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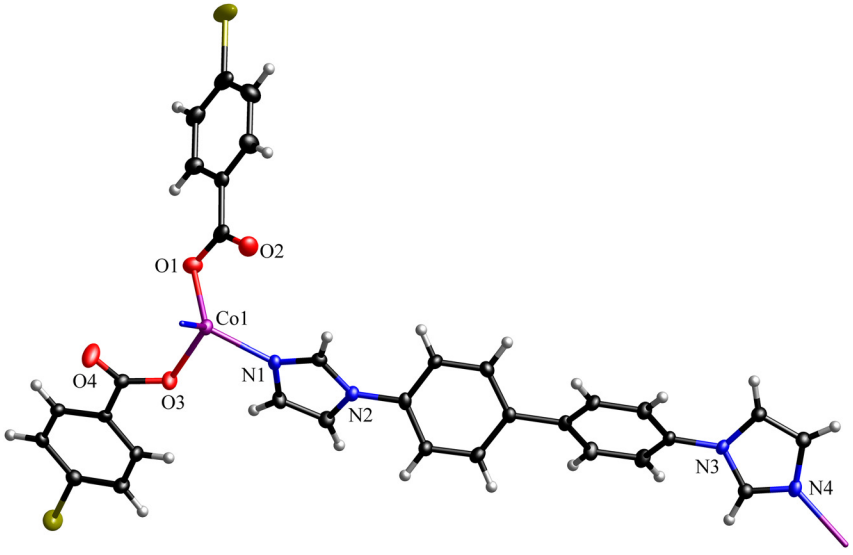
Crystal structure of *catena*-poly[(μ_2-1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol)-κ^2*N*:*N*′)-bis(4-bromobenzoate-κ^1*O*)cobalt(II)], $C_{32}H_{22}Br_2CoN_4O_4$



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Abstract

$C_{32}H_{22}Br_2CoN_4O_4$, monoclinic, $P2_1/c$ (no. 4), a = 6.5529(11) Å, b = 24.375(4) Å, c = 18.379(3) Å, β = 97.491(3)°, V = 2910.6(8) Å^3, Z = 4, $R_{gt}(F)$ = 0.0404, $wR_{ref}(F^2)$ = 0.1268, T = 296(2) K.

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A section of the chain-type title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All chemicals were used without further purification. A mixture of 1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol) (1 mmol, 286.3 mg), 4-bromobenzoic acid (2 mmol, 402.0 mg), $Co(CH_3COO)_2 \cdot 4H_2O$ (1 mmol, 249.1 mg), 1 mL *N*,*N*-dimethylacetamide and 3 mL H_2O in a 10 mL Teflon-lined autoclave was heated at 373 K under autogenous pressure for three days. After cooling to room temperature, purple block crystals were obtained.

Table 1: Data collection and handling.

Crystal:	Purple block
Size:	0.25 × 0.23 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	3.38 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14,779, 5119, 0.047
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 3545
$N(param)_{refined}$:	388
Programs:	Bruker [1], SHELX [2]

Experimental details

All H atoms were placed in calculated positions and were included in the refinement using the riding model approximation, with C–H = 0.93 Å and U_{iso}(H) set to 1.2U_{eq}(C).

