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

Re environment			
Re—P(1)	2·448 (2)	Re—C(53)	2·254 (8)
Re—P(2)	2·446 (2)	Re—C(54)	2·202 (7)
Re—Cl	2·502 (2)	Re—C(55)	3·344 (7)
Re—C(50)	2·244 (7)	Re—C(56)	3·744 (7)
Re—C(51)	2·219 (7)	Re—C(57)	3·369 (6)
Re—C(52)	2.264 (8)		
P(1)—Re—P(2)	98·09 (7)	Cl—Re—P(2)	88·53 (6)
Cl—Re—P(1)	85·90 (6)		
Cyclooctadienyl ring			
C(50)—C(51)	1·42 (1)	C(54)—C(55)	1·51 (1)
C(51)—C(52)	1·41 (1)	C(55)—C(56)	1·53 (1)
C(52)—C(53)	1·43 (1)	C(56)—C(57)	1·49 (1)
C(53)—C(54)	1·41 (1)	C(57)—C(50)	1·51 (9)
C(51)—C(50)—C(57)	126·4 (7)	C(53)—C(54)—C(55)	126·1 (6)
C(50)—C(51)—C(52)	123·6 (6)	C(54)—C(55)—C(56)	113·5 (6)
C(51)—C(52)—C(53)	129·2 (7)	C(55)—C(56)—C(57)	111·5 (6)
C(52)—C(53)—C(54)	121·2 (7)	C(56)—C(57)—C(50)	114·7 (7)
Triphenylphosphine group			
P(1)—C(1)	1·864 (7)	P(2)—C(19)	1·851 (7)
P(1)—C(7)	1·836 (6)	P(2)—C(25)	1·860 (8)
P(1)—C(13)	1·862 (8)	P(2)—C(31)	1·849 (8)
C(1)—P(1)—C(7)	101·5 (3)	C(19)—P(2)—C(25)	95·7 (3)
C(7)—P(1)—C(13)	101·1 (3)	C(19)—P(2)—C(31)	102·0 (3)
C(1)—P(1)—C(13)	102·1 (3)	C(25)—P(2)—C(31)	106·2 (3)

Related literature. Crystals of the title compound were formed by the reaction of HCl with the monohydridocyclooctatriene complex $ReH(PPh_3)_2(\eta^6\text{-}C_8H_{10})$, which was itself obtained by treatment of $ReH_7(PPh_3)_2$ with cyclooctatetraene (Boydell, 1984). This structure is to be compared with the structure of $ReH_2(PMe_2Ph)_2(\eta^5\text{-}C_8H_{11})$ (Trimarchi, Green, Huffman & Gaulton, 1985); the Re coordination is essentially the same with one H atom replaced by one Cl atom.

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Structure of (Histamine.2H$^+$)($ZnCl_4$)

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Abstract. 5-(2-Ammonioethyl)imidazolium tetrachlorozincate, $[C_5H_{11}N_3][ZnCl_4]$, $M_r = 320{\cdot}3$, orthorhombic, $P2_1nb$, $a = 7{\cdot}343\ (6)$, $b = 7{\cdot}619\ (2)$, $c = 21{\cdot}455\ (12)$ Å, $V = 1200\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}773$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 29{\cdot}58$ cm^{-1}, $F(000) = 640$, $T = 293$ K, $R = 6{\cdot}4\%$ for 738 observed reflections. The granular matrix which stores histamine in the mast cell contains zinc cations, but the nature of the cellular interaction between zinc and histamine is unknown. In the complex formed by zinc chloride and histamine.2H$^+$, zinc is tetrahedrally bound to four chloride atoms which are hydrogen bonded to the 5-(2-aminoethyl)imidazole molecule (protonated at N4 of the imidazole ring and N8 of the side chain) *via* the protons of the imidazole nitrogen atoms, N2 and N4.

Experimental. Clear plate with dimensions 0·2 × 0·2 × 0·1 mm; prepared from 0·3682 g (2 mmol) of histamine dissolved in 60 mL absolute EtOH containing 0·1110 g (1 mmol) anhydrous $CaCl_2$ and 0·1363 g (1 mmol) $ZnCl_2$; orthorhombic, space group $P2_1nb$ (No. 33). Intensities collected with a Syntex $P3m$ diffractometer; graphite monochromator; $\theta/2\theta$ scan, $2\theta_{max} = 45°$; $(\sin\theta/\lambda)_{max} = 0{\cdot}538$ Å^{-1}; variable scan rate; three standard reflections remeasured after every 100 reflections, variation 5%; 15 reflections with $10{\cdot}69 < 2\theta < 22{\cdot}97°$ used for refinement of lattice parameters; index range $0 \le h \le 10$, $0 \le k \le 10$, $0 \le l \le 22$; 1092 reflections measured, 738 unique reflections observed with $I > 3{\cdot}0\sigma(I)$, 354 unobserved; Lp corrected (absorption correction not applied); solution for non-hydrogen positions, *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); hydrogen atoms located from difference Fourier synthesis, hydrogen positional and isotropic thermal parameters fixed ($U = 0{\cdot}03$); final cycles of refinement including anisotropic thermal parameters for non-hydrogen atoms (function minimized $\sum w(|F_o| -$

