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Crystal Structure of Lignocaine Hydrochloride—Zinc Chloride Complex

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Crystal and molecular structure of lignocaine hydrochloride—zinc chloride complex, $ZnCl_4C_{28}N_4O_2H_{44}$, is reported. The sample cyrstallizes in the monoclinic space group $P2_1$ with a = 9.128(2) Å, b = 19.196(5) Å, c = 19.696(5) Å, β = 95.81(1)°, V = 3433.43(1) Å^3, Z = 4. The structure of the title compound was solved using 3527 counter intensities with $I > 2.5\sigma(I)$ using CuK_α radiation and refined to an R value of 0.071. Each metal group is associated with a pair of ligands. The planes of the phenyl groups of one of the pair are nearly perpendicular to the planes of the phenyl groups of the other.

Keywords: Charge-transfer complexes, crystal structure, lignocaine, zinc chloride

INTRODUCTION

Charge transfer complexes of lignocaine are of interest because of their role in medical applications. Lignocaine hydrochloride is the most common and important local anesthetic and antiarrhythmic drug. In addition to that they are also good organic semi-conductors.[1] We have undertaken the study of a series of complexes of lignocaine hydrochloride with various metals.[2–7] The results of the crystal structure analysis of the complex of lignocaine hydrochloride with zinc chloride are reported.

EXPERIMENTAL

Single crystals suitable for x-ray diffraction studies were obtained by slow evaporation in a mixture of ethanol and water. Cell dimensions were obtained from 25 reflections in the range $40° \leq 2\theta \leq 50°$. The crystal data are as follows: transparent single crystal of dimension 0.625 × 1.0 × 2.0 mm, monoclinic, $P2_1$, a = 9.128(2) Å, b = 19.196(5) Å, c = 19.696(5) Å, β = 95.81(1)°, V = 3433.43(1) Å^3, Z = 4, D_c = 1.308 Mg·m^{-3}, μ = 4.17 mm^{-1}, T = 293 K, FW = 675.87, F_{000} = 1415.76.

The data were collected on an Enraf Nonius diffractometer within the range $2° \leq 2\theta \leq 110°$ in $\omega - 2\theta$ mode of scanning using CuK_α radiation. 4010 counter intensities were obtained out of which 3527 intensities were greater than $2.5\sigma(I)$. Lorentz and polarization corrections were applied. Empirical absorption correction[8] was also applied. The minimum and maximum transmission factors are 0.669 and 0.997, respectively. The structure was solved by direct methods (MULTAN80)[9] and refined by block diagonal least-squares method (LSTSQ-NRCVAX).[10] The coordinates of the hydrogen atoms were generated using CDEDIT-NRCVAX.[10] These were placed at a distance of 1.08 Å from the parent atom and refined isotropically as riding with those of the atoms to which they are bonded. The final least-squares cycle was run for 166 atoms, 1055 parameters and 3523 reflections. The final residuals are $R_f = 0.071$, $R_w = 0.056$ where

$$R_f = \frac{\sum||F_o| - |F_c||}{\sum|F_o|}$$

and

$$R_w = \left[\frac{\sum w(|F_o| - |F_c|)^2}{\sum wF_o^2}\right]^{1/2}$$

The maximum value of $|\Delta|/\sigma = 0.652$. The goodness-of-fit indicator is 4.13. Extinction coefficient[11] was also refined and secondary extinction coefficient = 0.0255, $\sigma = 0.0115$. In the last difference Fourier map, the deepest hole was $-0.48\ eA^{-3}$ and the highest peak $0.54\ eA^{-3}$. All the computational work was carried out on a Zenith 386SX/387SX IBM compatible PC using NRCVAX SDP.

RESULTS AND DISCUSSION

The positional coordinates of the atoms, thermal parameters for the non-hydrogens, bond distances and angles are given in Tables I to IV, respectively. The bond lengths and angles are in good agreement with the standard values. The projection of the molecule on the plane with least overlap is shown in Figure 1. The atoms C1, C2, C3, C5, C6 & C8, C15, C16, C17, C19, C20 & C22, C29, C30, C31, C33, C34 & C36 and C43, C44, C45, C47, C48 & C50 constitute the four phenyl rings 1 to 4, respectively. The dihedral angles between the planes through phenyl rings 1 and 2 is 4.5(8)°, 1 and 3 is 73.9(7)°, 1 and 4 is 76.4(7)°, 2 and 3 is 78.0(7)°, 2 and 4 is 80.4(7)° and 3 and 4 is 2.5(7)°. The complex shows hydrogen bonding of the

TABLE I

Fractional atomic coordinates of the nonhydrogens. Quantities in the parentheses are respective e.s.d's.

