

structure with P constrained on the threefold axis. Anisotropic (non-H atoms) full-matrix least-squares refinement; $\sum w||F_o| - |F_c||^2$ minimized where $w = 1/[\sigma(F_o)]^2$. The H-atom positions were calculated (C—H bond length 1.0 Å) and included as fixed contributors with isotropic thermal parameters fixed to 5.0 Å². 67 parameters were refined; $R = 0.068$, $wR = 0.083$, $S = 3.23$; $(\Delta/\sigma)_{\max} = 0.017$; $\Delta\rho_{\max/\min} = 0.84/-1.00 \text{ e \AA}^{-3}$. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The *UCLA Crystallographic Program Package* (Strouse, 1985) was used throughout. The program *PLOTMD* (Luo, Ammon & Gilliland, 1989) was used to modify the labels of the *ORTEP* drawing (Johnson, 1976) displayed in Fig. 1. Positional parameters and isotropic temperature factors are listed in Table 1; selected bond lengths and angles are listed in Table 2.* In Fig. 2, the crystal packing is displayed.

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54971 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0566]

Related literature. The isomorphous structures P(SC₆H₅)₃ (Burford, Royan & White, 1990) and As(SC₆H₅)₃ (Papalardo, Chakravorty, Irgolic & Meyers, 1983) have been reported.

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Structure of 3,3-Bis(2-imidazolyl)propionic Acid Monohydrate

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Abstract. C₉H₁₀N₄O₂·H₂O, $M_r = 224.2$, triclinic, $P\bar{1}$, $a = 7.322$ (1), $b = 10.029$ (1), $c = 7.155$ (1) Å, $\alpha = 89.96$ (1), $\beta = 99.72$ (1), $\gamma = 95.14$ (1)°, $V = 515.8$ (4) Å³, $Z = 2$, $D_x = 1.44 \text{ Mg m}^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.1 \text{ mm}^{-1}$, $F(000) = 236$, $T = 295 \text{ K}$, final $R = 0.039$ for 1081 reflections. The molecule, abbreviated as HBIP, is a zwitterion containing —COO[−] and —(imidazole)H⁺ residues. The

dihedral angle between the two imidazole rings is 66.7 (1)°. There is no intramolecular hydrogen bond.

Experimental. Synthesis according to Joseph, Leigh & Swain (1977), colourless data-collection crystal of dimensions 0.35 × 0.20 × 0.08 mm. D_m not measured. Enraf–Nonius CAD-4 diffractometer; graphite-monochromated Mo $K\alpha$; cell dimensions from setting angles of 25 reflections having $10.6 < \theta < 13.1$ °; 1813 reflections measured using ω – 2θ scan with 2θ

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Table 1. Fractional atomic coordinates and isotropic or equivalent isotropic temperature factors ($\text{\AA}^2 \times 10^3$) with e.s.d.'s in parentheses

	$U_{\text{eq}} = \frac{1}{3} \text{trace } U$			$U_{\text{eq}}/U_{\text{iso}}$
	x	y	z	
O(1)	0.1023 (4)	0.2443 (3)	0.1485 (4)	5.0 (5)
O(2)	0.3315 (3)	0.1440 (2)	0.0592 (4)	4.1 (4)
C(1)	0.2680 (5)	0.2392 (3)	0.1275 (4)	3.0 (6)
C(2)	0.4025 (5)	0.3630 (3)	0.1890 (5)	3.0 (6)
C(3)	0.6028 (4)	0.3285 (3)	0.2502 (4)	2.7 (5)
C(4)	0.6200 (4)	0.2454 (3)	0.4263 (4)	2.7 (5)
N(1)	0.7141 (4)	0.1387 (3)	0.4539 (4)	3.3 (5)
C(5)	0.6973 (5)	0.0878 (4)	0.6302 (5)	4.1 (6)
C(6)	0.5899 (5)	0.1653 (3)	0.7067 (5)	3.8 (6)
N(2)	0.5420 (4)	0.2646 (3)	0.5782 (4)	3.2 (5)
C(7)	0.7392 (4)	0.4515 (3)	0.2749 (4)	2.6 (5)
N(3)	0.7063 (4)	0.5701 (3)	0.3340 (4)	3.4 (5)
C(8)	0.8683 (5)	0.6510 (4)	0.3280 (5)	3.8 (6)
C(9)	0.9936 (5)	0.5808 (4)	0.2672 (5)	3.9 (6)
N(4)	0.9106 (4)	0.4523 (3)	0.2316 (4)	3.4 (5)
Ow	-0.1251 (4)	0.0296 (3)	0.1980 (4)	5.5 (5)
H1(Ow)	-0.069 (6)	0.104 (3)	0.141 (6)	8.0
H2(Ow)	-0.202 (5)	-0.018 (4)	0.094 (4)	8.0

