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Crystal structure of diaqua-bis(*N,N*-dimethylformamide- κ^1O)-bis{3-((5-chloro-2-oxidobenzylidene)amino)-2-oxo-2*H*-chromen-4-olato- $\kappa^4N,O,O':O'$ }dinickel(II), $C_{38}H_{34}Ni_2Cl_2N_4O_{12}$

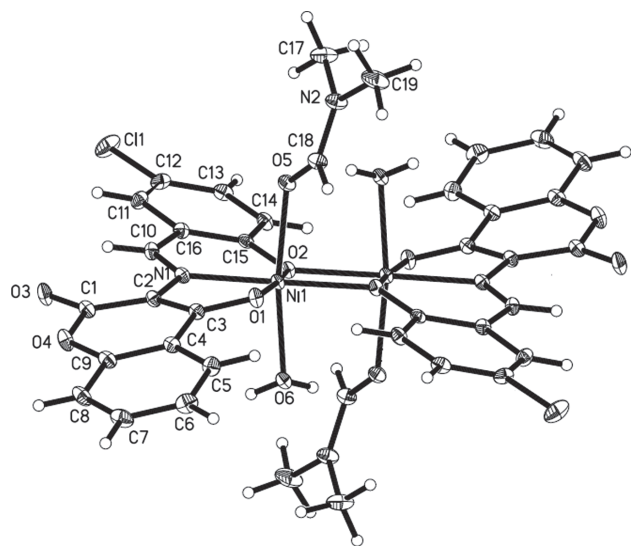


Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Ni1	0.702897(13)	0.21397(2)	0.540268(9)	0.01428(10)
Cl1	0.39857(3)	0.61158(6)	0.30916(2)	0.03601(16)
O6	0.70664(8)	−0.00198(14)	0.51499(6)	0.0196(3)
H6A	0.6612	−0.0300	0.4962	0.029*
H6B	0.7306	−0.0016	0.4916	0.029*
O4	0.48797(8)	0.00734(16)	0.61407(6)	0.0261(3)
O3	0.42914(8)	0.14707(17)	0.53779(7)	0.0293(3)
O1	0.71102(8)	0.13479(15)	0.62026(5)	0.0199(3)
O5	0.71768(8)	0.43212(14)	0.56753(6)	0.0208(3)
C13	0.55050(12)	0.5093(2)	0.34088(8)	0.0216(4)
H13	0.5522	0.5563	0.3079	0.026*
C11	0.47821(12)	0.4463(2)	0.40333(8)	0.0224(4)
H11	0.4318	0.4523	0.4121	0.027*
C3	0.64137(11)	0.0940(2)	0.61733(8)	0.0177(4)
C4	0.63238(11)	−0.0078(2)	0.66031(8)	0.0194(4)
N2	0.79546(11)	0.60014(18)	0.62958(7)	0.0256(4)
O2	0.68062(8)	0.28306(13)	0.45827(6)	0.0161(3)
C2	0.57100(11)	0.1386(2)	0.57212(8)	0.0180(4)
C16	0.54453(11)	0.3649(2)	0.43986(8)	0.0182(4)
C14	0.61668(11)	0.4312(2)	0.37636(8)	0.0200(4)
H14	0.6625	0.4274	0.3668	0.024*
C5	0.69776(13)	−0.0719(2)	0.70317(9)	0.0239(4)
H5	0.7495	−0.0424	0.7078	0.029*
C8	0.54307(13)	−0.1573(2)	0.69137(9)	0.0273(4)
H8	0.4914	−0.1846	0.6878	0.033*
C15	0.61601(10)	0.35798(19)	0.42641(7)	0.0160(3)
C6	0.68598(14)	−0.1797(2)	0.73890(9)	0.0292(5)
H6	0.7297	−0.2236	0.7669	0.035*
N1	0.58521(10)	0.21900(15)	0.52814(7)	0.0166(3)
C9	0.55524(12)	−0.0511(2)	0.65522(8)	0.0216(4)
C12	0.48215(11)	0.5166(2)	0.35502(8)	0.0223(4)
C19	0.86153(15)	0.6317(3)	0.68368(10)	0.0394(6)
H19A	0.8815	0.5422	0.7038	0.059*
H19B	0.8429	0.6936	0.7076	0.059*
H19C	0.9037	0.6801	0.6751	0.059*
C17	0.76193(17)	0.7237(2)	0.59160(11)	0.0363(6)
H17A	0.8008	0.7602	0.5764	0.054*
H17B	0.7479	0.7993	0.6132	0.054*
H17C	0.7149	0.6931	0.5602	0.054*
C7	0.60853(15)	−0.2219(2)	0.73269(10)	0.0295(5)
H7	0.6008	−0.2943	0.7566	0.035*
C1	0.49370(12)	0.1028(2)	0.57211(8)	0.0210(4)
C10	0.53063(11)	0.2894(2)	0.48728(8)	0.0195(4)
H10	0.4792	0.2918	0.4884	0.023*
C18	0.77108(12)	0.4655(2)	0.61437(8)	0.0221(4)
H18	0.7952	0.3908	0.6402	0.027*

N,N-dimethylformamide (DMF) molecules and two coordinated water molecules. Each Ni(II) center is coordinated by one N1 and two O atoms (O1, O2) from a tridentate ligand, as well as two O atoms (O5, O6) from one DMF and one water molecule to obtain two [NiL(DMF)(H₂O)] moieties. These two [NiL(DMF)(H₂O)] moieties are bridged via two μ₂-O2 atoms (phenolic oxygen) to form a hexa-coordinated binuclear structure (*cf.* the figure). The coordination geometry

of the Ni(II) centers can be described as slightly distorted octahedra with axial donor atoms (O5 and O6). The geometric parameters of the 3-((5-chloro-2-oxidobenzylidene)amino)-2-oxo-2*H*-chromen-4-olato ligand are similar to those we have recently reported [21, 22].

An infinite 2D supramolecular planar structure was formed by intermolecular O—H···O hydrogen bonds and π···π intermolecular interactions with the centroid-centroid distance of 4.224(3) Å.

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