

These data and the  $^1\text{H}$  NMR studies (Albano *et al.*, 1984) indicate that an equilibrium exists in solution between the five-coordinate and a square-planar complex while in the solid state only the former complex is isolated. Breaking of either of the N–Pt bonds in the five-coordinate complex should lead to the formation of the other species, as reported for a similar  $\text{Pt}^{\text{II}}$ -ethylene complex containing  $N,N,N',N'$ -tetramethyl-1,3-propanediamine (Cattalini, Maresca & Natile, 1979). The Pt–olefin, C=C, and both the Pt–N bond lengths are in the range reported for five-coordinate Pt complexes (see Table 3). The Pt–N bond lengths are significantly longer than the Pt–N( $sp^2$ ) values reported for square-planar Pt complexes, which range from 1.73 to 2.05 Å.

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## Structure of Bis(*meso*-1,2-diphenyl-1,2-ethanediamine)nickel(II) Dichloride Dihydrate, [Ni(C<sub>14</sub>H<sub>16</sub>N<sub>2</sub>)<sub>2</sub>]Cl<sub>2</sub>·2H<sub>2</sub>O

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**Abstract.**  $M_r = 590$ , orthorhombic,  $Pccn$ ,  $a = 26.831$  (5),  $b = 15.366$  (4),  $c = 7.1773$  (6) Å,  $V = 2959.1$  (6) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.32$  Mg m<sup>-3</sup>,  $\mu(\text{Mo } K\alpha) = 0.87$  mm<sup>-1</sup>,  $T = 298$  K,  $F(000) = 1240$ , final  $R = 0.046$  for 1075 observed reflections. The Ni coordination is square planar, with Ni–N distances 1.922 (4) and 1.921 (4) Å and N–Ni–N angle 86.4 (2)°. Bond lengths and angles are normal.

**Introduction.** The structure of the title compound was determined in order to provide further structural information on complexes of Ni with ethylenediamine and C-substituted ethylenediamines. In this case we have studied the complex with *meso*-1,2-diphenyl-1,2-ethanediamine (*meso*-stien). In previous work we determined the structures of two very similar Ni complexes, those formed by tetramethylethylenediamine (Alcalá-Aranda, Fernández, Gómez-Beltrán & Larena, 1977) and 1,2-cyclohexanediamine (Valero-Capilla, Alcalá-Aranda & Gómez-Beltrán, 1980), in which the environments of Ni are respectively square planar and octahedral. The molecular structures of two different

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bis(*meso*-stien)nickel(II) bis(dichloroacetates) have previously been determined by X-ray diffraction (Nyburg & Wood, 1964).

**Experimental.** Yellow crystal 0.27 × 0.15 × 0.27 mm.  $D_m$  not determined. Unit-cell parameters and intensity data obtained on an Enraf–Nonius CAD-4F diffractometer with graphite-monochromated Mo  $K\alpha$  radiation in  $\omega/2\theta$  scan mode ( $0 < \theta < 28^\circ$ ). Cell dimensions refined by least-squares fitting of the  $\theta$  values of 25 reflections. No appreciable drop in intensity of three standard reflections checked every hour. 3555 reflections collected in the  $hkl$  range 0,0,0 to 35,20,9; 1075 with  $I > 2\sigma(I)$  used in subsequent calculations. Intensities corrected for Lorentz and polarization effects, but not for absorption ( $\mu R = 0.23$ ). Scattering factors for neutral atoms and anomalous-dispersion corrections for Ni and Cl from *International Tables for X-ray Crystallography* (1974). A statistical test showed a centrosymmetric intensity distribution. Structure solved with *MULTAN77* (Main, Lessinger, Woolfson, Germain & Declercq, 1977) and standard Fourier

Table 1. Atomic coordinates and equivalent isotropic thermal parameters (Å<sup>2</sup> × 10<sup>4</sup>)

	$U_{eq} = \frac{1}{3} \sum U_{ii}$			
	x	y	z	$U_{eq}$
Ni	0.00000	0.00000	0.00000	440 (4)
Cl	0.03647 (6)	-0.12380 (10)	-0.48463 (29)	668 (6)
O	-0.02655 (15)	-0.21939 (23)	0.21305 (66)	954 (23)
N(1)	-0.04206 (14)	-0.03162 (27)	-0.20600 (53)	485 (19)
N(2)	-0.05456 (15)	-0.03375 (27)	0.15763 (55)	454 (19)
C(1)	-0.08446 (20)	-0.08498 (32)	-0.13799 (75)	457 (22)
C(2)	-0.10237 (18)	-0.04256 (32)	0.04562 (68)	468 (23)
C(11)	-0.12482 (19)	-0.09814 (36)	-0.28041 (75)	514 (24)
C(12)	-0.14124 (21)	-0.03123 (37)	-0.39693 (77)	662 (27)
C(13)	-0.18144 (20)	-0.04785 (36)	-0.52170 (95)	804 (27)
C(14)	-0.20412 (20)	-0.12823 (45)	-0.52681 (99)	934 (31)
C(15)	-0.18780 (23)	-0.19271 (38)	-0.40938 (87)	954 (34)
C(16)	-0.14750 (22)	-0.17768 (34)	-0.28993 (77)	642 (27)
C(21)	-0.12892 (17)	0.04467 (32)	0.02127 (82)	473 (20)
C(22)	-0.18105 (18)	0.04235 (31)	0.00450 (101)	666 (22)
C(23)	-0.20662 (19)	0.11891 (40)	-0.02843 (110)	893 (30)
C(24)	-0.18240 (24)	0.19670 (33)	-0.04354 (116)	1110 (38)
C(25)	-0.13085 (22)	0.19884 (34)	-0.02962 (107)	867 (30)
C(26)	-0.10469 (17)	0.12356 (33)	0.00415 (103)	606 (21)

