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Poly[bis(μ_3-benzene-1,3-dicarboxylato)-[μ_2-4,4′-(propane-1,3-diyl)dipyridine]-dizinc(II)]

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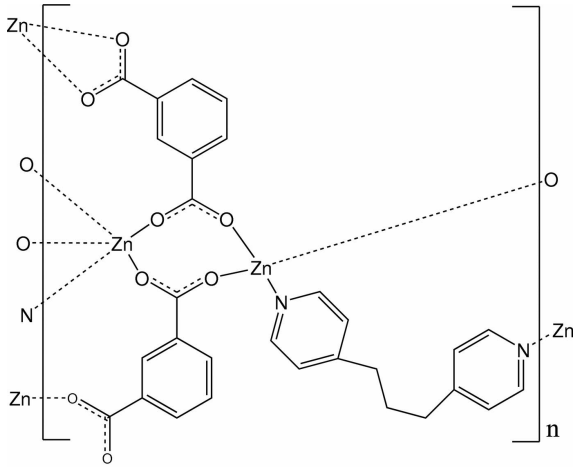
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.106; data-to-parameter ratio = 17.4.

The solvothermal reaction of zinc nitrate with 4,4′-(propane-1,3-diyl)dipyridine and benzene-1,3-dicarboxylic acid in water and ethanol gave the title complex, $[Zn_2(C_8H_4O_4)_2(C_{13}H_{14}N_2)]_n$. The structure displays distorted tetrahedral ZnO_3N and square-pyramidal ZnO_4N groups.

Related literature

For related literature, see: Chen *et al.* (2006); Kitagawa *et al.* (2004).



Experimental

Crystal data

$[Zn_2(C_8H_4O_4)_2(C_{13}H_{14}N_2)]$
M_r = 657.23
Triclinic, $P\overline{1}$
a = 9.4165 (3) Å
b = 9.8777 (3) Å
c = 15.2418 (5) Å
α = 80.705 (1)°
β = 72.990 (1)°
γ = 75.519 (1)°
V = 1306.61 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 295 (2) K
0.25 × 0.10 × 0.05 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.786, T_{max} = 0.952
9800 measured reflections
6441 independent reflections
4724 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.106
S = 0.90
6441 reflections
370 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2441).

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supplementary materials

Acta Cryst. (2007). E**63**, m2341 [**doi:10.1107/S160053680703509X**]

Poly[bis(μ_3-benzene-1,3-dicarboxylato)[μ_2-4,4'-(propane-1,3-diyl)dipyridine]dizinc(II)]

C.-H. Lin and T.-H. Tsao

Comment

The synthesis of coordination polymers, or so-called metal-organic framework (MOF), has been a subject of intense research owing to their interesting structural chemistry and potential applications in gas storage, separation, catalysis, magnetism, luminescence. A large number of these materials have been synthesized by hydro(solvo)thermal reactions with organic pyridines and carboxyl acids (Kitagawa *et al.*, 2004). They commonly adopt 3-D framework structures *via* employed metal ions as connectors and rigid or flexible organic ligands as linkers. As a further study of such complex, we report the title compound (Fig. 1) which is isotypic with $[ZnCo(C_{13}H_{14}N_2)(C_8H_4O_4)_2]_n$ (Chen *et al.*, 2006) (Fig. 2). All the geometric parameters are within normal ranges. The two Zn sites are four- and five-coordinated by the one N atoms of the 4,4'-(propane-1,3-diyl)dipyridines and three or four O atoms of the carboxylate anions, giving distorted tetrahedra and square pyramidal geometry.

Experimental

Solvothermal reactions were carried out at 150 °C for 2 d in a Teflon-lined acid digestion bomb with an internal volume of 23 ml followed by slow cooling at 6 °C/h to room temperature. A single-phase product consisting of transparent colorless crystals of was obtained from a mixture of 4,4'-(propane-1,3-diyl)dipyridine ($C_{14}H_{14}N_2$, 0.0861 g), $Zn(NO_3)\cdot 6H_2O$ (0.0891 g), 1, 3-benzene dicarboxyl acid ($C_8H_6O_4$, 0.0726 g), H_2O (5.0 ml), ethancol (5.0 ml). Powder X-ray diffraction measurements were performed to confirm the phase purity before all chemical and physical analyses. Thermal analyses, using a Perkin- Elmer TGA7 thermal analyzer, were performed on powder samples under flowing oxygen with a heating rate of 10 °C/min. A total weight loss of 67.81% was observed from 350 to 500 °C.

