Ting-Ting Zhang, Guan-Nan Li and Feng-Mei Nie*

Crystal structure of [tris(2-benzimidazolylmethyl)amine- κ^3N](isonicotinate- κO) cobalt(II) [tris(2-benzimidazolylmethyl)amine- κ^3N](isonicotinic acid- κO) cobalt(II) triperchlorate, $C_{60}H_{51}N_{16}O_{16}Cl_3Co_2$

Table 1: Data collection and handling.

Crystal:	Red blocks
	Size $0.50 \times 0.40 \times 0.10$ mm
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	7.6 cm^{-1}
Diffractometer, scan mode:	Bruker CCD, φ and ω
$2\theta_{\max}$, completeness:	55° , $>98\%$
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	94380, 27610, 0.054
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 21014
$N(\text{param})_{\text{refined}}$:	1815
Programs:	Bruker programs [6], SHELX [7]

Only one out of four crystallographically independent and pairwise differently protonated Co-complexes 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.

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Abstract

$C_{60}H_{51}N_{16}O_{16}Cl_3Co_2$, monoclinic, $P2_1/n$ (no. 14), $a = 35.652(4) \text{ \AA}$, $b = 14.1314(16) \text{ \AA}$, $c = 25.141(3) \text{ \AA}$, $\beta = 105.113(2)^\circ$, $V = 12228(3) \text{ \AA}^3$, $Z = 8$, $R_{\text{gt}}(F) = 0.0651$, $wR_{\text{ref}}(F^2) = 0.1663$, $T = 103(2) \text{ K}$.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.530264(12)	0.25683(3)	0.418056(18)	0.01648(10)
Co2	0.203987(12)	0.24756(3)	−0.178527(17)	0.01583(10)
Co3	1.024726(12)	0.27197(3)	0.922851(17)	0.01591(10)
Co4	0.709264(13)	0.25167(3)	0.317239(18)	0.01725(10)
O1	0.48454(7)	0.24273(16)	0.35326(9)	0.0215(5)
O2	0.52284(7)	0.31550(17)	0.30981(10)	0.0252(5)
O3	0.24983(7)	0.25994(17)	−0.11454(9)	0.0219(5)
O4	0.21395(7)	0.20554(19)	−0.06068(10)	0.0294(6)
O5	0.97922(7)	0.26027(16)	0.85853(10)	0.0216(5)
O6	1.01725(7)	0.31881(18)	0.80908(10)	0.0275(6)
O7	0.75302(7)	0.27675(17)	0.38349(9)	0.0224(5)
O8	0.71658(7)	0.19244(18)	0.42534(10)	0.0267(6)
N1	0.58401(8)	0.2654(2)	0.50008(11)	0.0201(6)
N2	0.53112(8)	0.3963(2)	0.44320(11)	0.0197(6)
N3	0.55581(8)	0.5149(2)	0.49911(12)	0.0246(6)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H3	0.5700	0.5451	0.5280	0.029*