Atom	x	y	z	Biso(A)²
MOLECULE A				
ZN1	.4238(2)	.6521(Ø)	.4530(1)	5.2(1)
CL1	.3531(7)	.7353(3)	.3738(3)	8.5(4)
CL2	.6420(5)	.6974(3)	.5032(2)	6.1(3)
CL3	.2730(5)	.6391(3)	.5360(2)	5.7(2)
CL4	.4467(7)	.5549(3)	.3926(3)	7.1(3)
C 1	.837(3)	.608(1)	.665(1)	13.9(2)
C 2	.683(3)	.601(1)	.675(1)	10.3(2)
C 3	.635(2)	.588(1)	.737(1)	9.Ø(1)
C 4	.483(3)	.583(1)	.750(1)	12.5(2)
C 5	.747(2)	.583(1)	.790(1)	6.2(1)
C 6	.891(2)	.590(1)	.787(1)	9.3(2)
C 7	.997(3)	.590(1)	.845(1)	14.1(2)
C 8	.941(3)	.602(1)	.720(1)	10.6(2)
N 1	.695(2)	.577(1)	.855(1)	8.1(1)
C 9	.639(2)	.517(1)	.881(1)	8.3(1)
O 1	.633(1)	.454(1)	.853(1)	8.Ø(8)
C10	.587(2)	.519(1)	.958(1)	8.4(1)
N 2	.482(2)	.461(1)	.961(1)	12.4(1)
C11	.325(2)	.490(1)	.916(1)	11.5(2)
C12	.235(3)	.436(1)	.923(2)	15.6(2)
C13	.506(3)	.427(1)	.999(2)	18.6(2)
C14	.630(2)	.388(1)	1.Ø39(1)	6.6(1)
C15	.260(3)	.750(1)	.832(1)	10.Ø(2)
C16	.138(3)	.756(1)	.783(1)	12.Ø(2)
C17	.171(2)	.766(1)	.715(1)	7.5(1)
C18	.Ø30(2)	.779(1)	.661(1)	9.6(2)
C19	.314(2)	.769(1)	.697(1)	7.1(1)
C20	.441(2)	.762(1)	.754(1)	10.6(2)
C21	.595(3)	.767(1)	.727(1)	11.5(2)
C22	.412(2)	.752(1)	.815(1)	9.1(1)
N 3	.339(2)	.782(1)	.628(1)	5.8(8)
C23	.367(2)	.843(1)	.607(1)	4.9(9)
O 2	.367(1)	.893(1)	.644(1)	7.2(7)
C24	.396(2)	.850(1)	.537(1)	6.5(1)
N 4	.464(1)	.914(1)	.523(1)	7.5(1)
C25	.403(2)	.939(1)	.444(1)	13.6(2)
C26	.378(2)	.928(1)	.391(1)	7.Ø(1)
C27	.630(2)	.917(1)	.504(1)	5.9(1)
C28	.715(2)	.888(1)	.576(1)	9.7(2)
MOLECULE B				
ZN2	.5756(3)	.6957(1)	.Ø462(1)	5.6(1)
CL5	.3527(5)	.6584(3)	-.ØØ23(2)	5.9(3)
CL6	.6691(6)	.6175(3)	.1243(3)	7.6(3)
CL7	.5199(7)	.7962(3)	.Ø971(3)	8.7(3)
CL8	.7267(5)	.7105(3)	-.Ø356(2)	5.9(2)
C29	.897(2)	.966(1)	.390(1)	9.5(1)
C30	.785(2)	.950(1)	.339(1)	9.Ø(1)
C31	.740(2)	.879(1)	.328(1)	4.4(8)
C32	.643(2)	.855(1)	.273(1)	8.4(1)
C33	.811(2)	.830(1)	.371(1)	4.1(8)
C34	.924(2)	.846(1)	.421(1)	5.4(9)
C35	1.ØØØ(2)	.792(1)	.462(1)	5.6(1)
C36	.962(2)	.917(1)	.429(1)	6.Ø(1)

.....continued

TABLE I (*Continued*)

Atom	x	y	z	Biso(Å)²
MOLECULE B				
N 5	.775(1)	.757(1)	.365(1)	3.7(6)
C37	.820(1)	.715(1)	.321(1)	2.8(7)
O 3	.915(1)	.732(1)	.287(1)	5.6(6)
C38	.762(1)	.643(1)	.317(1)	3.8(7)
N 6	.871(1)	.595(1)	.300(1)	3.9(6)
C39	.987(2)	.587(1)	.361(1)	5.8(1)
C40	.948(3)	.552(1)	.429(1)	8.5(1)
C41	.802(2)	.522(1)	.285(1)	4.9(9)
C42	.899(2)	.466(1)	.256(1)	6.4(1)
C43	.111(2)	.388(1)	.096(1)	7.7(1)
C44	.046(2)	.441(1)	.060(1)	8.5(1)
C45	.084(2)	.507(1)	.073(1)	6.1(1)
C46	.001(2)	.568(1)	.029(1)	9.6(2)
C47	.193(2)	.523(1)	.123(1)	5.4(1)
C48	.263(2)	.469(1)	.165(1)	7.5(1)
C49	.392(2)	.483(1)	.222(1)	8.1(1)
C50	.219(2)	.402(1)	.150(1)	8.0(1)
N 7	.252(1)	.592(1)	.140(1)	3.9(6)
C51	.184(2)	.632(1)	.184(1)	6.1(1)
O 4	.079(1)	.615(1)	.219(1)	5.3(6)
C52	.256(2)	.704(1)	.192(1)	5.1(9)
N 8	.122(1)	.759(1)	.196(1)	4.6(7)
C53	.003(2)	.765(1)	.137(1)	6.3(1)
C54	.072(2)	.787(1)	.078(1)	8.0(1)
C55	.203(2)	.825(1)	.224(1)	5.8(1)
C56	.080(2)	.878(1)	.231(1)	8.6(1)

TABLE II

Fractional atomic coordinates of the hydrogens. Quantities in the parentheses are respective e.s.d's.

Atom	x	y	z	Biso(Å)²
MOLECULE A				
H1	0.881(2)	0.607(1)	0.613(9)	13.7(7)
H2	0.609(1)	0.609(7)	0.631(7)	7.6(5)
H4A	0.434(2)	0.576(9)	0.801(8)	11.8(6)
H4B	0.426(2)	0.626(8)	0.733(8)	11.8(6)
H4C	0.419(2)	0.544(9)	0.726(8)	14.9(7)
H7A	1.102(2)	0.589(1)	0.817(1)	22.1(9)
H7B	0.996(1)	0.636(7)	0.869(6)	5.1(4)
H7C	0.995(2)	0.543(9)	0.868(8)	14.2(7)
HN1	1.046(2)	0.607(8)	0.722(8)	11.1(6)
H10	0.710(2)	0.622(8)	0.885(8)	11.2(6)
H10A	0.514(2)	0.574(8)	0.967(7)	10.3(5)
H10B	0.673(2)	0.512(8)	0.999(8)	9.7(5)
H11A	0.338(2)	0.505(8)	0.854(7)	8.5(5)
H11B	0.274(2)	0.551(8)	0.940(8)	11.7(6)
H12A	0.109(2)	0.447(9)	0.884(8)	13.0(6)
H12B	0.278(2)	0.386(9)	0.899(9)	14.9(7)
H12C	0.235(2)	0.426(1)	0.994(9)	15.7(7)
H13A	0.419(2)	0.436(9)	1.032(8)	11.2(6)

