perspective view of a copper-diiminodiamide moiety with the numbering scheme and deviations of atoms from the least-squares plane through O(1)—N(2)—N(1)—O(2) is shown in Fig. 1. The equation of the least-squares plane formed by atoms N(1), N(2), O(1) and O(2) is $-2{\cdot}707x + 25{\cdot}75y + 3{\cdot}097z = 2{\cdot}798$.

As shown in Fig. 1, the Cu is five-coordinate in a slightly distorted square-pyramidal geometry, and is slightly displaced from the best plane of the two amine nitrogens and the two amide oxygens towards the apex of the pyramid, which is formed by a perchlorato O atom with Cu—O distance 2·483 Å. This bond is significantly longer than the equatorial Cu—O bond distances (1·952 and 1·945 Å). The two methyl groups attached to the asymmetric nitrogens N(1) and N(2) are axial. The bond angles and distances of the complex are normal for square-pyramidal copper(II) complexes, with alternating five- and six-membered chelate rings.

Comparing the results between this crystal and the crystal of $[Cu(NO_3)(bcen)(H_2O)].NO_3.H_2O$ (Lee *et al.*, 1984), we found the following significant results: (1) For each of these two complexes, the two asymmetric nitrogens are of the same *R* or *S* configuration, and the five-membered chelate ring adopts a stable *gauche* conformation. However, the bond angles and bond distances of this crystal shown in Table 2 are significantly different from those of $[Cu(NO_3)(bcen)H_2O]^+$. (2) The coordination numbers of these two complexes are different. $[Cu(NO_3)(bcen)(H_2O)]^+$ is of the 4+2 type; on the other hand, the Cu of each of these moieties of the present crystal is five-coordinate. This difference is mainly due to the steric effect of the two *N*-methyl groups of $[\{Cu(N\text{-}Me_2bcen)\}_2(ClO_4)](ClO_4)_3$. As shown in Fig. 1, the two bulky methyl groups are axial. Thus the coordination of a sixth ligand is inhibited sterically by the picket-fence effect of the axial *N*-methyl groups. For the present crystal, the hydrogen-bond lengths N(3)—H(20)···O(22) and N(4)—H(21)···O(31) are 3·07 (1) and 2·93 (1) Å respectively, and their bond angles are 143·9 (2) and 154·6 (2)° respectively. The O atoms around Cl(2) are disordered in the present crystal.

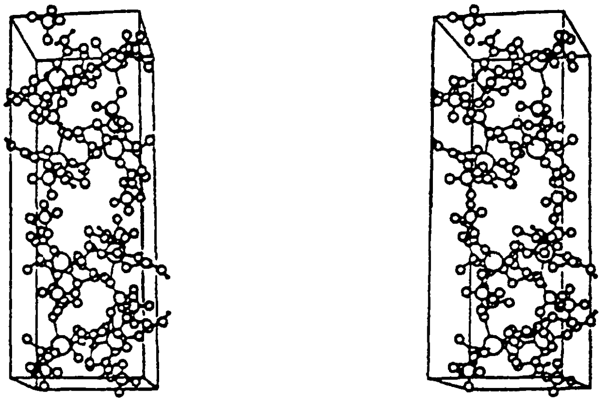

Fig. 2. Stereoview of the packing (viewed down the negative c direction).

Fig. 2 is a stereoview of the molecular packing.

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Structures of Three Copper Complexes with 2-Dimethylaminomethyl-4-phenylphenol

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Abstract. The crystal structures of three 2-dimethylaminomethyl-4-phenylphenolato (dapp) copper complexes were determined: (I) bis(2-dimethylaminomethyl-4-phenylphenolato)copper(II), $[Cu(C_{15}H_{16}NO)_2]$, $M_r = 516{\cdot}14$, monoclinic, $P2_1/n$, $a = 11{\cdot}051$ (2), $b = 9{\cdot}577$ (4), $c = 24{\cdot}436$ (12) Å, $\beta = 101{\cdot}29$ (3)°, V

