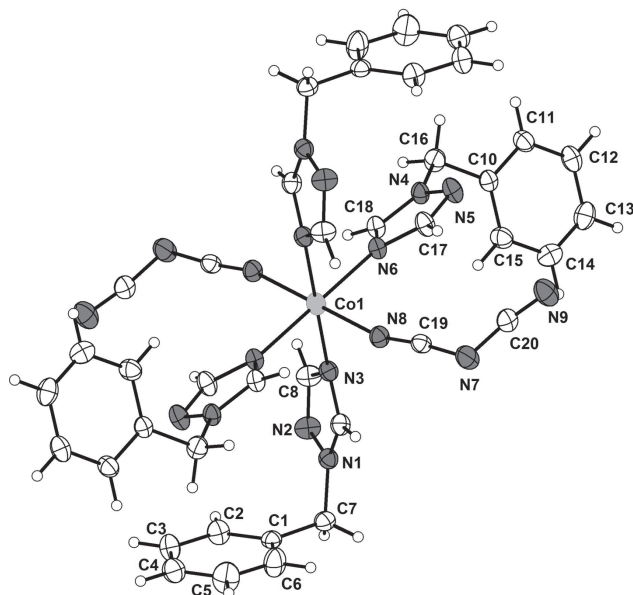


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Crystal structure of bis(dicyanamido- κ^1N)-tetrakis[1-benzyl-1*H*-1,2,4-triazole- κ^1N]cobalt(II), $\text{CoC}_{40}\text{H}_{36}\text{N}_{18}$

**Table 1:** Data collection and handling.

Crystal:	Light-orange block
Size:	0.62 × 0.50 × 0.30 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	4.8 cm ⁻¹
Diffractometer, scan mode:	Rigaku Mercury, ω
$2\theta_{\text{max}}$, completeness:	50.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	18996, 3661, 0.029
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3344
$N(\text{param})_{\text{refined}}$:	268
Programs:	SHELX [9], CrystalClear [10]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.0000	0.0000	0.02600(12)
N1	-0.17559(18)	-0.24249(11)	-0.11522(12)	0.0322(4)
N2	-0.30626(18)	-0.20427(12)	-0.12830(14)	0.0415(4)
N3	-0.12432(17)	-0.10699(10)	-0.08195(12)	0.0310(4)
N4	-0.21121(18)	0.16796(11)	-0.24788(12)	0.0327(4)
N5	-0.07281(19)	0.18201(12)	-0.24680(13)	0.0413(4)
N6	-0.07404(17)	0.08678(11)	-0.12713(11)	0.0306(4)
N7	0.3732(2)	-0.04851(13)	-0.11463(18)	0.0587(6)
N8	0.18400(18)	-0.03499(11)	-0.03853(13)	0.0345(4)
N9	0.4539(2)	0.06182(14)	-0.20710(16)	0.0540(5)
C1	-0.1157(2)	-0.36776(12)	-0.00516(15)	0.0315(4)
C2	-0.2117(2)	-0.36663(15)	0.04746(17)	0.0419(5)
H2A	-0.3085	-0.3483	0.0155	0.050*
C3	-0.1664(3)	-0.39230(16)	0.14661(18)	0.0489(6)
H3A	-0.2323	-0.3910	0.1820	0.059*
C4	-0.0259(3)	-0.41970(16)	0.19387(17)	0.0498(6)
H4A	0.0044	-0.4377	0.2613	0.060*
C5	0.0701(3)	-0.4208(2)	0.1426(2)	0.0637(8)
H5A	0.1669	-0.4390	0.1750	0.076*
C6	0.0250(3)	-0.39504(18)	0.04308(19)	0.0544(7)
H6A	0.0915	-0.3963	0.0081	0.065*
C7	-0.1611(2)	-0.33679(13)	-0.11227(15)	0.0371(5)
H7A	-0.0880	-0.3541	-0.1419	0.045*
H7B	-0.2547	-0.3631	-0.1517	0.045*
C8	-0.2693(2)	-0.12343(14)	-0.10789(16)	0.0393(5)
H8A	-0.3381	-0.0800	-0.1110	0.047*
C9	-0.0700(2)	-0.18444(13)	-0.08797(15)	0.0335(5)