N4	0.57600(8)	0.18676(19)	0.39968(11)	0.0183(6)
N5	0.63847(8)	0.1485(2)	0.41654(12)	0.0214(6)
H5N	0.6636	0.1480	0.4326	0.026*
N6	0.51346(8)	0.17783(19)	0.47547(11)	0.0184(6)
N7	0.52422(9)	0.1007(2)	0.55454(12)	0.0233(6)
H7N	0.5369	0.0768	0.5865	0.028*
N8	0.40332(8)	0.2503(2)	0.15902(12)	0.0239(6)
N9	0.15299(8)	0.23831(19)	−0.26182(12)	0.0198(6)
N10	0.22457(8)	0.31981(19)	−0.23508(11)	0.0179(6)
N11	0.21586(8)	0.3992(2)	−0.31330(11)	0.0210(6)
H11N	0.2041	0.4241	−0.3454	0.025*
N12	0.20274(8)	0.1076(2)	−0.20016(12)	0.0212(6)
N13	0.18540(8)	−0.0100(2)	−0.26005(12)	0.0247(6)
H13N	0.1738	−0.0400	−0.2905	0.030*
N14	0.15783(8)	0.31829(19)	−0.16266(11)	0.0167(5)
N15	0.09550(8)	0.3611(2)	−0.18508(11)	0.0209(6)
H15N	0.0707	0.3625	−0.2028	0.025*
N16	0.34345(9)	0.2544(2)	0.06934(12)	0.0243(6)
N17	1.07628(8)	0.28492(19)	1.00641(11)	0.0193(6)
N18	1.07162(8)	0.20587(19)	0.90694(11)	0.0174(6)
N19	1.13429(8)	0.1698(2)	0.92739(11)	0.0204(6)
H19N	1.1592	0.1707	0.9444	0.024*
N20	1.00768(8)	0.18710(19)	0.97758(11)	0.0176(6)
N21	1.01811(9)	0.1057(2)	1.05542(12)	0.0228(6)
H21N	1.0304	0.0823	1.0877	0.027*
N22	1.02591(8)	0.41301(19)	0.94368(11)	0.0188(6)
N23	1.05094(8)	0.5347(2)	0.99698(12)	0.0208(6)
H23N	1.0645	0.5663	1.0257	0.025*
N24	0.89196(10)	0.2606(2)	0.66828(13)	0.0316(8)
N25	0.65823(8)	0.2382(2)	0.23403(12)	0.0207(6)
N26	0.72788(8)	0.32604(19)	0.25983(11)	0.0200(6)
N27	0.71784(8)	0.4061(2)	0.18123(11)	0.0213(6)
H27N	0.7055	0.4308	0.1493	0.026*
N28	0.71078(8)	0.1121(2)	0.29600(12)	0.0215(6)
N29	0.69318(9)	−0.0076(2)	0.23789(13)	0.0269(7)
H29N	0.6813	−0.0388	0.2079	0.032*
N30	0.66238(8)	0.3185(2)	0.33262(11)	0.0201(6)
N31	0.59918(8)	0.3496(2)	0.31319(12)	0.0230(6)
H31N	0.5742	0.3466	0.2966	0.028*
N32	0.83372(9)	0.2600(2)	0.57584(13)	0.0256(7)
C1	0.57919(10)	0.3521(2)	0.53002(13)	0.0237(7)
H1A	0.6049	0.3796	0.5478	0.028*
H1B	0.5660	0.3370	0.5591	0.028*
C2	0.55560(10)	0.4211(2)	0.49032(14)	0.0216(7)
C3	0.52949(10)	0.5555(2)	0.45434(14)	0.0227(7)
C4	0.51959(11)	0.6494(3)	0.44153(17)	0.0303(8)
H4	0.5307	0.6999	0.4654	0.036*
C5	0.49252(12)	0.6649(3)	0.39171(17)	0.0329(9)
H5	0.4854	0.7280	0.3804	0.039*
C6	0.47537(12)	0.5896(3)	0.35751(16)	0.0307(8)
H6	0.4562	0.6032	0.3243	0.037*
