Because the charge on the anion is diffuse, there is a minimum of interaction between the anion and the hydrated cation in this compound. In fact, there are only three I—H distances which are less than the sum of the van der Waals distances of 3·15 Å (Bondi, 1964) and this lack of hydrogen bonding has resulted in high thermal parameters for the H atoms. Thus it would seem that, where a hydrated Ca^{2+} ion is free to fill an interstice in the structure with a minimum of interaction, it coordinates to seven water molecules rather than six which is normal for a hydrogen-bonded situation.

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The Structure of (o-Phthalato)bis(pyridine)copper(II) with Bridging and Chelating o-Phthalate Anions

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Abstract

$[Cu(C_5H_5N)_2(C_8H_4O_4)]$, $M_r = 385·9$, is monoclinic, space group $P2_1/c$, with $a = 18·199$ (6), $b = 11·991$ (14), $c = 17·923$ (8) Å, $\beta = 119·98$ (2)°, $V = 3388$ (4) Å^3, $Z = 8$, $D_x = 1·51$, $D_m = 1·51$ Mg m^{-3}, $F(000) = 1576$, $\lambda(Cu\ K\alpha) = 1·54178$ Å, $\mu(Cu\ K\alpha) = 1·999$ mm^{-1}. $R = 0·055$ for 5425 observed reflections.

The structure consists of two crystallographically independent square-pyramidal $[Cu(C_5H_5N)_2(C_8H_4O_4)]$ complexes linked in polymeric chains by bridging phthalate anions which also act as chelating ligands through two O atoms from one carboxylate group. Pentacoordination of Cu involves two N atoms (one at the apex of the pyramid) from two pyridine molecules, one O atom from the monodentate carboxylate of an

o-phthalate anion and two O atoms from the bidentate chelating carboxylate of another *o*-phthalate anion. In the chains, held together by normal van der Waals contacts, $C-H\cdots O$ interactions involving C atoms of pyridine and O atoms from chelating carboxylate groups are present.

Introduction

Investigations on the ligand behaviour of the *o*-phthalate anion (pht) in a series of Cu^{II} complexes, in the presence of other ionic or molecular species, have shown that the pht anion acts as a bridging ligand through two, three or four O atoms from both its carboxylate groups (Biagini Cingi, Manotti Lanfredi, Tiripicchio & Tiripicchio Camellini, 1977, 1978*a,b,c*, 1979). In strontium bis(*o*-phthalato)cuprate(II) trihydrate, pht shows bridging and chelating (through O atoms from both carboxylates) behaviour, so that seven-membered rings involving O atoms from both carboxylate groups of the same pht are formed. In the present compound, [Cu(pht)py$_2$], pht also behaves as a bridging and chelating ligand, but in a different way. Each pht connects two adjacent Cu atoms through both its carboxylate groups and chelates to one of the Cu atoms through both O atoms of the same carboxylate group, forming four-membered rings.

Experimental

Green-blue crystals of the title compound were prepared by evaporation at room temperature of solutions obtained by dissolving copper carbonate hydroxide and phthalic acid (in 1 : 1 ratio) in pyridine.

The crystal data are in the *Abstract*. Space group $P2_1/c$ was indicated by the systematic absences. Cell parameters were first determined from rotation and Weissenberg photographs and then refined from diffractometer data.

Intensities were collected on a Siemens AED diffractometer with Ni-filtered Cu $K\alpha$ radiation and the $\theta-2\theta$ scan technique. A crystal 0·26 × 0·40 × 0·56 mm was aligned with [010] along the φ axis of the diffractometer and all reflections with $3 < \theta < 70°$ were measured. Of the 6306 independent reflections collected, 5425 having $I > 2\sigma(I)$ were considered observed and used in the analysis. Corrections for Lorentz and polarization effects were applied, but no correction was made for absorption. The absolute scale and overall temperature factor were obtained by Wilson's method.