Refinement

H atoms were constrained to ideal geometries, with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

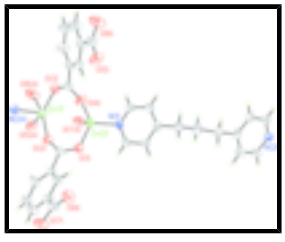

Fig. 1. *ORTEP* drawing of the building unit in $[Zn_2(C_{13}H_{14}N_2)(C_8H_4O_4)_2]_n$. Thermal ellipsoids are drawn at the 50% level.

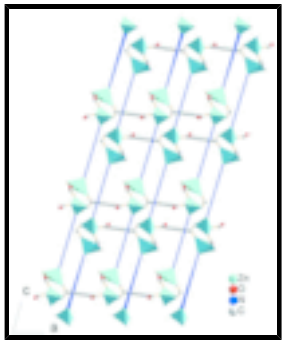

Fig. 2. View of $[Zn_2(C_{13}H_{14}N_2)(C_8H_4O_4)_2]_n$ along the [010] direction.

Poly[bis(μ$_3$-benzene-1,3-dicarboxylato)[μ$_2$-4,4'-(propane-1,3-\ diyl)dipyridine]dizinc(II)]

Crystal data

$[Zn_2(C_8H_4O_4)_2(C_{13}H_{14}N_2)]$	$Z = 2$
$M_r = 657.23$	$F_{000} = 668$
Triclinic, $P\overline{1}$	$D_x = 1.671$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 9.4165$ (3) Å	Cell parameters from 3205 reflections
$b = 9.8777$ (3) Å	θ = 2.4–28.1º
$c = 15.2418$ (5) Å	μ = 1.89 mm^{-1}
α = 80.7050 (10)º	$T = 295$ (2) K
β = 72.9900 (10)º	Tabular, colourless
γ = 75.5190 (10)º	0.25 × 0.10 × 0.05 mm
$V = 1306.61$ (7) Å^3	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer	6441 independent reflections
Radiation source: fine-focus sealed tube	4724 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 295(2)$ K	$\theta_{max} = 28.3$º
φ and ω scans	$\theta_{min} = 1.4$º
Absorption correction: ψ scan (SADABS; Sheldrick, 1996)	$h = -11\rightarrow12$
$T_{min} = 0.786$, $T_{max} = 0.952$	$k = -13\rightarrow13$
9800 measured reflections	$l = -20\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.106$	$w = 1/[\sigma^2(F_o^2) + (0.1083P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.90$	$(\Delta/\sigma)_{max} = 0.016$
6441 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
370 parameters	$\Delta\rho_{min} = -0.47$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.24424 (4)	0.91047 (3)	0.30445 (2)	0.03279 (10)
Zn2	0.30801 (3)	1.12768 (3)	0.10530 (2)	0.03108 (10)
O1	0.5236 (2)	1.0389 (2)	0.10058 (15)	0.0374 (5)
O2	0.4608 (2)	0.8956 (2)	0.22778 (14)	0.0370 (5)
O3	0.1155 (2)	1.10300 (19)	0.32168 (15)	0.0384 (5)
O4	0.2380 (2)	1.2418 (2)	0.21163 (15)	0.0430 (5)
O5	0.2433 (3)	0.7031 (2)	0.29929 (16)	0.0493 (6)
O6	0.0313 (3)	0.8241 (2)	0.3759 (2)	0.0635 (8)
O7	0.2099 (2)	0.9677 (2)	0.12935 (19)	0.0496 (6)
O8	0.0359 (3)	1.1476 (2)	0.09523 (18)	0.0514 (6)
N1	0.3400 (2)	1.2901 (2)	0.00864 (16)	0.0304 (5)
N2	0.3140 (3)	0.8916 (2)	0.42573 (18)	0.0366 (6)
C1	0.5553 (3)	0.9446 (3)	0.1619 (2)	0.0288 (6)
C2	0.3959 (3)	1.5303 (3)	−0.1078 (2)	0.0335 (6)
C3	0.1435 (3)	1.2198 (3)	0.2870 (2)	0.0310 (6)
C4	0.0580 (3)	1.3460 (3)	0.3379 (2)	0.0316 (6)
C5	0.7206 (3)	0.8859 (3)	0.15572 (19)	0.0290 (6)
C6	0.8239 (3)	0.9735 (3)	0.1293 (2)	0.0313 (6)
H6A	0.7918	1.0679	0.1107	0.038*
C7	0.9741 (3)	0.9211 (3)	0.1305 (2)	0.0325 (6)
C8	0.0772 (3)	1.0214 (3)	0.1158 (2)	0.0374 (7)
C9	0.2393 (3)	0.9684 (3)	0.4961 (2)	0.0386 (7)
H9A	0.1567	1.0402	0.4894	0.046*
C10	0.1208 (3)	1.4650 (3)	0.3214 (2)	0.0335 (6)
H10A	0.2167	1.4635	0.2811	0.040*
C11	0.0412 (3)	1.5849 (3)	0.3647 (2)	0.0357 (7)

