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Crystal structure of bis(acetylacetonato)bis(quinoline)nickel(II), $Ni(C_5H_{14}O_2N)_2(C_9H_7N)_2$

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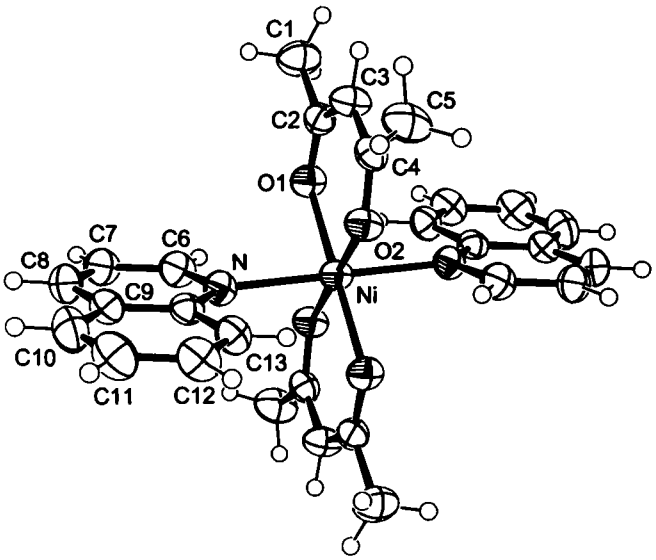

Abstract

$C_{28}H_{28}N_2NiO_4$, triclinic, $P\bar{1}$ (no. 2), a = 7.9202(6) Å, b = 8.0496(6) Å, c = 10.246(1) Å, α = 97.15(1)°, β = 106.68(1)°, γ = 94.686(9)°, V = 616.1 Å^3, Z = 1, $R_{gt}(F)$ = 0.028, $wR_{ref}(F^2)$ = 0.078, T = 293 K.

Source of material

The synthesis has been described elsewhere [1]. Crystals were obtained by slow evaporation from ethanol at 277 K.

Discussion

Adducts of Ni(II) acetylacetonate (acac) chelate with heterocyclic bases have been synthesized with the aim of establishing correlations between the bond energies and other thermodynamic parameters [1]. The title compound also belongs to these compounds of general formula $Ni(acac)_2L_2$ with L = quinoline. The structures of the compounds with L = 3- and 4-cyanopyridine have already been published [2].

The title compound crystallizes with the Ni(II) atom situated on a center of symmetry and bonded octahedrally to two equatorial acac groups and two quinoline groups axially coordinated in a *trans* configuration. The Ni—O_{acac} distances of 2.014(1) Å and 2.024(1) Å give rise to the so-called tetragonal distortion. The acac moiety is not planar, in fact the r.m.s. deviation of O1, O2, C2 – C5 being 0.014 Å, C1 being 0.098(3) Å and Ni(II) being 0.243(2) Å out of the plane, in opposite directions. In the solid state, there is a short intramolecular distance: d(C13···O2) = 3.165(2) Å, ∠C13–H13···O2 = 123°. In turn, the molecules are associated via a C–H···O and C–H···π interactions: d(C13···O1^{i}) = 3.151(2) Å, ∠C13–H13···O1^{i} = 134°; d(H5B···Cg1^{ii}(N,C6-C9, C14)) = 2.73 Å, ∠C5–H5B···Cg1^{ii} = 162°; d(H3···Cg2^{ii}(C9-C14) = 2.99 Å, ∠C3–H3···Cg2^{ii} = 178°. Cg is the centroid of the aromatic ring (symmetry operations i: –x,–y,–z; ii: –x,1–y,–z).

Table 1. Data collection and handling.