Structure determination and refinement

The structure was solved by Patterson and Fourier methods and refined by full-matrix least squares with

SHELX (Sheldrick, 1976), initially with isotropic and then anisotropic thermal parameters for the non-hydrogen atoms. All H atoms were located from a ΔF synthesis. Additional cycles were then computed including the H atoms with isotropic thermal parameters. Unit weights were used at every stage of the refinement by analysing the variation of $|\Delta F|$ with $|F_o|$. The final R was 0·055 (observed reflections

Table 1. *Fractional atomic coordinates* (×10⁴) *with e.s.d.'s in parentheses and isotropic B equivalent values* (*Hamilton*, 1959) *for the non-hydrogen atoms*

	x	y	z	B_{eq} (Å²)
Cu(1)	6835 (1)	6237 (1)	2581 (1)	2·59 (3)
Cu(2)	8252 (1)	1185 (1)	3372 (1)	2·76 (3)
O(11)	5872 (3)	5254 (3)	1897 (3)	3·97 (20)
O(21)	7085 (2)	4539 (3)	2172 (2)	3·05 (16)
O(31)	7650 (3)	2059 (4)	1718 (3)	3·93 (20)
O(41)	7225 (2)	2011 (3)	2682 (2)	3·29 (17)
O(12)	9184 (3)	102 (3)	3757 (3)	4·00 (19)
O(22)	8044 (2)	−440 (3)	2592 (2)	3·07 (17)
O(32)	7508 (2)	−3036 (3)	1633 (2)	3·72 (18)
O(42)	7892 (2)	−2981 (3)	3012 (2)	3·17 (17)
N(13)	6074 (3)	7581 (4)	2348 (3)	2·98 (20)
N(14)	7170 (3)	5642 (4)	3864 (3)	3·13 (20)
N(15)	9086 (3)	2453 (4)	3871 (3)	2·90 (20)
N(16)	7794 (3)	601 (4)	4184 (3)	3·06 (20)
C(11)	5823 (3)	3522 (4)	1223 (3)	2·65 (21)
C(21)	6212 (3)	2495 (4)	1259 (3)	2·49 (21)
C(31)	5756 (4)	1671 (5)	643 (4)	3·85 (26)
C(41)	4912 (4)	1863 (6)	39 (4)	5·10 (29)
C(51)	4520 (4)	2867 (6)	5 (4)	5·30 (32)
C(61)	4976 (4)	3694 (6)	600 (4)	4·10 (27)
C(71)	6298 (3)	4470 (4)	1810 (3)	2·58 (21)
C(81)	7103 (3)	2199 (4)	1919 (3)	2·67 (22)
C(12)	9311 (3)	−1503 (4)	3055 (3)	2·56 (21)
C(22)	8933 (3)	−2514 (4)	2639 (3)	2·42 (21)
C(32)	9416 (4)	−3304 (5)	2493 (4)	3·52 (26)
C(42)	10270 (4)	−3106 (6)	2784 (4)	2·76 (32)
C(52)	10654 (4)	−2106 (6)	3219 (5)	3·97 (32)
C(62)	10167 (3)	−1316 (5)	3347 (4)	3·05 (27)
C(72)	8803 (3)	−575 (4)	3131 (3)	3·93 (21)
C(82)	8044 (3)	−2837 (4)	2387 (3)	3·29 (21)
C(13)	6366 (4)	8640 (5)	2432 (4)	4·00 (26)
C(23)	5856 (4)	9565 (5)	2271 (5)	3·07 (31)
C(33)	5014 (5)	9418 (6)	2009 (5)	3·72 (38)
C(43)	4710 (5)	8325 (7)	1959 (6)	3·17 (42)
C(53)	5256 (4)	7432 (6)	2115 (5)	2·98 (32)
C(14)	7423 (4)	4609 (5)	4137 (4)	3·13 (26)
C(24)	7669 (5)	4238 (6)	4967 (4)	2·90 (33)
C(34)	7633 (5)	5010 (7)	5534 (4)	3·06 (36)
C(44)	7382 (5)	6075 (7)	5267 (4)	2·65 (37)
C(54)	7140 (5)	6384 (6)	4419 (4)	2·49 (32)
C(15)	9834 (4)	2255 (6)	4609 (4)	3·85 (28)
C(25)	10466 (4)	3039 (6)	4964 (5)	5·10 (33)
C(35)	10359 (5)	4058 (7)	4560 (5)	5·30 (39)
C(45)	9579 (5)	4274 (7)	3809 (5)	4·10 (39)
C(55)	8960 (4)	3456 (5)	3485 (4)	2·58 (28)
C(16)	8085 (4)	−336 (5)	4651 (4)	2·67 (28)
C(26)	7848 (5)	−656 (6)	5253 (4)	2·56 (33)
C(36)	7296 (5)	31 (6)	5367 (4)	2·42 (38)
C(46)	6984 (6)	998 (7)	4884 (5)	3·52 (44)
C(56)	7246 (5)	1246 (6)	4288 (4)	4·25 (32)

only).* Final atomic coordinates for the heavy and H atoms are given in Tables 1 and 2 respectively.