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= 2536 (3) Å^3, T = 293 K, Z = 4, D_x = 1·352, D_m(flotation) = 1·356 (5) g cm^{-3}, μ = 8·90 cm^{-1}, λ(Mo $K\alpha$) = 0·71069 Å, F(000) = 1084, R = 0·070 and wR = 0·046 for 4327 most intense reflections and 316 variables; (II) diacetato-bis-μ-(2-dimethylaminomethyl-4-phenylphenolato)-dicopper(II) [Cu($C_{15}H_{16}NO$)($C_2H_3O_2$)]$_2$, M_r = 697·78, monoclinic, $P2_1/c$, a = 12·585 (11), b = 8·421 (8), c = 18·175 (16) Å, β = 121·30 (7)°, V = 1646 (3) Å^3, T = 293 K, Z = 2, D_x = 1·408, D_m(flotation) = 1·413 (6) g cm^{-3}, μ = 13·39 cm^{-1}, λ(Mo $K\alpha$) = 0·71069 Å, F(000) = 724, R = 0·069 and wR = 0·040 for 3275 most intense reflections and 199 variables; (III) diacetato-bis-μ-(2-dimethylaminomethyl-4-phenylphenolato)-dimethanoldicopper(II), [Cu($C_{15}H_{16}NO$)($C_2H_3O_2$)(CH_4O)]$_2$, M_r = 761·86, orthorhombic, $Pbna$, a = 7·423 (7), b = 24·444 (28), c = 19·142 (7) Å, V = 3473 (7) Å^3, T = 293 K, Z = 4, D_x = 1·456, D_m(flotation) = 1·453 (8) g cm^{-3}, μ = 12·79 cm^{-1}, λ(Mo $K\alpha$) = 0·71069 Å, F(000) = 1592, R = 0·098 and wR = 0·061 for 4061 most intense reflections and 217 variables. Compound (I) is monomeric with the two dapp ligands coordinated *trans*-planar to the Cu atom; the average Cu—O and Cu—N distances are 1·89 (1) Å and 2·07 (1) Å, respectively. Compounds (II) and (III) are five-coordinate square-pyramidal dimers with the dapp O atoms bridging the Cu atoms. In compound (II) each acetate is bidentate but in compound (III) they are monodentate with MeOH molecules at the other coordination sites. The Cu—O and Cu—N distances for the dapp ligands are similar for (II) and (III), 1·926–1·987 and 2·028–2·044 Å, respectively. The apical Cu—O distances are 2·491 and 2·421 Å for (II) and (III), respectively.

Introduction. Although there are many known copper complexes of salicylaldimine (salicylideneamine) and its derivatives (Maslen & Waters, 1975; Hobday & Smith, 1972; Yamada, 1966) there has been little investigation of the coordinating properties of the corresponding amines. It would be expected from the similarity of their structures that both bases would form similar coordination complexes with copper(II) ions. In an effort to explore the structural chemistry of complexes with amine analogues of salicylaldimines, we have examined the crystal structures of three dapp copper complexes.

Experimental. *Preparation of* 2-*dimethylaminomethyl*-4-*phenylphenol*. The ligand, (Hdapp), was prepared by a slight modification of the procedure described by Goken (1962). 16·5 ml of 37% aqueous formaldehyde (0·22 mol) was added to a mixture of 10 ml (0·22 mol) anhydrous dimethylamine, 10 ml MeOH at 273·16 K. 34 g *p*-phenylphenol (0·20 mol) in 75 ml MeOH was added next and the reaction mixture refluxed for 12 h. The solvent was removed under reduced pressure and the resulting solid recrystallized (m.p. 362–363 K) from 95% ethanol and propanol.

Preparation of single crystals of Cu(dapp)$_2$. A mixture of 0·5 g Cu(OAc)$_2$.2H$_2$O (2·5 mmol) and 0·84 g NaHCO$_3$ (10·0 mmol) was added to 1·14 g Hdapp (5·0 mmol) in 50 ml of MeOH. The brown solution was warmed to 323 K and most of the MeOH was allowed to evaporate. The resulting reddish-brown residue was washed with water and ether and then dissolved in acetone at room temperature. A few drops of water were added to the solution and the solvent was then allowed to evaporate slowly. Small dark-brown crystals formed within a week. The melting point (480–483 K) was the same as that reported by Goken (1962).