Crystal:	blue, irregular, size 0.12 × 0.15 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.24 cm^{-1}
Diffractometer, scan mode:	Nonius CAD4, $\theta/2\theta$
$2\theta_{max}$:	50.94°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2437, 2296
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2152
$N(param)_{refined}$:	162
Programs:	SIR92 [3], SHELXL-97 [4], PARST95 [5], PLATON [6], WinGX [7], ORTEP-3 [8]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(6)	2*i*	0.3408	0.0439	–0.0509	0.052
H(7)	2*i*	0.5041	0.1383	–0.1876	0.059
H(8)	2*i*	0.3617	0.2400	–0.3840	0.062
H(10)	2*i*	0.0736	0.2947	–0.5481	0.066
H(11)	2*i*	–0.2283	0.2777	–0.6083	0.068
H(12)	2*i*	–0.3804	0.1674	–0.4687	0.058
H(13)	2*i*	–0.2313	0.0802	–0.2678	0.048
H(1A)	2*i*	0.4208	0.3043	0.3553	0.083
H(1B)	2*i*	0.3363	0.4735	0.3602	0.083
H(1C)	2*i*	0.4423	0.4310	0.2551	0.083
H(3)	2*i*	0.0537	0.4855	0.2264	0.053
H(5A)	2*i*	–0.3150	0.4501	–0.0326	0.083
H(5B)	2*i*	–0.2205	0.5414	0.1184	0.083
H(5C)	2*i*	–0.3587	0.3806	0.0918	0.083

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni	1*a*	0	0	0	0.0250(2)	0.0330(2)	0.0371(2)	0.0089(1)	0.0054(1)	0.0010(1)
O(1)	2*i*	0.2049(2)	0.1535(2)	0.1366(1)	0.0300(6)	0.0401(6)	0.0433(7)	0.0071(5)	0.0053(5)	0.0018(5)
O(2)	2*i*	−0.1568(2)	0.1872(2)	−0.0094(1)	0.0321(6)	0.0370(6)	0.0402(6)	0.0115(5)	0.0055(5)	0.0005(5)
N	2*i*	0.1068(2)	0.0773(2)	−0.1627(2)	0.0282(7)	0.0424(8)	0.0408(8)	0.0083(6)	0.0103(6)	0.0050(6)
C(6)	2*i*	0.2810(2)	0.0817(2)	−0.1318(2)	0.0307(8)	0.052(1)	0.047(1)	0.0099(8)	0.0099(8)	0.0034(8)
C(7)	2*i*	0.3817(2)	0.1398(3)	−0.2133(2)	0.0297(9)	0.059(1)	0.059(1)	0.0045(8)	0.0182(8)	−0.0027(9)
C(8)	2*i*	0.2971(3)	0.1980(3)	−0.3299(2)	0.046(1)	0.058(1)	0.057(1)	0.0000(9)	0.029(1)	0.0011(9)
C(9)	2*i*	0.1109(3)	0.1950(2)	−0.3695(2)	0.044(1)	0.0412(9)	0.0427(9)	0.0053(7)	0.0184(8)	0.0015(7)
C(10)	2*i*	0.0136(3)	0.2508(3)	−0.4918(2)	0.065(1)	0.061(1)	0.047(1)	0.011(1)	0.027(1)	0.015(1)
C(11)	2*i*	−0.1657(3)	0.2410(3)	−0.5277(2)	0.065(1)	0.065(1)	0.044(1)	0.022(1)	0.013(1)	0.017(1)
C(12)	2*i*	−0.2571(3)	0.1751(3)	−0.4428(2)	0.042(1)	0.059(1)	0.046(1)	0.0183(9)	0.0093(8)	0.0082(9)
C(13)	2*i*	−0.1685(2)	0.1223(2)	−0.3231(2)	0.0341(9)	0.046(1)	0.0422(9)	0.0122(7)	0.0130(7)	0.0067(7)
C(14)	2*i*	0.0186(2)	0.1314(2)	−0.2832(2)	0.0339(8)	0.0335(8)	0.0370(8)	0.0079(6)	0.0117(7)	0.0010(6)
C(2)	2*i*	0.1946(2)	0.2975(2)	0.1952(2)	0.0362(9)	0.0396(9)	0.0303(8)	0.0023(7)	0.0084(7)	0.0057(7)
C(1)	2*i*	0.3640(3)	0.3845(3)	0.3011(2)	0.043(1)	0.055(1)	0.056(1)	0.0019(9)	0.0005(9)	−0.003(1)
C(3)	2*i*	0.0443(3)	0.3818(2)	0.1717(2)	0.045(1)	0.0374(9)	0.043(1)	0.0090(8)	0.0070(8)	−0.0045(7)
C(4)	2*i*	−0.1196(2)	0.3237(2)	0.0727(2)	0.0380(9)	0.0356(8)	0.0354(8)	0.0117(7)	0.0143(7)	0.0072(7)
C(5)	2*i*	−0.2668(3)	0.4340(3)	0.0615(2)	0.049(1)	0.051(1)	0.062(1)	0.0231(9)	0.011(1)	−0.003(1)

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