All the calculations were carried out on the Cyber 76 computer of the Centro di Calcoló Interuniversitario dell'Italia Nord-Orientale (Bologna) with the financial support of the University of Parma.

Discussion

The crystal structure consists of two crystallographically independent [Cu(pht)py$_2$] complexes linked in zigzag polymeric chains, running along **b**, by bridging pht anions (Fig. 1). Bond distances and angles are given in Table 3. Each pht anion behaves as a tridentate ligand bridging two adjacent Cu atoms through O atoms from both carboxylate groups, one of which acts as a chelate to a metal atom. The Cu—O lengths [Cu(1)—O(11) = 1·954 (5), Cu(1)—O(21) = 2·285 (4) and Cu(2)—O(12) = 1·967 (5), Cu(2)—O(22) = 2·316 (4) Å] and the values of the Cu—O—C angles [Cu(1)—O(11)—C(71) = 96·4, Cu(1)—O(21)—C(71) =

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* Lists of structure factors and anisotropic thermal parameters are available from the authors and have also been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36060 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

82·2 and Cu(2)—O(12)—C(72) = 96·7, Cu(2)—O(22)—C(72) = 81·8°] involving the bidentate carboxylates support their asymmetric chelation; the O—C—O bite angles [O(11)—C(71)—O(21) = 119·9, O(12)—C(72)—O(22) = 120·5°] and the corresponding O···O distances [O(11)···O(21) = 2·183, O(12)···O(22) = 2·181 Å] are in good agreement with those found in nearly symmetrically chelating carboxylate groups (Venkatasubramanian, Chiesi Villa, Gaetani Manfredotti & Guastini, 1972; Drew, Othman, Edwards & Richards, 1975; Alcock & Tracy, 1979). The coordination polyhedron of both independent Cu atoms can be described as a square pyramid: the base is formed by a pyridine N atom, by two O atoms from the chelating carboxylate of one pht anion and by an O atom from the monodentate carboxylate of the other pht anion. The constrained geometry of the chelating carboxylate group justifies the values of the corresponding O—Cu—O angles [O(11)—Cu(1)—O(21) = 61·4 (2) and O(12)—Cu(2)—O(22) = 60·6 (2)°] in the basal coordination plane. The apex of the pyramid is occupied by one N atom from a second pyridine molecule at a distance longer than that found in the basal plane [2·183 (5) against 2·028 (5) and 2·125 (6) against 2·015 (5) Å respectively]. The four atoms forming the base of the pyramid show a tetrahedral distortion (Table 4), with the Cu atom displaced from

Table 2. *Fractional coordinates* ($\times 10^3$) *and isotropic thermal parameters* ($\times 10^3$) *of the* H *atoms, with e.s.d.'s in parentheses*