Table 2. Bond lengths (\AA) and angles ($^\circ$) with e.s.d.'s in parentheses

C(1)—O(1)	1.253 (4)	C(1)—O(2)	1.235 (4)
C(1)—C(2)	1.530 (4)	C(2)—C(3)	1.529 (5)
C(3)—C(4)	1.504 (4)	C(3)—C(7)	1.507 (4)
C(4)—N(1)	1.321 (4)	C(7)—N(3)	1.319 (4)
N(1)—C(5)	1.381 (5)	N(3)—C(8)	1.383 (4)
C(5)—C(6)	1.333 (6)	C(8)—C(9)	1.333 (6)
C(6)—N(2)	1.383 (4)	C(9)—N(4)	1.379 (4)
N(2)—C(4)	1.332 (4)	N(4)—C(7)	1.342 (4)
Ow—H1(Ow)	0.95 (3)	Ow—H2(Ow)	0.95 (3)
O(1)—C(1)—O(2)	125.8 (3)	C(6)—N(2)—C(4)	108.1 (3)
O(1)—C(1)—C(2)	117.0 (3)	C(2)—C(3)—C(4)	110.8 (3)
O(2)—C(1)—C(2)	117.2 (3)	C(2)—C(3)—C(7)	112.1 (3)
C(1)—C(2)—C(3)	112.5 (3)	C(4)—C(3)—C(7)	111.6 (2)
C(3)—C(4)—N(1)	125.0 (3)	C(3)—C(7)—N(3)	125.6 (3)
C(3)—C(4)—N(2)	126.4 (3)	C(3)—C(7)—N(4)	122.5 (3)
N(2)—C(4)—N(1)	108.6 (3)	N(4)—C(7)—N(3)	111.9 (3)
C(4)—N(1)—C(5)	108.7 (3)	C(7)—N(3)—C(8)	104.8 (3)
N(1)—C(5)—C(6)	107.1 (3)	N(3)—C(8)—C(9)	110.2 (3)
C(5)—C(6)—N(2)	107.4 (3)	C(8)—C(9)—N(4)	106.5 (3)
C(9)—N(4)—C(7)	106.6 (3)	H1(Ow)—Ow—H2(Ow)	104 (3)

from 3 to 50° ; $-8 \leq h \leq 8$, $-11 \leq k \leq 11$, $0 \leq l \leq 8$; ω -scan width $(1.1 + 0.35 \tan \theta)^\circ$, scan speed $1-10^\circ \text{ min}^{-1}$. Intensities of three reflections ($1\bar{1}4$, $4\bar{1}1$, $1\bar{1}4$) measured every hour showed only random variations, no decay correction. Corrections for Lp, no absorption corrections, no redundant data. 1813 unique data. Direct methods followed by Fourier and least-squares techniques using 1081 reflections having $F_o^2 > 3\sigma(F_o^2)$. Full-matrix least-squares refinement minimizing $\sum w(|F_o| - |F_c|)^2$, with anisotropic thermal parameters for all non-H atoms. All H atoms located by ΔF map, water-molecule H atoms refined, other H atoms in constrained geometry (C—H = N—H = 0.97\AA). Isotropic U_{H} first allowed to vary, then kept fixed. $R = 0.039$, $wR = 0.041$, 160 variables, $S = 0.54$, unit weights. Mean and max. parameter shifts 0.001σ and 0.012σ ,

respectively. Max. and min. heights in final ΔF map 0.27 and -0.23 e \AA^{-3} . Scattering factors including real and imaginary parts of anomalous dispersion from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 99–101, 149) and from Stewart, Davidson & Simpson (1965) for H atoms. Micro-VAX 3400 DEC computer. *MolEN* (Fair, 1990), *SHELXS86* (Sheldrick, 1986), *SHELX76* (Sheldrick, 1976), *ORFFE* (Busing, Martin & Levy, 1964) and *NRC* (Ahmed, Hall, Pippy & Huber, 1966) programs.

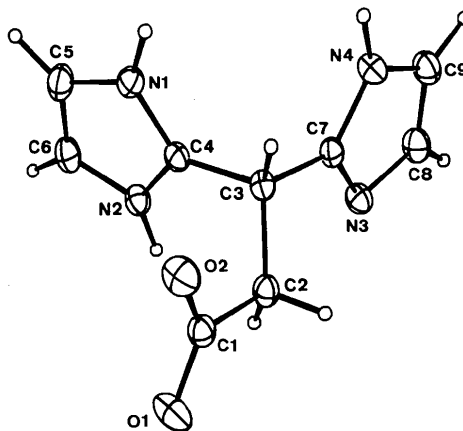


Fig. 1. ORTEP plot showing 35% probability thermal ellipsoids. H atoms are drawn at an arbitrary scale.

