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Aqua(2,2′-bipyridyl)bis(furan-2-carboxylato)zinc(II)

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Key indicators

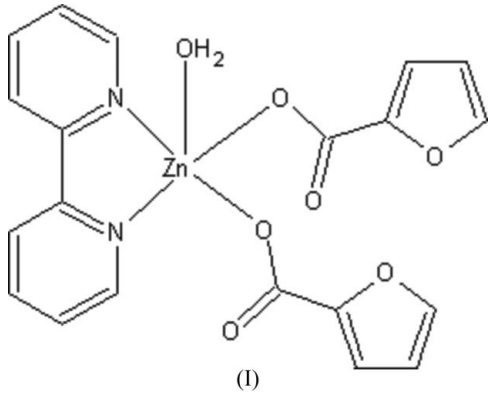
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.087
Data-to-parameter ratio = 14.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title complex, $[Zn(C_5H_3O_3)_2(C_{10}H_8N_2)(H_2O)]$, has a slightly distorted square-pyramidal geometry around the Zn^{II} ion and forms a three-dimensional supramolecular structure *via* O—H···O, C—H···O and π–π interactions.

Comment

The construction of supramolecular complexes is a rapidly growing field of research due to their intriguing potential applications such as magnetism, nonlinear optics, molecular recognition and biological simulation (Lehn, 1995). Supramolecular interactions, such as hydrogen bonds (Hunter, 1994), π–π interactions (Janiak, 2000) and weak C—H···O interactions (Steiner, 1997), are important and play dominant roles in determining the crystal packing in many instances. Zinc is an important element of life, participating in various metabolic processes, including the synthesis and catabolism of sugars, fats, proteins and nucleic acids (Wang, 1988). We present here the title new Zn^{II} complex, (I).



(I)

The Zn^{II} ion of (I) is coordinated by two O atoms from two furancarboxylate ligands, two N atoms from the 2,2′-bipyridyl ligand and one O atom from a water molecule in a distorted square-pyramidal geometry (Fig. 1).

Molecules of (I) are connected by strong O7—H7*A*···O5^{i} [symmetry code: (i) $x-1, y, z$] hydrogen bonds to form a chain structure along the *a* axis, as shown in Fig. 2. The shortest plane-to-plane (3.358 Å) and centroid-to-centroid (3.6093 Å) distances between 2,2′-bipyridyl ligands of two neighbouring chains suggest π–π stacking interactions between them, which link the two chains together. The chains then form a three-dimensional supramolecular network *via* weaker C—H···O and π–π stacking interactions between the furan rings, with plane-to-plane and centroid-to-centroid distances of 3.574 and 3.7508 Å, respectively.

Experimental

A mixture of $Zn(CH_3COO)_2{\cdot}2H_2O$ (0.1098 g, 0.5 mmol), La_2O_3 (0.0878 g, 0.25 mmol), 2,2′-bipyridyl (0.1556 g, 1.0 mmol), furan 2-carboxylic acid (0.2803 g, 2.5 mmol) and distilled water (0.2 ml) was mixed in a Teflon-lined autoclave and heated at 353 K for 3 d. The brown liquid obtained was dissolved in distilled water and kept at room temperature. Brown crystals of (I) suitable for X-ray single-crystal diffraction were obtained after several days.

Crystal data

$[Zn(C_5H_3O_3)_2(C_{10}H_8N_2)(H_2O)]$
M_r = 461.72
Monoclinic, $P2_1/c$
a = 6.8540 (5) Å
b = 17.028 (1) Å
c = 16.370 (1) Å
β = 96.016 (1)°
V = 1900.1 (2) Å^3
Z = 4
D_x = 1.614 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.34 mm^{-1}
T = 293 (2) K
Block, brown
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.689, T_{max} = 0.878
10995 measured reflections
4134 independent reflections
3489 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.087
S = 1.05
4134 reflections
279 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.0586P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20···O1^{i}	0.93	2.48	3.182 (3)	132
C9—H9···O6^{ii}	0.93	2.57	3.434 (3)	154
C4—H4···O5^{iii}	0.93	2.55	3.461 (2)	167
O7—H7*A*···O5^{iv}	0.87 (3)	1.84 (3)	2.706 (2)	171 (3)
O7—H7*B*···O2	0.76 (3)	1.93 (4)	2.656 (2)	160 (3)

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y+1, -z$; (iv) $x-1, y, z$.

H atoms bonded to C atoms were placed in idealized positions, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). Water H atoms were located in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

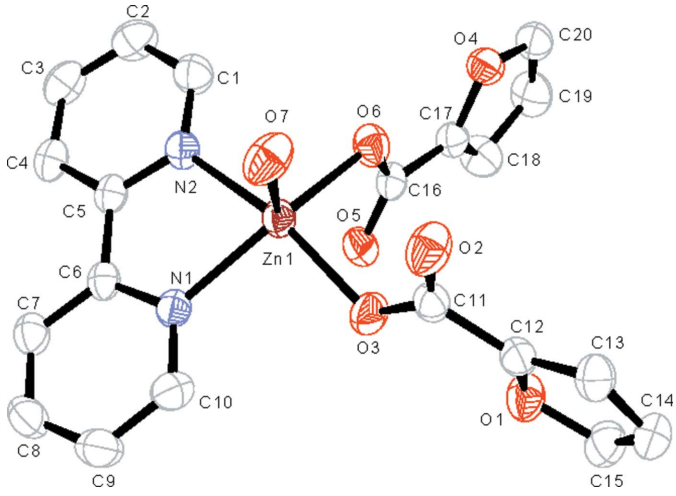


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

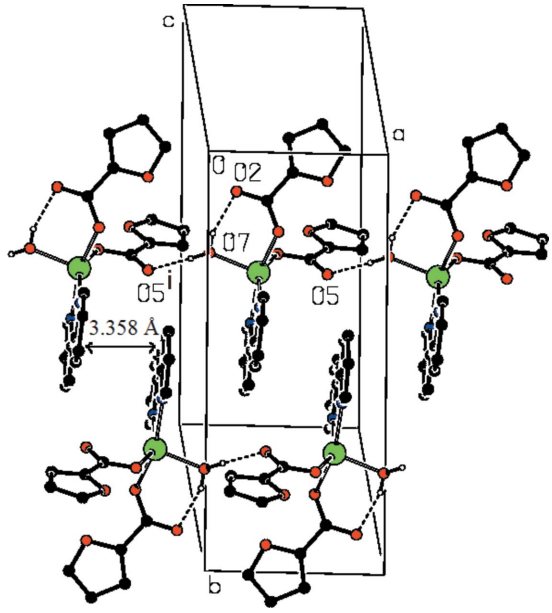


Figure 2
A partial packing view, showing the O—H···O hydrogen bonds linking the molecules of (I) into a chain and the occurrence of π–π stacking. Hydrogen bonds are represented as dashed lines and H atoms as small spheres of arbitrary radius. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) $x-1, y, z$].

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