|	x	y	z	U (Å^2)
H(31)	603 (3)	98 (4)	62 (3)	44 (14)
H(41)	462 (3)	135 (5)	−43 (3)	94 (15)
H(51)	392 (4)	303 (5)	−43 (4)	56 (16)
H(61)	466 (3)	454 (4)	58 (3)	75 (14)
H(32)	915 (3)	−404 (4)	224 (3)	47 (14)
H(42)	1059 (3)	−361 (5)	267 (3)	58 (16)
H(52)	1138 (3)	−199 (5)	355 (3)	59 (16)
H(62)	1045 (3)	−51 (4)	367 (3)	68 (14)
H(13)	698 (3)	875 (4)	260 (3)	47 (14)
H(23)	609 (3)	1036 (5)	232 (3)	55 (16)
H(33)	460 (4)	1009 (5)	187 (4)	82 (19)
H(43)	406 (4)	818 (6)	180 (4)	104 (22)
H(53)	503 (4)	664 (5)	204 (4)	62 (17)
H(14)	749 (3)	414 (4)	378 (3)	69 (15)
H(24)	788 (3)	339 (5)	517 (4)	111 (17)
H(34)	776 (4)	481 (5)	608 (4)	65 (18)
H(44)	737 (4)	668 (5)	571 (4)	100 (19)
H(54)	696 (4)	719 (5)	423 (4)	60 (17)
H(15)	993 (3)	146 (4)	492 (3)	72 (14)
H(25)	1103 (3)	291 (4)	556 (3)	96 (16)
H(35)	1086 (4)	467 (5)	481 (4)	103 (18)
H(45)	947 (4)	507 (5)	349 (4)	104 (19)
H(55)	841 (3)	363 (4)	301 (3)	47 (14)
H(16)	849 (3)	−87 (4)	455 (3)	53 (15)
H(26)	813 (3)	−134 (5)	563 (4)	63 (17)
H(36)	711 (4)	−19 (5)	583 (4)	72 (20)
H(46)	641 (4)	137 (6)	481 (4)	93 (23)
H(56)	700 (4)	199 (5)	390 (4)	96 (18)
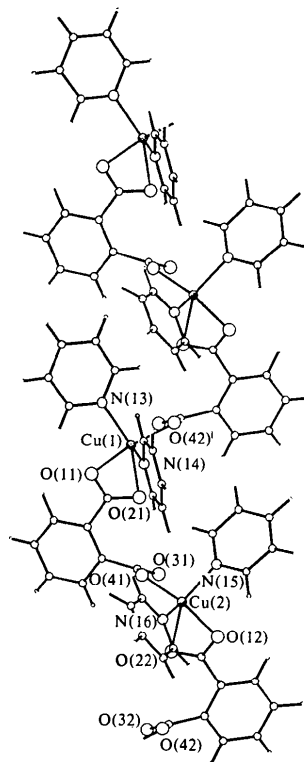
Fig. 1. View of the two independent Cu^{II} complexes linked by bridging phthalate anions in zigzag polymeric chains running along **b**.

Table 3. Bond distances (Å) and angles (°) (not involving H atoms) with e.s.d.'s

(a) The Cu coordination polyhedra

Cu(1)–O(11)	·1·954 (5)	Cu(2)–O(12)	1·967 (5)
Cu(1)–O(21)	2·285 (4)	Cu(2)–O(22)	2·316 (4)
Cu(1)–N(13)	2·028 (5)	Cu(2)–N(15)	2·015 (5)
Cu(1)–N(14)	2·183 (5)	Cu(2)–N(16)	2·125 (6)
Cu(1)–O(42^i)	1·921 (4)	Cu(2)–O(41)	1·922 (4)

O(11)–Cu(1)–O(21)	61·4 (2)	O(12)–Cu(2)–O(22)	60·6 (2)
O(11)–Cu(1)–N(13)	92·5 (2)	O(12)–Cu(2)–N(15)	90·9 (2)
O(11)–Cu(1)–N(14)	98·9 (2)	O(12)–Cu(2)–N(16)	96·1 (2)
O(21)–Cu(1)–N(13)	150·1 (2)	O(22)–Cu(2)–N(15)	139·7 (2)
O(21)–Cu(1)–N(14)	92·9 (2)	O(22)–Cu(2)–N(16)	97·7 (2)
N(13)–Cu(1)–N(14)	106·2 (2)	N(15)–Cu(2)–N(16)	114·3 (2)
O(11)–Cu(1)–O(42^i)	161·9 (2)	O(12)–Cu(2)–O(41)	163·1 (2)
O(21)–Cu(1)–O(42^i)	104·1 (2)	O(22)–Cu(2)–O(41)	103·4 (2)
N(13)–Cu(1)–O(42^i)	98·0 (2)	N(15)–Cu(2)–O(41)	99·9 (2)
N(14)–Cu(1)–O(42^i)	92·3 (2)	N(16)–Cu(2)–O(41)	91·3 (2)

(b) The o-phthalate anions

C(11)–C(21)	1·406 (7)	C(12)–C(22)	1·409 (7)
C(21)–C(31)	1·403 (8)	C(22)–C(32)	1·403 (9)
C(31)–C(41)	1·387 (10)	C(32)–C(42)	1·391 (11)
C(41)–C(51)	1·385 (10)	C(42)–C(52)	1·411 (10)
C(51)–C(61)	1·387 (10)	C(52)–C(62)	1·392 (10)
C(11)–C(61)	1·395 (9)	C(12)–C(62)	1·391 (9)
C(11)–C(71)	1·496 (7)	C(12)–C(72)	1·496 (8)
C(71)–O(11)	1·277 (7)	C(72)–O(12)	1·273 (6)
C(71)–O(21)	1·245 (7)	C(72)–O(22)	1·238 (7)
C(21)–C(81)	1·496 (8)	C(22)–C(82)	1·497 (8)
C(81)–O(31)	1·228 (8)	C(82)–O(32)	1·232 (6)
C(81)–O(41)	1·291 (6)	C(82)–O(42)	1·293 (6)