Preparation of single crystals of [Cu(dapp)(OAc)]$_2$ *and* [Cu(dapp)(OAc)(MeOH)]$_2$. Cu(OAc)$_2$.2H$_2$O (0·5 g; 2·5 mmol) was added to a solution of Hdapp (0·57 g; 2·5 mmol) in 50 ml of MeOH. The dark-green solution was heated at 323 K for one hour and then cooled to room temperature. After two weeks of slow evaporation of the MeOH, dark-green crystals had formed, leaving a light-green solution. Further evaporation of the solvent over an additional week yielded some light-green crystals. The dark-green crystals are [Cu(dapp)(OAc)]$_2$. Calculated: C, 58·52; H, 5·49; N, 4·01%. Found: C, 58·51; H, 5·64; N, 3·99%. The light-green crystals are [Cu(dapp)(OAc)-

Table 1. *Summary of crystallographic data and data collection parameters*

	Cu(dapp)$_2$	[Cu(dapp)(OAc)]$_2$	[Cu(dapp)(OAc)(MeOH)]$_2$
Crystal size, mm	0·36 × 0·21 × 0·21	0·48 × 0·27 × 0·14	0·40 × 0·29 × 0·13
μ(Mo $K\alpha$), cm^{-1}	8·89	13·35	12·76
$T_{\min}$, $T_{\max}$*	0·81–0·66	0·85–0·76	0·86–0·65
Scan speed, ° min^{-1}	1·0	1·0	1·0
$2\theta_{\max}$,°	60	60	60
hkl range	$+h, +k, \pm l$	$+h, +k, \pm l$	$+h, +k, +l$
Number of unique data	5435	4606	4550
Number of data used	4327	3275	4061
Number of variables	316	199	217
R	0·070	0·069	0·098
wR	0·046	0·040	0·061
$\rho_{\max}$, e Å^{-3}	0·9	0·6	1·2
Δ/σ†	0·11	0·07	0·27

* Range of transmission coefficients.

† Maximum shift (Δ) over e.s.d. (σ) for last refinement.

(MeOH)]$_2$. Calculated: C, 56·76; H, 6·08; N, 3·68%. Found: C, 56·61; H, 6·01; N, 3·62%.

X-ray data collection. Preliminary Weissenberg photographs indicated the lattices and space groups for all three compounds listed in the *Abstract*. Other crystallographic data are also given in the *Abstract* and Table 1 along with a summary of the data collections and structure refinements. In all cases the lattice parameters were obtained by a least-squares fit to the setting angles ($2\theta < 25°$) for 15 reflections from each crystal performed on a Syntex $P\bar{1}$ autodiffractometer. The data collections, preliminary data analyses and assignment of weights were completed using methods described by Post, Von Dreele & Buseck (1982). Analytical absorption corrections (de Meulenaer & Tompa, 1965) were applied using the linear absorption coefficients (*International Tables for X-ray Crystallography,* 1974) listed in the table; the ranges of transmission coefficients ($T_{\min}$–$T_{\max}$) are also indicated. No extinction corrections were applied. The periodic monitoring of four reflections was used to correct for slight (1–1·5%) intensity variations during the collections. In all three cases examination of ω scans for selected reflections showed that the crystals were single and of good quality.

Structure solution and refinement. In all three cases the Cu atom positions were obtained from Patterson maps;* subsequent difference maps gave the positions of the other non-hydrogen atoms. Neutral-atom scattering factors including the anomalous scattering for Cu (*International Tables for X-ray Crystallography,* 1974) were used. After isotropic refinement by full-matrix least squares on F, H atoms were placed at idealized positions with fixed $U = 0{\cdot}05$ Å^2 in accord with peaks found in difference maps. The final anisotropic refinements were by large-block least squares on F; Cu atom and scale factor in one block, other atom coordinates in a second block and remaining thermal parameters in a third block. The H parameters were fixed. The numerical details of these last refinements are given in Table 1.† The high residuals listed for these refinements arise from our use of nearly all the data collected; we rejected only the weakest reflections ($F < 1{\cdot}0\sigma$). A stiffer rejection criterion would have produced lower residuals but not changed the result. In any case the weighted residuals given here indicate that the refinements are satisfactory.

Discussion. Atomic coordinates and equivalent thermal parameters for the non-hydrogen atoms in Cu(dapp)$_2$, [Cu(dapp)(OAc)]$_2$ and [Cu(dapp)(OAc)(MeOH)]$_2$ are given in Tables 2, 3 and 4, respectively. Figs. 1 to 3 show the essential features of these three molecules.

