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catena-Poly[zinc(II)-bis[μ_2-3-(3-pyridyl)-benzoato]-$\kappa^2O{:}N;\kappa^2N{:}O$]

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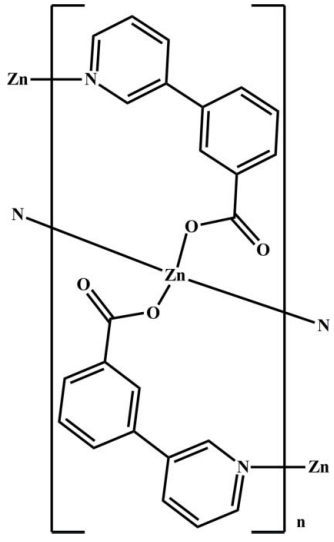
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.095; data-to-parameter ratio = 12.9.

In the title compound, $[Zn(C_{12}H_8NO_2)_2]_n$, the Zn^{2+} cation is coordinated by a pair of carboxylate O atoms as well as two pyridyl N atoms to afford a distorted tetrahedral environment. Adjacent Zn^{2+} cations, with a separation of 8.807 (2) Å, are linked by two 3-(3-pyridyl)benzoate ligand bridges, generating an infinite ribbon extending parallel to [001].

Related literature

For the use of 3-(pyridin-3-yl)benzoate units in the construction of framework structures, see: Guo (2009). For a similar structure, see: Zhong *et al.* (2008).



Experimental

Crystal data

$[Zn(C_{12}H_8NO_2)_2]$
M_r = 461.76
Monoclinic, $P2_1/c$
a = 10.0512 (8) Å
b = 12.0809 (10) Å
c = 17.4872 (14) Å
β = 105.631 (1)°
V = 2044.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 273 K
0.15 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.836, T_{max} = 0.908
10620 measured reflections
3616 independent reflections
2253 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.095
S = 1.08
3616 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: NG5177).

References

Bruker (1997). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Guo, F. (2009). *J. Coord. Chem.* **62**, 3621–3628.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhong, R.-Q., Zou, R.-Q., Du, M., Jiang, L., Yamada, T., Maruta, G., Takeda, S. & Xu, Q. (2008). *CrystEngComm*, **10**, 605–613.

supporting information

Acta Cryst. (2011). E**67**, m894 [doi:10.1107/S1600536811021404]

catena-Poly[zinc(II)-bis[μ_2-3-(3-pyridyl)benzoato]-κ^2O:N;κ^2N:O]

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S1. Comment

In the structure of the title compound, the Zn^{2+} center is located at the general site and coordinated by a pair of carboxylate oxygen atoms as well as two pyridyl nitrogen donors to afford a tetrahedral environment (see Fig. 1). As a result, the Zn^{2+} ions are connected by the 3-(pyridin-3-yl)benzoate spacers to result in a in?nite 1D double-strand chain motif, with the Zn···Zn separation of 8.807Å, as shown in Fig. 2.

S2. Experimental

The title compound was prepared by hydrothermal method. An aqueous solution (20 mL) containing 3-(pyridin-3-yl)benzoate acid (0.10 mmol) and Zinc nitrate hexahydrate (0.10 mmol) was placed in a Parr Te?on-lined stainless steel vessel (25 mL) under autogenous pressure, which was heated to 433 K for 72 h and subsequently cooled to room temperature at a rate of 5 K an hour. Colorless single crystals were obtained from the reaction mixture (yield ca 46% based on Zn).

S3. Refinement

The C-bound H atoms were geometrically placed (C—H = 0.93 Å) and refined as riding with U_{iso}(H) =1.2U_{eq}(C).

