observed for estradiol hemihydrate (Busetta & Hospital, 1972) and 4-fluoroestradiol (Go, Kartha & Neeman, 1982). The O(3)$\cdots$O(17) distances were 2·774 and 2·77 Å in these structures. In this study, however, no H atoms corresponding to this link could be found.

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The Structure of N^1,N^2-Diphenylbenzamidine and a Comparison with its Transition-Metal Complexes

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Abstract. N^1,N^2-Diphenylbenzenecarboximidamide, $C_{19}H_{16}N_2$, $M_r = 272\cdot4$, monoclinic, $P2_1/a$, $a = 31\cdot340$ (8), $b = 10\cdot259$ (3), $c = 9\cdot527$ (3) Å, $\beta = 92\cdot34$ (3)°, $U = 3060\cdot5$ (2) Å³, $Z = 8$, $D_x = 1\cdot18$ g cm⁻³, Mo $K\alpha$ radiation, $\lambda = 0\cdot71069$ Å, $\mu = 0\cdot65$ cm⁻¹, $F(000) = 1151\cdot79$, $T = 298$ K, $R = 0\cdot055$ for 1490 unique observed $[I/\sigma(I) \geq 3\cdot0]$ reflections. The two molecules of the asymmetric unit are linked by a single hydrogen bond [N(4)—H$\cdots$N(1) $(x, y, 1+z)$ 2·46 (5) Å]. The C—N bonds show distinct amine [1·360 (8) Å average] and imine [1·302 (7) Å average] characteristics, which on complexation become near-equivalent C$\rightleftharpoons$N bonds with a high degree of delocalization. The change in the N—C—N 'bite' angle on complexation is determined by the bonding mode adopted; the angle changes by a mean value of 3·9° where the ligand bridges two metals, and by a mean value of 13·1° for bidentate bonding to a single metal.

Introduction. Recently, a number of structural papers concerning the structures of amidines have appeared (Tykarska, Jaskólski & Kosturkiewicz, 1986a; Thailambal, Pattabhi & Guru Row, 1986; Tykarska, Jaskólski & Kosturkiewicz, 1986b; Barker, Gould & Kilner, 1987; Barker, Cameron, Mahmoud, Kilner & Wallwork, 1986), reflecting the widespread interest in

such compounds because of their pharmaceutical, bonding and ligand properties, and their biological importance. This structural investigation was undertaken to investigate the effect of diaryl substitution on the central benzamidine fragment, the possibility of hydrogen bonding, and to examine the structural changes which occur to an amidine upon complexation with a transition metal to form an important pseudo-allyl group (Fig. 1).

Experimental. N^1,N^2-Diphenylbenzamidine was prepared by the method of Kroehnke (Kroehnke & Steuernagel, 1963) and crystals were obtained by slow recrystallization from acetone in darkness. A large colourless elongated plate 1·7 × 0·14 × 0·26 mm was used. (Despite the unusual length of the crystal, it appeared to be satisfactorily located within the beam and refinement encountered no problems.) Syntex $P2_1$
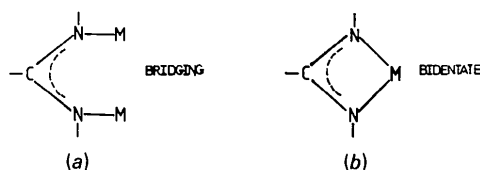

Fig. 1. Amidino bonding modes.

four-circle diffractometer, $2\theta_{max} = 45°$, scan range $\pm1.25°$ (2θ) around the $K\alpha_1-K\alpha_2$ angles, scan speed $2.5-29°$ min^{-1}, depending on the intensity of a 2 s pre-scan; backgrounds measured at each end of the scan for 0.25 of the scan time. hkl ranges: $-32/+31$; $0/10$; $0/10$. Three standard reflections monitored every 100 reflections showed no significant changes. Unit-cell dimensions and standard deviations by least-squares fit to 15 medium-angle reflections $(15 < 2\theta < 18°)$. Reflections 3998 unique, 1490 observed $[I/\sigma(I) > 3.0]$. No absorption correction. Systematic absences $h0l$, $h \neq 2n$; $0k0$, $k \neq 2n$ indicated space group $P2_1/a$. Structure solution was readily achieved using the *SOLV* link of *SHELXTL* (Sheldrick, 1983). Anisotropic temperature factors were used for non-H atoms. The ring H atoms (fixed isotropic temperature factors of 0.07-0.12 Å^2) were inserted at calculated positions. The coordinates of H atoms attached to N atoms were refined. Final refinement was on F by cascaded least-squares method refining 385 parameters. Largest positive and negative peaks on a final ΔF synthesis were ±0.2 e Å^{-3}. A weighting scheme of the form $w = 1/[\sigma^2(F_o) + g(F_o)^2]$ with $g = 0.0019$ was used and shown to be satisfactory by a weight analysis. Final $R = 0.055$, $wR = 0.058$. Max. Δ/σ in final cycle 0.04. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Computing with *SHELXTL* (Sheldrick, 1983) on a Data General DG30. Final atomic coordinates are given in Table 1, and selected bond lengths and angles in Table 2.*

