Bis(1-naphthylacetato-κ^2O,O)(1,10-phenanthroline-κ^2N,N)zinc(II)

Y.-F Liu,[a]* H.-T Xia,[a] S.-P Yang[a] and D.-Q Wang[b]

[a]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang, Jiangsu 222005, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China

Correspondence e-mail: liu222005@hhit.edu.cn

Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.012 Å
R factor = 0.082
wR factor = 0.276
Data-to-parameter ratio = 12.8

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

In the crystal structure of the title compound, [Zn(C₁₂H₉O₂)₂(C₁₂H₈N₂)], there are two molecules in the asymmetric unit. The molecules are linked into a sandwiched sheet by six C—H···O hydrogen bonds.

Comment

As a part of our investigation of the reactions of 1-naphthylacetic acid and phenanthroline with metals, we report here the crystal structure of the title compound, (I) (Fig. 1).

(I)
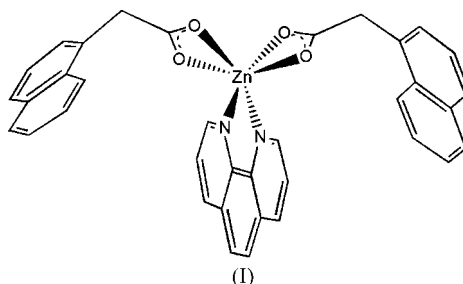
In the crystal structure, there are two molecules in the asymmetric unit. Compound (I) has a distorted octahedral configuration, in which the central Zn^{II} atom is coordinated by carboxylate O atoms and N atoms from two 1-naphthylacetic acid ligands and one 1,10-phenanthroline ligand. The molecules are linked into sheets through six independent C—H···O hydrogen bonds (Figs. 2–4 and Table 2), and neighbouring sheets are connected by van der Waals forces (Fig. 4), thereby joining the molecules into a three-dimensional network structure.