Table 2. *Fractional coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3) *for* Cu(dapp)$_2$

The value in parentheses in this and all succeeding tables is the standard deviation in the last figure given.

$$U_{\rm eq} = (U_1U_2U_3)^{1/3}.$$

	x	y	z	$U_{\rm eq}$
Cu	3390·1 (5)	−1382·9 (6)	6195·9 (2)	37
O(1*a*)	2912 (3)	−414 (3)	5517 (1)	49
N(1*a*)	4703 (3)	−2563 (4)	5900 (1)	36
C(1*a*)	3069 (4)	−812 (4)	5017 (2)	38
C(2*a*)	2198 (4)	−433 (5)	4538 (2)	41
C(3*a*)	2371 (4)	−781 (4)	4012 (2)	36
C(4*a*)	3387 (4)	−1554 (4)	3927 (2)	36
C(5*a*)	4240 (4)	−1941 (4)	4405 (2)	36
C(6*a*)	4106 (4)	−1574 (4)	4937 (2)	35
C(7*a*)	3565 (4)	−1937 (4)	3359 (2)	36
C(8*a*)	4090 (4)	−3206 (5)	3258 (2)	45
C(9*a*)	4288 (4)	−3543 (5)	2734 (2)	59
C(10*a*)	3958 (4)	−2639 (6)	2297 (2)	58
C(11*a*)	3424 (4)	−1392 (6)	2384 (2)	50
C(12*a*)	3236 (4)	−1036 (4)	2909 (2)	39
C(13*a*)	5114 (4)	−1840 (4)	5432 (2)	39
C(14*a*)	4167 (4)	−3926 (5)	5721 (2)	52
C(15*a*)	5809 (4)	−2773 (5)	6341 (2)	51
O(1*b*)	3669 (2)	−2493 (3)	6852 (1)	43
N(1*b*)	2298 (3)	17 (4)	6525 (1)	36
C(1*b*)	3983 (4)	−1843 (4)	7338 (2)	53
C(2*b*)	5041 (4)	−2225 (5)	7729 (2)	46
C(3*b*)	5356 (4)	−1528 (5)	8230 (2)	46
C(4*b*)	4675 (4)	−413 (5)	8376 (2)	41
C(5*b*)	3602 (4)	−61 (5)	7989 (2)	43
C(6*b*)	3263 (4)	−760 (5)	7489 (2)	39
C(7*b*)	5047 (4)	369 (5)	8906 (2)	44
C(8*b*)	4229 (5)	1133 (6)	9137 (2)	67
C(9*b*)	4598 (6)	1860 (6)	9630 (2)	80
C(10*b*)	5790 (6)	1829 (5)	9903 (2)	71
C(11*b*)	6628 (5)	1082 (6)	9682 (2)	77
C(12*b*)	6275 (5)	359 (6)	9186 (2)	66
C(13*b*)	2082 (4)	−424 (5)	7087 (2)	44
C(14*b*)	1071 (4)	194 (5)	6163 (2)	53
C(15*b*)	2958 (4)	1374 (5)	6574 (2)	53

Table 3. *Fractional coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3) *for* [Cu(dapp)(OAc)]$_2$

	x	y	z	$U_{\rm eq}$
Cu	−935·4 (4)	288·7 (5)	286·3 (3)	42·9
O(1)	474 (2)	1254 (3)	316 (2)	52
N(1)	−1548 (2)	2337 (3)	527 (2)	37
C(1)	1128 (3)	2473 (4)	857 (2)	41
C(2)	2430 (3)	2504 (4)	1325 (2)	46
C(3)	3068 (3)	3751 (5)	1872 (2)	45
C(4)	2434 (3)	5001 (4)	1980 (2)	39
C(5)	1132 (3)	4949 (4)	1516 (2)	39
C(6)	466 (3)	3714 (4)	951 (2)	36
C(7)	3135 (3)	6344 (4)	2562 (2)	43
C(8)	4220 (4)	6097 (5)	3358 (3)	53
C(9)	4864 (4)	7351 (6)	3901 (3)	61
C(10)	4441 (4)	8861 (6)	3658 (3)	78
C(11)	3369 (4)	9141 (5)	2869 (3)	66
C(12)	2716 (3)	7897 (5)	2327 (2)	50
C(13)	−935 (3)	3773 (4)	396 (2)	47
C(14)	−1302 (4)	2353 (5)	1417 (2)	62
C(15)	−2895 (4)	2450 (5)	−86 (3)	50
O(2)	−2149 (2)	−982 (3)	374 (2)	49
O(3)	−335 (3)	−1438 (4)	1557 (2)	64
C(16)	−1465 (4)	−1672 (5)	1102 (3)	53
C(17)	−2143 (4)	−2711 (5)	1401 (3)	71

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* From this point on in all three structure analyses the crystallographic computer system *CRYSTALS* was used for all calculations (Rollett & Carruthers, 1974).