Discussion. The asymmetric unit consists of a hydrogen-bonded dimer (Fig. 2) linked by a single $N-H\cdots N$ interaction $[N(4)-H\cdots N(1)$ $(x, y, 1+z)$ 2.46 (5) Å] (Fig. 3). The absence of a second interaction in the dimer clearly relates to the conformation of the molecule in which the N—H bond and N lone pairs point in opposite directions.

The skeletal C—N bond lengths are clearly differentiated in terms of single- and double-bond character, with a mean C=N of 1.302 (7) Å and a mean C—N of 1.360 (8) Å. They are similar to those found in N^2-(m-chlorophenyl)-N^1,N^1-pentamethylenebenzamidine [1.290 (6) and 1.365 (6) Å respectively: Tykarska, Jaskólski & Kosturkiewicz (1986a)]; N^2-(p-methoxyphenyl)-N^1,N^1-pentamethylenebenzamidine [1.283 (5) and 1.372 (5) Å: Tykarska, Jaskólski & Kosturkiewicz (1986b)] and acetamidine [1.298 (1) and 1.344 (1) Å: Norrestam, Mertz & Crossland (1983)]; but differ somewhat from those found for benzamidine hydrochloride monohydrate [1.293 (7)

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and all bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44643 (13 pp.). Copies may be obtained through The Executive Secretary. International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates* $(\times 10^4)$ *and equivalent isotropic thermal parameters* (Å$^2 \times 10^3$)

	x	y	z	U_{eq}*
N(1)	4092 (2)	6523 (5)	5388 (4)	67 (2)
C(11)	4366 (2)	7541 (6)	5861 (6)	64 (2)
C(12)	4222 (2)	8496 (8)	6749 (7)	75 (3)
C(13)	4501 (3)	9432 (8)	7253 (7)	99 (4)
C(14)	4912 (3)	9465 (10)	6906 (9)	107 (5)
C(15)	5063 (3)	8514 (11)	6049 (10)	106 (4)
C(16)	4790 (3)	7547 (7)	5518 (7)	84 (3)
C(1)	3953 (2)	6507 (6)	4072 (7)	62 (2)
C(21)	4001 (2)	7556 (5)	3021 (5)	52 (2)
C(22)	4167 (2)	7263 (6)	1716 (7)	64 (2)
C(23)	4196 (2)	8234 (7)	715 (6)	74 (3)
C(24)	4057 (2)	9466 (6)	980 (6)	75 (3)
C(25)	3892 (2)	9754 (6)	2258 (7)	68 (3)
C(26)	3864 (2)	8791 (6)	3265 (6)	66 (2)
N(2)	3731 (2)	5456 (5)	3542 (5)	73 (2)
C(31)	3650 (3)	4228 (7)	4122 (8)	79 (3)
C(32)	3904 (3)	3701 (8)	5192 (8)	103 (4)
C(33)	3815 (4)	2489 (10)	5682 (12)	149 (6)
C(34)	3481 (5)	1772 (11)	5181 (15)	168 (8)
C(35)	3232 (3)	2291 (10)	4075 (14)	143 (6)
C(36)	3309 (3)	3511 (8)	3561 (9)	100 (4)
C(2)	3372 (2)	6056 (5)	-1103 (5)	55 (2)
N(3)	3242 (1)	5892 (4)	158 (4)	54 (2)
C(41)	2836 (2)	6368 (6)	496 (6)	51 (2)
C(42)	2461 (2)	5934 (6)	-191 (6)	66 (3)
C(43)	2073 (2)	6391 (8)	159 (7)	82 (3)
C(44)	2035 (2)	7287 (8)	1218 (8)	83 (3)
C(45)	2394 (2)	7703 (7)	1912 (6)	74 (3)
C(46)	2792 (2)	7273 (6)	1566 (5)	57 (2)
C(51)	3158 (2)	6875 (5)	-2211 (5)	50 (2)
C(52)	3069 (2)	6381 (6)	-3547 (6)	64 (2)
C(53)	2894 (2)	7169 (8)	-4593 (7)	77 (3)
C(54)	2807 (2)	8449 (7)	-4333 (6)	77 (3)
C(55)	2891 (2)	8962 (6)	-2998 (6)	70 (2)
C(56)	3066 (2)	8167 (5)	-1954 (6)	61 (2)
N(4)	3737 (2)	5520 (5)	-1546 (5)	64 (2)
C(61)	4025 (2)	4641 (6)	-871 (6)	60 (2)
C(62)	3936 (2)	3907 (6)	309 (6)	66 (3)
C(63)	4242 (3)	3099 (7)	903 (7)	84 (3)
C(64)	4626 (3)	2968 (9)	337 (10)	140 (5)
C(65)	4713 (3)	3694 (11)	-837 (11)	168 (6)
C(66)	4415 (2)	4536 (8)	-1432 (8)	116 (4)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2. *Selected bond lengths* (Å) *and bond angles* (°) *and torsion angles* (°)