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$|F_c|)^2$] (*XRAY*78; Stewart, 1978); scattering factors and f', f'' from *International Tables for X-ray Crystallography* (1974); 117 parameters refined in final least-squares cycle; final $(\text{shift/e.s.d.})_{max} = 0{\cdot}36$; max. positive electron density in final difference Fourier synthesis 0·36 e Å^{-3}, final $R = 6{\cdot}4$, $wR = 8{\cdot}3\%$; $w = 1/\sigma^2(F_o)$, σ from counting statistics; GOF = 0·4.

The numbering of atoms is shown in Fig. 1. Fractional atomic coordinates for non-hydrogen atoms are in Table 1;* bond distances and angles are in Table 2.

Related literature. Histamine release from mast cells is mediated by the presence of calcium (Kazimierczak & Diamant, 1978; Lichtenstein 1972; Cochrane & Douglas, 1974). Calcium binds directly to the allergens, penicillin V (Cole & Holt, 1987) and nicotinic acid (Cole & Holt, 1985) as well as to histamine itself. [(Histamine.H$^+$)$_2$CaCl$_4$(H$_2$O)$_2$CaCl$_2$(H$_2$O)$_2$] crystallizes with a calcium atom bound to two molecules of histamine *via* the nitrogen atom α to the side chain. The histamine is in monocationic form, being protonated at the side-chain amine group (Cole & Holt, 1986).

Zinc is present in mast cells (Pepys & Edwards, 1979) and it has been reported that (lidocaine.H$^+$)$_2$(ZnCl$_4$) exhibits an inhibitory effect on histamine release (Nosal, Pecivova & Drabikova, 1981). However the crystalline material (histamine.2H$^+$)(ZnCl$_4$), isolated from a mixture of zinc chloride and histamine shows only a weak interaction between zinc tetrachloride and the histamine dication: see Fig. 2; N2—H2···Cl1 2·23; N4—H4···Cl1′ 2·35 Å ($' = -1 + x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$). This hydrogen bonding extends parallel to the *ab* diagonal of the cell linking ZnCl$_4$ anions to histamine.2H$^+$

* Lists of structure amplitudes, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52754 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

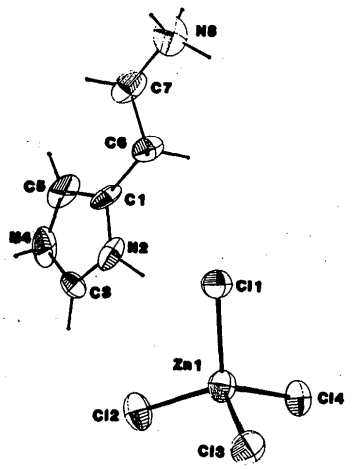

Fig. 1. View of the asymmetric unit of (histamine.2H$^+$)(ZnCl$_4$). Ellipsoids are shown at 50% probability level.

Table 1. *Positional parameters for* (*histamine*.2H$^+$)(ZnCl$_4$)

	x	y	z	U_{eq} (Å^2)*
Zn1	0·6882	0·2275 (3)	0·1129 (1)	4·2 (1)
Cl1	0·6941 (9)	0·1440 (6)	0·2151 (3)	4·2 (1)
Cl2	0·4033 (8)	0·2878 (7)	0·0840 (4)	5·6 (2)
Cl3	0·8242 (8)	0·0080 (6)	0·0574 (3)	4·6 (1)
Cl4	0·8665 (8)	0·4728 (6)	0·0979 (3)	4·9 (1)
C1	0·293 (3)	0·306 (2)	0·312 (1)	3·4 (11)
N2	0·310 (2)	0·304 (2)	0·251 (1)	4·6 (9)
C3	0·162 (3)	0·358 (3)	0·220 (1)	4·4 (9)
N4	0·046 (2)	0·398 (3)	0·263 (1)	6·3 (10)
C5	0·122 (4)	0·373 (3)	0·322 (2)	6·0 (12)
C6	0·446 (3)	0·252 (3)	0·357 (1)	4·3 (9)
C7	0·383 (4)	0·259 (3)	0·423 (1)	5·6 (11)
N8	0·532 (3)	0·206 (2)	0·467 (1)	5·5 (8)

* $U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$; $\sigma(U_{eq}) = \frac{1}{2}[\sigma(U_{11})^2 + \sigma(U_{22})^2 + \sigma(U_{33})^2]^{1/2}$.