C12	0.4767 (3)	1.2924 (3)	−0.0497 (2)	0.0320 (6)
H12A	0.5540	1.2125	−0.0501	0.038*
C13	0.4312 (4)	1.6593 (3)	−0.1683 (2)	0.0388 (7)
H13A	0.5396	1.6541	−0.1822	0.047*
H13B	0.3797	1.7403	−0.1341	0.047*
C14	0.3868 (4)	1.6832 (3)	−0.2583 (2)	0.0458 (8)
H14A	0.2770	1.7006	−0.2455	0.055*
H14B	0.4296	1.5994	−0.2907	0.055*
C15	0.2786 (4)	0.9464 (3)	0.5782 (2)	0.0410 (7)
H15A	0.2233	1.0031	0.6253	0.049*
C16	0.7711 (3)	0.7437 (3)	0.1791 (2)	0.0360 (7)
H16A	0.7021	0.6852	0.1996	0.043*
C17	0.2297 (3)	1.4065 (3)	0.0089 (2)	0.0381 (7)
H17A	0.1340	1.4056	0.0489	0.046*
C18	1.0247 (3)	0.7780 (3)	0.1493 (2)	0.0413 (7)
H18A	1.1268	0.7414	0.1467	0.050*
C19	0.3998 (3)	0.8405 (3)	0.5909 (2)	0.0383 (7)
C20	0.5074 (3)	1.4081 (3)	−0.1089 (2)	0.0346 (6)
H20A	0.6032	1.4045	−0.1498	0.042*
C21	0.9238 (4)	0.6891 (3)	0.1719 (3)	0.0449 (8)
H21A	0.9589	0.5927	0.1823	0.054*
C22	0.2527 (3)	1.5271 (3)	−0.0475 (2)	0.0399 (7)
H22A	0.1736	1.6057	−0.0454	0.048*
C23	−0.1021 (4)	1.5875 (3)	0.4233 (3)	0.0504 (9)
H23A	−0.1569	1.6685	0.4514	0.061*
C24	0.4332 (4)	0.7888 (3)	0.4376 (2)	0.0486 (8)
H24A	0.4881	0.7343	0.3893	0.058*
C25	0.4438 (4)	1.8087 (3)	−0.3196 (2)	0.0458 (8)
H25A	0.4035	1.8912	−0.2858	0.055*
H25B	0.5538	1.7896	−0.3329	0.055*
C26	0.4765 (4)	0.7614 (3)	0.5178 (2)	0.0489 (8)
H26A	0.5588	0.6886	0.5233	0.059*
C27	−0.0833 (4)	1.3491 (3)	0.3989 (3)	0.0459 (8)
H27A	−0.1243	1.2693	0.4124	0.055*
C28	−0.1645 (4)	1.4701 (3)	0.4403 (3)	0.0610 (11)
H28A	−0.2612	1.4724	0.4797	0.073*
C29	0.1086 (4)	0.7124 (3)	0.3468 (2)	0.0399 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03078 (18)	0.02288 (16)	0.0417 (2)	−0.01015 (13)	−0.00201 (15)	−0.00176 (13)
Zn2	0.02863 (18)	0.02833 (17)	0.0366 (2)	−0.01020 (13)	−0.00876 (14)	0.00277 (13)
O1	0.0292 (10)	0.0389 (11)	0.0433 (13)	−0.0121 (8)	−0.0106 (9)	0.0084 (9)
O2	0.0273 (10)	0.0429 (11)	0.0391 (12)	−0.0130 (8)	−0.0049 (9)	0.0024 (9)
O3	0.0415 (12)	0.0244 (9)	0.0452 (13)	−0.0114 (8)	−0.0043 (10)	0.0013 (9)
O4	0.0519 (13)	0.0372 (11)	0.0392 (13)	−0.0224 (10)	0.0025 (10)	−0.0082 (9)
O5	0.0537 (14)	0.0450 (12)	0.0490 (14)	−0.0304 (11)	0.0059 (11)	−0.0095 (11)