N(1)-C(11)	1.416 (8)	N(1)-C(1)	1.310 (8)
C(1)-C(21)	1.481 (8)	C(1)-N(2)	1.369 (8)
N(2)-H(2)	0.720 (49)	N(2)-C(31)	1.403 (9)
C(2)-N(3)	1.295 (6)	C(2)-C(51)	1.488 (7)
C(2)-N(4)	1.351 (7)	N(3)-C(41)	1.412 (7)
N(4)-H(4)	0.878 (54)	N(4)-C(61)	1.412 (8)

C(11)-N(1)-C(1)	119.2 (5)	N(1)-C(1)-C(21)	126.8 (5)
N(1)-C(11)-N(2)	120.4 (5)	C(21)-C(1)-N(2)	112.7 (5)
C(1)-N(2)-H(2)	120.9 (39)	C(1)-N(2)-C(31)	131.2 (6)
H(2)-N(2)-C(31)	107.9 (39)	N(3)-C(2)-C(51)	125.5 (5)
N(3)-C(2)-N(4)	122.7 (5)	C(51)-C(2)-N(4)	111.7 (4)
C(2)-N(3)-C(41)	119.2 (4)	C(2)-N(4)-H(4)	113.7 (36)
C(2)-N(4)-C(61)	130.6 (5)	H(4)-N(4)-C(61)	115.3 (36)

C(1)-N(1)-C(11)-C(12)	108.8 (6)	C(2)-N(3)-C(41)-C(42)	60.7 (7)
C(1)-N(1)-C(11)-C(16)	-75.5 (8)	C(2)-N(3)-C(41)-C(46)	-121.1 (6)
C(1)-N(2)-C(31)-C(32)	-22.3 (7)	N(3)-C(2)-C(51)-C(52)	-129.6 (6)
C(1)-N(2)-C(31)-C(36)	159.6 (7)	N(3)-C(2)-C(51)-C(56)	54.0 (7)
N(1)-C(1)-C(21)-C(22)	128.5 (6)	N(4)-C(2)-C(51)-C(52)	52.6 (7)
N(1)-C(1)-C(21)-C(26)	-55.1 (7)	N(4)-C(2)-C(51)-C(56)	-123.7 (6)
N(2)-C(1)-C(21)-C(22)	-52.7 (6)	C(2)-N(4)-C(61)-C(62)	15.48 (8)
N(2)-C(1)-C(21)-C(26)	123.6 (6)	C(2)-N(4)-C(61)-C(66)	-163.9 (6)

and 1.328 (7) Å: Thailambal, Pattabhi & Guru Row (1986)]; and N^1,N^1-hexamethylene-N^2-(p-nitrophenyl)-formamidine [1.302 (6) and 1.334 (5) Å: Krajewski *et al.* (1981)]. The C—N double-bond lengths vary little, but a clear difference may be noted in the C—N

single-bond lengths. Further, the difference between the C—N and C=N distances is a guide to the degree of delocalization around the N—C—N skeleton. This difference is 0·058 Å in the title compound, 0·075 and 0·089 Å in the pentamethylenebenzamidines, 0·046 Å in the acetamidine, 0·035 in the benzamidine hydrochloride, and 0·032 Å in the formamidine. Hence, the degree of delocalization in N^1,N^2-diphenylbenzamidine is similar to that of acetamidine, less than that of benzamidine hydrochloride or the formamidine, but more than the pentamethylenebenzamidines. The degree of delocalization clearly depends upon the substituents on the N and the central C atom.

