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The crystal structure of *cis*-diaqua-bis(*N*-butyl-*N*-(pyridin-2-yl)pyridin-2-amine- $\kappa^2 N, N'$)cobalt(II)] dichloride trihydrate, $C_{28}H_{44}Cl_2N_6O_5Co$

Table 1: Data collection and handling.

Crystal:	Colourless cuboid
Size:	0.27 × 0.22 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.73 mm ⁻¹
Diffractometer, scan mode:	BRUKER APEX-II, φ and ω
$\theta_{\max}$, completeness:	28.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	26,921, 8038, 0.049
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 6746
$N(\text{param})_{\text{refined}}$:	421
Programs:	BRUKER [1], SIR97 [2], WinGX [3], SHELX [4], DIAMOND [5]

and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

To a stirred solution of *N*-butyl-*N*-(pyridin-2-yl)pyridin-2-amine (nBut-DPA) (50 mg, 0.2 mmol) in methanol/water (80/20 ratio), a stoichiometric amount of sodium hydroxide (NaOH) was added at room temperature. After stirring for *ca.* 10 min, a solution of cobalt(II) chloride (52.3 mg, 0.2 mmol) was added drop-wise over 5 min. The reaction was left to stir for another hour. The reaction mixture was filtered and dried *in vacuo*. The dried product yielded reddish crystals, from a methanol/DCM solvent mixture, suitable for X-ray diffraction analysis.

Experimental details

The aromatic H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H = 0.95 and 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ and $1.2 U_{\text{eq}}(\text{C})$, respectively. The placement of the H atoms on the butyl groups was that of an idealised methylene and methyl group according to the electron-density map (HFIX 23, 137).

Comment

The use of organometallic complexes across many scientific disciplines, in attempt to analyse potential synergistic

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Abstract

$C_{28}H_{44}Cl_2N_6O_5Co$, triclinic, $P\bar{1}$ (no. 2), $a = 11.20(2)$ Å, $b = 12.70(3)$ Å, $c = 12.80(4)$ Å, $\alpha = 100.30(12)^\circ$, $\beta = 103.18(9)^\circ$, $\gamma = 106.77(6)^\circ$, $V = 1638(8)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0372$, $wR_{\text{ref}}(F^2) = 0.0890$, $T = 100$ K.

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The molecular structure is shown in figure (the chloride counter anions and uncoordinated water molecules are omitted for clarity). Table 1 contains crystallographic data

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
C1	0.44687(18)	0.21909(17)	0.34586(16)	0.0219(4)
H1	0.437968	0.291082	0.344727	0.026*
C2	0.36548(19)	0.14787(18)	0.38800(17)	0.0277(4)
H2	0.303145	0.170000	0.417329	0.033*
C3	0.37728(19)	0.04307(18)	0.38632(17)	0.0277(4)
H3	0.322273	−0.009110	0.414668	0.033*
C4	0.46914(19)	0.01331(17)	0.34342(16)	0.0232(4)
H4	0.476677	−0.059649	0.341019	0.028*
C5	0.55030(17)	0.09108(15)	0.30388(14)	0.0176(3)
C6	0.65536(16)	0.07428(15)	0.15508(15)	0.0169(3)
C7	0.65246(17)	−0.01831(15)	0.07429(15)	0.0191(4)
H7	0.640584	−0.090435	0.089785	0.023*
C8	0.66678(17)	−0.00493(16)	−0.02730(15)	0.0208(4)
H8	0.664981	−0.067276	−0.081922	0.025*
C9	0.68366(17)	0.09999(16)	−0.04821(15)	0.0200(4)
H9	0.696205	0.112818	−0.116441	0.024*
C10	0.68174(17)	0.18639(15)	0.03383(15)	0.0178(3)
H10	0.689847	0.258200	0.018501	0.021*
C11	0.69594(19)	−0.02121(16)	0.30369(16)	0.0218(4)
H11A	0.643870	−0.098037	0.253643	0.026*
H11B	0.684834	−0.020932	0.378278	0.026*
C12	0.83923(19)	0.00300(16)	0.31130(17)	0.0239(4)
H12A	0.852723	0.016742	0.240425	0.029*
H12B	0.892490	0.073398	0.371081	0.029*
C13	0.8862(2)	−0.0927(2)	0.3346(2)	0.0365(5)
H13A	0.832480	−0.163421	0.275422	0.044*
H13B	0.874393	−0.105671	0.406135	0.044*
C14	1.0291(2)	−0.0673(2)	0.3401(3)	0.0487(7)
H14A	1.040989	−0.056057	0.268893	0.073*
H14B	1.055558	−0.131489	0.355519	0.073*
H14C	1.082908	0.001901	0.399539	0.073*
C15	0.83187(19)	0.31527(16)	0.47229(15)	0.0208(4)
H15	0.751412	0.306097	0.488534	0.025*
C16	0.9373(2)	0.31636(16)	0.55451(16)	0.0243(4)
H16	0.928799	0.306468	0.624612	0.029*
C17	1.0552(2)	0.33221(17)	0.53185(17)	0.0269(4)
H17	1.129187	0.332552	0.586001	0.032*
C18	1.06387(18)	0.34758(17)	0.42907(17)	0.0244(4)
H18	1.144667	0.360566	0.412734	0.029*
C19	0.95238(17)	0.34384(15)	0.34905(15)	0.0177(3)
C20	0.91515(17)	0.43934(15)	0.20201(14)	0.0176(3)
C21	0.99754(19)	0.51915(16)	0.16566(16)	0.0227(4)
H21	1.083005	0.519026	0.168582	0.027*
C22	0.9532(2)	0.59821(17)	0.12544(17)	0.0280(4)
H22	1.007423	0.652870	0.098787	0.034*
C23	0.8286(2)	0.59823(17)	0.12373(17)	0.0269(4)
H23	0.796912	0.653197	0.097105	0.032*
C24	0.75329(19)	0.51762(16)	0.16112(15)	0.0217(4)
H24	0.668243	0.517561	0.160271	0.026*
C25	1.05597(18)	0.32351(16)	0.19778(17)	0.0222(4)
H25A	1.144388	0.370681	0.247691	0.027*
H25B	1.049360	0.338889	0.123906	0.027*
C26	1.03853(19)	0.19962(16)	0.18676(18)	0.0247(4)
H26A	0.946759	0.152703	0.144892	0.030*
H26B	1.056676	0.186184	0.261697	0.030*
C27	1.1294(2)	0.16229(18)	0.12673(18)	0.0285(4)