† Tables of observed and calculated structure factors with phase angles, anisotropic thermal parameters and hydrogen-atom positions for all three structures have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43124 (83 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystalllography, 5 Abbey Square, Chester CH1 2HU, England.

Table 4. *Fractional coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3) *for* [Cu(dapp)(OAc)(MeOH)]$_2$

	x	*y*	*z*	U_{eq}
Cu	179·8 (13)	485·7 (4)	502·2 (4)	24·6
O(1)	614 (7)	290 (2)	−491 (3)	30
N(1)	976 (10)	1280 (2)	375 (3)	29
C(1)	786 (11)	663 (3)	−1028 (4)	27
C(2)	46 (12)	547 (3)	−1686 (3)	32
C(3)	128 (13)	924 (3)	−2209 (4)	33
C(4)	869 (11)	1444 (3)	−2091 (4)	25
C(5)	1606 (11)	1552 (3)	−1435 (4)	28
C(6)	1568 (11)	1173 (3)	−903 (4)	26
C(7)	842 (11)	1881 (3)	−2641 (4)	29
C(8)	340 (13)	2414 (3)	−2463 (5)	43
C(9)	310 (15)	2825 (4)	−2976 (5)	53
C(10)	797 (14)	2704 (4)	−3649 (5)	57
C(11)	1252 (14)	2175 (4)	−3834 (4)	47
C(12)	1323 (12)	1763 (4)	−3329 (4)	41
C(13)	2349 (11)	1313 (3)	−199 (4)	28
C(14)	−633 (12)	1628 (4)	214 (4)	39
C(15)	1860 (14)	1484 (4)	1026 (4)	41
O(2)	−947 (8)	648 (2)	1388 (2)	27
O(3)	−3623 (9)	766 (3)	939 (3)	46
C(16)	−2607 (13)	677 (4)	1443 (4)	30
C(17)	−3366 (13)	606 (5)	2152 (4)	56
O(4)	3159 (8)	227 (3)	896 (3)	44
C(18)	3847 (15)	−291 (4)	805 (5)	56

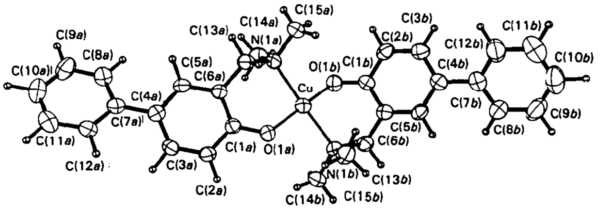

Fig. 1. Perspective representation of Cu(dapp)$_2$.

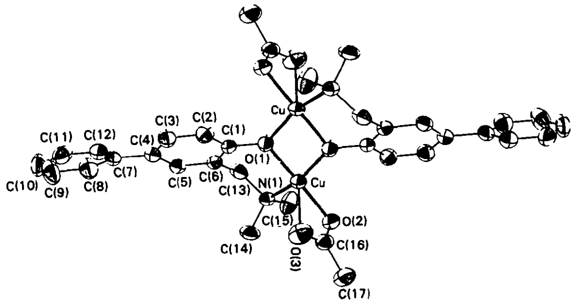

Fig. 2. Perspective representation of [Cu(dapp)(OAc)]$_2$.

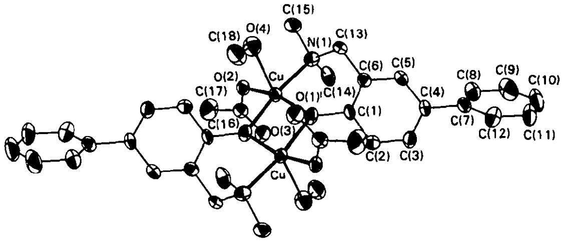

Fig. 3. Perspective representation of [Cu(dapp)(OAc)(MeOH)]$_2$.

Bond distances and angles within the coordination sphere of each Cu atom and those unique to each complex are given in Table 5. All the common distances and angles with their averages for the dapp ligands are collected in Table 6.