The N—C—N angle [121·5 (5)° average] deviates from that found for acetamidine [125·5 (1)°: Norrestam, Mertz & Crossland (1983)]; the isoelectronic diphenyltriazene [115°: Gladkova & Kondrashev (1972)]; and surprisingly the substituted benzamidines: N^2-(p-methoxyphenyl)-N^1,N^1-pentamethylenebenzamidine [119·4 (3)°: Tykarska, Jaskólski & Kosturkiewicz (1986b); N^2-(m-chlorophenyl)-N^1,N^1-pentamethylenebenzamidine [118·4 (4)°: Tykarska, Jaskólski & Kosturkiewicz (1986a)]. However, the angle is similar to that found for benzamidine hydrochloride hydrate [121·6 (4)°: Thailambal, Pattabhi & Guru Row (1986)], and N^1,N^1-hexamethylene-N^2-(p-
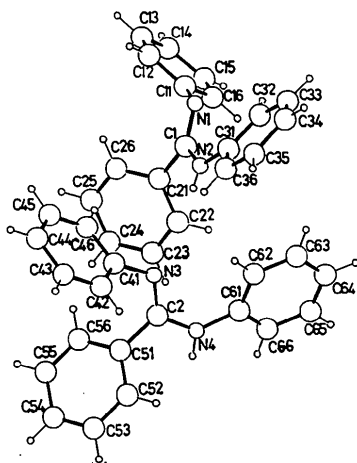

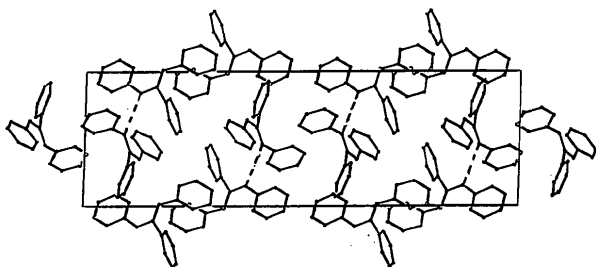Fig. 2. Molecular structure and atomic labels of N^1,N^2-diphenylbenzamidine (ORTEP; Johnson, 1976).

Fig. 3. Projection of structure down c.

Table 3. *Comparison of N^1,N^2-diphenylbenzamidine complexes*

Complex	C—N(Å)	N—C—N(°)	Bonding mode	Reference
[Pt(Am)₂]	1·331 (8) 1·340 (8)	106·7 (5)	Bidentate	Barker et al. (1987)
[Cu₂(Am)₄]	1·328 (7) 1·334 (8)	120·0 (5)	Bridging	Halfpenny, Kilner & Pietryzkowski (1982)
[Mo₂(Am)₄]	1·32 (1) 1·38 (1) 1·36 (1) 1·33 (1)	118 (1) 114 (1) 118 (1)	Bridging	Cotton, Inglis, Kilner & Webb (1975)
[Re₂(Am)₂Cl₄]	1·34 (3) 1·37 (3)	116 (2)	Bridging	Cotton & Shive (1975)
[Re₂(Am)₂Cl₄(THF)]	1·34 (2) 1·32 (2) 1·31 (2) 1·37 (2)	116 (2) 118 (1)	Bridging	Cotton & Shive (1975)
[Rh(Am)(1,5-cyclooctadiene)]	1·356 (9) 1·331 (9)	110·0 (6)	Bidentate	Lahoz et al. (1985)
[Rh₂(Am)₂(tetrafluorobenzo[5,6]bicyclo[2.2.2]octa-2,5,9-triene)]	1·350 (7) 1·317 (9) 1·346 (7) 1·339 (7)	118·1 (5) 120·4 (5)	Bridging	Lahoz et al. (1985)

Abbreviations: Am = N^1,N^2-diphenylbenzamidinate;   THF = tetrahydrofuran.

nitrophenyl)formamidine [122·1 (4)°: Krajewski et al. (1981)]. The substituted benzamidine N—C—N angles may differ from that of N^1,N^2-diphenylbenzamidine because one of their skeletal N atoms is contained within a piperidine ring.