TABLE II (*Continued*)

Atom	x	y	z	Biso(A)*
MOLECULE A				
H13B	Ø.484(2)	Ø.375(1)	Ø.961(1)	23.7(9)
H14A	Ø.588(2)	Ø.354(8)	1.Ø59(7)	9.6(6)
H14B	Ø.732(2)	Ø.386(8)	1.ØØØ(7)	11.2(5)
H14C	Ø.662(1)	Ø.425(5)	1.Ø9Ø(4)	Ø.3(2)
H15	Ø.24Ø(2)	Ø.749(1)	Ø.87Ø(8)	15.Ø(7)
H16	Ø.Ø46(2)	Ø.753(8)	Ø.798(7)	8.Ø(5)
H18A	Ø.Ø44(2)	Ø.786(8)	Ø.625(7)	9.1(5)
H18B	-Ø.Ø38(2)	Ø.74Ø(9)	Ø.661(7)	11.1(6)
H18C	-Ø.Ø34(2)	Ø.829(8)	Ø.683(7)	8.6(5)
H21A	Ø.659(1)	Ø.757(8)	Ø.769(7)	8.1(5)
H21B	Ø.61Ø(2)	Ø.734(8)	Ø.696(7)	9.8(5)
H21C	Ø.63Ø(1)	Ø.818(7)	Ø.713(7)	7.3(4)
H22	Ø.486(1)	Ø.746(7)	Ø.85Ø(6)	6.7(4)
HN3	Ø.329(1)	Ø.744(7)	Ø.598(6)	6.9(4)
H24A	Ø.465(2)	Ø.816(7)	Ø.528(7)	7.5(4)
H24B	Ø.249(2)	Ø.852(8)	Ø.5Ø6(7)	9.7(5)
H25A	Ø.461(2)	Ø.976(9)	Ø.441(8)	15.2(7)
H25B	Ø.275(2)	Ø.958(8)	Ø.465(7)	9.4(5)
H26A	Ø.329(1)	Ø.96Ø(6)	Ø.358(6)	4.Ø(3)
H26B	Ø.465(1)	Ø.912(7)	Ø.371(6)	7.Ø(4)
H26C	Ø.289(2)	Ø.882(8)	Ø.39Ø(7)	11.Ø(5)
H27A	Ø.65Ø(1)	Ø.881(7)	Ø.454(7)	8.2(4)
H27B	Ø.669(1)	Ø.975(7)	Ø.492(6)	6.7(4)
H28A	Ø.848(2)	Ø.888(8)	Ø.565(7)	9.1(5)
H28B	Ø.691(2)	Ø.926(9)	Ø.624(8)	1Ø.7(6)
H28C	Ø.673(2)	Ø.848(1)	Ø.588(9)	13.7(7)
MOLECULE B				
H29	Ø.925(2)	1.ØØ6(9)	Ø.4ØØ(8)	11.4(6)
H3Ø	Ø.736(2)	Ø.983(8)	Ø.3Ø6(7)	9.Ø(5)
H32A	Ø.62Ø(1)	Ø.8Ø6(7)	Ø.266(7)	7.3(4)
H32B	Ø.57Ø(1)	Ø.876(6)	Ø.276(6)	2.9(3)
H32C	Ø.669(2)	Ø.861(8)	Ø.23Ø(8)	12.3(6)
H35A	1.Ø79(1)	Ø.82Ø(6)	Ø.49Ø(6)	4.1(3)
H35B	Ø.916(1)	Ø.754(7)	Ø.479(6)	6.6(4)
H35C	1.Ø78(1)	Ø.755(7)	Ø.436(6)	5.1(4)
H36	1.Ø5Ø(1)	Ø.922(7)	Ø.46Ø(6)	7.2(4)
HN5	Ø.734(1)	Ø.735(6)	Ø.4Ø3(6)	4.7(4)
H38A	Ø.686(1)	Ø.643(6)	Ø.29Ø(6)	4.Ø(3)
H38B	Ø.726(1)	Ø.631(6)	Ø.366(5)	3.Ø(3)
H39A	1.Ø26(2)	Ø.628(8)	Ø.37Ø(7)	9.5(5)
H39B	1.Ø8Ø(1)	Ø.561(6)	Ø.351(5)	3.Ø(3)
H4ØA	1.Ø5Ø(2)	Ø.558(9)	Ø.463(8)	13.1(6)
H4ØB	Ø.84Ø(2)	Ø.578(7)	Ø.451(7)	7.7(4)
H4ØC	Ø.918(2)	Ø.518(8)	Ø.423(7)	8.2(5)
H41A	Ø.77Ø(1)	Ø.51Ø(6)	Ø.326(6)	4.9(4)
H41B	Ø.7Ø9(1)	Ø.529(6)	Ø.257(6)	3.5(3)
H42A	Ø.862(1)	Ø.432(7)	Ø.247(6)	5.5(4)
H42B	Ø.941(1)	Ø.487(6)	Ø.213(6)	5.5(4)
H42C	Ø.995(1)	Ø.462(6)	Ø.287(6)	4.5(3)
H43	Ø.Ø73(2)	Ø.342(8)	Ø.Ø84(7)	8.9(5)
H44	-Ø.Ø77(2)	Ø.435(8)	Ø.Ø18(7)	9.7(5)
H46A	Ø.Ø61(2)	Ø.615(9)	Ø.Ø35(8)	13.2(6)
H46B	Ø.Ø34(2)	Ø.556(9)	-Ø.Ø13(8)	11.9(6)
H46C	-Ø.118(2)	Ø.575(9)	Ø.Ø4Ø(8)	12.1(6)
H49A	Ø.4Ø5(2)	Ø.43Ø(9)	Ø.251(8)	12.7(6)
H49B	Ø.48Ø(2)	Ø.514(8)	Ø.194(8)	11.7(5)