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

Atom	x	y	z	U_{iso}*/U_{eq}
Br1	−0.04722 (13)	0.44795 (3)	−0.11975 (3)	0.0748 (3)
Br2	−0.26590 (9)	0.21135 (2)	0.58923 (3)	0.0523 (2)
C1	0.4254 (8)	0.3956 (2)	0.1840 (3)	0.0388 (13)
C2	0.3095 (8)	0.40888 (18)	0.1106 (3)	0.0323 (11)
C3	0.0996 (8)	0.4024 (2)	0.0975 (3)	0.0411 (13)
H3	0.028120	0.390337	0.134969	0.049*
C4	−0.0070 (9)	0.4139 (2)	0.0285 (3)	0.0496 (15)
H4	−0.148761	0.408910	0.019628	0.060*
C5	0.0986 (10)	0.4325 (2)	−0.0263 (3)	0.0500 (15)
C6	0.3077 (10)	0.4406 (2)	−0.0140 (3)	0.0576 (16)
H6	0.378197	0.453931	−0.050991	0.069*
C7	0.4124 (9)	0.4282 (2)	0.0553 (3)	0.0521 (15)
H7	0.554190	0.433178	0.064050	0.062*
C8	0.2672 (7)	0.36459 (19)	0.4252 (3)	0.0293 (11)
C9	0.1421 (7)	0.32758 (18)	0.4671 (2)	0.0263 (10)
C10	0.2090 (7)	0.27521 (18)	0.4883 (3)	0.0318 (11)
H10	0.335891	0.263137	0.477065	0.038*
C11	0.0930 (8)	0.2409 (2)	0.5253 (3)	0.0372 (12)
H11	0.141683	0.206377	0.540634	0.045*
C12	−0.0995 (8)	0.2588 (2)	0.5395 (3)	0.0349 (12)
C13	−0.1713 (7)	0.31044 (19)	0.5183 (2)	0.0327 (11)
H13	−0.300445	0.322073	0.527744	0.039*
C14	−0.0482 (7)	0.34428 (19)	0.4830 (2)	0.0301 (11)
H14	−0.094522	0.379341	0.469416	0.036*
C15	0.9204 (7)	0.29608 (18)	0.2901 (2)	0.0282 (11)
H15	0.992174	0.321479	0.265502	0.034*
C16	0.6920 (7)	0.25802 (18)	0.3478 (3)	0.0323 (11)
H16	0.574231	0.253015	0.370306	0.039*
C17	0.8356 (7)	0.21942 (18)	0.3425 (3)	0.0331 (11)
H17	0.836226	0.183664	0.360221	0.040*
C18	1.1569 (7)	0.21489 (18)	0.2843 (3)	0.0278 (11)
C19	1.2334 (7)	0.22701 (19)	0.2198 (3)	0.0317 (11)
H19	1.183683	0.257015	0.191692	0.038*
C20	1.3849 (7)	0.19405 (19)	0.1975 (3)	0.0337 (11)
H20	1.437829	0.202712	0.154409	0.040*
C21	1.4603 (7)	0.14880 (18)	0.2370 (2)	0.0276 (10)
C22	1.3848 (7)	0.13839 (18)	0.3034 (3)	0.0336 (11)
H22	1.435020	0.108588	0.331878	0.040*
C23	1.2369 (7)	0.17171 (18)	0.3272 (3)	0.0315 (11)
H23	1.191254	0.165033	0.372245	0.038*
C24	1.6195 (7)	0.11214 (18)	0.2124 (2)	0.0273 (10)
C25	1.7839 (7)	0.13342 (18)	0.1814 (3)	0.0305 (11)
H25	1.793263	0.171181	0.175427	0.037*
C26	1.9340 (7)	0.10017 (18)	0.1593 (3)	0.0345 (12)
H26	2.044677	0.115400	0.139481	0.041*
C27	1.9188 (7)	0.04376 (18)	0.1668 (2)	0.0273 (10)
C28	1.7549 (7)	0.02150 (19)	0.1961 (3)	0.0346 (12)
H28	1.743202	−0.016368	0.200235	0.042*
C29	1.6078 (7)	0.05532 (18)	0.2195 (3)	0.0322 (11)
H29	1.499081	0.039995	0.240290	0.039*
C30	2.1511 (7)	−0.03533 (18)	0.1812 (3)	0.0306 (11)
H30	2.106454	−0.048207	0.224038	0.037*
C31	2.1788 (7)	0.01502 (19)	0.0851 (3)	0.0322 (11)
H31	2.160369	0.042525	0.049762	0.039*
C32	2.3133 (7)	−0.02731 (18)	0.0878 (3)	0.0319 (11)
H32	2.403014	−0.034063	0.053563	0.038*
Co1	0.55196 (9)	0.37176 (2)	0.31765 (3)	0.02741 (18)
N1	0.7435 (6)	0.30611 (15)	0.3151 (2)	0.0277 (9)
N2	0.9829 (6)	0.24381 (15)	0.3053 (2)	0.0280 (9)
N3	2.0757 (6)	0.00929 (14)	0.1445 (2)	0.0278 (9)
N4	2.2970 (6)	−0.05869 (14)	0.1486 (2)	0.0287 (9)
O1	0.3236 (5)	0.38113 (14)	0.23528 (19)	0.0429 (9)
O2	0.6156 (6)	0.39836 (15)	0.1940 (2)	0.0506 (10)
O3	0.4103 (5)	0.34085 (13)	0.39622 (19)	0.0399 (9)
O4	0.2285 (6)	0.41350 (14)	0.4202 (2)	0.0553 (11)

Comment

In recent years, 1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol) has been widely applied in the formation of coordination polymers due to its excellent coordination ability and versatile coordination modes [3–10]. To further explore this area, 1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol) was selected as the organic ligand, together with the auxiliary ligand 4-bromobenzoate to synthesize a new Co(II) coordination polymer.

The title structure is a *zigzag* one-dimensional chain structure. As shown in Figure, the asymmetric unit consists one cobalt cation, one 1,1′-(biphenyl-4,4′-diyl) bis(1*H*-imidazol) ligand, and two 4-bromobenzoate ligands. The Co(II) cation is surrounded by two nitrogen atoms from two symetry related 1,1′-(biphenyl-4,4′-diyl) bis(1*H*-imidazol) ligands and two oxygen atoms from two 4-bromobenzoate ligands. Its coordination geometry is a distorted tetrahedron. The Co–O bond lengths range from 1.966(3) to 1.998(3) Å. The Co–N bond lengths range from 2.019(4) to 2.038(4) Å. The bridging 1,1′-(biphenyl-4,4′-diyl)bis(1*H*-imidazol) ligands link Co(II) cations to form a chain with the Co–Co distance of 17.808 Å and Co–Co–Co angel of 86.37°.

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