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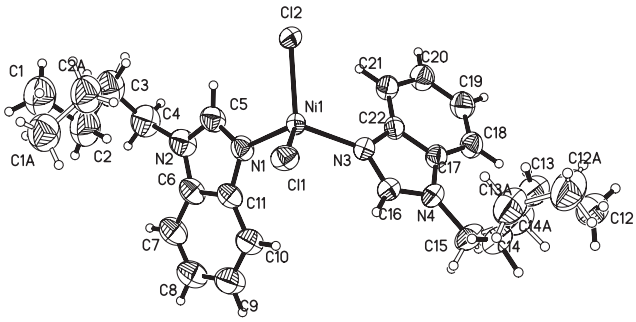
Crystal structure of dichloro-bis-(1-butyl-1*H*-benzo[*d*]imidazole)-nickel(II), $C_{22}H_{28}Cl_2N_4Ni$



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Abstract

$C_{22}H_{28}Cl_2N_4Ni$, monoclinic, $P2_1/c$ (no. 14), $a = 9.7332(19)$ Å, $b = 14.886(3)$ Å, $c = 18.623(5)$ Å, $\beta = 117.45(2)°$, $V = 2394.5(10)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0450$, $wR_{ref}(F^2) = 0.1466$, $T = 293.0$ K.

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The molecular 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

Sodium ethanolide (0.05 mol) was added to 50 mL ethanol, 1*H*-benzo[*d*]imidazole (0.05 mol); bromobutane (0.05 mol) was subsequently added, and the mixture was heated and stirred for 10 h, then nickel chloride (0.03 mol) was added,

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Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.34 × 0.25 × 0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.05 mm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD-4, ω
θ_{max}, completeness:	27.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	23163, 5478, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3720
$N(param)_{refined}$:	312
Programs:	CAD-4 [1, 2], Olex2 [3]

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

Atom	x	y	z	U_{iso}*/U_{eq}
Ni1	1.13167(4)	0.80476(2)	0.476128(18)	0.05323(14)
Cl1	1.23583(9)	0.92719(4)	0.55403(5)	0.0720(2)
Cl2	1.28090(9)	0.68027(4)	0.51326(5)	0.0678(2)
N1	1.0916(3)	0.82524(17)	0.36048(14)	0.0731(7)
N2	1.1128(4)	0.80461(19)	0.24874(16)	0.0922(10)
N3	0.9296(3)	0.78285(16)	0.47886(14)	0.0638(6)
N4	0.7224(3)	0.81044(16)	0.49549(18)	0.0765(7)
C1[a]	1.5499(13)	0.8674(10)	0.2634(7)	0.165(3)
H1a[a]	1.565(2)	0.901(5)	0.224(3)	0.248(5)*
H1b[a]	1.6092(17)	0.894(6)	0.316(3)	0.248(5)*
H1c[a]	1.583(3)	0.8066(12)	0.264(6)	0.248(5)*
C1A[b]	1.489(2)	0.9245(9)	0.2558(9)	0.154(4)
H1Aa[b]	1.417(9)	0.968(2)	0.257(6)	0.231(5)*
H1Ab[b]	1.593(4)	0.945(4)	0.288(4)	0.231(5)*
H1Ac[b]	1.472(13)	0.916(2)	0.201(3)	0.231(5)*
C2[a]	1.3772(13)	0.8682(6)	0.2419(8)	0.152(3)
H2a[a]	1.3595(13)	0.8931(6)	0.2851(8)	0.182(3)*
H2b[a]	1.3149(13)	0.9000(6)	0.1918(8)	0.182(3)*
C2A[b]	1.4657(18)	0.8352(8)	0.2894(7)	0.145(3)
H2Aa[b]	1.5658(18)	0.8058(8)	0.3160(7)	0.174(3)*
H2Ab[b]	1.4358(18)	0.8492(8)	0.3312(7)	0.174(3)*
C3	1.3498(7)	0.7660(4)	0.2331(3)	0.1376(14)
H3aa[a]	1.3863(7)	0.7393(4)	0.1975(3)	0.1651(17)*
H3ab[a]	1.3962(7)	0.7355(4)	0.2849(3)	0.1651(17)*
H3bc[b]	1.3730(7)	0.7602(4)	0.1879(3)	0.1651(17)*
H3bd[b]	1.3802(7)	0.7095(4)	0.2622(3)	0.1651(17)*
C4	1.1728(6)	0.7678(4)	0.1950(2)	0.1177(13)
H4a	1.1341(6)	0.7071(4)	0.1797(2)	0.1412(16)*
H4b	1.1330(6)	0.8036(4)	0.1460(2)	0.1412(16)*
C5	1.1535(4)	0.7778(2)	0.32425(18)	0.0836(9)
H5	1.2198(4)	0.7297(2)	0.34867(18)	0.1003(11)*
C6	1.0161(5)	0.8770(2)	0.23431(18)	0.0836(9)
C7	0.9346(5)	0.9308(3)	0.1646(2)	0.1032(11)
H7	0.9430(5)	0.9219(3)	0.1173(2)	0.1239(13)*
C8	0.8437(6)	0.9957(3)	0.1709(3)	0.1139(12)

