039(3)
O(16)	2*i*	1.2982(3)	0.1422(4)	0.2069(3)	0.043(3)	0.089(4)	0.064(4)	−0.014(3)	−0.005(3)	−0.017(3)
O(17)	2*i*	1.3107(3)	0.1490(4)	0.0869(3)	0.037(3)	0.085(4)	0.083(4)	−0.017(3)	0.011(2)	−0.056(3)
O(18)	2*i*	1.0130(3)	0.4588(3)	0.1269(3)	0.046(3)	0.058(3)	0.146(5)	−0.032(3)	0.014(3)	−0.058(3)
O(19)	2*i*	0.6827(3)	0.7420(3)	0.1392(3)	0.051(3)	0.034(3)	0.087(4)	−0.018(2)	0.004(3)	−0.025(3)
O(20)	2*i*	0.8287(3)	0.7126(3)	0.1781(3)	0.048(3)	0.039(3)	0.075(3)	−0.018(2)	0.008(2)	−0.028(2)
O(21)	2*i*	0.7219(3)	0.4760(3)	0.0909(3)	0.032(3)	0.049(3)	0.164(6)	−0.013(2)	−0.005(3)	−0.048(3)
O(22)	2*i*	0.1354(3)	0.6450(3)	0.2917(2)	0.083(3)	0.041(3)	0.039(3)	−0.016(3)	0.008(2)	−0.016(2)
O(23)	2*i*	0.1456(3)	0.6688(3)	0.4360(3)	0.068(3)	0.046(3)	0.059(3)	−0.030(3)	0.017(3)	−0.030(2)
O(24)	2*i*	0.0363(3)	0.5751(3)	0.4123(3)	0.045(3)	0.041(3)	0.082(4)	−0.023(2)	0.011(2)	−0.029(2)
O(25)	2*i*	0.2070(3)	0.4351(3)	0.3675(2)	0.038(2)	0.043(3)	0.070(3)	−0.021(2)	0.009(2)	−0.033(2)
O(26)	2*i*	0.0639(3)	0.4444(3)	0.3522(3)	0.038(3)	0.044(3)	0.105(4)	−0.019(2)	0.010(3)	−0.041(3)
O(27)	2*i*	0.1341(3)	0.1348(3)	0.4010(3)	0.034(3)	0.049(3)	0.085(4)	−0.020(2)	0.014(2)	−0.033(3)
O(28)	2*i*	0.0648(3)	−0.0696(3)	0.2589(3)	0.066(3)	0.055(3)	0.062(3)	−0.040(3)	−0.003(3)	−0.018(3)
O(29)	2*i*	0.1610(4)	−0.1694(3)	0.3651(3)	0.098(4)	0.040(3)	0.085(4)	−0.044(3)	−0.038(3)	0.008(3)
O(30)	2*i*	0.3814(3)	−0.0926(3)	0.3427(3)	0.042(3)	0.041(3)	0.092(4)	−0.014(2)	0.007(2)	−0.040(3)
O(31)	2*i*	0.7401(3)	−0.1956(3)	0.4090(2)	0.030(2)	0.045(3)	0.059(3)	−0.012(2)	0.007(2)	−0.018(2)
O(32)	2*i*	0.6695(3)	−0.0986(3)	0.2911(3)	0.043(3)	0.082(4)	0.044(3)	−0.014(3)	0.011(2)	−0.022(3)
O(33)	2*i*	0.4182(3)	0.1419(3)	0.3789(3)	0.049(3)	0.064(3)	0.147(5)	−0.040(3)	0.027(3)	−0.061(3)
O(34)	2*i*	0.4003(7)	0.310(1)	0.404(1)	0.095(7)	0.29(2)	0.60(3)	−0.140(8)	0.19(1)	−0.39(2)
O(35)	2*i*	0.3967(6)	0.3471(7)	0.2873(7)	0.075(6)	0.115(7)	0.32(1)	−0.052(5)	0.053(8)	−0.031(9)
O(36)	2*i*	0.7116(3)	0.2593(3)	0.4324(3)	0.052(3)	0.055(3)	0.126(5)	−0.028(3)	0.023(3)	−0.058(3)
O(37)	2*i*	0.9572(4)	0.3166(4)	0.4414(3)	0.096(4)	0.089(4)	0.069(4)	−0.069(3)	0.032(3)	−0.049(3)
O(38)	2*i*	0.9682(3)	0.3640(3)	0.3177(3)	0.063(3)	0.056(3)	0.070(3)	−0.038(3)	0.004(3)	−0.023(3)
O(39)	2*i*	0.9752(3)	0.0195(3)	0.4028(3)	0.038(3)	0.063(3)	0.105(4)	−0.025(3)	0.015(3)	−0.048(3)
O(40)	2*i*	0.9981(3)	−0.1891(3)	0.2821(2)	0.036(2)	0.039(2)	0.060(3)	−0.019(2)	0.007(2)	−0.024(2)
O(41)	2*i*	0.9033(3)	−0.2387(3)	0.3519(2)	0.032(2)	0.032(2)	0.071(3)	−0.013(2)	0.008(2)	−0.022(2)
O(42)	2*i*	0.6957(3)	0.0020(3)	0.4239(3)	0.060(3)	0.058(3)	0.084(4)	−0.042(3)	0.019(3)	−0.035(3)

geometry can be described as a distorted octahedron. The Co—N and Co—O bond distances are comparable to those reported for other cobalt complexes. There are four unique TTA anions in the asymmetric unit. Two carboxyl groups of BTB ligand are protonated, so each TTA ligand carries a charge of −1, satisfying the charge balance. Two BTB anions do not participate in the coordination of the Co(II) atoms. In comparable structures, TTA can adopt a μ_5-mode to bind metal centers [4, 5], and all carboxyl oxygen atoms are involved in metal coordination. In the title compound, the complex cations and dihydrogen TTA ligands align in neat alternating mode, which is made possible by the well matched ionic size, and interact with each other O—H···O hydrogen bonds between the carboxyl groups and coordinated water molecules resulting in the formation of infinite chains. Adjacent chains are linked by O—H···O hydrogen bonds formed between the carboxyl groups and coordinated water molecules to create three dimensional networks.

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