.....continued

TABLE II (*Continued*)

Atom	x	y	z	Biso(A)*
MOLECULE B				
H49C	Ø.367(2)	Ø.522(7)	Ø.264(7)	8.7(5)
H5Ø	Ø.267(2)	Ø.375(9)	Ø.183(8)	13.6(6)
HN7	Ø.331(1)	Ø.6Ø6(7)	Ø.13Ø(7)	7.6(5)
H52A	Ø.348(1)	Ø.7Ø4(7)	Ø.24Ø(7)	7.7(4)
H52B	Ø.313(1)	Ø.719(6)	Ø.154(6)	5.3(4)
H53A	-Ø.Ø8Ø(1)	Ø.8Ø2(6)	Ø.143(6)	5.3(4)
H53B	-Ø.Ø6Ø(2)	Ø.729(8)	Ø.13Ø(7)	1Ø.2(5)
H54A	-Ø.Ø05(2)	Ø.79Ø(8)	Ø.Ø45(7)	9.3(5)
H54B	Ø.115(2)	Ø.825(8)	Ø.Ø84(7)	8.7(5)
H54C	Ø.178(1)	Ø.748(8)	Ø.Ø6Ø(7)	7.9(4)
H55A	Ø.261(2)	Ø.817(9)	Ø.274(8)	14.Ø(6)
H55B	Ø.262(1)	Ø.833(7)	Ø.188(6)	5.3(4)
H56A	Ø.Ø92(2)	Ø.918(9)	Ø.258(8)	11.Ø(6)
H56B	Ø.Ø11(2)	Ø.893(8)	Ø.188(8)	11.Ø(6)
H56C	Ø.Ø14(1)	Ø.865(7)	Ø.27Ø(7)	7.2(4)

(Hydrogen atoms have been labelled with the number of the atom to which they are bonded. Multiple atoms have an additional suffix).

TABLE III

$u(i, j)$ of U values *100 of the hydrogens. Quantities in the parentheses are respective e.s.d's.

Atom	u11(U)	u22	u33	u12	u13	u23
MOLECULE A						
ZN1	8.6(2)	5.5(1)	5.8(1)	-Ø.4(1)	1.2(1)	-Ø.1(1)
CL1	14.3(6)	9.8(5)	7.4(4)	Ø.8(4)	-1.8(4)	3.1(3)
CL2	6.3(3)	9.7(4)	7.2(3)	-1.2(3)	-Ø.1(3)	Ø.5(3)
CL3	7.7(3)	7.5(3)	6.5(3)	-2.Ø(3)	1.9(3)	-Ø.9(3)
CL4	13.8(5)	5.6(3)	7.7(4)	Ø.1(3)	2.3(3)	-1.7(3)
C 1	32.5(4)	8.9(2)	11.Ø(2)	3.4(2)	Ø.4(2)	-3.6(2)
C 2	18.5(3)	7.Ø(2)	12.5(2)	-Ø.9(2)	-3.8(2)	-1.1(2)
C 3	18.2(2)	4.4(1)	1Ø.8(2)	3.Ø(2)	-2.9(2)	-Ø.8(1)
C 4	21.1(3)	5.2(2)	19.3(3)	-2.4(2)	-6.8(2)	1.1(2)
C 5	13.3(2)	5.3(1)	4.9(1)	Ø.8(1)	Ø.8(1)	-Ø.5(1)
C 6	13.7(2)	9.3(2)	12.Ø(2)	1.7(2)	Ø.8(2)	1.1(2)
C 7	17.4(3)	19.2(3)	16.5(2)	3.5(2)	-Ø.4(2)	13.7(2)
C 8	17.Ø(2)	16.4(2)	7.2(2)	3.6(2)	3.1(2)	2.5(2)
N 1	11.6(2)	6.9(1)	12.2(2)	Ø.1(1)	1.3(1)	-4.3(1)
C 9	8.5(2)	18.4(2)	4.5(1)	2.7(2)	-Ø.6(1)	-4.4(1)
O 1	15.Ø(1)	5.8(8)	1Ø.7(1)	Ø.1(9)	6.2(1)	-3.9(8)
C1Ø	7.9(2)	9.4(2)	14.6(2)	-3.7(1)	1.4(1)	-6.2(2)
N 2	17.1(2)	15.2(2)	14.3(2)	5.4(2)	-1.9(2)	-4.2(2)
C11	11.7(2)	17.7(3)	13.2(2)	4.1(2)	-3.1(2)	-3.4(2)
C12	2Ø.6(3)	1Ø.1(2)	3Ø.3(4)	5.6(2)	11.9(3)	4.7(2)
C13	21.5(3)	5.3(1)	4Ø.8(4)	-4.4(2)	-12.2(3)	13.1(2)
C14	5.1(1)	9.1(2)	1Ø.9(2)	3.5(1)	1.Ø(1)	5.2(1)
C15	27.3(3)	6.5(2)	4.2(1)	2.1(2)	1.8(2)	1.3(1)
C16	25.6(3)	7.5(2)	12.8(2)	3.3(2)	3.7(2)	-Ø.8(2)
C17	16.8(2)	5.5(1)	6.1(1)	1.Ø(1)	1.1(1)	2.Ø(1)
C18	14.1(2)	13.7(2)	8.4(2)	-1.6(2)	-Ø.4(2)	2.1(2)
C19	12.5(2)	4.6(1)	9.7(2)	1.8(1)	Ø.1(1)	-Ø.6(1)