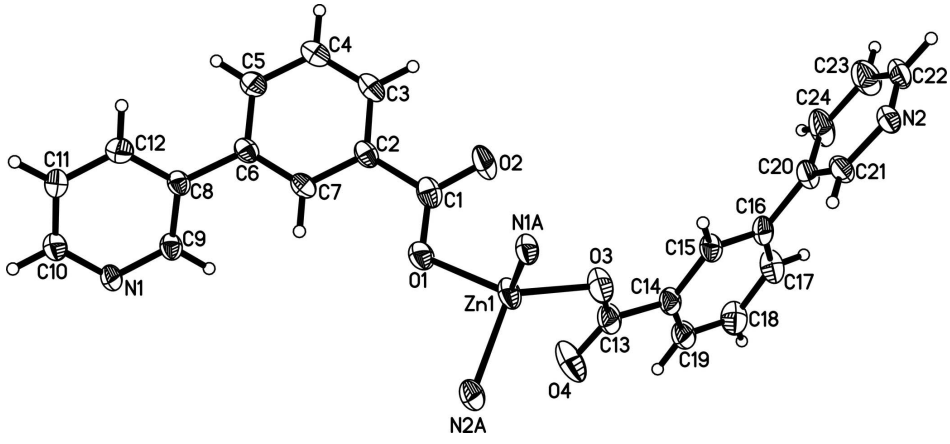

Figure 1

Thermal ellipsoid plot of the title compound at the 30% probability level, hydrogen atoms are drawn as sphere of arbitrary radius.

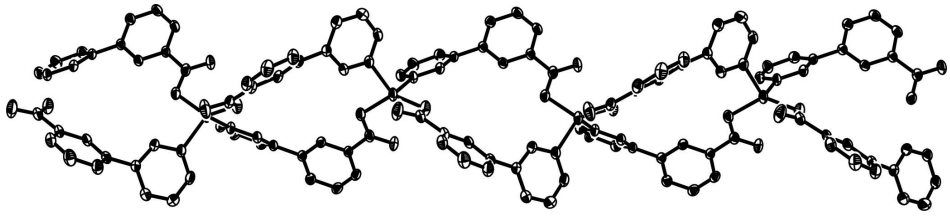

Figure 2

The 1D chain of the title compound, viewed down the c axis.

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$b = 12.0809$ (10) Å
$c = 17.4872$ (14) Å
$\beta = 105.631$ (1)°
$V = 2044.9$ (3) Å^3
$Z = 4$
$F(000) = 944$
$D_x = 1.500$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1527 reflections
$\theta = 2.4$–$21.1°$
$\mu = 1.24$ mm^{-1}
$T = 273$ K
Block, colourless
0.15 × 0.10 × 0.08 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.836$, $T_{max} = 0.908$
10620 measured reflections
3616 independent reflections
2253 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.1°$
$h = -5\rightarrow11$
$k = -14\rightarrow14$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.095$
$S = 1.08$
3616 reflections
280 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.54736 (4)	0.79354 (4)	0.82510 (2)	0.04985 (17)
C1	0.4220 (4)	0.6225 (3)	0.8717 (2)	0.0479 (9)
C2	0.3496 (3)	0.5541 (3)	0.92062 (18)	0.0401 (9)
C3	0.2852 (4)	0.4556 (3)	0.8909 (2)	0.0478 (10)
H3	0.2882	0.4309	0.8410	0.057*
C4	0.2170 (4)	0.3943 (3)	0.9347 (2)	0.0525 (10)
H4	0.1750	0.3279	0.9146	0.063*
C5	0.2105 (4)	0.4308 (3)	1.0087 (2)	0.0473 (9)
H5	0.1635	0.3893	1.0379	0.057*
C6	0.2743 (3)	0.5295 (3)	1.03928 (18)	0.0389 (9)
C7	0.3441 (3)	0.5902 (3)	0.99507 (18)	0.0415 (9)
H7	0.3879	0.6558	1.0155	0.050*
C8	0.2645 (4)	0.5697 (3)	1.11789 (18)	0.0379 (8)
C9	0.3784 (4)	0.6111 (3)	1.17361 (18)	0.0415 (9)
H9	0.4620	0.6142	1.1604	0.050*
C10	0.2537 (4)	0.6462 (3)	1.2631 (2)	0.0519 (10)
H10	0.2495	0.6732	1.3123	0.062*
C11	0.1359 (4)	0.6076 (3)	1.2119 (2)	0.0556 (11)
H11	0.0529	0.6080	1.2259	0.067*
C12	0.1416 (4)	0.5679 (3)	1.1389 (2)	0.0512 (10)
H12	0.0624	0.5397	1.1037	0.061*
C13	0.7782 (4)	0.7247 (3)	0.7844 (2)	0.0525 (10)
C14	0.8517 (4)	0.6655 (3)	0.73188 (19)	0.0444 (9)
C15	0.7794 (4)	0.6278 (3)	0.65703 (19)	0.0449 (9)
H15	0.6856	0.6430	0.6380	0.054*
C16	0.8458 (4)	0.5675 (3)	0.6104 (2)	0.0474 (10)
C17	0.9861 (4)	0.5446 (3)	0.6400 (2)	0.0607 (11)
H17	1.0310	0.5021	0.6102	0.073*
C18	1.0589 (4)	0.5845 (3)	0.7132 (2)	0.0664 (12)
H18	1.1535	0.5719	0.7317	0.080*
C19	0.9909 (4)	0.6432 (3)	0.7588 (2)	0.0553 (10)
H19	1.0400	0.6683	0.8087	0.066*
C20	0.7694 (4)	0.5294 (3)	0.52977 (19)	0.0475 (9)
C21	0.6937 (4)	0.6032 (3)	0.47544 (19)	0.0494 (10)
H21	0.6875	0.6758	0.4918	0.059*
C22	0.6343 (4)	0.4723 (4)	0.3773 (2)	0.0625 (12)
H22	0.5881	0.4524	0.3256	0.075*
C23	0.7069 (5)	0.3932 (4)	0.4277 (3)	0.0826 (15)
H23	0.7096	0.3207	0.4102	0.099*
C24	0.7762 (5)	0.4218 (4)	0.5045 (2)	0.0742 (13)