O6	0.0561 (15)	0.0274 (11)	0.107 (2)	−0.0089 (11)	−0.0170 (15)	−0.0150 (13)
O7	0.0226 (10)	0.0428 (12)	0.0868 (19)	−0.0120 (9)	−0.0108 (11)	−0.0146 (12)
O8	0.0489 (14)	0.0424 (12)	0.0679 (17)	−0.0229 (10)	−0.0192 (12)	0.0085 (11)
N1	0.0292 (12)	0.0281 (11)	0.0324 (13)	−0.0063 (9)	−0.0070 (10)	−0.0002 (9)
N2	0.0374 (14)	0.0303 (12)	0.0376 (14)	−0.0067 (10)	−0.0042 (11)	−0.0025 (10)
C1	0.0249 (13)	0.0296 (13)	0.0361 (16)	−0.0107 (11)	−0.0091 (12)	−0.0055 (11)
C2	0.0398 (16)	0.0302 (14)	0.0329 (15)	−0.0106 (12)	−0.0123 (13)	0.0001 (11)
C3	0.0273 (14)	0.0290 (13)	0.0384 (16)	−0.0084 (11)	−0.0101 (12)	−0.0015 (12)
C4	0.0303 (14)	0.0245 (13)	0.0392 (17)	−0.0093 (11)	−0.0065 (12)	−0.0005 (11)
C5	0.0256 (13)	0.0323 (14)	0.0315 (15)	−0.0101 (11)	−0.0092 (11)	−0.0010 (11)
C6	0.0270 (13)	0.0307 (13)	0.0362 (16)	−0.0093 (11)	−0.0063 (12)	−0.0020 (11)
C7	0.0263 (14)	0.0378 (15)	0.0361 (16)	−0.0116 (11)	−0.0065 (12)	−0.0066 (12)
C8	0.0257 (14)	0.0468 (17)	0.0417 (18)	−0.0153 (12)	−0.0022 (13)	−0.0107 (14)
C9	0.0388 (16)	0.0299 (14)	0.0434 (18)	−0.0033 (12)	−0.0084 (14)	−0.0041 (13)
C10	0.0341 (15)	0.0271 (13)	0.0370 (16)	−0.0132 (11)	−0.0026 (13)	0.0011 (12)
C11	0.0369 (16)	0.0246 (13)	0.0439 (18)	−0.0117 (11)	−0.0045 (13)	−0.0014 (12)
C12	0.0284 (14)	0.0280 (13)	0.0368 (16)	−0.0027 (11)	−0.0073 (12)	−0.0024 (11)
C13	0.0461 (18)	0.0315 (14)	0.0405 (18)	−0.0148 (13)	−0.0127 (14)	0.0050 (13)
C14	0.057 (2)	0.0438 (17)	0.0442 (19)	−0.0259 (15)	−0.0205 (17)	0.0104 (14)
C15	0.0496 (18)	0.0342 (15)	0.0372 (17)	−0.0087 (13)	−0.0072 (15)	−0.0062 (13)
C16	0.0339 (15)	0.0327 (14)	0.0478 (19)	−0.0138 (12)	−0.0168 (14)	−0.0003 (13)
C17	0.0267 (14)	0.0403 (16)	0.0392 (17)	−0.0045 (12)	−0.0001 (13)	−0.0011 (13)
C18	0.0276 (15)	0.0423 (16)	0.059 (2)	−0.0053 (12)	−0.0186 (15)	−0.0076 (15)
C19	0.0435 (17)	0.0345 (15)	0.0368 (17)	−0.0176 (13)	−0.0082 (14)	0.0065 (13)
C20	0.0308 (15)	0.0367 (15)	0.0325 (16)	−0.0092 (12)	−0.0020 (12)	−0.0008 (12)
C21	0.0403 (17)	0.0327 (15)	0.069 (2)	−0.0052 (13)	−0.0287 (17)	−0.0048 (15)
C22	0.0340 (16)	0.0306 (14)	0.0487 (19)	0.0018 (12)	−0.0089 (14)	−0.0029 (13)
C23	0.0416 (18)	0.0315 (16)	0.069 (2)	−0.0091 (13)	0.0055 (17)	−0.0150 (15)
C24	0.0465 (19)	0.0460 (18)	0.042 (2)	0.0059 (15)	−0.0057 (16)	−0.0095 (15)
C25	0.058 (2)	0.0431 (17)	0.0401 (19)	−0.0219 (15)	−0.0161 (16)	0.0071 (14)
C26	0.0408 (18)	0.0487 (19)	0.046 (2)	0.0058 (15)	−0.0097 (16)	0.0005 (15)
C27	0.0411 (17)	0.0290 (14)	0.064 (2)	−0.0169 (13)	−0.0002 (16)	−0.0052 (14)
C28	0.0400 (19)	0.0398 (18)	0.087 (3)	−0.0165 (15)	0.0186 (19)	−0.0128 (18)
C29	0.0487 (19)	0.0289 (14)	0.0449 (19)	−0.0182 (13)	−0.0102 (15)	0.0001 (13)