TABLE III (*Continued*)

Atom	u11(U)	u22	u33	u12	u13	u23
MOLECULE A						
C2Ø	15.6(2)	7.6(2)	17.8(3)	-Ø.8(2)	4.5(2)	-1.8(2)
C21	18.3(2)	8.5(2)	15.2(2)	2.2(2)	-6.6(2)	Ø.Ø(2)
C22	2Ø.8(2)	7.4(2)	5.5(1)	1.7(2)	-3.1(2)	Ø.4(1)
N 3	11.3(1)	5.2(1)	5.2(9)	Ø.1(9)	-1.6(9)	-1.9(8)
C23	5.9(1)	3.3(1)	9.Ø(1)	Ø.2(9)	-Ø.5(1)	-2.4(1)
O 2	1Ø.4(1)	6.3(9)	1Ø.3(1)	Ø.8(8)	Ø.2(9)	-2.4(8)
C24	1Ø.3(2)	6.4(1)	7.7(1)	-Ø.9(1)	Ø.6(1)	-5.5(1)
N 4	5.3(1)	13.1(2)	1Ø.7(1)	-3.1(1)	4.3(9)	-6.4(1)
C25	1Ø.9(2)	17.6(3)	22.6(3)	-4.7(2)	-2.Ø(2)	9.9(2)
C26	12.8(2)	8.4(2)	4.9(1)	2.1(1)	-1.6(1)	-2.Ø(1)
C27	5.2(1)	9.4(2)	8.2(1)	2.7(1)	3.6(1)	1.5(1)
C28	13.1(2)	6.4(2)	18.5(3)	Ø.4(2)	7.6(2)	2.7(2)
MOLECULE B						
ZN2	9.1(2)	6.1(2)	6.2(1)	-Ø.1(1)	1.1(1)	-Ø.2(1)
CL5	6.8(3)	1Ø.Ø(4)	5.4(3)	-1.9(3)	Ø.3(2)	1.1(3)
CL6	13.6(5)	8.6(4)	6.4(3)	1.3(4)	-Ø.6(3)	3.6(3)
CL7	15.9(6)	5.2(3)	13.3(5)	-2.2(4)	8.4(4)	-3.5(3)
CL8	7.8(4)	8.3(4)	6.7(3)	-2.1(3)	2.9(3)	-Ø.9(3)
C29	15.6(2)	6.4(2)	15.1(2)	-4.9(2)	7.1(2)	-1.9(2)
C3Ø	11.1(2)	6.5(1)	17.6(2)	1.3(1)	5.9(2)	3.1(2)
C31	5.4(1)	5.7(1)	5.7(1)	Ø.7(9)	1.4(9)	1.9(9)
C32	11.3(2)	1Ø.Ø(2)	11.Ø(2)	4.7(2)	2.3(1)	6.7(2)
C33	6.8(1)	3.7(1)	5.7(1)	-2.2(9)	3.Ø(9)	-1.2(9)
C34	4.1(1)	8.5(1)	8.4(1)	Ø.4(1)	3.1(1)	-1.8(1)
C35	6.3(1)	9.9(2)	4.6(1)	Ø.1(1)	-Ø.9(9)	-Ø.8(1)
C36	7.3(1)	6.6(1)	9.1(2)	-2.2(1)	Ø.8(1)	-3.4(1)
N 5	3.6(8)	5.1(8)	5.5(9)	-Ø.8(7)	1.1(6)	-Ø.8(7)
C37	3.2(9)	4.Ø(9)	3.6(9)	-Ø.9(7)	Ø.8(7)	Ø.Ø(7)
O 3	9.6(1)	4.8(7)	7.5(9)	-1.3(7)	3.7(7)	-1.3(7)
C38	3.2(9)	5.3(1)	5.9(1)	-Ø.5(8)	-Ø.2(8)	1.4(9)
N 6	5.3(9)	3.8(8)	5.2(8)	-Ø.2(7)	-1.2(7)	-Ø.4(7)
C39	6.5(1)	3.9(1)	11.9(2)	Ø.5(1)	2.9(1)	Ø.6(1)
C4Ø	18.1(2)	1Ø.1(2)	3.5(1)	-Ø.9(2)	-1.3(1)	2.4(1)
C41	9.1(1)	4.8(1)	4.9(1)	-1.7(1)	1.7(1)	Ø.4(9)
C42	9.Ø(2)	4.4(1)	11.1(2)	2.Ø(1)	2.4(1)	-1.3(1)
C43	1Ø.1(2)	6.6(1)	12.3(2)	-Ø.3(1)	-Ø.6(1)	-1.1(1)
C44	1Ø.1(2)	1Ø.1(2)	12.2(2)	-2.1(2)	2.2(2)	-1.9(2)
C45	9.9(2)	4.9(1)	8.9(2)	-2.8(1)	2.6(1)	-1.4(1)
C46	1Ø.7(2)	1Ø.1(2)	15.Ø(2)	-Ø.9(2)	-2.2(2)	3.3(2)
C47	6.8(1)	9.Ø(2)	5.Ø(1)	1.6(1)	1.Ø(1)	-Ø.6(1)
C48	14.1(2)	8.2(2)	6.3(1)	-Ø.2(2)	Ø.8(1)	-2.1(1)
C49	1Ø.6(2)	11.9(2)	7.3(2)	5.5(2)	-2.8(1)	-1.2(1)
C5Ø	13.1(2)	5.9(1)	11.2(2)	2.5(1)	-Ø.1(2)	2.4(1)
N 7	6.2(9)	4.3(8)	4.8(8)	Ø.8(7)	3.Ø(7)	-Ø.1(7)
C51	12.6(2)	4.2(1)	6.Ø(1)	Ø.9(1)	-Ø.1(1)	Ø.8(1)
O 4	8.7(9)	3.8(7)	8.4(9)	-Ø.1(7)	3.8(7)	-Ø.1(6)
C52	7.1(1)	6.5(1)	6.2(1)	-Ø.3(1)	2.4(1)	-2.8(1)
N 8	8.7(1)	3.1(8)	5.9(9)	-Ø.4(8)	1.8(8)	Ø.1(7)
C53	1Ø.9(2)	7.1(1)	5.6(1)	-1.6(1)	-Ø.4(1)	-Ø.2(1)
C54	9.9(2)	8.Ø(2)	11.4(2)	Ø.5(1)	-4.7(1)	Ø.9(1)
C55	7.2(1)	5.1(1)	9.7(2)	-1.6(1)	Ø.3(1)	-Ø.2(1)
C56	17.Ø(2)	5.1(1)	11.3(2)	-5.4(2)	4.7(2)	-2.2(1)