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Abstract

$\text{CoC}_{40}\text{H}_{36}\text{N}_{18}$, monoclinic, $P2_1/c$ (no. 14), $a = 9.7410(15)$ Å, $b = 15.511(2)$ Å, $c = 14.162(2)$ Å, $\beta = 110.00(3)^\circ$, $V = 2010.7(5)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0395$, $wR_{\text{ref}}(F^2) = 0.0869$, $T = 223(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H9A	0.0295	−0.1963	−0.0747	0.040*
C10	−0.3679(2)	0.18563(13)	−0.42672(15)	0.0314(4)
C11	−0.4196(2)	0.24648(14)	−0.50231(15)	0.0387(5)
H11A	−0.4284	0.3044	−0.4857	0.046*
C12	−0.4584(3)	0.22231(16)	−0.60204(16)	0.0458(6)
H12A	−0.4946	0.2637	−0.6530	0.055*
C13	−0.4441(2)	0.13782(17)	−0.62700(17)	0.0463(6)
H13A	−0.4692	0.1217	−0.6948	0.056*
C14	−0.3931(2)	0.07730(16)	−0.55242(17)	0.0447(5)
H14A	−0.3839	0.0195	−0.5694	0.054*
C15	−0.3551(2)	0.10083(14)	−0.45237(16)	0.0409(5)
H15A	−0.3206	0.0590	−0.4018	0.049*
C16	−0.3358(2)	0.21305(15)	−0.31880(15)	0.0411(5)
H16A	−0.3164	0.2752	−0.3133	0.049*
H16B	−0.4224	0.2024	−0.3002	0.049*
C17	0.0044(2)	0.13195(14)	−0.17307(15)	0.0375(5)
H17A	0.1066	0.1277	−0.1535	0.045*
C18	−0.2093(2)	0.11214(13)	−0.17685(14)	0.0328(5)
H18A	−0.2925	0.0931	−0.1635	0.039*
C19	0.2727(2)	−0.03709(13)	−0.07476(15)	0.0319(4)
C20	0.4116(2)	0.01356(14)	−0.16206(16)	0.0363(5)

the atoms including atomic coordinates and displacement parameters.

Source of material

A methanolic solution (10 mL) of 1-benzyl-1*H*-1,2,4-triazole (1.0 mmol) was added slowly to an aqueous solution (10 mL) of Co(NO₃)₂·6H₂O (0.5 mmol) and Na[N(CN)₂] (1.0 mmol) with stirring. The mixture was stirred at room temperature and the resultant solution was filtered. The filtrate was allowed to stand for several days, yielding colorless crystals of the title compound.

Experimental details

All hydrogen atoms were placed in idealized positions and refined using a riding model.

Discussion

Design, synthesis and characterization of coordination polymers have drawn great interest not only because of their versatile structural motifs and intriguing structures, but also mainly due to their various applications in the areas of optics, magnetism, electronics, catalysis, molecular recognition and adsorption and biological activity [1–4]. The ligands and metal centers both are the key to the design and construction of metal-organic frameworks. A large number of mononuclear, oligonuclear, and polynuclear transition metal

complexes of 1- and 4-substituted 1,2,4-triazole derivatives have been synthesized and characterized due to their interesting properties and novel topologies [5–8]. In this paper, we select 1-benzyl-1*H*-1,2,4-triazole to react with Co(II) ions to obtain a new MOFs.

The asymmetric unit of the title structure consists of one half of a Co²⁺ ion, two 1-benzyl-1*H*-1,2,4-triazole and one [N(CN)₂][−]. Each Co(II) atom is coordinated by four nitrogen atoms from four 1-benzyl-1*H*-1,2,4-triazole ligands and two nitrogen atoms from two [N(CN)₂][−] anionic ligands in octahedral geometry. The bond lengths and angles around the Co(II) are in the ranges of 2.1152(17)–2.1646(15) Å and 86.26(6)–180.00(12)°, respectively. These findings are all in the normal range for a distorted octahedral Co complex.

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