C7	0.48536(10)	0.4970(3)	0.37040(15)	0.0259(8)
H7	0.4736	0.4467	0.3468	0.031*
C8	0.51363(10)	0.4798(2)	0.41975(14)	0.0205(7)
C9	0.61900(9)	0.2680(2)	0.47901(14)	0.0209(7)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H9A	0.6422	0.2482	0.5080	0.025*
H9B	0.6234	0.3328	0.4669	0.025*
C10	0.61157(9)	0.2010(2)	0.43162(14)	0.0195(7)
C11	0.61951(10)	0.0950(2)	0.37108(14)	0.0215(7)
C12	0.63267(11)	0.0272(2)	0.34037(16)	0.0275(8)
H12	0.6593	0.0093	0.3486	0.033*
C13	0.60510(11)	−0.0130(2)	0.29713(15)	0.0279(8)
H13	0.6129	−0.0590	0.2746	0.033*
C14	0.56578(11)	0.0130(2)	0.28595(15)	0.0274(8)
H14	0.5476	−0.0159	0.2559	0.033*
C15	0.55272(10)	0.0786(2)	0.31702(14)	0.0228(7)
H15	0.5260	0.0951	0.3092	0.027*
C16	0.58016(9)	0.1202(2)	0.36050(13)	0.0183(7)
C17	0.58167(10)	0.1783(2)	0.53124(14)	0.0241(7)
H17A	0.5931	0.1890	0.5711	0.029*
H17B	0.5962	0.1266	0.5190	0.029*
C18	0.53968(10)	0.1520(2)	0.52082(13)	0.0198(7)
C19	0.48482(10)	0.0919(2)	0.53014(14)	0.0219(7)
C20	0.45509(11)	0.0495(3)	0.54822(16)	0.0280(8)
H20	0.4599	0.0166	0.5823	0.034*
C21	0.41802(11)	0.0583(3)	0.51344(17)	0.0312(9)
H21	0.3967	0.0320	0.5244	0.037*
C22	0.41116(10)	0.1047(3)	0.46273(16)	0.0287(8)
H22	0.3854	0.1074	0.4397	0.034*
C23	0.44096(10)	0.1470(2)	0.44519(15)	0.0231(7)
H23	0.4361	0.1792	0.4109	0.028*
C24	0.47832(10)	0.1404(2)	0.47994(14)	0.0189(7)
C25	0.49209(9)	0.2746(2)	0.31007(13)	0.0195(7)
C26	0.43786(10)	0.2867(3)	0.15952(14)	0.0253(7)
H26	0.4423	0.3087	0.1260	0.030*
C27	0.46761(10)	0.2933(3)	0.20760(14)	0.0234(7)
H27A	0.4921	0.3189	0.2068	0.028*
C28	0.46126(9)	0.2625(2)	0.25659(13)	0.0177(6)
C29	0.42538(10)	0.2236(3)	0.25570(14)	0.0252(8)
H29	0.4203	0.2009	0.2887	0.030*
C30	0.39711(10)	0.2183(3)	0.20622(15)	0.0280(8)
H30	0.3726	0.1913	0.2057	0.034*
C31	0.15700(10)	0.3244(2)	−0.29317(13)	0.0215(7)
H31A	0.1424	0.3774	−0.2823	0.026*
H31B	0.1465	0.3130	−0.3331	0.026*
C32	0.19916(9)	0.3482(2)	−0.28073(13)	0.0182(6)
C33	0.25508(10)	0.4056(2)	−0.28716(14)	0.0209(7)
C34	0.28575(11)	0.4481(2)	−0.30290(15)	0.0253(8)
H34	0.2820	0.4819	−0.3366	0.030*
C35	0.32220(10)	0.4383(2)	−0.26629(15)	0.0260(8)
H35	0.3441	0.4655	−0.2754	0.031*