H24	0.8270	0.3691	0.5390	0.089*
N1	0.3752 (3)	0.6471 (2)	1.24571 (15)	0.0437 (7)
N2	0.6278 (3)	0.5766 (3)	0.39999 (16)	0.0497 (8)
O1	0.4801 (2)	0.7115 (2)	0.90317 (13)	0.0540 (7)
O2	0.4192 (3)	0.5923 (2)	0.80425 (14)	0.0648 (8)
O3	0.6515 (3)	0.7467 (2)	0.75352 (14)	0.0635 (8)
O4	0.8408 (3)	0.7481 (3)	0.85317 (16)	0.0880 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0573 (3)	0.0665 (3)	0.0242 (2)	0.0047 (2)	0.00805 (19)	0.0020 (2)
C1	0.050 (2)	0.059 (3)	0.031 (2)	0.013 (2)	0.0045 (18)	0.0057 (19)
C2	0.043 (2)	0.047 (2)	0.0264 (18)	0.0099 (18)	0.0020 (16)	0.0005 (16)
C3	0.054 (3)	0.052 (3)	0.032 (2)	0.013 (2)	0.0025 (18)	−0.0080 (18)
C4	0.057 (3)	0.051 (3)	0.044 (2)	0.000 (2)	0.004 (2)	−0.0111 (19)
C5	0.047 (2)	0.053 (3)	0.039 (2)	−0.0027 (19)	0.0055 (17)	−0.0026 (18)
C6	0.038 (2)	0.046 (2)	0.0277 (19)	0.0053 (18)	0.0002 (16)	−0.0003 (16)
C7	0.046 (2)	0.045 (2)	0.0298 (19)	0.0021 (17)	0.0026 (17)	−0.0033 (16)
C8	0.040 (2)	0.044 (2)	0.0280 (18)	0.0017 (17)	0.0063 (16)	0.0005 (15)
C9	0.041 (2)	0.052 (2)	0.031 (2)	0.0046 (18)	0.0090 (16)	0.0023 (16)
C10	0.062 (3)	0.057 (3)	0.040 (2)	−0.008 (2)	0.021 (2)	−0.0050 (19)
C11	0.053 (3)	0.067 (3)	0.055 (3)	−0.008 (2)	0.028 (2)	−0.013 (2)
C12	0.049 (3)	0.056 (3)	0.047 (2)	−0.008 (2)	0.0096 (19)	−0.0052 (19)
C13	0.068 (3)	0.056 (3)	0.033 (2)	0.005 (2)	0.014 (2)	0.0092 (18)
C14	0.051 (3)	0.052 (2)	0.0290 (19)	0.0014 (19)	0.0089 (18)	0.0098 (16)
C15	0.049 (2)	0.052 (2)	0.031 (2)	0.0046 (19)	0.0079 (17)	0.0097 (17)
C16	0.059 (3)	0.052 (2)	0.034 (2)	0.004 (2)	0.0172 (19)	0.0094 (17)
C17	0.062 (3)	0.080 (3)	0.043 (2)	0.019 (2)	0.018 (2)	0.005 (2)
C18	0.051 (3)	0.095 (4)	0.053 (3)	0.012 (2)	0.013 (2)	0.010 (2)
C19	0.058 (3)	0.070 (3)	0.035 (2)	−0.003 (2)	0.007 (2)	0.005 (2)
C20	0.064 (3)	0.047 (3)	0.033 (2)	0.005 (2)	0.0150 (18)	0.0004 (18)
C21	0.064 (3)	0.050 (2)	0.032 (2)	−0.003 (2)	0.0087 (18)	−0.0055 (17)
C22	0.094 (3)	0.062 (3)	0.035 (2)	−0.015 (3)	0.024 (2)	−0.011 (2)
C23	0.142 (5)	0.050 (3)	0.057 (3)	−0.003 (3)	0.029 (3)	−0.007 (2)
C24	0.123 (4)	0.058 (3)	0.044 (3)	0.018 (3)	0.026 (3)	0.010 (2)
N1	0.049 (2)	0.055 (2)	0.0286 (16)	−0.0032 (15)	0.0128 (14)	−0.0033 (14)
N2	0.061 (2)	0.056 (2)	0.0307 (17)	−0.0053 (16)	0.0102 (15)	−0.0023 (15)
O1	0.0694 (18)	0.0601 (18)	0.0311 (13)	−0.0095 (15)	0.0109 (12)	−0.0004 (12)
O2	0.088 (2)	0.078 (2)	0.0307 (15)	0.0024 (15)	0.0201 (14)	−0.0066 (13)
O3	0.0587 (19)	0.092 (2)	0.0411 (16)	0.0112 (16)	0.0162 (14)	−0.0029 (14)
O4	0.100 (2)	0.121 (3)	0.0370 (17)	0.028 (2)	0.0069 (16)	−0.0116 (17)

