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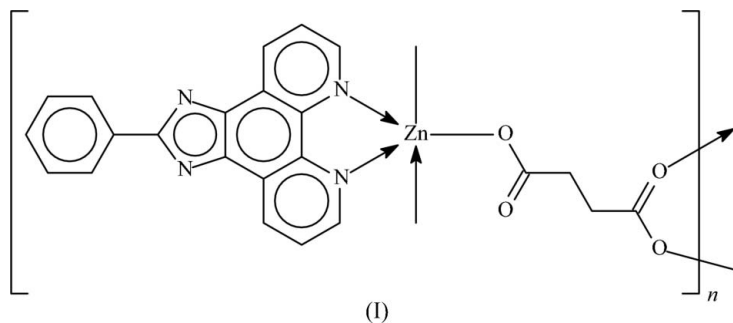
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$
 R factor = 0.055
 wR factor = 0.152
Data-to-parameter ratio = 14.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Poly[[*(2-phenyl-1H-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene)zinc(II)*]- μ_3 -succinato]The *N*-heterocycle in the title compound, $[\text{Zn}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_{19}\text{H}_{12}\text{N}_4)]_n$, chelates to the Zn^{II} ion; adjacent Zn ions are linked through three O atoms of the succinate anions into a ribbon. Adjacent ribbons are further linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonding, forming layers. The Zn center shows a square-pyramidal coordination.

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Comment

A recent study on the manganese isophthalate adduct of 2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]phenanthrene documents a ribbon structure that arises from one carboxylate $-\text{CO}_2$ end of the dianion chelating to the metal atom whereas the other carboxylate end bridges two other metal atoms. As the *N*-heterocycle binds in a chelating mode, the Mn atom is connected to six atoms in an octahedral geometry (Che *et al.*, 2006).

The present zinc succinate adduct, (I), adopts a ribbon structure; however, of the two carboxylate ends, one engages in binding in a monodentate mode although the other functions like that in the manganese compound (Fig. 1). The geometry is square-pyramidal, but is distorted towards octa-

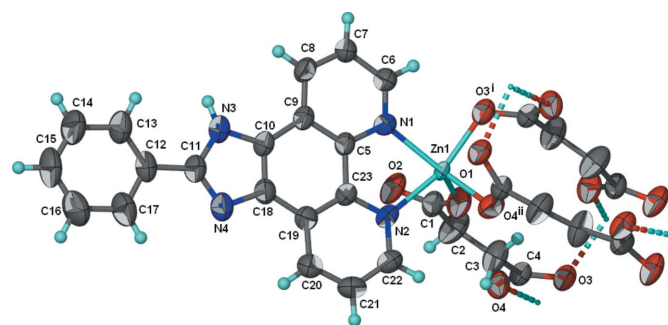


Figure 1

Displacement ellipsoid plot (50% probability level) showing a portion of the ribbon structure of (I); symmetry codes are as given in Table 1. Dashed lines indicate the bridging O–Zn bonds.

hedral owing to the proximity of the double-bond carbonyl O atom of the monodentate carboxylate unit (Table 1).

Experimental

The organic ligand was synthesized according to a literature method (Steck & Day, 1943). The ligand (0.5 mmol, 148 mg) was dissolved in methanol (12 ml) and this solution was added to an aqueous solution (8 ml) of zinc nitrate hexahydrate (0.5 mmol, 149 mg) and succinic acid (0.5 mmol, 59 mg). The mixture was filtered and the solution allowed to stand for several days for the formation of single crystals of (I) (yield 45%).

Crystal data

$[\text{Zn}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_{19}\text{H}_{12}\text{N}_4)]$	$Z = 8$
$M_r = 477.77$	$D_x = 1.675 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pcca</i>	Mo $K\alpha$ radiation
$a = 13.819 (2) \text{ \AA}$	$\mu = 1.34 \text{ mm}^{-1}$
$b = 9.757 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 28.098 (2) \text{ \AA}$	Block, pale yellow
$V = 3788.5 (10) \text{ \AA}^3$	$0.33 \times 0.31 \times 0.27 \text{ mm}$

Data collection

Rigaku RAXIS-RAPID IP diffractometer	32856 measured reflections
ω scans	4342 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	2419 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.666, T_{\max} = 0.714$	$R_{\text{int}} = 0.088$
	$\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.055$	
$wR(F^2) = 0.152$	$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2]$
$S = 0.96$	where $P = (F_o^2 + 2F_c^2)/3$
4342 reflections	$(\Delta/\sigma)_{\max} = 0.001$
293 parameters	$\Delta\rho_{\max} = 0.69 \text{ e \AA}^{-3}$
	$\Delta\rho_{\min} = -0.62 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Zn1—O1	1.955 (3)	Zn1—N1	2.099 (3)
Zn1—O3 ⁱ	2.052 (3)	Zn1—N2	2.106 (3)
Zn1—O4 ⁱⁱ	2.025 (3)		
O1—Zn1—O4 ⁱⁱ	93.8 (1)	O3 ⁱ —Zn1—N1	86.7 (1)
O1—Zn1—O3 ⁱ	99.5 (1)	O3 ⁱ —Zn1—N2	160.1 (1)
O1—Zn1—N1	124.8 (1)	O4 ⁱⁱ —Zn1—N1	141.0 (1)
O1—Zn1—N2	99.4 (1)	O4 ⁱⁱ —Zn1—N2	92.7 (1)
O3 ⁱ —Zn1—O4 ⁱⁱ	92.3 (1)	N1—Zn1—N2	77.3 (1)

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

The carbon-bound H atoms were positioned geometrically ($\text{C—H} = 0.93\text{--}0.96 \text{ \AA}$) and were included in the refinement in the riding-

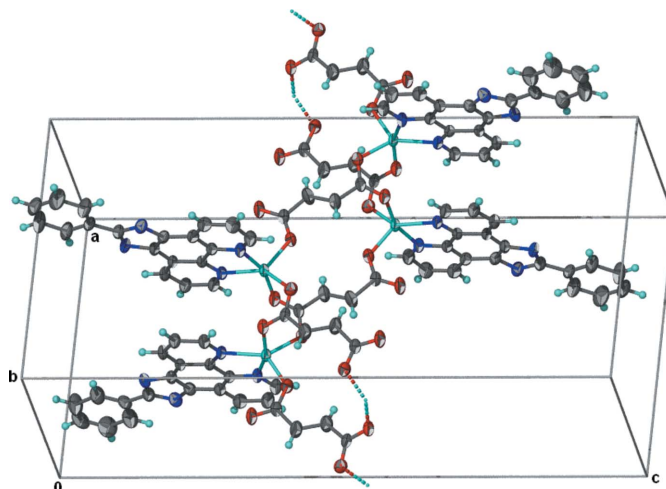


Figure 2

The ribbon structure of (I). Dashed lines indicate hydrogen bonds.

model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The amino H atom was located in a difference Fourier map and was refined with an N—H distance restraint of $0.86 (1) \text{ \AA}$; its displacement parameter was freely refined.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2006).

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