C36	0.32768(10)	0.3892(2)	−0.21625(15)	0.0255(8)
H36	0.3531	0.3849	−0.1923	0.031*
C37	0.29699(10)	0.3470(2)	−0.20085(15)	0.0226(7)
H37	0.3007	0.3139	−0.1670	0.027*
C38	0.26045(9)	0.3555(2)	−0.23757(13)	0.0179(6)
C39	0.15877(10)	0.1515(2)	−0.29039(14)	0.0236(7)
H39A	0.1726	0.1663	−0.3188	0.028*
H39B	0.1333	0.1235	−0.3090	0.028*
C40	0.18188(10)	0.0827(2)	−0.25008(14)	0.0221(7)
C41	0.21028(10)	−0.0495(3)	−0.21428(16)	0.0256(8)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
C42	0.22347(11)	−0.1416(3)	−0.20200(17)	0.0305(8)
H42	0.2158	−0.1915	−0.2279	0.037*
C43	0.24834(12)	−0.1572(3)	−0.15027(18)	0.0337(9)
H43	0.2581	−0.2191	−0.1404	0.040*
C44	0.25930(12)	−0.0830(3)	−0.11238(17)	0.0349(9)
H44	0.2763	−0.0961	−0.0773	0.042*
C45	0.24630(11)	0.0078(3)	−0.12429(16)	0.0297(8)
H45	0.2540	0.0574	−0.0982	0.036*
C46	0.22131(10)	0.0246(2)	−0.17614(15)	0.0223(7)
C47	0.11692(9)	0.2384(2)	−0.24389(14)	0.0204(7)
H47A	0.1114	0.1742	−0.2321	0.024*
H47B	0.0947	0.2589	−0.2743	0.024*
C48	0.12312(9)	0.3059(2)	−0.19696(13)	0.0186(7)
C49	0.11366(9)	0.4153(2)	−0.13966(13)	0.0197(7)
C50	0.09973(11)	0.4876(2)	−0.11246(15)	0.0253(8)
H50	0.0735	0.5084	−0.1240	0.030*
C51	0.12608(11)	0.5277(3)	−0.06769(16)	0.0275(8)
H51	0.1178	0.5766	−0.0475	0.033*
C52	0.16508(11)	0.4970(2)	−0.05149(15)	0.0261(8)
H52	0.1822	0.5249	−0.0200	0.031*
C53	0.17900(10)	0.4280(2)	−0.07988(14)	0.0214(7)
H53	0.2055	0.4090	−0.0691	0.026*
C54	0.15272(9)	0.3868(2)	−0.12520(13)	0.0184(7)
C55	0.24451(10)	0.2363(2)	−0.06802(14)	0.0209(7)
C56	0.34850(10)	0.2519(2)	0.01845(14)	0.0232(7)
H56	0.3740	0.2532	0.0136	0.028*
C57	0.31677(10)	0.2475(2)	−0.02736(14)	0.0233(7)
H57	0.3204	0.2465	−0.0635	0.028*
C58	0.27982(9)	0.2446(2)	−0.01950(14)	0.0194(7)
C59	0.27546(10)	0.2476(3)	0.03381(15)	0.0276(8)
H59	0.2503	0.2460	0.0400	0.033*
C60	0.30783(11)	0.2528(3)	0.07741(15)	0.0309(9)
H60	0.3049	0.2552	0.1139	0.037*
C61	1.11203(9)	0.2885(2)	0.98732(14)	0.0211(7)
H61A	1.1348	0.2698	1.0174	0.025*
H61B	1.1164	0.3534	0.9754	0.025*
C62	1.10675(9)	0.2215(2)	0.94036(13)	0.0176(6)
C63	1.11663(10)	0.1141(2)	0.88222(14)	0.0207(7)
C64	1.13114(11)	0.0442(3)	0.85452(15)	0.0265(8)
H64	1.1578	0.0265	0.8648	0.032*