The compound Cu(dapp)$_2$ is monomeric with each dapp ligand bonded *via* an O and an N atom to give a nearly planar (r.m.s. deviation 0·14 Å) Cu coordination geometry; the two dapp ligands are *trans* to each other. A very similar structure was found for bis(salicylaldiminato)copper(II) (Baker, Hall & Waters, 1966). The other two compounds, [Cu(dapp)(OAc)]$_2$ and [Cu(dapp)(OAc)(MeOH)]$_2$, are dimers consisting of two distorted square-pyramidal Cu^{II} polyhedra sharing a square base edge with their pyramid apices *trans* to each other. This shared edge is formed by the O atoms from the dapp ligands, the N atom from each dapp occupying another square apex. In both cases the center of this common edge is a crystallographic inversion center so that only one half of each dimer is unique. The corresponding salicylaldimine copper complexes are apparently unknown. The Cu—O bonds

Table 5. *Selected bond distances* (Å) *and angles* (°)

Cu(dapp)$_2$			
Cu—O(1*a*)	1·884 (3)	O(1*a*)—Cu—O(1*b*)	172·28 (7)
Cu—O(1*b*)	1·897 (3)	N(1*a*)—Cu—N(1*b*)	171·14 (7)
Cu—N(1*a*)	2·078 (3)	O(1*a*)—Cu—N(1*a*)	93·19 (11)
Cu—N(1*b*)	2·069 (3)	O(1*b*)—Cu—N(1*b*)	92·60 (11)
		O(1*a*)—Cu—N(1*b*)	86·50 (11)
		O(1*b*)—Cu—N(1*a*)	88·88 (11)
[Cu(dapp)(OAc)]$_2$			
Cu—Cu	3·067 (1)		
Cu—O(1)	1·926 (2)	O(1)—Cu—O(1′)	76·16 (4)
Cu—O(1′)	1·971 (2)	O(1)—Cu—N(1)	94·76 (10)
Cu—N(1)	2·028 (3)	N(1)—Cu—O(1′)	159·28 (6)
		Cu—O(1)—Cu	103·84 (16)
Cu—O(2)	1·938 (2)	O(2)—Cu—O(3)	58·26 (6)
Cu—O(3)	2·491 (3)	O(2)—Cu—O(1)	169·81 (6)
		O(2)—Cu—O(1′)	98·86 (8)
		O(2)—Cu—N(1)	92·74 (9)
		O(3)—Cu—O(1)	112·89 (7)
		O(3)—Cu—O(1′)	95·49 (8)
		O(3)—Cu—N(1)	105·22 (8)
O(2)—C(16)	1·283 (4)	O(2)—C(16)—O(3)	122·8 (3)
O(3)—C(16)	1·234 (4)	C(16)—O(2)—Cu	101·5 (3)
C(16)—C(17)	1·507 (5)	C(16)—O(3)—Cu	77·4 (2)
		O(2)—C(16)—C(17)	115·6 (4)
		O(3)—C(16)—C(17)	121·4 (4)
[Cu(dapp)(OAc)(MeOH)]$_2$			
Cu—Cu	3·067 (2)		
Cu—O(1)	1·987 (5)	O(1)—Cu—O(1′)	78·89 (10)
Cu—O(1′)	1·985 (5)	O(1)—Cu—N(1)	93·93 (21)
Cu—N(1)	2·044 (6)	N(1)—Cu—O(1′)	172·54 (11)
		Cu—O(1)—Cu	101·1 (3)
Cu—O(2)	1·932 (5)	O(2)—Cu—O(4)	100·11 (17)
Cu—O(4)	2·421 (6)	O(2)—Cu—O(1)	163·65 (12)
		O(2)—Cu—O(1′)	94·42 (19)
		O(2)—Cu—N(1)	91·99 (21)
		O(4)—Cu—O(1)	95·00 (18)
		O(4)—Cu—O(1′)	91·42 (19)
		O(4)—Cu—N(1)	91·21 (22)
O(2)—C(16)	1·239 (9)	O(2)—C(16)—O(3)	123·2 (7)
O(3)—C(16)	1·244 (9)	C(16)—O(2)—Cu	121·2 (5)
C(16)—C(17)	1·478 (10)	O(2)—C(16)—C(17)	116·8 (7)
		O(3)—C(16)—C(17)	120·1 (7)
O(4)—C(18)	1·376 (11)	C(18)—O(4)—Cu	122·7 (5)

The values for the dapp ligands are collected in Table 6.