TABLE IV

Bond lengths (Å) and bond angles (°) involving non-hydrogens. Quantities in the parentheses are respective e.s.d's.

MOLECULE A		MOLECULE B	
ZN(1)-CL(1)	2.28Ø(5)	ZN(2)-CL(5)	2.274(5)
ZN(1)-CL(2)	2.3Ø3(5)	ZN(2)-CL(6)	2.254(5)
ZN(1)-CL(3)	2.254(5)	ZN(2)-CL(7)	2.257(5)
ZN(1)-CL(4)	2.234(5)	ZN(2)-CL(8)	2.243(5)
C(1)-C(2)	1.44(4)	C(29)-C(3Ø)	1.39(3)
C(1)-C(8)	1.38(3)	C(29)-C(36)	1.32(3)
C(2)-C(3)	1.36(3)	C(3Ø)-C(31)	1.43(3)
C(3)-C(4)	1.44(4)	C(31)-C(32)	1.4Ø(3)
C(3)-C(5)	1.4Ø(3)	C(31)-C(33)	1.38(2)
C(5)-C(6)	1.33(3)	C(33)-C(34)	1.39(2)
C(5)-N(1)	1.4Ø(2)	C(33)-N(5)	1.44(2)
C(6)-C(7)	1.42(3)	C(34)-C(35)	1.45(3)
C(6)-C(8)	1.44(3)	C(34)-C(36)	1.4Ø(2)
N(1)-C(9)	1.38(3)	N(5)-C(37)	1.27(2)
C(9)-O(1)	1.32(2)	C(37)-O(3)	1.2Ø(2)
C(9)-C(1Ø)	1.65(3)	C(37)-C(38)	1.46(2)
C(1Ø)-N(2)	1.48(3)	C(38)-N(6)	1.43(2)
N(2)-C(11)	1.7Ø(3)	N(6)-C(39)	1.54(2)
N(2)-C(13)	1.ØØ(3)	N(6)-C(41)	1.55(2)
C(11)-C(12)	1.33(4)	C(39)-C(4Ø)	1.58(3)
C(13)-C(14)	1.51(3)	C(41)-C(42)	1.53(2)
C(15)-C(16)	1.41(3)	C(43)-C(44)	1.35(3)
C(15)-C(22)	1.45(3)	C(43)-C(5Ø)	1.4Ø(3)
C(16)-C(17)	1.42(3)	C(44)-C(45)	1.33(3)
C(17)-C(18)	1.6Ø(3)	C(45)-C(46)	1.59(3)
C(17)-C(19)	1.38(3)	C(45)-C(47)	1.36(3)
C(19)-C(2Ø)	1.54(3)	C(47)-C(48)	1.43(3)
C(19)-N(3)	1.42(2)	C(47)-N(7)	1.46(2)
C(2Ø)-C(21)	1.56(3)	C(48)-C(49)	1.57(3)
C(2Ø)-C(22)	1.28(3)	C(48)-C(5Ø)	1.37(3)
N(3)-C(23)	1.29(2)	N(7)-C(51)	1.35(2)
C(23)-O(2)	1.2Ø(2)	C(51)-O(4)	1.28(2)
C(23)-C(24)	1.42(3)	C(51)-C(52)	1.54(2)
C(24)-N(4)	1.42(2)	C(52)-N(8)	1.62(2)
N(4)-C(25)	1.68(3)	N(8)-C(53)	1.51(2)
N(4)-C(27)	1.6Ø(2)	N(8)-C(55)	1.54(2)
C(25)-C(26)	1.Ø8(3)	C(53)-C(54)	1.44(3)
C(27)-C(28)	1.64(3)	C(55)-C(56)	1.54(3)
CL(1)-ZN(1)-CL(2)	1Ø1.64(2)	CL(5)-ZN(2)-CL(6)	1Ø9.79(2)
CL(1)-ZN(1)-CL(3)	115.ØØ(2)	CL(5)-ZN(2)-CL(7)	1Ø2.89(2)
CL(1)-ZN(1)-CL(4)	1Ø4.85(2)	CL(5)-ZN(2)-CL(8)	1Ø9.1Ø(2)
CL(2)-ZN(1)-CL(3)	1Ø7.2Ø(2)	CL(6)-ZN(2)-CL(7)	11Ø.64(2)
CL(2)-ZN(1)-CL(4)	114.84(2)	CL(6)-ZN(2)-CL(8)	11Ø.93(2)
CL(3)-ZN(1)-CL(4)	112.97(2)	CL(7)-ZN(2)-CL(8)	113.17(2)
C(2)-C(1)-C(8)	119.Ø(2)	C(3Ø)-C(29)-C(36)	121.4(2)
C(1)-C(2)-C(3)	123.1(2)	C(29)-C(3Ø)-C(31)	12Ø.Ø(2)
C(2)-C(3)-C(4)	125.3(2)	C(3Ø)-C(31)-C(32)	125.5(2)
C(2)-C(3)-C(5)	114.6(2)	C(3Ø)-C(31)-C(33)	116.3(2)
C(4)-C(3)-C(5)	12Ø.Ø(2)	C(32)-C(31)-C(33)	117.7(2)
C(3)-C(5)-C(6)	126.7(2)	C(31)-C(33)-C(34)	123.Ø(1)
C(3)-C(5)-N(1)	114.Ø(2)	C(31)-C(33)-N(5)	121.8(1)
C(6)-C(5)-N(1)	119.Ø(2)	C(34)-C(33)-N(5)	115.1(1)
C(5)-C(6)-C(7)	123.2(2)	C(33)-C(34)-C(35)	12Ø.6(2)
C(5)-C(6)-C(8)	118.2(2)	C(33)-C(34)-C(36)	117.6(2)
C(7)-C(6)-C(8)	118.5(2)	C(35)-C(34)-C(36)	121.8(2)
C(1)-C(8)-C(6)	118.4(2)	C(29)-C(36)-C(34)	121.6(2)
C(5)-N(1)-C(9)	124.6(1)	C(33)-N(5)-C(37)	125.7(1)