C65	1.10453(11)	0.0015(3)	0.81100(15)	0.0273(8)
H65	1.1133	−0.0459	0.7903	0.033*
C66	1.06481(11)	0.0264(2)	0.79651(15)	0.0252(8)
H66	1.0475	−0.0045	0.7663	0.030*
C67	1.05067(10)	0.0948(2)	0.82542(14)	0.0212(7)
H67	1.0239	0.1112	0.8160	0.025*
C68	1.07722(9)	0.1389(2)	0.86908(13)	0.0188(7)
C69	1.07419(10)	0.1984(2)	1.03861(14)	0.0223(7)
H69A	1.0830	0.2125	1.0785	0.027*
H69B	1.0914	0.1490	1.0300	0.027*
C70	1.03322(10)	0.1641(2)	1.02429(13)	0.0183(7)
C71	0.97974(10)	0.0889(2)	1.02778(15)	0.0229(7)
C72	0.95049(11)	0.0374(2)	1.04198(16)	0.0283(8)
H72	0.9549	0.0036	1.0757	0.034*
C73	0.91452(11)	0.0387(2)	1.00395(17)	0.0293(8)
H73	0.8937	0.0043	1.0118	0.035*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
C74	0.90772(10)	0.0890(3)	0.95408(17)	0.0279(8)
H74	0.8826	0.0874	0.9291	0.033*
C75	0.93700(10)	0.1410(2)	0.94058(15)	0.0226(7)
H75	0.9325	0.1754	0.9071	0.027*
C76	0.97328(10)	0.1402(2)	0.97848(14)	0.0198(7)
C77	1.06978(10)	0.3721(2)	1.03416(13)	0.0216(7)
H77A	1.0949	0.3991	1.0551	0.026*
H77B	1.0539	0.3587	1.0603	0.026*
C78	1.04919(9)	0.4400(2)	0.99139(13)	0.0188(7)
C79	1.02745(10)	0.5733(2)	0.94918(14)	0.0198(7)
C80	1.02072(11)	0.6673(3)	0.93201(15)	0.0257(8)
H80	1.0327	0.7188	0.9544	0.031*
C81	0.99548(11)	0.6807(3)	0.88030(15)	0.0269(8)
H81	0.9899	0.7433	0.8667	0.032*
C82	0.97803(11)	0.6044(3)	0.84773(15)	0.0291(8)
H82	0.9606	0.6166	0.8128	0.035*
C83	0.98543(11)	0.5116(3)	0.86482(14)	0.0265(8)
H83	0.9734	0.4602	0.8425	0.032*
C84	1.01130(10)	0.4968(2)	0.91618(13)	0.0198(7)
C85	0.98630(9)	0.2860(2)	0.81347(14)	0.0193(7)
C86	0.88614(11)	0.2488(3)	0.71797(16)	0.0366(10)
H86	0.8606	0.2350	0.7204	0.044*
C87	0.91544(11)	0.2557(3)	0.76637(16)	0.0336(9)
H87	0.9102	0.2472	0.8012	0.040*
C88	0.95271(10)	0.2752(2)	0.76241(14)	0.0207(7)
C89	0.95884(11)	0.2885(3)	0.71080(15)	0.0296(8)
H89	0.9840	0.3033	0.7071	0.036*
C90	0.92791(12)	0.2799(3)	0.66489(16)	0.0360(9)
H90	0.9323	0.2879	0.6295	0.043*
C91	0.66038(10)	0.3251(2)	0.20288(14)	0.0234(7)
H91A	0.6452	0.3761	0.2144	0.028*
H91B	0.6495	0.3137	0.1630	0.028*
C92	0.70221(10)	0.3531(2)	0.21434(13)	0.0191(7)
C93	0.75727(10)	0.4146(2)	0.20690(14)	0.0202(7)
C94	0.78750(10)	0.4576(2)	0.19088(15)	0.0235(7)
