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# Bis(N-cyclohexylsalicylideneaminato)nickel(II), [Ni(C13H16NO)2]*

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**Abstract.** $M_r = 463.3$, triclinic, $P\bar{1}$, $a = 7.939$ (8), $b = 12.261$ (10), $c = 6.578$ (10) Å, $\alpha = 105.2$ (1), $\beta = 74.2$ (1), $\alpha = 102.1$ (1)°, $V = 587.93$ Å$^3$, $D_m = 1.30$, $D_x = 1.308$ Mg m$^{-3}$, $Z = 1$, $\lambda(\text{Cu } K\alpha) = 1.5418$ Å, $\mu(\text{Cu } K\alpha) = 1.34$ mm$^{-1}$, $R = 0.054$ for 1769 observed reflexions $[I > 3\sigma(I)]$. The structure comprises two centrosymmetrically related organic ligands coordinated to Ni through two N and two O atoms arranged in a planar square. The molecular units are discrete with no intermolecular bonding other than van der Waals forces. The cyclohexane group has a stable chair shape and all the bonds and angles are normal.

**Introduction.** The reaction of salicylaldehyde with cyclohexylamine produces a Schiff's base which is of importance in enzyme reactions (Leussing & Stanfield, 1966). These bases coordinate to various metals such as Cu, Ni, Co and Pd, and this work was undertaken as part of a programme to study the structural changes caused by varying the substituent groups and the metal coordination.

**Experimental.** Crystals grown from material synthesized according to Sacconi, Paoletti & Ciampolini (1963) and Holm & Swaminathan (1963); cell dimensions determined photographically and refined from measurements of high-angle reflexions on a diffractometer; needle-shaped crystal 0·40 × 0·23 × 0·11 mm

used to obtain intensities on an integrating Weissenberg camera for layers $hk0 \rightarrow hk4$ and $0hl \rightarrow 1kl$, intensities estimated visually, corrections applied for Lp effects but not for absorption or anomalous dispersion, 1837 measured reflexions; structure determined by successive Fourier syntheses (Blount, 1966) using phases calculated for the Ni atom at the origin, all non-hydrogen atoms located and their parameters refined by least squares using the NRC programs (Ahmed, 1970); initially isotropic temperature parameters were refined, and these were changed to anisotropic in the later stages of the refinement; calculated H-atom positions included but not refined; $w = 1/F_o$; final $R = 0.054$, $R_w = 0.075$ (all parameter shifts $< 0.3\sigma$); $F(000) = 246$; scattering factors from *International Tables for X-ray Crystallography* (1962).

**Discussion.** The final positional and equivalent isotropic thermal parameters are listed in Table 1.† The numbering of the atoms used and the packing of the molecules in the unit cell are shown as a (001) projection in Fig. 1. The thermal-ellipsoid plot of the molecule (Johnson, 1965) is shown in Fig. 2. Bond lengths and bond angles are listed in Table 2.

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† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38218 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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* Preliminary communication: Kashyap, Bindlish, Bhatia & Jain (1975).

The mean C—C bond length in the cyclohexyl ring is 1·536 Å, and the mean C—C—C angle 110·1°. In the benzene ring the mean C—C bond length is 1·422 Å, and the mean C—C—C angle 120·0°. The square

### Table 1. *Final atomic parameters and e.s.d.'s*

$$B_{eq} = \tfrac{1}{3}(B_{11} + B_{22} + B_{33}).$$

|        | x | y | z | $B_{eq}$ (Å$^2$) |
|--------|--------|--------|--------|--------|
| Ni(1)  | 0·0000 | 0·0000 | 0·0000 | 3·04 |
| O(1)   | 0·1098 (2) | 0·1550 (1) | 0·0227 (3) | 2·59 (3) |
| N(1)   | 0·1456 (2) | −0·0087 (1) | 0·1976 (3) | 1·62 (3) |
| C(1)   | 0·1561 (3) | 0·2324 (2) | 0·2088 (4) | 2·32 (3) |
| C(2)   | 0·1731 (3) | 0·3518 (2) | 0·2312 (5) | 3·17 (4) |
| C(3)   | 0·2275 (4) | 0·4332 (2) | 0·4146 (6) | 3·31 (4) |
| C(4)   | 0·2682 (4) | 0·4014 (2) | 0·5861 (6) | 3·27 (4) |
| C(5)   | 0·2546 (3) | 0·2858 (2) | 0·5618 (5) | 2·60 (4) |
| C(6)   | 0·1983 (3) | 0·2018 (2) | 0·3787 (4) | 2·09 (3) |
| C(7)   | 0·2070 (3) | 0·0819 (2) | 0·3472 (4) | 2·18 (3) |
| C(8)   | 0·1816 (3) | −0·1214 (2) | 0·1885 (4) | 2·11 (3) |
| C(9)   | 0·2643 (3) | −0·1249 (2) | 0·3686 (4) | 2·36 (3) |
| C(10)  | 0·2840 (4) | −0·2500 (2) | 0·3351 (5) | 3·23 (4) |
| C(11)  | 0·3969 (3) | −0·2957 (2) | 0·1115 (5) | 3·05 (4) |
| C(12)  | 0·3165 (3) | −0·2868 (2) | −0·0770 (6) | 3·07 (4) |
| C(13)  | 0·2948 (4) | −0·1625 (2) | −0·0407 (4) | 2·57 (4) |