C(61)–C(11)–C(21)	119·7 (5)	C(62)–C(12)–C(22)	119·8 (5)
C(61)–C(11)–C(71)	118·0 (5)	C(62)–C(12)–C(72)	118·2 (5)
C(21)–C(11)–C(71)	122·2 (5)	C(22)–C(12)–C(72)	121·8 (5)
C(11)–C(21)–C(31)	119·6 (5)	C(12)–C(22)–C(32)	119·6 (6)
C(11)–C(21)–C(81)	124·5 (4)	C(12)–C(22)–C(82)	123·4 (5)
C(31)–C(21)–C(81)	115·9 (5)	C(32)–C(22)–C(82)	116·9 (5)
C(21)–C(31)–C(41)	119·1 (6)	C(22)–C(32)–C(42)	120·1 (6)
C(31)–C(41)–C(51)	121·6 (6)	C(32)–C(42)–C(52)	120·3 (7)
C(41)–C(51)–C(61)	119·4 (7)	C(42)–C(52)–C(62)	119·3 (7)
C(11)–C(61)–C(51)	120·5 (6)	C(12)–C(62)–C(52)	120·9 (6)
C(11)–C(71)–O(11)	118·2 (5)	C(12)–C(72)–O(12)	117·7 (5)
C(11)–C(71)–O(21)	121·8 (5)	C(12)–C(72)–O(22)	121·7 (4)
O(11)–C(71)–O(21)	119·9 (5)	O(12)–C(72)–O(22)	120·5 (5)
C(21)–C(81)–O(31)	121·2 (5)	C(22)–C(82)–O(32)	121·7 (5)
C(21)–C(81)–O(41)	115·1 (5)	C(22)–C(82)–O(42)	116·1 (4)
O(31)–C(81)–O(41)	123·5 (5)	O(32)–C(82)–O(42)	122·0 (5)

(c) The pyridine ligands

N(13)–C(13)	1·356 (8)	N(14)–C(14)	1·327 (8)
C(13)–C(23)	1·381 (10)	C(14)–C(24)	1·395 (9)
C(23)–C(33)	1·371 (13)	C(24)–C(34)	1·400 (11)
C(33)–C(43)	1·408 (12)	C(34)–C(44)	1·360 (12)
C(43)–C(53)	1·391 (12)	C(44)–C(54)	1·404 (9)
C(53)–N(13)	1·342 (10)	C(54)–N(14)	1·456 (9)

C(13)–N(13)–C(53)	118·1 (6)	C(14)–N(14)–C(54)	118·4 (5)
N(13)–C(13)–C(23)	122·9 (7)	N(14)–C(14)–C(24)	123·9 (6)
C(13)–C(23)–C(33)	119·2 (6)	C(14)–C(24)–C(34)	117·2 (6)
C(23)–C(33)–C(43)	118·5 (8)	C(24)–C(34)–C(44)	119·6 (6)
C(33)–C(43)–C(53)	119·0 (9)	C(34)–C(44)–C(54)	119·8 (7)
C(43)–C(53)–N(13)	122·0 (7)	C(44)–C(54)–N(14)	121·0 (7)

N(15)–C(15)	1·364 (8)	N(16)–C(16)	1·342 (8)
C(15)–C(25)	1·371 (11)	C(16)–C(26)	1·401 (11)
C(25)–C(35)	1·384 (11)	C(26)–C(36)	1·391 (13)
C(35)–C(45)	1·409 (12)	C(36)–C(46)	1·387 (11)
C(45)–C(55)	1·384 (11)	C(46)–C(56)	1·402 (13)
C(55)–N(15)	1·349 (8)	C(56)–N(16)	1·347 (11)

C(15)–N(15)–C(55)	119·0 (6)	C(16)–N(16)–C(56)	118·9 (6)
N(15)–C(15)–C(25)	122·0 (6)	N(16)–C(16)–C(26)	122·2 (7)
C(15)–C(25)–C(35)	119·8 (7)	C(16)–C(26)–C(36)	118·3 (6)
C(25)–C(35)–C(45)	118·3 (8)	C(26)–C(36)–C(46)	120·2 (8)
C(35)–C(45)–C(55)	119·4 (7)	C(36)–C(46)–C(56)	117·6 (9)
C(45)–C(55)–N(15)	121·5 (6)	C(46)–C(56)–N(16)	122·7 (7)

Symmetry code: (i) x, $1 + y$, z.