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Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
H8	0.7889(6)	1.0329(3)	0.1267(3)	0.1367(14)*
C9	0.8287(6)	1.0092(3)	0.2417(3)	0.1139(12)
H9	0.7641(6)	1.0545(3)	0.2429(3)	0.1366(14)*
C10	0.9074(5)	0.9569(2)	0.3088(2)	0.0922(9)
H10	0.8984(5)	0.9662(2)	0.3558(2)	0.1107(11)*
C11	1.0008(4)	0.8897(2)	0.30403(18)	0.0772(8)
C12[c]	0.604(4)	0.819(2)	0.695(2)	0.122(4)
H12a[c]	0.565(4)	0.762(2)	0.701(2)	0.184(6)*
H12b[c]	0.673(4)	0.843(2)	0.747(2)	0.184(6)*
H12c[c]	0.520(4)	0.860(2)	0.667(2)	0.184(6)*
C12A[d]	0.7722(9)	0.8459(6)	0.7422(4)	0.159(3)
H12d[d]	0.742(7)	0.7839(13)	0.7383(17)	0.239(4)*
H12e[d]	0.871(2)	0.854(4)	0.7886(5)	0.239(4)*
H12f[d]	0.696(5)	0.883(3)	0.748(2)	0.239(4)*
C13[e]	0.7057(11)	0.8127(5)	0.6512(6)	0.117(2)
H13a[e]	0.8141(11)	0.8088(5)	0.6907(6)	0.140(3)*
H13b[e]	0.6790(11)	0.7594(5)	0.6175(6)	0.140(3)*
C13A[f]	0.7832(15)	0.8733(11)	0.6653(6)	0.139(3)
H13c[f]	0.7918(15)	0.9380(11)	0.6623(6)	0.166(3)*
H13d[f]	0.8714(15)	0.8451(11)	0.6634(6)	0.166(3)*
C14[e]	0.6775(8)	0.8977(5)	0.5987(4)	0.1036(18)
H14a[e]	0.6047(8)	0.9378(5)	0.6045(4)	0.124(2)*
H14b[e]	0.7736(8)	0.9298(5)	0.6134(4)	0.124(2)*
C14A[f]	0.6301(15)	0.8388(11)	0.5966(6)	0.122(2)
H14c[f]	0.6250(15)	0.7742(11)	0.6017(6)	0.147(3)*
H14d[f]	0.5447(15)	0.8651(11)	0.6026(6)	0.147(3)*
C15	0.6103(5)	0.8610(3)	0.5117(3)	0.1050(11)
H15a[e]	0.5716(5)	0.9109(3)	0.4741(3)	0.1260(13)*
H15b[e]	0.5232(5)	0.8222(3)	0.5017(3)	0.1260(13)*
H15c[f]	0.6254(5)	0.9248(3)	0.5078(3)	0.1260(13)*
H15d[f]	0.5060(5)	0.8458(3)	0.4714(3)	0.1260(13)*
C16	0.8509(4)	0.8435(2)	0.49583(19)	0.0708(7)
H16	0.8812(4)	0.9033(2)	0.50693(19)	0.0850(9)*
C17	0.7152(4)	0.7199(2)	0.47599(18)	0.0688(7)
C18	0.6093(4)	0.6529(3)	0.4678(2)	0.0834(8)
H18	0.5227(4)	0.6644(3)	0.4752(2)	0.1001(10)*
C19	0.6399(4)	0.5687(2)	0.4483(2)	0.0900(9)
H19	0.5716(4)	0.5220(2)	0.4418(2)	0.1080(11)*
C20	0.7697(4)	0.5514(2)	0.4378(2)	0.0864(9)
H20	0.7866(4)	0.4935(2)	0.4250(2)	0.1037(10)*
C21	0.8736(4)	0.6179(2)	0.44596(18)	0.0729(7)
H21	0.9597(4)	0.6061(2)	0.43823(18)	0.0875(9)*
C22	0.8459(3)	0.70308(18)	0.46605(17)	0.0620(6)

[a]Occupancy: 0.561(9), [b]Occupancy: 0.439(9), [c]Occupancy: 0.128(8), [d]Occupancy: 0.872(8), [e]Occupancy: 0.626(8), [f]Occupancy: 0.374(8).

and the mixture was heated and stirred for 3 h. The mixture after the reaction was filtered, washed with distilled water and finally the title compound was obtained from the acetonitrile solution.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. Both terminal butyl groups are disordered with occupancies refining to 0.561(9) : 0.439(9) and to 0.626(8) : 0.374(8) for C1—C3 and C12—C14, respectively.

Comment

Benzimidazoles are a class of benzoheterocyclic compounds containing two nitrogen atoms. Compounds containing benzimidazole structural units are for example useful in anti-HIV, anticancer, antimicrobial agents and show excellent biological activity [4–6]. Benzimidazole compounds can also be used in the fields of corrosion inhibitors [7], transition metal ligands [8] and fluorescence [9].

The molecular structure of the title compound is shown in the figure, bond lengths and angles are within normal ranges [10]. In the complex, the N1—Ni1 bond length is 2.027(2) Å and the N3—Ni1 bond length is 2.017(2) Å. The Cl1—Ni1 bond length is 2.2579(8) Å and the Cl2—Ni1 bond length is 2.2575(8) Å.

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