H94	0.7833	0.4910	0.1571	0.028*
C95	0.82415(11)	0.4493(3)	0.22665(15)	0.0262(8)
H95	0.8458	0.4768	0.2169	0.031*
C96	0.83012(10)	0.4009(2)	0.27731(15)	0.0245(7)
H96	0.8555	0.3986	0.3014	0.029*
C97	0.79996(10)	0.3569(2)	0.29273(14)	0.0206(7)
H97	0.8042	0.3233	0.3265	0.025*
C98	0.76314(9)	0.3640(2)	0.25665(13)	0.0176(6)
C99	0.66584(11)	0.1523(3)	0.20567(14)	0.0256(8)
H99A	0.6799	0.1689	0.1779	0.031*
H99B	0.6410	0.1220	0.1865	0.031*
C100	0.68966(10)	0.0854(2)	0.24694(14)	0.0221(7)
C101	0.71866(10)	−0.0453(3)	0.28382(15)	0.0250(8)
C102	0.73155(11)	−0.1372(3)	0.29687(17)	0.0304(8)
H102	0.7233	−0.1881	0.2719	0.036*
C103	0.75709(11)	−0.1508(3)	0.34837(17)	0.0304(8)
H103	0.7665	−0.2127	0.3591	0.036*
C104	0.76925(11)	−0.0758(3)	0.38469(16)	0.0298(8)
H104	0.7871	−0.0877	0.4193	0.036*
C105	0.75605(10)	0.0155(3)	0.37169(15)	0.0261(8)
H105	0.7646	0.0663	0.3966	0.031*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C106	0.72981(10)	0.0302(2)	0.32080(14)	0.0218(7)
C107	0.62225(10)	0.2326(3)	0.25256(14)	0.0232(7)
H10A	0.6182	0.1674	0.2643	0.028*
H10B	0.5995	0.2511	0.2224	0.028*
C108	0.62749(9)	0.2995(2)	0.29990(13)	0.0195(7)
C109	0.61637(10)	0.4064(2)	0.35749(14)	0.0216(7)
C110	0.60134(11)	0.4748(3)	0.38568(16)	0.0291(8)
H110	0.5744	0.4897	0.3761	0.035*
C111	0.62732(11)	0.5201(3)	0.42821(17)	0.0306(9)
H111	0.6180	0.5670	0.4487	0.037*
C112	0.66738(11)	0.4987(3)	0.44222(16)	0.0282(8)
H112	0.6844	0.5309	0.4722	0.034*
C113	0.68247(10)	0.4317(2)	0.41316(14)	0.0228(7)
H113	0.7095	0.4176	0.4224	0.027*
C114	0.65621(10)	0.3858(2)	0.36967(14)	0.0201(7)
C115	0.74594(9)	0.2385(2)	0.42582(13)	0.0183(7)
C116	0.83846(12)	0.3036(3)	0.53136(16)	0.0377(10)
H116	0.8617	0.3381	0.5336	0.045*
C117	0.81034(11)	0.2999(3)	0.48203(16)	0.0319(9)
H117	0.8139	0.3316	0.4504	0.038*
C118	0.77693(9)	0.2494(2)	0.47949(14)	0.0183(7)
C119	0.77219(10)	0.2059(3)	0.52654(15)	0.0282(8)
H119	0.7489	0.1726	0.5258	0.034*
C120	0.80148(10)	0.2114(3)	0.57427(15)	0.0277(8)
H120	0.7987	0.1802	0.6065	0.033*
Cl2	0.69398(2)	0.02254(6)	0.54238(4)	0.02591(19)
Cl3	0.19681(2)	0.05858(7)	0.04730(4)	0.02645(19)
Cl5	0.86531(3)	0.39337(7)	0.89342(4)	0.0311(2)
Cl1 ^a	0.55539(6)	0.47133(16)	0.19547(8)	0.0208(3)