Table 4. Equations of least-squares planes in the form $AX + BY + CZ = D$, where X, Y, and Z are co-ordinates in Å referred to orthogonal axes and obtained from fractional coordinates by applying the matrix

$$\|a, 0, c \cos \beta | 0, b, 0 | 0, 0, c \sin \beta\|$$

Deviations (Å) of relevant atoms from the planes are in square brackets.

A	B	C	D

Plane (I): O(11)O(21)N(13)O(42^i)
| 0·3730 | 0·2791 | −0·8848 | 2·5846 |

[O(11) −0·080 (5), O(21) 0·035 (3), N(13) 0·066 (5), O(42^i) −0·022 (3), Cu(1) −0·265 (2), N(14) −2·428 (5)]

Plane (II): O(12)O(22)N(15)O(41)
| 0·6353 | 0·3027 | −0·7104 | 4·6764 |

[O(12) −0·302 (5), O(22) 0·131 (4), N(15) 0·247 (5), O(41) −0·077 (4), Cu(2) −0·343 (2), N(16) −2·442 (5)]

Plane (III): C(11)C(21)C(31)C(41)C(51)C(61)
| 0·6941 | 0·3698 | −0·6177 | 6·9765 |

[C(11) 0·008 (5), C(21) −0·013 (5), C(31) 0·019 (7), C(41) −0·007 (7), C(51) −0·004 (7), C(61) −0·001 (7), C(71) 0·100 (5), O(11) −0·228 (5), O(21) 0·552 (4), C(81) −0·062 (5), O(31) 0·884 (5), O(41) −1·198 (4)]

Plane (IV): C(11)C(71)O(11)O(21)
| 0·3828 | 0·4896 | −0·7835 | 4·2093 |

[C(11) 0·008 (5), C(71) −0·020 (5), O(11) 0·008 (5), O(21) 0·004 (3)]

Plane (V): C(21)C(81)O(31)O(41)
| −0·1580 | −0·9639 | −0·2142 | −4·9204 |

[C(21) 0·010 (5), C(81) −0·030 (5), O(31) 0·013 (5), O(41) 0·007 (4)]

Plane (VI): C(12)C(22)C(32)C(42)C(52)C(62)
| 0·2232 | 0·4258 | −0·8768 | −1·7638 |

[C(12) 0·009 (5), C(22) −0·011 (5), C(32) 0·010 (6), C(42) 0·004 (6), C(52) −0·009 (8), C(62) −0·003 (6), C(72) 0·158 (5), O(12) −0·318 (5), O(22) 0·760 (3), C(82) −0·143 (5), O(32) 0·714 (3), O(42) −1·255 (3)]

Plane (VII): C(12)C(72)O(12)O(22)
| 0·6010 | 0·5799 | −0·5500 | 4·8807 |

[C(12) 0·004 (5), C(72) −0·011 (5), O(12) 0·004 (5), O(22) 0·003 (4)]

Plane (VIII): C(22)C(82)O(32)O(42)
| −0·2680 | 0·9586 | −0·0964 | −6·9959 |

[C(22) −0·012 (5), C(82) 0·027 (5), O(32) −0·008 (4), O(42) −0·007 (4)]

Plane (IX): N(13)C(13)C(23)C(33)C(43)C(53)
| 0·2798 | −0·0148 | −0·9600 | −1·1373 |

[N(13) 0·008 (5), C(13) −0·008 (6), C(23) −0·004 (8), C(33) 0·026 (8), C(43) −0·022 (9), C(53) −0·001 (8)]

Plane (X): N(14)C(14)C(24)C(34)C(44)C(54)
| −0·9146 | −0·2654 | −0·3052 | −12·3942 |

[N(14) −0·001 (6), C(14) 0·001 (8), C(24) −0·004 (9), C(34) 0·006 (9), C(44) −0·007 (9), C(54) 0·004 (9)]