Geometric parameters (Å, °)

Zn1—O3	1.9944 (19)	C9—H9A	0.9300
Zn1—O2	2.0142 (19)	C10—C11	1.385 (4)
Zn1—O5	2.065 (2)	C10—H10A	0.9300
Zn1—N2	2.103 (3)	C11—C23	1.380 (4)
Zn1—O6	2.283 (2)	C11—C29^{iii}	1.501 (4)
Zn1—C29	2.497 (3)	C12—C20	1.372 (4)
Zn2—O7	1.957 (2)	C12—H12A	0.9300
Zn2—O4	1.981 (2)	C13—C14	1.514 (4)
Zn2—O1	1.9848 (19)	C13—H13A	0.9700
Zn2—N1	2.014 (2)	C13—H13B	0.9700
Zn2—C8	2.595 (3)	C14—C25	1.537 (4)
O1—C1	1.255 (3)	C14—H14A	0.9700

O2—C1	1.253 (3)	C14—H14B	0.9700
O3—C3	1.246 (3)	C15—C19	1.378 (4)
O4—C3	1.256 (3)	C15—H15A	0.9300
O5—C29	1.252 (4)	C16—C21	1.382 (4)
O6—C29	1.229 (4)	C16—H16A	0.9300
O7—C8	1.292 (3)	C17—C22	1.376 (4)
O8—C8	1.227 (4)	C17—H17A	0.9300
N1—C12	1.336 (3)	C18—C21	1.385 (4)
N1—C17	1.342 (3)	C18—H18A	0.9300
N2—C9	1.332 (4)	C19—C26	1.378 (5)
N2—C24	1.347 (4)	C19—C25^{iv}	1.503 (4)
C1—C5	1.499 (3)	C20—H20A	0.9300
C2—C20	1.387 (4)	C21—H21A	0.9300
C2—C22	1.397 (4)	C22—H22A	0.9300
C2—C13	1.496 (4)	C23—C28	1.383 (4)
C3—C4	1.500 (4)	C23—H23A	0.9300
C4—C27	1.378 (4)	C24—C26	1.366 (5)
C4—C10	1.400 (4)	C24—H24A	0.9300
C5—C16	1.390 (4)	C25—C19^{v}	1.503 (4)
C5—C6	1.392 (3)	C25—H25A	0.9700
C6—C7	1.383 (4)	C25—H25B	0.9700
C6—H6A	0.9300	C26—H26A	0.9300
C7—C18	1.385 (4)	C27—C28	1.384 (5)
C7—C8^{i}	1.502 (4)	C27—H27A	0.9300
C8—C7^{ii}	1.502 (4)	C28—H28A	0.9300
C9—C15	1.377 (4)	C29—C11^{vi}	1.501 (4)
O3—Zn1—O2	117.24 (8)	C4—C10—H10A	119.8
O3—Zn1—O5	144.99 (9)	C23—C11—C10	119.6 (2)
O2—Zn1—O5	94.47 (8)	C23—C11—C29^{iii}	120.0 (3)
O3—Zn1—N2	94.66 (9)	C10—C11—C29^{iii}	120.4 (3)
O2—Zn1—N2	90.59 (9)	N1—C12—C20	122.6 (2)
O5—Zn1—N2	99.74 (10)	N1—C12—H12A	118.7
O3—Zn1—O6	88.02 (8)	C20—C12—H12A	118.7
O2—Zn1—O6	153.83 (8)	C2—C13—C14	115.5 (2)
O5—Zn1—O6	59.36 (8)	C2—C13—H13A	108.4
N2—Zn1—O6	94.23 (10)	C14—C13—H13A	108.4
O3—Zn1—C29	116.59 (9)	C2—C13—H13B	108.4
O2—Zn1—C29	124.47 (10)	C14—C13—H13B	108.4
O5—Zn1—C29	30.00 (9)	H13A—C13—H13B	107.5
N2—Zn1—C29	97.81 (10)	C13—C14—C25	111.1 (3)
O6—Zn1—C29	29.37 (9)	C13—C14—H14A	109.4
O7—Zn2—O4	111.71 (10)	C25—C14—H14A	109.4
O7—Zn2—O1	103.59 (8)	C13—C14—H14B	109.4
O4—Zn2—O1	104.62 (9)	C25—C14—H14B	109.4
O7—Zn2—N1	138.30 (10)	H14A—C14—H14B	108.0
O4—Zn2—N1	95.43 (9)	C19—C15—C9	120.1 (3)
O1—Zn2—N1	99.11 (8)	C19—C15—H15A	119.9