The interaction between the N—C—N skeleton and the substituent aromatic rings may be rationalized in terms of the cosine of the dihedral angle between the N—C—N skeleton and the aryl ring atoms, since the superposition integral of the two p_π orbitals located on adjacent atoms is proportional to the cosine of the angle between them. The dihedral angles listed in Table 2 indicate a considerable interaction between the C—N(amine) part of the skeleton and its associated phenyl ring, with a tendency towards planarity, but very little interaction between the C=N(imine) fragment and its phenyl group. Clearly, the phenyl group on the C=N(imine) fragment has orientated its π system so that it may interact with the lone pair of the sp^2-hybridized imino N atom.

Similar bond lengths [C=N(imine), C(1)—N(1) 1·310 (8) and C(2)—N(3) 1·295 (6) Å; C—N(amine) C(1)—N(2) 1·369 (8) and C(2)—N(4) 1·351 (7) Å; C(skeletal)—C(ring) C(1)—C(21) 1·481 (8) and C(2)—C(51) 1·488 (7) Å] and angles [N—C—N, N(1)—C(1)—N(2) 120·4 (5) and N(3)—C(2)—N(4) 122·7 (5)°] were found for the two molecules in the dimer.

The determination of the structure of N^1,N^2-diphenylbenzamidine has allowed the comparison of an amidine ligand in its coordinated and non-coordinated forms for the first time. The structural parameters of the complexes of N^1,N^2-diphenylbenzamidine are given in Table 3. On complexation the C—N bond becomes shorter and the C=N bond longer to yield a C⚊⚊N bond indicative of the delocalization which occurs on complexation. The N—C—N angle is seen to be sensitive to the bonding mode adopted. In the bridging

(Fig. 1a) case a reduction of 3·9° (average) is found whereas for the bidentate mode (Fig. 1b) a considerable change of 13·1° (average) is involved. These changes reflect the relative lack of strain in the five-membered ring compared with the considerable strain involved in the four-membered ring.

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Structure and Absolute Configuration of (−)-Sclareol-8-acetate†

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Abstract. Natural (−)-sclareol, of which the principal source is clary sage (*Salvia sclarea* L.), was recently used for a new synthesis of Ambrox®, one of the most important ambergris fragrance chemicals [Decorzant, Vial, Näf & Whitesides (1987). *Tetrahedron*, **43**, 1871–1879]. (−)-Sclareol-8-acetate: $C_{22}H_{38}O_3$, m.p. 395–396 K, $[\alpha]_D^{20°C} = -35\cdot8°$ ($c = 1\cdot2\%$ in $CHCl_3$), $M_r = 350\cdot5$, orthorhombic, $P2_12_12_1$, $a = 6\cdot5001$ (7), $b = 16\cdot287$ (5), $c = 19\cdot497$ (6) Å, $V = 2064\cdot1$ (9) Å³, $Z = 4$, $F(000) = 776$, $D_x = 1\cdot128$ Mg m⁻³, $\lambda(Mo\ K\alpha) = 0\cdot71069$ Å, $\mu = 0\cdot068$ mm⁻¹, $T = 180$ K, $R = 0\cdot066$ for 1299 observed reflections [$|F_o| \geq 3\sigma(F_o)$ and $|F_o| \geq 9\cdot0$]. The (13R) configuration has been confirmed in spite of the presence of 9% of 13-*epi*-sclareol-8-acetate in the crystal. The hydroxyl group attached to C(13) is involved in an intermolecular hydrogen bond with the carbonyl of the acetate. The six-membered rings are *trans*-fused and both are in the chair conformation.

Introduction. Sclareol is a diterpene widely distributed in nature. It is a major component in the oil of clary sage (*Salvia sclarea* L.) and is present in several species of tobacco. It has been used to prepare a series of ambra odorants (Ohloff, 1982), Ambrox®(III) (Decorzant, Vial, Näf & Whitesides, 1987), drim-9(11)-8-ol (Leite, Sarragiotto, Imamura & Marsaioli, 1986), olean-11,12;13,18-diene, a pentacyclic triterpene derived from β-amyrin (Corey, Hess & Proskow, 1963), a vitamin K analog (Orgiyan & Lazurevskii, 1965), and other diterpenes such as manool (Büchi & Biemann, 1957; Ohloff 1958) and labdanolic acid (Bory & Lederer, 1957). Sclareol shows some interesting biological activity. It inhibited wheat coleoptiles

† {1R-[1α(R*),2β,4aβ,4aα]}-2-(Acetyloxy)-α-ethenyldecahydro-α,2,5,5,8a-pentamethyl-1-naphthalenepropanol; (13R)-8α-acetoxy-labd-14-en-13-ol.