Experimental

Equimolar quantities (1 mmol) of sodium naphthylacetate and 1,10-phenanthroline were mixed in methanol (20 ml), and a solution of
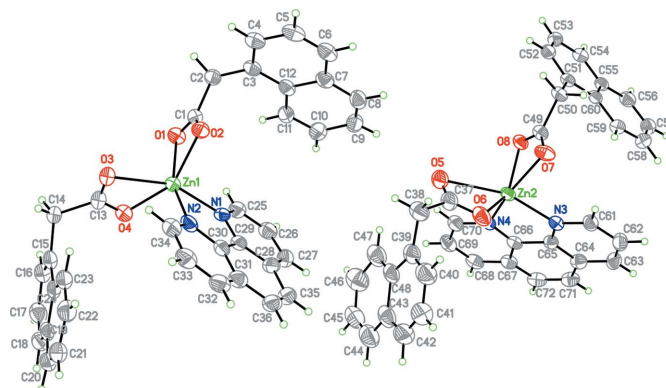
Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.
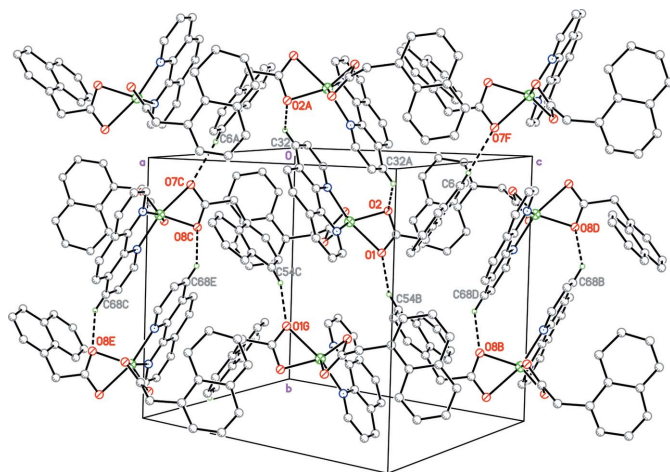
Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded sheet built from C—H···O interactions. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) $1 - x$, $-y$, $1 - z$; (B) $-1 + x$, y, z; (C) x, y, $-1 + z$; (D) $-1 + x$, y, z; (E) $2 - x$, $1 - y$, $1 - z$; (F) $1 - x$, $-y$, $2 - z$; (G) $1 - x$, $1 - y$, $1 - z$.]
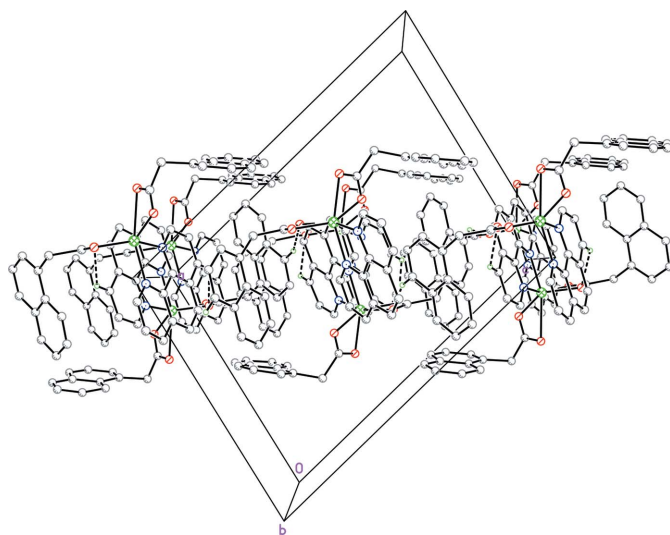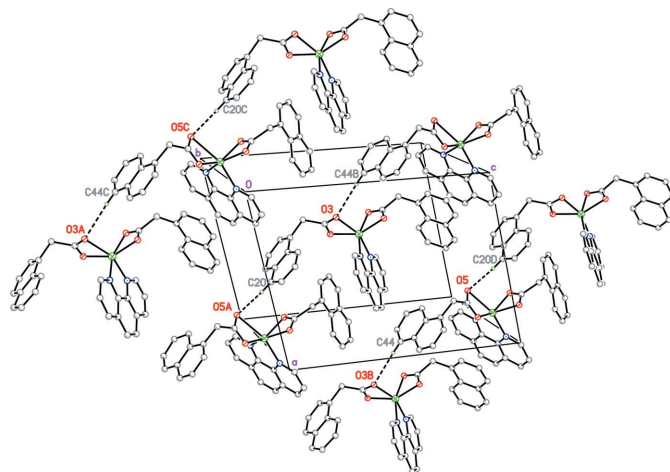

Figure 3
A view of the packing of (I), along the b axis, showing the formation of a hydrogen-bonded (dashed lines) sheet built from C—H···O interactions. H atoms not involved in hydrogen bonding have been omitted.

zinc nitrate (1 mmol) in methanol (20 ml) was added. The mixture was stirred for 1 h before being filtered. X-ray quality crystals of (I) were obtained by slow evaporation of the solution over a period of about one month.

Crystal data

[Zn(C₁₂H₉O₂)₂(C₁₂H₈N₂)]	$V = 2822$ (2) Å³
$M_r = 615.96$	$Z = 4$
Triclinic, $P\bar{1}$	$D_x = 1.450$ Mg m⁻³
$a = 12.964$ (6) Å	Mo $K\alpha$ radiation
$b = 13.055$ (6) Å	$\mu = 0.92$ mm⁻¹
$c = 17.128$ (8) Å	$T = 298$ (2) K
$\alpha = 89.403$ (8)°	Block, white
$\beta = 77.192$ (7)°	$0.38 \times 0.34 \times 0.30$ mm
$\gamma = 86.657$ (9)°	

Figure 4
A packing diagram of (I), showing the van der Waals interactions between adjacent sheets. Dashed lines indicate hydrogen bonds in a sheet. For clarity, H atoms not involved in the hydrogen bonding have been omitted. [Symmetry codes: (A) x, y, $-1 + z$; (B) $1 + x$, y, x.]