TABLE IV (*Continued*)

MOLECULE A		MOLECULE B	
N(1)-C(9)-O(1)	128.2(2)	N(5)-C(37)-O(3)	120.7(1)
N(1)-C(9)-C(10)	118.1(2)	N(5)-C(37)-C(38)	119.3(1)
O(1)-C(9)-C(10)	113.3(2)	O(3)-C(37)-C(38)	119.9(1)
C(9)-C(10)-N(2)	105.1(2)	C(37)-C(38)-N(6)	111.6(1)
C(10)-N(2)-C(11)	104.3(2)	C(38)-N(6)-C(39)	108.3(1)
C(10)-N(2)-C(13)	115.2(2)	C(38)-N(6)-C(41)	111.0(1)
C(11)-N(2)-C(13)	135(3)	C(39)-N(6)-C(41)	107.6(1)
N(2)-C(11)-C(12)	100.7(2)	N(6)-C(39)-C(40)	120.7(1)
N(2)-C(13)-C(14)	143(3)	N(6)-C(41)-C(42)	117.5(1)
C(16)-C(15)-C(22)	123.6(2)	C(44)-C(43)-C(50)	120.0(2)
C(15)-C(16)-C(17)	115.2(2)	C(43)-C(44)-C(45)	121.6(2)
C(16)-C(17)-C(18)	114.5(2)	C(44)-C(45)-C(46)	119.3(2)
C(16)-C(17)-C(19)	123.2(2)	C(44)-C(45)-C(47)	120.6(2)
C(18)-C(17)-C(19)	122.2(2)	C(46)-C(45)-C(47)	120.1(2)
C(17)-C(19)-C(20)	117.8(2)	C(45)-C(47)-C(48)	120.1(2)
C(17)-C(19)-N(3)	120.3(2)	C(45)-C(47)-N(7)	126.3(2)
C(20)-C(19)-N(3)	121.8(2)	C(48)-C(47)-N(7)	113.6(1)
C(19)-C(20)-C(21)	112.5(2)	C(47)-C(48)-C(49)	122.9(2)
C(19)-C(20)-C(22)	119.4(2)	C(47)-C(48)-C(50)	117.5(2)
C(21)-C(20)-C(22)	128.0(2)	C(49)-C(48)-C(50)	119.5(2)
C(15)-C(22)-C(20)	120.7(2)	C(43)-C(50)-C(48)	120.1(2)
C(19)-N(3)-C(23)	121.8(1)	C(47)-N(7)-C(51)	118.9(1)
N(3)-C(23)-O(2)	120.8(2)	N(7)-C(51)-O(4)	127.9(2)
N(3)-C(23)-C(24)	117.0(1)	N(7)-C(51)-C(52)	110.8(1)
O(2)-C(23)-C(24)	122.2(2)	O(4)-C(51)-C(52)	121.2(1)
C(23)-C(24)-N(4)	112.8(1)	C(51)-C(52)-N(8)	105.7(1)
C(24)-N(4)-C(25)	108.9(1)	C(52)-N(8)-C(53)	119.2(1)
C(24)-N(4)-C(27)	121.0(1)	C(52)-N(8)-C(55)	102.5(1)
C(25)-N(4)-C(27)	90.5(1)	C(53)-N(8)-C(55)	119.6(1)
N(4)-C(25)-C(26)	150(3)	N(8)-C(53)-C(54)	107.5(1)
N(4)-C(27)-C(28)	99.6(1)	N(8)-C(55)-C(56)	104.5(1)

type NH . . CL with the following bond distances between N—H and H—CL and the angle N—H—CL:

N3—HN3 . . . CL3: 0.93(14) Å, 2.39(14) Å, 168.84(3)°

N5—HN5 . . . CL2: 0.96(11) Å, 2.35(11) Å, 171.95(11)°

N7—HN7 . . . CL5: 0.81(13) Å, 2.82(14) Å, 118.62(5)°

It can be seen that the planes of the phenyl groups of one of the pair are nearly perpendicular to the planes of the phenyl groups of the other. In the complex, each zinc chloride molecule is associated with two lignocaine molecules through hydrogen bonds. The packing of the molecules down **a** axis is shown in Figure 2. A herringbone packing is observed parallel to **c** axis and the stacks appear parallel to the **b** axis when viewed down **a**.