### Table 2. *Bond lengths (Å) and angles (°)*

| | | | |
|---|---|---|---|
| Ni(1)—O(1) | 1·903 (2) | C(4)—C(5) | 1·368 (4) |
| Ni(1)—N(1) | 1·995 (2) | C(5)—C(6) | 1·470 (4) |
| O(1)—C(1) | 1·423 (3) | C(6)—C(7) | 1·443 (3) |
| N(1)—C(7) | 1·379 (3) | C(8)—C(9) | 1·516 (4) |
| N(1)—C(8) | 1·451 (3) | C(8)—C(13) | 1·546 (4) |
| C(1)—C(2) | 1·413 (3) | C(9)—C(10) | 1·526 (4) |
| C(1)—C(6) | 1·407 (4) | C(10)—C(11) | 1·530 (4) |
| C(2)—C(3) | 1·453 (5) | C(11)—C(12) | 1·577 (4) |
| C(3)—C(4) | 1·418 (5) | C(12)—C(13) | 1·518 (4) |
| | | | |
| O(1)—Ni(1)—N(1) | 85·9 (1) | C(1)—C(6)—C(5) | 123·3 (2) |
| Ni(1)—O(1)—C(1) | 127·4 (2) | C(1)—C(6)—C(7) | 115·2 (2) |
| Ni(1)—N(1)—C(7) | 125·5 (2) | C(5)—C(6)—C(7) | 121·0 (2) |
| Ni(1)—N(1)—C(8) | 116·5 (1) | N(1)—C(7)—C(6) | 128·5 (2) |
| C(7)—N(1)—C(8) | 117·9 (2) | N(1)—C(8)—C(9) | 113·6 (2) |
| O(1)—C(1)—C(2) | 120·9 (2) | N(1)—C(8)—C(13) | 106·8 (2) |
| O(1)—C(1)—C(6) | 125·5 (2) | C(9)—C(8)—C(13) | 113·6 (2) |
| C(2)—C(1)—C(6) | 113·5 (2) | C(8)—C(9)—C(10) | 105·2 (2) |
| C(1)—C(2)—C(3) | 122·3 (3) | C(9)—C(10)—C(11) | 112·4 (2) |
| C(2)—C(3)—C(4) | 123·8 (3) | C(10)—C(11)—C(12) | 112·1 (2) |
| C(3)—C(4)—C(5) | 113·8 (3) | C(11)—C(12)—C(13) | 106·9 (2) |
| C(4)—C(5)—C(6) | 123·4 (2) | C(8)—C(13)—C(12) | 110·6 (2) |



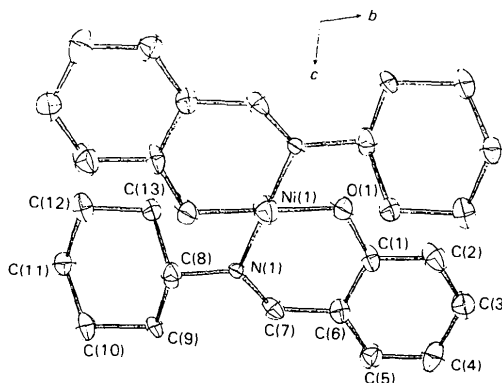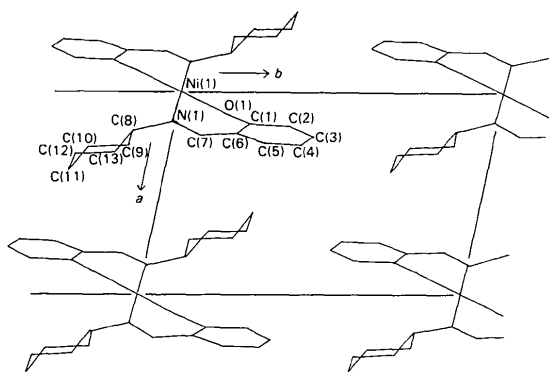Fig. 1. Projection of unit-cell contents on (001).



Fig. 2. *ORTEP* (Johnson, 1965) plot on (100) showing 50% probability contours for the thermal ellipsoids of the non-hydrogen atoms.

coordination around the Ni atom involves two N atoms at 1·995 (2) Å and two O atoms at 1·903 (2) Å with the included angle 85·9 (1)°.

The mean deviation from planarity of the benzene ring C(1–6) is 0·004 Å. The O atom is 0·055 (2) Å out of this plane, and C(7) is 0·180 (2) Å out.

Ni, O(1), C(1), C(6), C(7) and N(1) are not strictly coplanar but the mean plane through them makes a dihedral angle of 8·54 (5)° with the plane of the benzene ring, and the mean distance of the atoms out of this plane is 0·15 Å.

The closest intermolecular distances are C(5)···O(1) = 3·600 (3), C(2)···C(11) = 3·631 (4), C(6)···C(9)=3·631(4) and C(1)···C(11)=3·642(4)Å.

Generally dimensions are in agreement with those found in bis(*N*-methylsalicylideneaminato)nickel (Frasson, Panattoni & Sacconi, 1959) and bis[*N*-(3-dimethylaminopropyl)salicylideneaminato]nickel (Di Vaira & Orioli, 1967). There would appear to be no unusual stereochemical features present in this crystal structure.

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