Plane (XI): N(15)C(15)C(25)C(35)C(45)C(55)
| 0·7571 | −0·3591 | −0·5458 | 5·5502 |

[N(15) 0·007 (5), C(15) −0·003 (7), C(25) −0·011 (8), C(35) 0·019 (9), C(45) −0·003 (9), C(55) −0·009 (7)]

Plane (XII): N(16)C(16)C(26)C(36)C(46)C(56)
| −0·4838 | −0·5126 | −0·7094 | −10·0207 |

[N(16) −0·006 (5), C(16) 0·002 (7), C(26) 0·005 (7), C(36) −0·007 (7), C(46) −0·004 (9), C(56) 0·011 (7)]

the mean plane passing through them towards the apex of the pyramid [displacements are 0·265 and 0·343 Å for Cu(1) and Cu(2) respectively]. Each Cu atom is also involved in a long contact [Cu(1)···O(32^i) = 2·688 and Cu(2)···O(31) = 2·800 Å] with the uncoordinated O atom from a pht anion; these Cu···O interactions make angles of 30·4 and 31·6° with the normal to the basal coordination plane around Cu(1) and Cu(2) respectively. The distances between the bridged Cu atoms (alternately 6·46 and 6·34 Å) are much longer than that found in strontium bis(o-phthalato)cuprate(II) trihydrate (4·54 Å) (Biagini Cingi, Manotti Lanfredi, Tiripicchio & Tiripicchio Camellini, 1978b). In both independent pht anions of the present compound the carboxylate groups are rotated on the same side around their C—C bonds with respect to the benzene ring [21·5° for C(11)C(71)-O(11)O(21) and 70·5° for C(21)C(81)O(31)O(41); 30·3° for C(12)C(72)O(12)O(22) and 64·3° for C(22)C(82)O(32)O(42)] as found in all the compounds where pht acts as a bridging ligand, whereas in strontium bis(o-phthalato)cuprate(II) trihydrate they are rotated on opposite sides (−14·1 and 78·5°). In both independent complexes the pyridine molecules,

bonded in the apical positions, are nearly orthogonal with respect to the mean basal coordination plane [the angles formed by the planes through N(14)C(14)-C(24)C(34)C(44)C(54) and N(15)C(15)C(25)C(35)-C(45)C(55) with those through O(11)O(21)N(13)-O(42^i) and O(12)O(22)N(15)O(31) are 81·6 and 87·6° respectively] while the pyridine molecules bonded in the basal plane, N(13)C(13)C(23)C(33)C(43)-C(53) and N(15)C(15)C(25)C(35)C(45)C(55), are rotated with respect to this plane by different angles (18·3 and 40·5° respectively). The two pyridine ligands coordinated to Cu(1) make an angle of 87·6° and those coordinated to Cu(2) an angle of 78·2°. Fig. 2, representing the projection of the structure along b, shows the packing of the chains in the crystals, determined by normal van der Waals contacts. In a chain, C—H···O interactions involving C atoms of pyridine and the weaker coordinated O atoms of chelating carboxylate groups satisfy the geometrical requirements for hydrogen bonding [H(13)···O(22^i) 2·17 Å, C(13)—H(13)—O(22^i) 156°; H(55)···O(21) 2·38 Å, C(55)—H(55)—O(21) 161°].
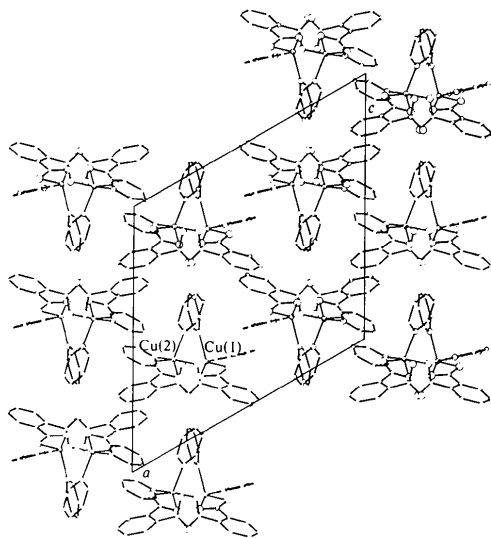

Fig. 2. Projection of the crystal structure along b, showing the packing of the chains.

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