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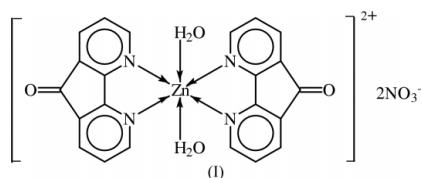
Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.047
 wR factor = 0.106
Data-to-parameter ratio = 14.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diaquabis(4,5-diazafluoren-9-one- κ^2N,N')-
zinc(II) dinitrate

The Zn atom in the crystal structure of $[\text{Zn}(\text{C}_{11}\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$ lies on an inversion center; it is chelated by the 4,5-diazafluoren-9-one entity in a nearly isobidentate manner. The coordinated water molecules link the nitrate anions to produce a linear hydrogen-bonded chain that runs along the a axis.

Comment

4,5-Diazafluoren-9-one also chelates to the Cu atom of a copper dinitrate adduct that crystallizes as a dihydrate, in which the two water molecules coordinate to the metal atom. Unfortunately, $[\text{Cu}(\text{C}_{11}\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$ was refined in the $P1$ space group (Hu *et al.*, 2001) rather than the correct space group $P\bar{1}$ space group, so that the reported bond dimensions may not be reliable. Nevertheless, one Cu–N distance (*ca.* 2.0 Å) is distinctly shorter than the other (*ca.* 2.6 Å).



The present Zn analog, (I) (Fig. 1), is not isomorphous with the Cu compound. In this case, the ligand chelates to the Zn atom, which lies on an inversion center, in a nearly isobidentate manner [$\text{Zn}-\text{N} = 2.201(3)$ and $2.290(3)\text{ \AA}$]. The two other coordination sites of the octahedron are occupied by the water molecules [$\text{Zn}-\text{O} = 2.061(3)\text{ \AA}$]. Hydrogen bonds link the cations to the nitrate anions [$\text{O}\cdots\text{O} = 2.702(4)$ and $2.744(4)\text{ \AA}$], leading to the formation of a chain motif running along the a axis of the crystal (Fig. 2). Nearly isobidentate chelation by the ligand is also noted in the dihydrated copper perchlorate complex (Gu *et al.*, 2002; Zhang *et al.*, 2003).

Experimental

4,5-Diazafluoren-9-one (Henderson *et al.*, 1984) (0.18 g, 1 mmol) was reacted with lithium hydride (0.01 g, 0.5 mmol) in tetrahydrofuran solvent (10 ml) in a Schlenk apparatus. The yellow solution was refluxed for 1 h, after which zinc nitrate (0.09 g, 0.5 mmol) dissolved in tetrahydrofuran (10 ml) was added. Reflux was continued for another hour. Yellow crystals separated from the solution after several days, m.p. 552 K. Analysis: calculated for $\text{C}_{22}\text{H}_{16}\text{N}_6\text{O}_{10}\text{Zn}$: C 44.76, H 2.71, N 14.24%; found C 44.60, H 2.72, N 13.78%.

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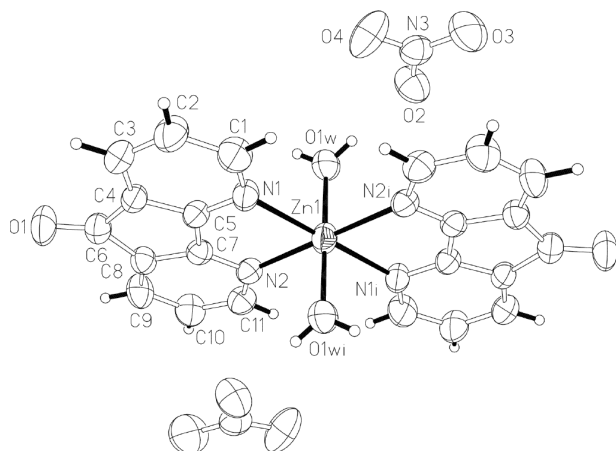


Figure 1
ORTEPII (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Crystal data

[Zn(C₁₁H₆N₂O)₂(H₂O)₂](NO₃)₂
M_r = 589.78
 Triclinic, *P*1̄
a = 6.989 (2) Å
b = 8.283 (3) Å
c = 10.222 (3) Å
 α = 94.909 (4)°
 β = 91.394 (4)°
 γ = 99.860 (4)°
V = 580.4 (3) Å³

Z = 1
D_x = 1.69 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 583 reflections
 θ = 3.0–23.3°
 μ = 1.13 mm⁻¹
T = 298 (2) K
 Block, yellow
 0.28 × 0.22 × 0.15 mm

Data collection

Bruker SMART 1K CCD diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.724, *T_{max}* = 0.844
 3777 measured reflections

2623 independent reflections
 1462 reflections with *I* > 2σ(*I*)
R_{int} = 0.034
 θ_{\max} = 28.3°
h = -9 → 9
k = -5 → 10
l = -13 → 13

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.047
wR (*F*²) = 0.106
S = 0.78
 2623 reflections
 186 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0431P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.69 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.68 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Zn1—O1w	2.061 (3)	Zn1—N2	2.201 (3)
Zn1—N1	2.290 (3)		
O1w—Zn1—O1w ⁱ	180	N1—Zn1—N1 ⁱ	180
O1w—Zn1—N1	90.5 (1)	N1—Zn1—N2	81.3 (1)
O1w—Zn1—N1 ⁱ	89.5 (1)	N1—Zn1—N2 ⁱ	98.7 (1)
O1w—Zn1—N2	89.3 (1)	N2—Zn1—N2 ⁱ	180
O1w—Zn1—N2 ⁱ	90.8 (1)		

Symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*.

The water H atoms were located and refined. The aromatic H atoms were positioned geometrically (C—H = 0.93 Å) and refined in the riding-model approximation; *U*_{iso}(H) was set to 1.2*U*_{eq} of the parent C atoms. The crystal used for data collection was a weak

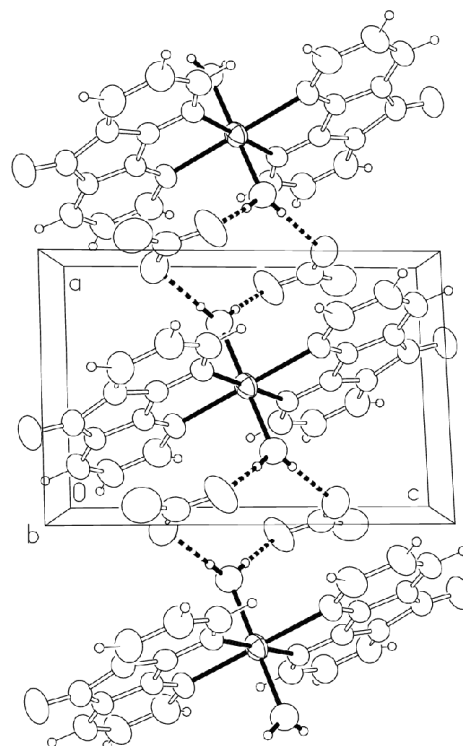


Figure 2
ORTEPII (Johnson, 1976) plot of the hydrogen-bonded chain structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Hydrogen bonds are indicated by dashed lines.

scatterer such that high-angle reflections, particularly those beyond θ of 25°, were not included in any calculations.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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