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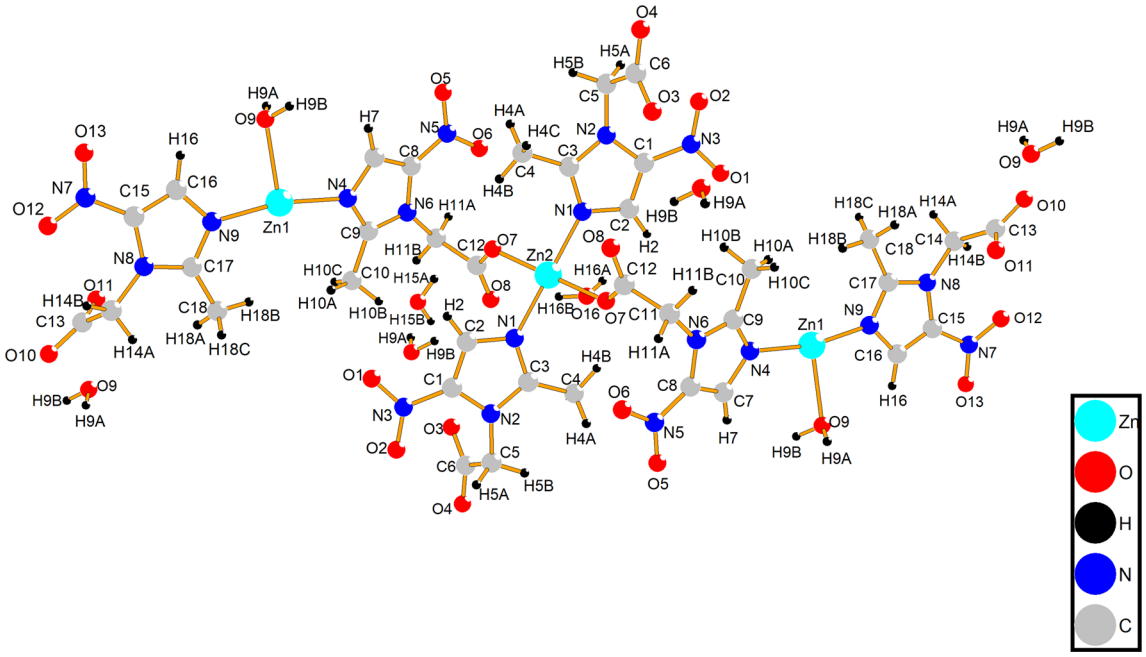
The crystal structure of tetraaqua-bis(2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)acetato-k^2*O:N*)-tetrakis(2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)acetato-k^1*N*) trizinc(II) hexahydrate $C_{36}H_{52}N_{18}O_{32}Zn_3$



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Abstract

$C_{36}H_{52}N_{18}O_{32}Zn_3$, monoclinic, $P2_1/n$ (no. 14), a = 8.9375(11) Å, b = 18.668(2) Å, c = 17.193(2) Å, β = 93.746(4)°, V = 2862.4(6) Å^3, Z = 2, $R_{gt}(F)$ = 0.0470, w$R_{ref}(F^2)$ = 0.1195, T = 296.15 K.

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1 Source of materials

2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)acetic acid (0.185 g, 1 mmol) and zinc nitrate hexahydrate (0.30 g, 1 mmol) were mixed in methanol/water 1:1 (20 mL) and stirred for 1 h, and the solution was kept at room temperature for 3 d. Colourless block crystals were obtain by slow evaporation (Table 1).

Table 1: Data collection and handling.

Crystal:	Colourless block
Size	0.42 × 0.33 × 0.22 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	1.36 mm^{-1}
Diffractometer, scan mode:	Bruker APEX 3, φ and ω scan
θ_{max}, completeness:	28.4°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	25315, 7189, 0.047
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5,680
$N(param)_{refined}$:	413
Programs:	Bruker,[1] Olex2,[2] SHELX[3,4]

2 Experimental details

Absorption corrections were applied by using multi-scan program.[1] Using Olex2,[2] the structure was solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with the ShelXL[4] refinement package using least squares minimisation.

3 Comment

Researchers have long exhibited a profound interest in nitrogen-containing heterocycles and their coordination with metal atoms.[5,6] In the crystal structure of the title compound, the unit consists of six formula units of the 2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)acetato ligands, three zinc ions and four water molecules. This compound's structure is novel and has been reported for the first time. The molecular structure is composed of three zinc ions linked to two imidazolate ligands. Among these units, the dihedral angle between any two adjacent ones is 13.83°, while the non-adjacent units are parallel to each other as the trinuclear title complex is located on an inversion center. This particular spatial arrangement significantly influences the overall conformation and properties of the complex molecule. There are intramolecular hydrogen bonds (O9–H9B…O8, O16–H16B…O8) in the complex molecules. The single-crystal structure analysis confirms that all bond lengths and bond angles of the compound fall within a reasonable range.[7]

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