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
H27A	1.219657	0.216334	0.162739	0.034*
H27B	1.128310	0.086180	0.135547	0.034*
C28	1.0923(3)	0.1567(2)	0.0033(2)	0.0398(6)
H28A	1.148355	0.125078	−0.031284	0.060*
H28B	1.103878	0.233584	−0.006140	0.060*
H28C	1.000858	0.107930	−0.032088	0.060*
Cl1	0.47781(5)	0.31888(4)	−0.11558(4)	0.02823(11)
Cl2	0.64532(5)	0.43755(5)	0.60652(4)	0.03053(12)
Co1	0.66479(2)	0.31584(2)	0.25061(2)	0.01468(7)
H1A	0.493(2)	0.307(2)	0.066(2)	0.035(7)*
H1B	0.452(3)	0.357(3)	0.145(3)	0.062(9)*
H2A	0.643(2)	0.448(2)	0.428(2)	0.030(6)*
H2B	0.639(3)	0.509(3)	0.358(2)	0.051(9)*
H3A	0.386(3)	0.501(3)	0.128(2)	0.049(8)*
H3B	0.359(3)	0.476(3)	0.215(3)	0.056(9)*
H4A	0.562(3)	0.643(2)	0.377(2)	0.053(9)*
H4B	0.615(3)	0.670(2)	0.302(3)	0.048(8)*
H5A	0.683(3)	0.298(3)	−0.284(2)	0.046(9)*
H5B	0.635(4)	0.285(3)	−0.200(3)	0.087(12)*
N1	0.53957(14)	0.19313(13)	0.30556(12)	0.0175(3)
N2	0.64645(15)	0.06351(13)	0.26165(12)	0.0181(3)
N3	0.66903(14)	0.17531(12)	0.13467(12)	0.0154(3)
N4	0.83724(14)	0.32653(12)	0.37037(12)	0.0167(3)
N5	0.95761(15)	0.35721(13)	0.24248(13)	0.0188(3)
N6	0.79397(15)	0.43790(13)	0.19929(12)	0.0176(3)
O1	0.49629(13)	0.31181(12)	0.13010(12)	0.0216(3)
O2	0.64032(14)	0.44669(12)	0.36299(12)	0.0225(3)
O3	0.35491(15)	0.44747(13)	0.15145(14)	0.0269(3)
O4	0.63318(15)	0.65980(13)	0.36378(13)	0.0263(3)
O5	0.6914(2)	0.26774(17)	−0.2365(2)	0.0541(5)

effects therein, has become a norm. Moreover, derivatizing organic compounds as ligand systems has become a necessity to allow appropriate functionalities to be built-in [6–9]. Herein, *N*-butyl-*N*-(pyridin-2-yl)pyridin-2-amine (nBut-DPA), a derivative of 2,2'-dipyridylamine is used. This ligand and its derivative analogs with metal centres have been found to be efficient in many biological media [10–12]. Its complexes with different transition metal ions cover broad scientific fields [12–17].

The crystal structure is comprised of two nBut-DPA bidentate ligands inducing a distorted octahedral coordination mode to a cobalt(II) metal ion. Furthermore, there are two coordinated aqua ligands in a *cis* configuration completing the distorted octahedral molecular geometry for the title structure. In the second coordination sphere, there are further three water molecules and two charge balancing chloride anions in the asymmetric unit. The structure is further held in tact by intramolecular hydrogen interactions between the water (O1 and O2) molecules in the first coordination sphere and the chloride anions

(Cl1 and Cl2) and other water molecules (O3, O4 and O5) in the second coordination sphere.

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