O9 ^a	0.55327(16)	0.3707(4)	0.1829(2)	0.0311(10)
O10 ^a	0.53476(11)	0.5219(2)	0.14690(14)	0.0365(8)
O11 ^a	0.53762(9)	0.4885(2)	0.23917(12)	0.0349(8)
O12 ^a	0.59515(9)	0.4999(2)	0.21158(16)	0.0429(9)
Cl4 ^b	1.05134(5)	0.47734(15)	0.69561(8)	0.0208(3)
O21 ^b	1.0301(3)	0.5223(5)	0.6459(3)	0.0306(12)
O22 ^b	1.04839(10)	0.3769(2)	0.68680(15)	0.0469(10)
O23 ^b	1.03462(10)	0.4990(3)	0.73990(13)	0.0454(9)
O24 ^b	1.09128(10)	0.5037(3)	0.71024(18)	0.0519(11)
Cl6 ^c	0.62324(4)	0.60935(11)	0.62377(6)	0.0273(3)
O29 ^c	0.60914(16)	0.6464(4)	0.56805(19)	0.0396(12)
O30 ^c	0.61413(16)	0.5101(3)	0.62293(19)	0.0475(12)
O31 ^c	0.66499(12)	0.6215(4)	0.6406(2)	0.0466(13)
O32 ^c	0.60648(16)	0.6577(4)	0.6612(2)	0.0893(18)
Cl1 ^d	0.5609(5)	0.4607(14)	0.1887(7)	0.0208(3)
O9 ^d	0.5598(15)	0.362(4)	0.1960(19)	0.0311(10)
O10 ^d	0.5235(8)	0.5014(18)	0.1657(10)	0.0365(8)
O11 ^d	0.5795(6)	0.5019(14)	0.2429(9)	0.028(5)
O12 ^d	0.5837(6)	0.4791(17)	0.1505(11)	0.0429(9)
Cl4 ^e	1.0573(5)	0.4689(13)	0.6884(7)	0.0208(3)
O21 ^e	1.029(3)	0.541(5)	0.652(3)	0.0306(12)
O22 ^e	1.0792(7)	0.4212(15)	0.6616(11)	0.0469(10)
O23 ^e	1.0335(7)	0.411(2)	0.7153(9)	0.0454(9)
O24 ^e	1.0762(7)	0.528(2)	0.7308(13)	0.0519(11)
Cl6 ^f	0.6341(3)	0.5849(7)	0.6052(5)	0.040(3)
O29 ^f	0.6015(11)	0.645(3)	0.5811(14)	0.0396(12)
O30 ^f	0.6120(11)	0.537(2)	0.6383(13)	0.0475(12)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
O31 ^f	0.6549(9)	0.638(3)	0.6497(15)	0.0466(13)
O32 ^f	0.6509(9)	0.529(2)	0.5754(12)	0.0893(18)
O13	0.68659(8)	0.12278(19)	0.53929(12)	0.0337(6)
O14	0.73502(8)	0.0075(2)	0.55514(14)	0.0457(8)
O15	0.67494(8)	−0.0219(2)	0.49134(11)	0.0363(7)
O16	0.67919(9)	−0.0155(2)	0.58632(11)	0.0424(8)
O17	0.18560(8)	0.15616(19)	0.04991(11)	0.0342(6)
O18	0.18006(8)	0.0210(2)	−0.00634(11)	0.0353(6)
O19	0.18262(8)	0.00479(19)	0.08699(11)	0.0359(7)
O20	0.23805(8)	0.0517(2)	0.06106(13)	0.0468(8)
O25	0.84553(10)	0.3425(2)	0.84508(13)	0.0503(9)
O26	0.90546(9)	0.3671(2)	0.90913(14)	0.0562(10)
O27	0.86166(9)	0.4917(2)	0.88121(14)	0.0493(8)
O28	0.84852(13)	0.3726(3)	0.93792(15)	0.0755(12)
H16N	0.3651(10)	0.255(4)	0.0997(14)	0.074(18)*
H32N	0.8531(11)	0.263(4)	0.6088(12)	0.078(19)*