Table 2. Bond lengths (Å) and angles (°) with e.s.d.'s in parentheses

Ni—N(1)	1.922 (4)	C(15)—C(16)	1.399 (8)
Ni—N(2)	1.921 (4)	C(16)—C(11)	1.367 (7)
N(1)—C(1)	1.485 (6)	C(2)—C(21)	1.528 (6)
N(2)—C(2)	1.519 (6)	C(21)—C(22)	1.404 (6)
C(1)—C(2)	1.546 (7)	C(22)—C(23)	1.382 (7)
C(1)—C(11)	1.502 (7)	C(23)—C(24)	1.365 (8)
C(11)—C(12)	1.396 (7)	C(24)—C(25)	1.387 (8)
C(12)—C(13)	1.425 (8)	C(25)—C(26)	1.374 (7)
C(13)—C(14)	1.377 (8)	C(26)—C(21)	1.381 (7)
C(14)—C(15)	1.372 (9)		
N(1)—Ni—N(2)	86.4 (2)	C(13)—C(14)—C(15)	119.3 (5)
Ni—N(1)—C(1)	109.6 (3)	C(14)—C(15)—C(16)	120.2 (5)
Ni—N(2)—C(2)	110.8 (2)	C(11)—C(16)—C(15)	121.5 (4)
N(1)—C(1)—C(2)	106.5 (3)	C(2)—C(21)—C(26)	124.1 (4)
N(2)—C(2)—C(1)	103.1 (3)	C(2)—C(21)—C(22)	116.9 (4)
N(1)—C(1)—C(11)	113.7 (3)	C(22)—C(21)—C(26)	118.9 (4)
N(2)—C(2)—C(21)	112.1 (3)	C(21)—C(22)—C(23)	119.2 (4)
C(1)—C(11)—C(12)	122.3 (4)	C(22)—C(23)—C(24)	121.5 (4)
C(1)—C(11)—C(16)	118.3 (4)	C(23)—C(24)—C(25)	119.3 (4)
C(12)—C(11)—C(16)	119.2 (4)	C(24)—C(25)—C(26)	120.1 (4)
C(11)—C(12)—C(13)	118.9 (4)	C(21)—C(26)—C(25)	120.9 (4)
C(12)—C(13)—C(14)	120.8 (5)		

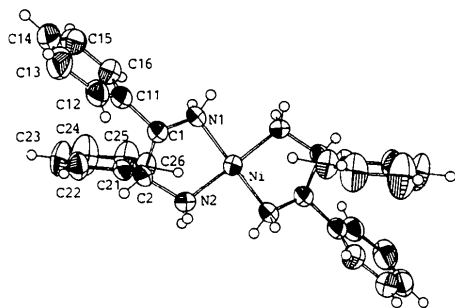


Fig. 1. ORTEP (Johnson, 1965) drawing of the centrosymmetric complex cation, showing the atom numbering.

techniques. H atoms located by  $\Delta F$  synthesis. Full-matrix least-squares refinement on  $F$ ; anisotropic thermal parameters for all non-hydrogen atoms and isotropic ones for H; final  $R = 0.046$  and  $R_w = 0.026$ , with  $w = 1/\sigma^2(F_o)$ ;  $S = 2.05$ . In final cycle  $(\Delta/\sigma)_{\max} = 0.26$ . Residual electron density within  $\pm 0.3 \text{ e \AA}^{-3}$ . Most calculations carried out with the *CRYSTAN* system (Burzlaff, Böhme & Gomm, 1977) on the HP-1000-F minicomputer of the Computing Center of the University of Oviedo.

**Discussion.** Atomic parameters are listed in Table 1.\* Interatomic distances and angles are in Table 2; all are normal for this type of compound. Fig. 1 (Johnson, 1965) shows the geometry of the complex cation and the atom labelling.

The centrosymmetric  $[\text{NiN}_4]$  chromophore has a square-planar structure with Ni—N distances of 1.92 Å and N(1)—Ni—N(2) angle of 86.4 (2)°. The spatial disposition of the amine ligands does not indicate steric hindrance for octahedral coordination. The H<sub>2</sub>O molecule contributes to the packing through hydrogen bonds. A listing of the geometrical features of the hydrogen bonds and values of the angles between the best least-squares planes for various portions of the molecule and principal torsion angles computed by *PARST5* (Nardelli, Musatti, Domiano & Andreotti, 1965) have been deposited.\*

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\* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters, distances and angles involving H atoms, H-bond distances and angles and least-squares-planes' data and principal torsion angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39679 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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