Geometric parameters (Å, º)

Zn1—O3	1.921 (2)	C12—H12	0.9300
Zn1—O1	1.949 (2)	C13—O4	1.230 (4)
Zn1—N1^{i}	2.035 (3)	C13—O3	1.270 (4)

Zn1—N2^{ii}	2.064 (3)	C13—C14	1.506 (5)
C1—O2	1.227 (4)	C14—C19	1.377 (5)
C1—O1	1.276 (4)	C14—C15	1.392 (4)
C1—C2	1.510 (5)	C15—C16	1.391 (5)
C2—C3	1.387 (5)	C15—H15	0.9300
C2—C7	1.388 (4)	C16—C17	1.393 (5)
C3—C4	1.374 (5)	C16—C20	1.485 (5)
C3—H3	0.9300	C17—C18	1.380 (5)
C4—C5	1.385 (4)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.379 (5)
C5—C6	1.391 (4)	C18—H18	0.9300
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.385 (4)	C20—C21	1.373 (5)
C6—C8	1.486 (4)	C20—C24	1.380 (5)
C7—H7	0.9300	C21—N2	1.346 (4)
C8—C12	1.380 (4)	C21—H21	0.9300
C8—C9	1.382 (4)	C22—N2	1.327 (4)
C9—N1	1.343 (4)	C22—C23	1.370 (5)
C9—H9	0.9300	C22—H22	0.9300
C10—N1	1.335 (4)	C23—C24	1.381 (5)
C10—C11	1.361 (5)	C23—H23	0.9300
C10—H10	0.9300	C24—H24	0.9300
C11—C12	1.380 (5)	N1—Zn1^{ii}	2.035 (3)
C11—H11	0.9300	N2—Zn1^{i}	2.064 (3)