Table 2. *Bond distances* (Å) *and bond angles* (°) *for* (*histamine*.2H$^+$)(ZnCl$_4$)

Zn1—Cl1	2·285 (6)	Cl1—Zn1—Cl2	110·0 (3)
Zn1—Cl2	2·230 (7)	Cl1—Zn1—Cl3	106·8 (2)
Zn1—Cl3	2·283 (7)	Cl1—Zn1—Cl4	110·4 (2)
Zn1—Cl4	2·304 (5)	Cl2—Zn1—Cl3	114·6 (2)
C1—N2	1·30 (4)	Cl2—Zn1—Cl4	109·1 (2)
N2—C3	1·34 (3)	Cl3—Zn1—Cl4	105·9 (2)
C3—N4	1·29 (3)	C5—C1—N2	105 (2)
N4—C5	1·40 (4)	C1—N2—C3	115 (2)
C5—C1	1·37 (4)	N2—C3—N4	104 (2)
C1—C6	1·54 (4)	C3—N4—C5	111 (2)
C6—C7	1·48 (4)	N4—C5—C1	105 (3)
C7—N8	1·50 (4)	C5—C1—C6	131 (3)
		N2—C1—C6	124 (2)
		C1—C6—C7	111 (2)
		C6—C7—N8	111 (2)

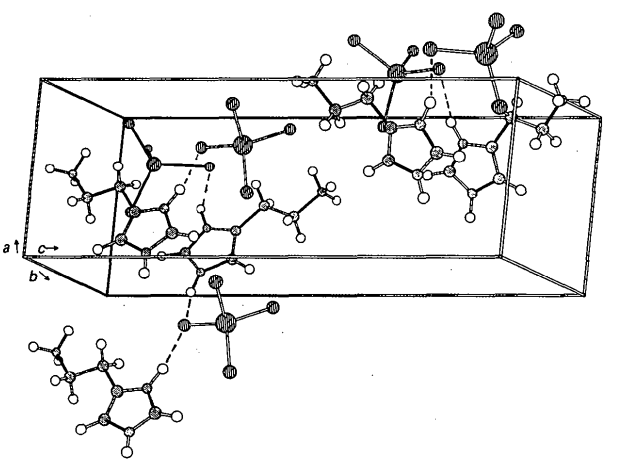

Fig. 2. Packing view with hydrogen bonding indicated by dashed lines.

cations in series. The lack of interaction between chains is reflected in the poor quality of the crystals.

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Structure of Diaqua[1,6-bis(2-benzimidazolyl)-2,5-dithiahexane]nickel(II) Diperchlorate Monohydrate

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Abstract. $[Ni(C_{18}H_{18}N_4S_2)(OH_2)_2](ClO_4)_2.H_2O$, M_r = 666·16, monoclinic, $C2/c$, a = 19·502 (3), b = 11·048 (3), c = 12·878 (5) Å, β = 109·96 (3)°, V = 2607·8 Å^3, Z = 4, D_x = 1·697 g cm^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, μ = 50·4 cm^{-1}, $F(000)$ = 1368, T = 293 K. The final R value is 0·063 for 1763 observed [$I > 3\sigma(I)$] reflections. The Ni atom is octahedrally coordinated to the two pyridine N atoms of the benzimidazolyl groups, the two thioether S atoms and the two water O atoms. The anions, cations and hydrated water molecules are linked by a network of hydrogen bonds.

Experimental. A bluish green crystal of approximate dimensions 0·50 × 0·10 × 0·08 mm was mounted on a glass fibre. The observed systematic absences determined the space group to be Cc or $C2/c$, the latter being confirmed by the subsequent refinement. In the final full-matrix least-squares refinement all non-H atoms were assigned anisotropic thermal parameters; the H atoms were included in the structure-factor calculation with fixed isotropic temperature factors (B_{iso} = 4·0 Å^2). More details of the intensity data collection, structure solution and refinement are listed in Table 1. Final atomic coordinates are given in Table 2, distances and angles in Table 3.* Figs. 1 and 2 show the numbering scheme and a stereoview of the $[Ni(C_{18}H_{18}N_4S_2)(OH_2)_2]^{2+}$ cation, respectively.

Related literature. The structure determination is part of our studies of transition-metal complexes derived from open-chain tetradentate ligands containing NSSN donor atoms (Birker, Helder, Henkel, Krebs & Reedijk, 1982; Castiñeiras, Hiller, Strähle, Paredes & Sordo, 1985; Smits, Janssen, Beurskens, Van Rijn & Reedijk, 1987; Castiñeiras, Carballo,

* Lists of structure factors, anisotropic thermal parameters, least-squares planes, further distances and angles, torsion angles, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52874 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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