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μ-Benzene-1,4-dicarboxylato-bis[aquachloro-(2-phenyl-1*H*-1,3,7,8-tetraazacyclopenta[*l*]-phenanthrene)zinc(II)]

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In the title compound, $[Zn_2(C_8H_4O_4)Cl_2(C_{19}H_{12}N_4)_2(H_2O)_2]$ or $[Zn_2(BDC)Cl_2(L)_2(H_2O)_2]$ (where BDC is benzene-1,4-dicarboxylate and *L* is 2-phenyl-1*H*-1,3,7,8,-tetraaza-cyclopenta[*l*]phenanthrene), the two Zn^{II} atoms are bridged by the BDC ligand to form a dinuclear compound in which each Zn^{II} atom is five-coordinated by two N atoms from one *L* ligand, one chloride ion, and two O atoms, one from the BDC and one from the water molecule. The molecule is centrosymmetric. Neighbouring dinuclear complexes interact through π–π contacts to form stacks, leading to a two-dimensional supramolecular structure.

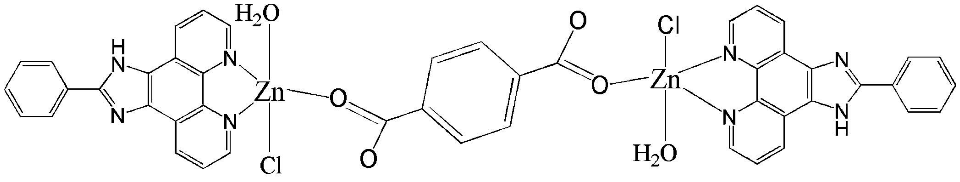
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.011 Å
R factor = 0.071
wR factor = 0.235
Data-to-parameter ratio = 14.9

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

Comment

The synthesis and design of supramolecular complexes exhibiting novel structures and properties has provided exciting new prospects for chemists (Eddaoudi *et al.*, 2001). A common and successful approach to the preparation of supramolecular frameworks is *via* direct chemical combination of functional inorganic and organic components. 1,10-Phenanthroline (phen) and its derivatives are one type of important organic ligand widely used in the construction of metal-organic complexes. 2-Phenyl-1*H*-1,3,7,8,-tetraazacyclopenta[*l*]phenanthrene (*L*) is one such phen derivative and, to date, the chemistry of supramolecular architectures based on *L* has received little attention (Collins *et al.*, 1998). We present here a new compound $[Zn_2(BDC)Cl_2(L)_2(H_2O)_2]$, (I), incorporating the *L* ligand (BDC is benzene-1,4-dicarboxylate).



(I)

Selected bond lengths and angles for (I) are given in Table 1. There is a centre of symmetry at the centre of the BDC ligand. In compound (I), the Zn^{II} atom is five-coordinated by two N atoms from one *L* ligand, one chlorine ion, and two O atoms from one BDC and one water molecule (Fig. 1). The two Zn^{II} atoms are bridged by the BDC ligand to form a dinuclear compound.

The water molecule, NH group, chloride ion and carboxylate O atoms form hydrogen bonds (Table 2).

Neighbouring dinuclear complexes interact through π–π contacts, leading to a two-dimensional supramolecular structure (Fig. 2). There are two types of π–π interactions: one

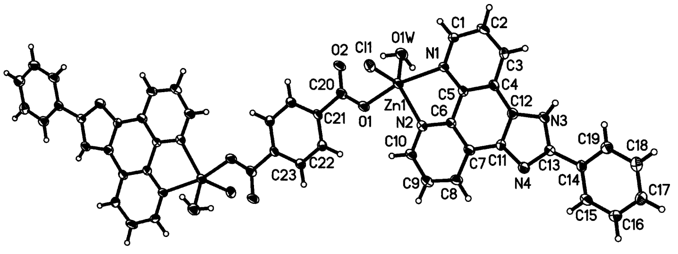


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by ($-x, 1-y, 1-z$).

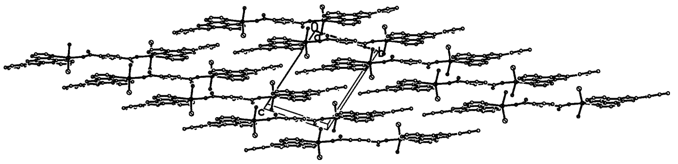


Figure 2
View of the two-dimensional supramolecular structure of (I), generated by intermolecular π–π interactions.

exists between two *L* ligands (*ca* 3.442 Å), while the other exists between the *L* and BDC ligands (*ca* 3.709 Å). It is clear that aromatic–aromatic interactions help to stabilize this and related architectures (Noveron *et al.*, 2002).

Experimental

The *L* ligand was synthesized according to the reported method (Collins *et al.*, 1998). Complex (I) was self-assembled from *L*, $ZnCl_2 \cdot H_2O$ and H_2BDC. A methanol solution (10 ml) of *L* (0.5 mmol) was added slowly to an aqueous solution (10 ml) of $ZnCl_2 \cdot H_2O$ (0.5 mmol) and H_2BDC (1 mmol) with stirring. The resulting solution was filtered and the filtrate allowed to stand in air at room temperature for several days, yielding pale-yellow crystals of (I) (68% yield based on Zn).

Crystal data

$[Zn_2(C_8H_4O_4)Cl_2(C_{19}H_{12}N_4)_2(H_2O)_2]$
$M_r = 994.44$
Triclinic, $P\overline{1}$
$a = 9.0702$ (18) Å
$b = 9.1815$ (18) Å
$c = 12.642$ (3) Å
$\alpha = 103.54$ (3)°
$\beta = 98.01$ (3)°
$\gamma = 100.49$ (3)°
$V = 988.0$ (4) Å^3
$Z = 1$
$D_x = 1.671$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.42$ mm^{-1}
$T = 292$ (2) K
Block, pale yellow
0.34 × 0.30 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.651$, $T_{max} = 0.744$
9673 measured reflections
4441 independent reflections
2309 reflections with $I > 2\sigma(I)$
$R_{int} = 0.093$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.235$
$S = 0.98$
4441 reflections
298 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1295P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.08$ e Å^{-3}
$\Delta\rho_{min} = -0.85$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Zn1	2.157 (5)	O1*W*—Zn1	2.084 (6)
N2—Zn1	2.088 (6)	Zn1—Cl1	2.275 (2)
O1—Zn1	2.051 (5)		
O1—Zn1—O1*W*	87.8 (2)	N2—Zn1—N1	78.2 (2)
O1—Zn1—N2	90.7 (2)	O1—Zn1—Cl1	99.75 (17)
O1*W*—Zn1—N2	127.5 (2)	O1*W*—Zn1—Cl1	117.30 (18)
O1—Zn1—N1	163.8 (2)	N2—Zn1—Cl1	114.64 (18)
O1*W*—Zn1—N1	89.7 (2)	N1—Zn1—Cl1	95.60 (17)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H*W*11···O2	0.84 (6)	1.96 (4)	2.769 (7)	160 (9)
N3—H3*B*···Cl1^{i}	0.81 (11)	2.57 (11)	3.264 (6)	144 (9)

Symmetry code: (i) $x, y+1, z$.

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Aqua H atoms were located in difference Fourier maps and refined with O—H = 0.85 Å and $U_{iso}(H) = 1.2U_{eq}(O)$. The N-bound H atom was located in a difference Fourier map and refined freely, with $U_{iso}(H) = 1.2U_{eq}(N)$. The highest residual density peak was located 0.87 Å from atom H2.

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: *SHELXTL-Plus* (Siemens, 1990); software used to prepare material for publication: *SHELXL97*.

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