O7—Zn2—C8	28.87 (9)	C9—C15—H15A	119.9
O4—Zn2—C8	103.93 (9)	C21—C16—C5	120.1 (3)
O1—Zn2—C8	131.74 (9)	C21—C16—H16A	120.0
N1—Zn2—C8	115.91 (10)	C5—C16—H16A	120.0
C1—O1—Zn2	120.01 (17)	N1—C17—C22	122.6 (3)
C1—O2—Zn1	148.88 (18)	N1—C17—H17A	118.7
C3—O3—Zn1	130.23 (19)	C22—C17—H17A	118.7
C3—O4—Zn2	126.95 (18)	C7—C18—C21	120.3 (3)
C29—O5—Zn1	94.45 (18)	C7—C18—H18A	119.9
C29—O6—Zn1	84.99 (19)	C21—C18—H18A	119.9
C8—O7—Zn2	104.15 (18)	C15—C19—C26	116.5 (3)
C12—N1—C17	118.1 (2)	C15—C19—C25^{iv}	122.2 (3)
C12—N1—Zn2	120.91 (18)	C26—C19—C25^{iv}	121.2 (3)
C17—N1—Zn2	120.47 (19)	C12—C20—C2	120.1 (3)
C9—N2—C24	117.0 (3)	C12—C20—H20A	119.9
C9—N2—Zn1	123.8 (2)	C2—C20—H20A	119.9
C24—N2—Zn1	119.0 (2)	C16—C21—C18	120.0 (3)
O1—C1—O2	125.6 (2)	C16—C21—H21A	120.0
O1—C1—C5	117.0 (2)	C18—C21—H21A	120.0
O2—C1—C5	117.4 (2)	C17—C22—C2	119.4 (3)
C20—C2—C22	117.1 (2)	C17—C22—H22A	120.3
C20—C2—C13	120.4 (3)	C2—C22—H22A	120.3
C22—C2—C13	122.5 (3)	C11—C23—C28	120.2 (3)
O3—C3—O4	125.4 (3)	C11—C23—H23A	119.9
O3—C3—C4	118.4 (3)	C28—C23—H23A	119.9
O4—C3—C4	116.3 (2)	N2—C24—C26	122.5 (3)
C27—C4—C10	119.0 (3)	N2—C24—H24A	118.8
C27—C4—C3	121.5 (2)	C26—C24—H24A	118.8
C10—C4—C3	119.4 (3)	C19^{v}—C25—C14	113.8 (3)
C16—C5—C6	119.3 (2)	C19^{v}—C25—H25A	108.8
C16—C5—C1	120.1 (2)	C14—C25—H25A	108.8
C6—C5—C1	120.6 (2)	C19^{v}—C25—H25B	108.8
C7—C6—C5	120.5 (2)	C14—C25—H25B	108.8
C7—C6—H6A	119.8	H25A—C25—H25B	107.7
C5—C6—H6A	119.8	C24—C26—C19	120.8 (3)
C6—C7—C18	119.4 (2)	C24—C26—H26A	119.6
C6—C7—C8^{i}	119.2 (2)	C19—C26—H26A	119.6
C18—C7—C8^{i}	121.3 (3)	C4—C27—C28	120.4 (3)
O8—C8—O7	122.0 (3)	C4—C27—H27A	119.8
O8—C8—C7^{ii}	121.9 (3)	C28—C27—H27A	119.8
O7—C8—C7^{ii}	116.0 (3)	C27—C28—C23	120.2 (3)
O8—C8—Zn2	75.05 (16)	C27—C28—H28A	119.9
O7—C8—Zn2	46.98 (13)	C23—C28—H28A	119.9
C7^{ii}—C8—Zn2	163.0 (2)	O6—C29—O5	121.2 (3)
N2—C9—C15	123.1 (3)	O6—C29—C11^{vi}	120.4 (3)
N2—C9—H9A	118.5	O5—C29—C11^{vi}	118.4 (3)