O3—Zn1—O1	131.25 (11)	O4—C13—C14	120.0 (4)
O3—Zn1—N1^{i}	99.90 (11)	O3—C13—C14	116.1 (3)
O1—Zn1—N1^{i}	105.38 (11)	C19—C14—C15	118.8 (3)
O3—Zn1—N2^{ii}	116.65 (12)	C19—C14—C13	120.3 (3)
O1—Zn1—N2^{ii}	95.30 (11)	C15—C14—C13	120.8 (3)
N1^{i}—Zn1—N2^{ii}	106.30 (12)	C16—C15—C14	120.8 (3)
O2—C1—O1	123.7 (4)	C16—C15—H15	119.6
O2—C1—C2	119.4 (4)	C14—C15—H15	119.6
O1—C1—C2	116.8 (3)	C15—C16—C17	118.9 (3)
C3—C2—C7	119.3 (3)	C15—C16—C20	120.8 (3)
C3—C2—C1	120.3 (3)	C17—C16—C20	120.3 (3)
C7—C2—C1	120.4 (3)	C18—C17—C16	120.4 (4)
C4—C3—C2	120.4 (3)	C18—C17—H17	119.8
C4—C3—H3	119.8	C16—C17—H17	119.8
C2—C3—H3	119.8	C17—C18—C19	119.7 (4)
C3—C4—C5	120.4 (4)	C17—C18—H18	120.2
C3—C4—H4	119.8	C19—C18—H18	120.2
C5—C4—H4	119.8	C14—C19—C18	121.3 (4)
C4—C5—C6	119.9 (4)	C14—C19—H19	119.4
C4—C5—H5	120.0	C18—C19—H19	119.4
C6—C5—H5	120.0	C21—C20—C24	117.1 (3)
C7—C6—C5	119.3 (3)	C21—C20—C16	120.3 (3)
C7—C6—C8	120.9 (3)	C24—C20—C16	122.5 (3)

C5—C6—C8	119.8 (3)	N2—C21—C20	123.9 (3)
C6—C7—C2	120.7 (3)	N2—C21—H21	118.0
C6—C7—H7	119.6	C20—C21—H21	118.0
C2—C7—H7	119.6	N2—C22—C23	122.1 (4)
C12—C8—C9	116.7 (3)	N2—C22—H22	119.0
C12—C8—C6	121.9 (3)	C23—C22—H22	119.0
C9—C8—C6	121.4 (3)	C22—C23—C24	119.5 (4)
N1—C9—C8	123.6 (3)	C22—C23—H23	120.3
N1—C9—H9	118.2	C24—C23—H23	120.3
C8—C9—H9	118.2	C20—C24—C23	119.5 (4)
N1—C10—C11	122.7 (3)	C20—C24—H24	120.3
N1—C10—H10	118.7	C23—C24—H24	120.3
C11—C10—H10	118.7	C10—N1—C9	117.8 (3)
C10—C11—C12	118.8 (4)	C10—N1—Zn1^{ii}	120.6 (2)
C10—C11—H11	120.6	C9—N1—Zn1^{ii}	121.5 (2)
C12—C11—H11	120.6	C22—N2—C21	117.9 (3)
C11—C12—C8	120.3 (3)	C22—N2—Zn1^{i}	125.1 (3)
C11—C12—H12	119.9	C21—N2—Zn1^{i}	116.5 (3)
C8—C12—H12	119.9	C1—O1—Zn1	109.3 (2)
O4—C13—O3	123.9 (4)	C13—O3—Zn1	116.4 (2)

Symmetry codes: (i) x, $-y+3/2$, $z-1/2$; (ii) x, $-y+3/2$, $z+1/2$.