to the shared O atoms in the dimers are much longer, 1·93–1·99 Å, than found in Cu(dapp)$_2$, 1·89 Å. In contrast, the Cu—N bonds are shorter for the dimers, 2·03–2·04 Å, than for Cu(dapp)$_2$, 2·07 Å; evidently crowding is not appreciable in the five-coordinate complexes. The Cu—Cu distances are identical for both dimers, 3·067 Å, and indicate an absence of any appreciable metal–metal bonding. In the case of [Cu(dapp)(OAc)]$_2$, the remaining two coordination sites on each Cu atom are taken by an acetate ion acting as a bidentate ligand. The bonding of the two acetate O atoms to Cu is distinctly asymmetric; the apical Cu—O distance is 2·491 Å while the other Cu—O distance is 1·938 Å. For [Cu(dapp)(OAc)(MeOH)]$_2$ the coordination polyhedra are similar but the acetate is monodentate with the apical position occupied by the O atom of MeOH; the uncoordinated acetate O atom forms a hydrogen bond with MeOH on a neighboring molecule. In this case the Cu—O bond lengths for the acetate group and MeOH are very similar (1·932 and 2·421 Å, respectively) to each of those for the asymmetrically bonded acetate in [Cu(dapp)(OAc)]$_2$. These apical Cu—O distances are at the short end of the usual range for this bond, 2·4–2·8 Å, and are more like those of some aqua copper salicyldimine complexes (Maslen & Waters, 1975). The bite of the dapp ligand, 2·88–2·95 Å, on Cu^{II} is larger than that for salicylaldimines, 2·75 Å (Lingafelter & Braun, 1966); this may account for the easy dimer formation.

Table 6. *Bond distances* (Å) *and angles* (°) *within the 2-dimethylaminomethyl-4-phenylphenol ligands*