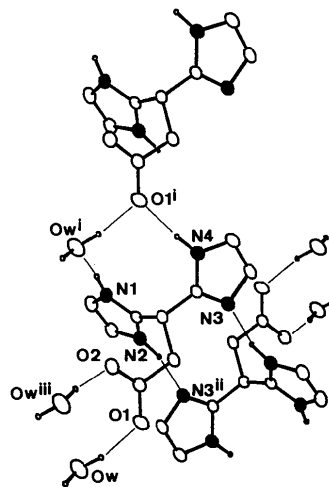


Fig. 2. An ORTEP view of the hydrogen-bonding scheme (thin lines) in the unit cell [$\text{N}(1) \cdots \text{Ow}^i = 2.627 (4)$, $\text{H}(\text{N}1) \cdots \text{Ow}^i = 1.66 \text{\AA}$, $\text{N}(1) \cdots \text{H}(\text{N}1) \cdots \text{Ow}^i = 172^\circ$; $\text{N}(2) \cdots \text{N}(3^{ii}) = 2.716 (4)$, $\text{H}(\text{N}2) \cdots \text{N}(3^{ii}) = 1.77 \text{\AA}$, $\text{N}(2) \cdots \text{H}(\text{N}2) \cdots \text{N}(3^{ii}) = 163^\circ$; $\text{N}(4) \cdots \text{O}(1^i) = 2.736 (4)$, $\text{H}(\text{N}4) \cdots \text{O}(1^i) = 1.78 \text{\AA}$, $\text{N}(4) \cdots \text{H}(\text{N}4) \cdots \text{O}(1^i) = 167^\circ$; $\text{Ow} \cdots \text{O}(1) = 2.663 (4)$, $\text{H}1(\text{Ow}) \cdots \text{O}(1) = 1.79 \text{\AA}$, $\text{Ow} \cdots \text{H}1(\text{Ow}) \cdots \text{O}(1) = 151 (3)^\circ$; $\text{Ow}^{iii} \cdots \text{O}(2) = 2.701 (3)$, $\text{H}2(\text{Ow}^{iii}) \cdots \text{O}(2) = 1.77 (3) \text{\AA}$, $\text{Ow}^{iii} \cdots \text{H}2(\text{Ow}^{iii}) \cdots \text{O}(2) = 165 (3)^\circ$]. Symmetry operations are: (i) $1 + x, y, z$; (ii) $1 - x, 1 - y, 1 - z$; (iii) $-x, -y, -z$.

Related literature. Final atomic parameters are listed in Table 1.* The bond lengths and angles are listed in Table 2. Fig. 1 shows a thermal-ellipsoid plot (Johnson, 1965) of the molecule with atom labelling and Fig. 2 displays the hydrogen-bond network in the crystal.

The title compound is one of the ligands used to model the active centre of the metalloprotein of Fe^{II} called the ferroquinone complex (Boinnard, Cassoux, Petrouleas, Savariault & Tuchagues, 1990). It contains two imidazole rings and a carboxylic group and represents a simplification of the fundamental structural elements that are believed to make up the ferroquinone complex. The HBIP molecule is a zwitterion, the predominant form for the amino acids. The two imidazole rings of the same molecule make a dihedral angle of 66.7 (1)°; the relative spatial positions of the N atoms and the carboxylic group are such that the molecule is expected to act as a tridentate ligand after removal of a proton and yield

* Lists of structure factors, H-atom parameters, anisotropic thermal parameters and least-squares-planes equations have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54980 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA0265]

neutral $M^{II}(\text{BIP})_2$ complexes containing $M^{II}\text{N}_4\text{O}_2$ chromophores.

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Structure of *tert*-Butylammonium Hexachlorotellurate(IV)

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Abstract. $[(\text{CH}_3)_3\text{CNH}_3]_2\text{TeCl}_6$, $M_r = 488.6$, monoclinic, $P2_1/a$, $a = 12.620$ (3), $b = 15.719$ (5), $c = 9.945$ (2) Å, $\beta = 90.14$ (2)°, $V = 1973.0$ (9) Å³, $Z = 4$, $D_x = 1.645$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 2.318$ mm⁻¹, $F(000) = 960$, $T = 289$ K, final $R = 0.051$ for 2630 unique reflections with $I > 3\sigma(I)$. The structure may be regarded as having monoclinically distorted *anti*-CdI₂-type packing of the composite ions forming puckered layers parallel to the *ab* plane. Each complex anion is surrounded by six cations, while each cation has three anion neighbours with Cl...N distances in the range 3.233 (7)–3.584 (8) Å. The C—N axes of the cations are almost parallel to

the *c* axis, the N atoms pointing in the layers. The TeCl_6^{2-} octahedron is distorted and noncentrosymmetric.

Experimental. Crystals of $[(\text{CH}_3)_3\text{CNH}_3]_2\text{TeCl}_6$ were grown by slow evaporation of a concentrated HCl solution. A yellow prismatic crystal with dimensions 0.35 × 0.30 × 0.40 mm was mounted in a glass capillary. Measurements were made on a Rigaku AFC-5R diffractometer with graphite-monochromated Mo $K\alpha$ radiation (40 kV, 200 mA) at the X-ray Laboratory of Okayama University. Cell constants were obtained from a least-squares refinement