C15—C9—H9A	118.5	O6—C29—Zn1	65.64 (16)
C11—C10—C4	120.5 (3)	O5—C29—Zn1	55.55 (14)
C11—C10—H10A	119.8	C11^{vi}—C29—Zn1	173.8 (2)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*−1, *y*, *z*; (iii) *x*, *y*+1, *z*; (iv) *x*, *y*−1, *z*+1; (v) *x*, *y*+1, *z*−1; (vi) *x*, *y*−1, *z*.

Fig. 1

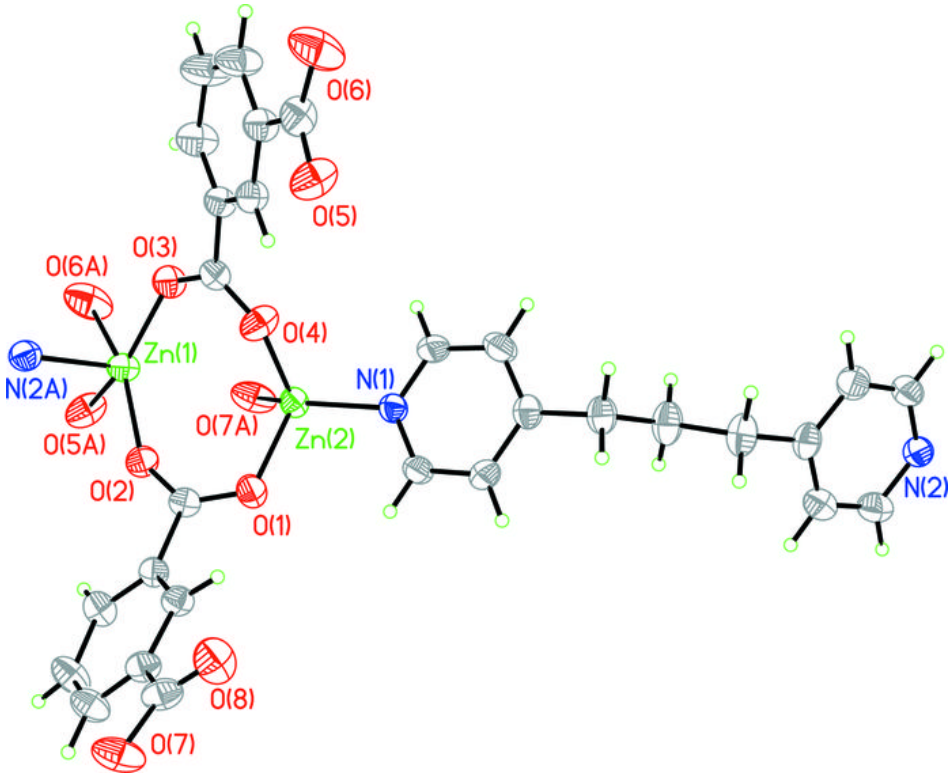

Fig. 2