	*A**	*B*	*C*	*D*	Average†
O(1)—C(1)	1·323 (4)	1·326 (4)	1·363 (4)	1·381 (8)	–
C(1)—C(2)	1·409 (5)	1·406 (5)	1·401 (5)	1·401 (9)	1·404 (4)
C(2)—C(3)	1·378 (5)	1·377 (5)	1·380 (5)	1·361 (9)	1·374 (9)
C(3)—C(4)	1·394 (5)	1·393 (6)	1·395 (5)	1·402 (10)	1·396 (4)
C(4)—C(5)	1·400 (5)	1·404 (5)	1·402 (4)	1·395 (10)	1·400 (4)
C(5)—C(6)	1·383 (5)	1·380 (5)	1·394 (4)	1·378 (10)	1·384 (7)
C(6)—C(1)	1·404 (5)	1·401 (5)	1·401 (4)	1·396 (10)	1·401 (3)
C(6)—C(13)	1·497 (5)	1·505 (5)	1·511 (5)	1·505 (10)	1·505 (6)
C(13)—N(1)	1·482 (5)	1·500 (5)	1·518 (4)	1·502 (9)	–
N(1)—C(14)	1·465 (5)	1·477 (5)	1·481 (4)	1·499 (10)	
N(1)—C(15)	1·477 (5)	1·484 (5)	1·470 (4)	1·494 (9)	1·481 (11)
C(4)—C(7)	1·484 (5)	1·485 (5)	1·486 (5)	1·501 (9)	1·489 (8)
C(7)—C(8)	1·390 (5)	1·367 (6)	1·396 (5)	1·398 (11)	
C(7)—C(12)	1·389 (5)	1·395 (6)	1·392 (5)	1·395 (10)	1·390 (10)
C(8)—C(9)	1·378 (5)	1·382 (6)	1·383 (5)	1·404 (11)	
C(11)—C(12)	1·382 (5)	1·383 (6)	1·379 (5)	1·397 (11)	1·386 (9)
C(9)—C(10)	1·368 (6)	1·355 (7)	1·361 (6)	1·371 (13)	
C(10)—C(11)	1·367 (6)	1·362 (7)	1·387 (6)	1·383 (13)	1·369 (11)
Cu—O(1)—C(1)	127·3 (2)	117·6 (2)	122·7 (2)	124·6 (4)	123·0 (41)
Cu′—O(1)—C(1)			131·0 (2)	130·6 (4)	130·8 (3)
Cu—N(1)—C(13)	110·8 (3)	112·5 (3)	111·3 (2)	109·5 (5)	111·0 (12)
Cu—N(1)—C(14)	108·6 (3)	112·2 (2)	110·8 (2)	109·4 (6)	
Cu—N(1)—C(15)	110·8 (2)	106·5 (3)	108·0 (2)	110·1 (5)	109·6 (18)
C(13)—N(1)—C(14)	107·0 (3)	109·6 (3)	109·2 (3)	111·1 (6)	
C(13)—N(1)—C(15)	110·8 (3)	112·5 (3)	108·0 (2)	107·2 (6)	109·4 (20)
C(14)—N(1)—C(15)	109·0 (3)	109·1 (3)	109·4 (2)	109·5 (6)	109·2 (2)
N(1)—C(13)—C(6)	114·2 (3)	112·6 (3)	112·4 (3)	112·4 (6)	112·9 (9)
O(1)—C(1)—C(6)	122·4 (3)	121·4 (3)	118·4 (3)	120·0 (6)	120·6 (17)
C(1)—C(6)—C(13)	118·4 (3)	116·8 (4)	120·3 (3)	121·2 (6)	119·2 (20)
O(1)—C(1)—C(2)	120·0 (3)	121·6 (3)	122·0 (3)	119·9 (6)	120·8 (12)
C(1)—C(2)—C(3)	121·0 (3)	120·6 (3)	120·7 (3)	120·4 (7)	120·7 (2)
C(2)—C(3)—C(4)	122·1 (3)	122·9 (3)	121·0 (3)	120·8 (6)	121·7 (10)
C(3)—C(4)—C(5)	116·5 (3)	116·1 (4)	117·8 (3)	118·0 (6)	117·1 (9)
C(4)—C(5)—C(6)	122·6 (3)	121·8 (3)	122·2 (3)	122·0 (6)	122·2 (3)
C(5)—C(6)—C(1)	120·3 (3)	121·5 (3)	118·6 (3)	118·8 (6)	119·8 (14)
C(5)—C(6)—C(13)	121·1 (3)	121·6 (3)	121·0 (3)	120·0 (6)	120·9 (7)
C(2)—C(1)—C(6)	117·5 (3)	117·0 (4)	119·6 (3)	119·9 (6)	118·5 (15)
C(3)—C(4)—C(7)	122·0 (3)	122·6 (3)	120·2 (3)	121·9 (6)	
C(5)—C(4)—C(7)	121·6 (3)	121·3 (4)	121·9 (3)	120·0 (6)	
C(4)—C(7)—C(8)	121·3 (3)	122·5 (4)	121·6 (3)	119·8 (6)	
C(4)—C(7)—C(12)	121·6 (3)	120·1 (4)	120·4 (3)	120·7 (6)	121·2 (9)
C(8)—C(7)—C(12)	117·1 (3)	117·4 (4)	118·0 (3)	119·4 (6)	118·0 (10)
C(7)—C(8)—C(9)	121·2 (4)	121·5 (4)	121·4 (4)	120·0 (7)	
C(7)—C(12)—C(11)	121·2 (4)	120·4 (4)	120·3 (3)	119·7 (8)	120·7 (7)
C(8)—C(9)—C(10)	120·7 (4)	120·7 (5)	119·8 (4)	120·0 (8)	
C(10)—C(11)—C(12)	120·4 (4)	120·8 (4)	120·6 (3)	120·3 (7)	120·4 (4)
C(9)—C(10)—C(11)	119·3 (4)	119·2 (4)	120·0 (3)	120·5 (7)	119·8 (6)

* Dapp ligands *A–D* are ligands *A* and *B* in Cu(dapp)$_2$, the ligand in [Cu(dapp)(OAc)]$_2$ and the ligand in [Cu(dapp)(OAc)(MeOH)]$_2$, respectively.

† Averages and estimated standard deviations calculated for chemically equivalent bonds and angles.

It has been proposed that the color isomerism of salicylaldimine Cu^{II} complexes is related to the coordination number of the Cu atom; four-coordinate Cu complexes are brown or violet and five-coordinate complexes are green (Baker, Hall & Waters, 1970). This relationship appears also to hold for these amine complexes; four-coordinate Cu(dapp)$_2$ is brown and the two five-coordinate Cu–dapp complexes examined here are green.

Bond lengths and angles for dapp ligands are all within the normally expected ranges. There may be a slight difference in the C—O bond lengths for the unbridged Cu(dapp)$_2$ complex, 1·32 Å, compared with that for the bridged compounds, 1·37 Å, but no other systematic differences were noted.

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