^aOccupancy: 0.876(4); ^boccupancy: 0.875(4); ^coccupancy: 0.851(5); ^doccupancy: 0.124(4); ^eoccupancy: 0.125(4); ^foccupancy: 0.149(5).

Source of material

Tris(2-benzimidazolylmethyl)amine (*ntb*) was prepared according to the literature method [1]. A methanol solution (10 mL) containing Co(ClO₄)₂·6H₂O (0.092 g, 0.25 mmol) was added to a methanol solution (10 mL) of *ntb* (0.102 g, 0.25 mmol). The reaction mixture was stirred for 30 min, then a methanol solution (20 mL) of isonicotinic acid (0.031 g, 0.25 mmol) was added dropwise. After stirring for 3 h, the solution was filtered and allowed to stand at room temperature for slow evaporation. Red crystals suitable for X-ray structure determination were formed.

Experimental details

The methyl groups were idealized and refined using rigid groups allowed to rotate about the N—C bond (with the SHELX program). The U_{iso} values of the hydrogen atoms of methyl groups were set to $1.5U_{eq}(C)$ and the U_{iso} values of all other hydrogen atoms were set to $1.2U_{eq}(C)$. The three perchlorate anions (Cl1, Cl4, Cl6) are disordered with occupancies of 0.876(4) and 0.124(4), 0.875(4) and 0.125(4), 0.851(5) and 0.149(5), respectively.

Discussion

The tripodal ligand tris(2-benzimidazolylmethyl)amine and their complexes with metal ions have attracted much attention in recent years. These complexes may not only exhibit special supramolecular networks [2], but also serve as model compounds for the active site of metalloproteins [3, 4]. Isonicotinate (*isonic*) is a ligand with two types of binding site. It can coordinate with transition metal ion *via* one or two O atoms from the carboxylate group or the N atom from the pyridine ring or both of them [5].

Some cobalt(II) complexes of *ntb* were structurally characterized with H_2O , NCS^- , and Cl^- used as coligands. However, isonicotinate as coligand has never been reported. In this paper, we synthesized and characterized a cobalt(II) complex $[Co(ntb)(Hisonic)][Co(ntb)(isonic)](ClO_4)_3$ in which *Hisonic* and isonicotinate anionic ligands are present.

The title crystal structure shows the presence of two asymmetric double molecular structure units containing $[Co(ntb)(Hisonic)]^{2+}$ cation and $[Co(ntb)(isonic)]^+$ cation in 1:1 ratio along with three perchlorate anions. The two units are connected by hydrogen bonds, and the hydrogen bonds are probably caused by the transfer of hydrogen atom of *Hisonic* from the oxygen atom of carboxylate to the nitrogen atom of pyridine. This is a huge difference from the commonly found example in which isonicotinic acid functions as a coligand. In the title structure, the coordination of Co can be viewed as a 4+2 coordination (*cf.* the figure) onal bipyramidal geometry with a N_4O_1 donor set, formed by a tetradentate *ntb* and a monodentate isonicotinate/isonicotinic acid. The three nitrogen atoms of benzimidazole groups of *ntb* constitute the equatorial plane. The axial sites are occupied by O atom of isonicotinate and tertiary amine nitrogen atom of *ntb*. The distance between Co1 and N1 is 2.425(3) Å, significantly longer than the average bond length between Co and the nitrogen donors which is about 2 Å. It largely deviates from the ideal trigonal bipyramid equatorial plane bond angle (120°), thus the title structure in a distorted trigonal bipyramidal geometry. Co2 has the same distorted trigonal bipyramidal geometry and N_4O_1 donor set as Co1 even though it is coordinated by the protonated *Hisonic*. The axial distance between Co2 and N9 is 2.392(3) Å, which is slightly shorter than the mentioned axial distance $Co1-N1 = 2.425(3)$ Å. The coordination environment, bond length and bond angle of Co3, Co4 are similar to Co1, Co2.

In addition, extensive hydrogen bonds are existed in the title complex, a one-dimensional chain structure is formed by

intermolecular H-bonds between adjacent complexes. They are two pairs of $N-H-N(N16-H16N-N8$ and $N32-H32N-N24)$ and four pairs of $N-H-O$ ($N31-H31N-O2$, $N5-H5N-O8$, $N15-H15N-O6$ and $N19-H19N-O4$). The chain is further expanded to form a 2D network through $N-H-O$ hydrogen bonds, which are linked between N atoms of benzimidazole and O atoms of perchlorate anion.

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