Data collection

Bruker SMART CCD area-detector diffractometer	14796 measured reflections
	9785 independent reflections
φ and ω scans	4949 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.043$
$T_{min} = 0.722$, $T_{max} = 0.771$	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1469P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.082$	$+ 0.4533P]$
$wR(F^2) = 0.276$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
9785 reflections	$\Delta\rho_{max} = 1.53$ e Å⁻³
763 parameters	$\Delta\rho_{min} = -0.72$ e Å⁻³
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	2.061 (5)	Zn2—O6	1.998 (6)
Zn1—O4	2.070 (6)	Zn2—O8	2.067 (5)
Zn1—N1	2.110 (6)	Zn2—N4	2.100 (6)
Zn1—N2	2.119 (6)	Zn2—N3	2.104 (6)
Zn1—O1	2.273 (5)	Zn2—O7	2.268 (5)
Zn1—O3	2.323 (5)		
O2—Zn1—O4	147.8 (2)	O6—Zn2—O8	138.3 (2)
O2—Zn1—N1	99.4 (2)	O6—Zn2—N4	106.6 (2)
O4—Zn1—N1	104.1 (2)	O8—Zn2—N4	103.7 (2)
O2—Zn1—N2	103.4 (2)	O6—Zn2—N3	113.6 (2)
O4—Zn1—N2	102.6 (2)	O8—Zn2—N3	99.7 (2)
N1—Zn1—N2	78.9 (2)	N4—Zn2—N3	78.8 (2)
O2—Zn1—O1	60.32 (19)	O6—Zn2—O7	94.4 (2)
O4—Zn1—O1	96.5 (2)	O8—Zn2—O7	60.40 (19)
N1—Zn1—O1	92.6 (2)	N4—Zn2—O7	158.6 (2)
N2—Zn1—O1	160.5 (2)	N3—Zn2—O7	89.5 (2)
O2—Zn1—O3	102.6 (2)	O6—Zn2—O5	56.6 (2)
O4—Zn1—O3	58.8 (2)	O8—Zn2—O5	96.7 (2)
N1—Zn1—O3	157.0 (2)	N4—Zn2—O5	88.9 (2)
N2—Zn1—O3	89.6 (2)	N3—Zn2—O5	161.4 (2)
O1—Zn1—O3	104.0 (2)	O7—Zn2—O5	106.3 (2)

Table 2
Hydrogen-bond geometry (Å, °).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
C54—H54$\cdots$O1^i	0.93	2.43	3.320 (9)	161
C20—H20$\cdots$O5^{ii}	0.93	2.58	3.493 (11)	166
C44—H44$\cdots$O3^{iii}	0.93	2.70	3.627 (14)	176
C68—H68$\cdots$O8^{iv}	0.93	2.67	3.407 (10)	137
C32—H32$\cdots$O2^v	0.93	2.68	3.350 (10)	130
C6—H6$\cdots$O7^{vi}	0.93	2.54	3.275 (10)	136

Symmetry codes: (i) $-x + 1, -y + 1, -z + 2$; (ii) $x, y, z - 1$; (iii) $x + 1, y, z$; (iv) $-x + 2, -y + 1, -z + 2$; (v) $-x + 1, -y, -z + 1$; (vi) $-x + 1, -y, -z + 2$.

All H atoms were located in a difference Fourier map and were subsequently treated as riding, with C—H distances of 0.93 (aryl) and 0.97 Å (methylene), and with $U_{iso}(H) = 1.2U_{eq}(C)$. The maximum electron-density peak is located 1.14 Å from the N4 atom and the deepest hole 0.21 Å from the C46 atom.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

References

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen,Germany.
Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.