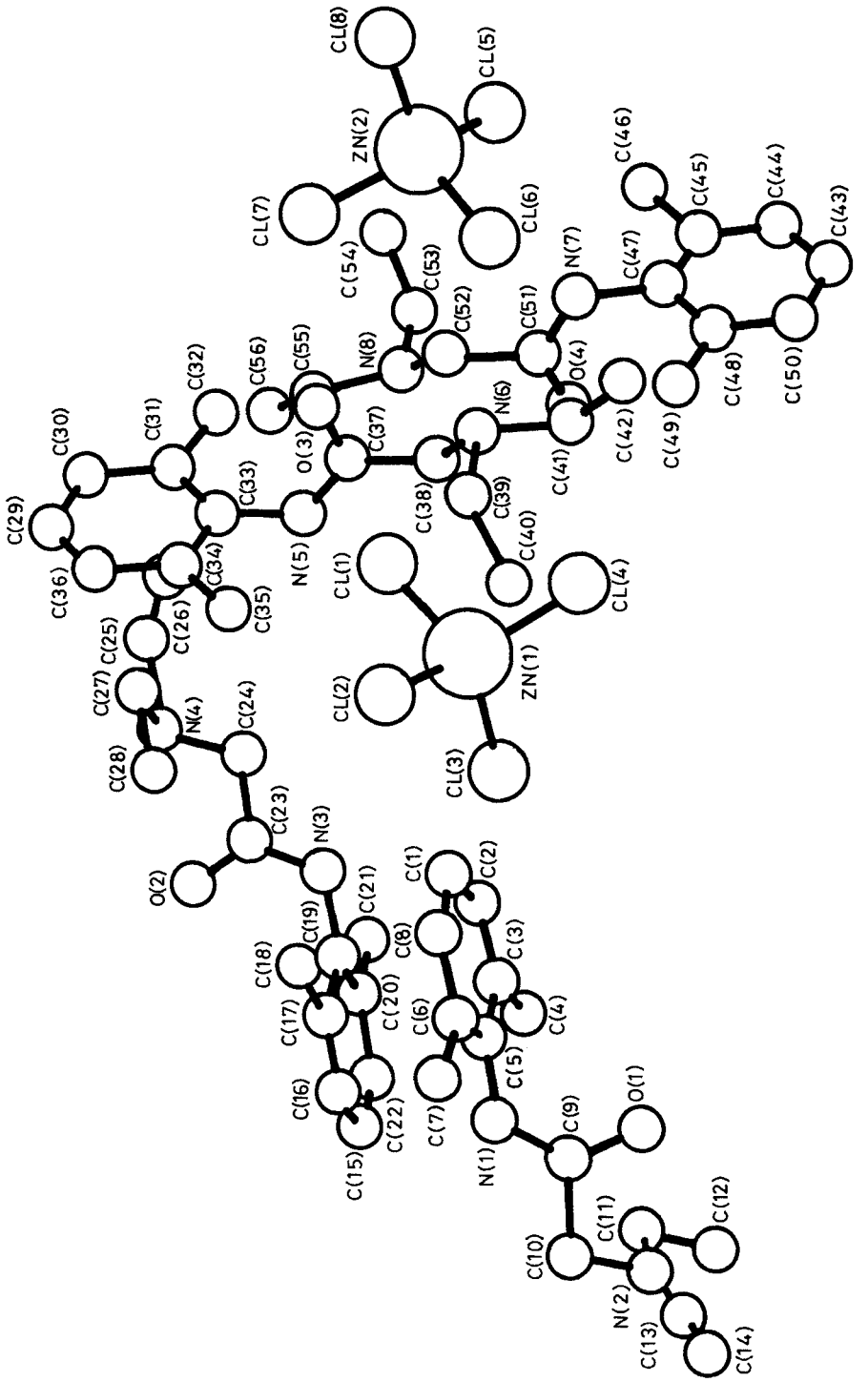

FIGURE 1

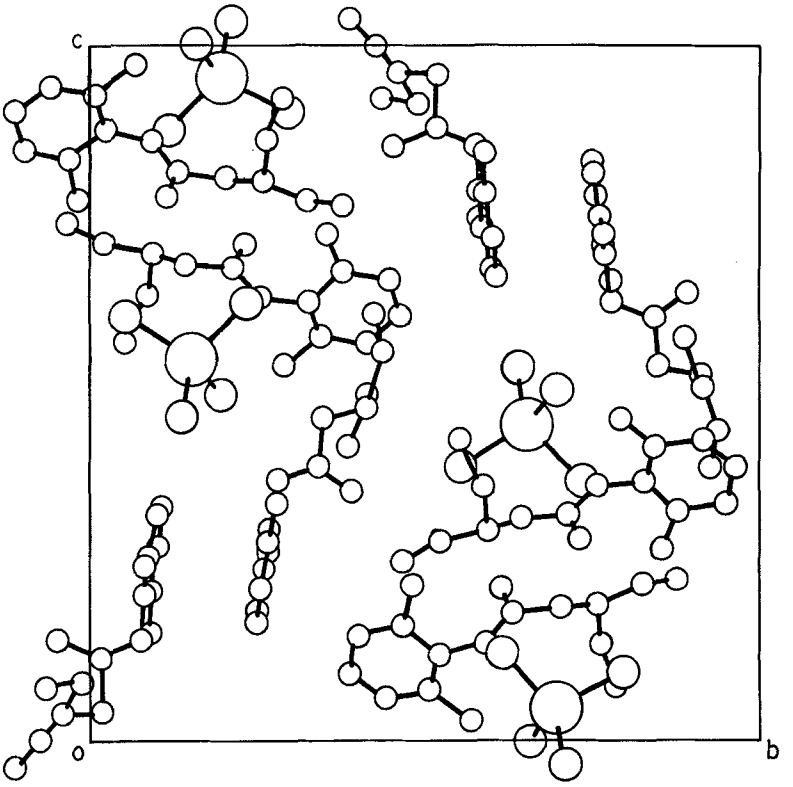

FIGURE 2

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