

# Crystal structure of (4,4'-bis(imidazol-1-ylmethyl)biphenyl)-(5-hydroxyisophthalato)zinc(II), $\text{Zn}(\text{C}_{20}\text{H}_{18}\text{N}_4)(\text{C}_8\text{H}_4\text{O}_5)$

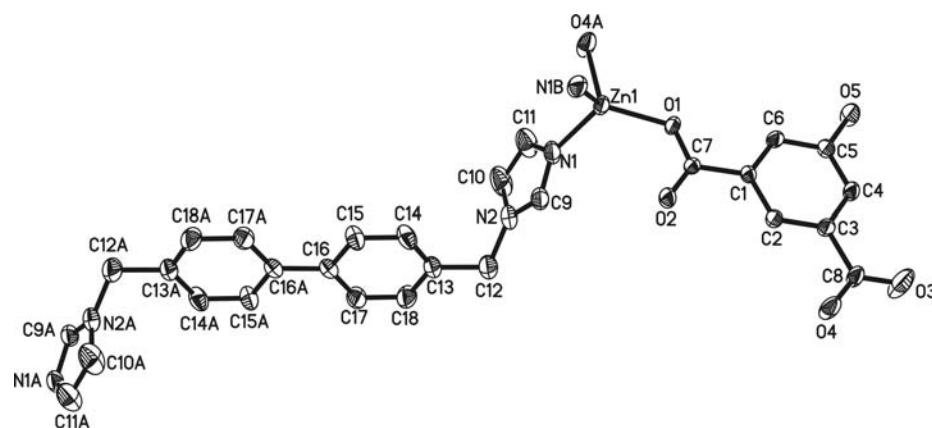
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## Abstract

$\text{C}_{28}\text{H}_{22}\text{N}_4\text{O}_5\text{Zn}$ , orthorhombic,  $Pnma$  (no. 62),  $a = 14.829 \text{ \AA}$ ,  $b = 18.184 \text{ \AA}$ ,  $c = 9.493 \text{ \AA}$ ,  $V = 2559.8 \text{ \AA}^3$ ,  $Z = 4$ ,  $R_{\text{gt}}(F) = 0.035$ ,  $wR_{\text{ref}}(F^2) = 0.094$ ,  $T = 293 \text{ K}$ .

## Source of material

Chemicals were purchased from commercial sources and used without further purification except 4,4'-bis(imidazol-1-ylmethyl)biphenyl which was prepared according to [1]. A mixture of 5-hydroxyisophthalic acid (0.018 g, 0.1 mmol),  $\text{Zn}(\text{OH})_2$  (0.01 g, 0.1 mmol), 4,4'-bis(imidazol-1-ylmethyl)biphenyl (0.031 g, 0.1 mmol) and 8 mL water was stirred for 1 h and then sealed in a 25 mL Teflon-lined stainless steel container, which was heated at  $140^\circ\text{C}$  for 3 days and then cooled to ambient temperature at  $10^\circ\text{C/h}$ . Colorless block-shaped crystals of the title compound were collected in 22 % yield.

## Experimental details

All hydrogen were generated geometrically with  $d(\text{C}—\text{H}) = 0.93 - 0.97 \text{ \AA}$ ,  $d(\text{O}—\text{H}) = 0.82 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ ,  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$

## Discussion

The asymmetric unit consists of half a  $\text{Zn}(\text{II})$  ion, half a 4,4'-bis(imidazol-1-ylmethyl)biphenyl molecule and half a 5-hydroxyisophthalate anion. The  $\text{Zn}(\text{II})$  ion is tetrahedrally four-coordinated by two N atoms from two different 4,4'-bis(imidazol-1-ylmethyl)biphenyl molecules ( $d(\text{Zn1}—\text{N1}) = 2.009(2) \text{ \AA}$  and  $d(\text{Zn1}—\text{N1B}) = 2.009(2) \text{ \AA}$ ) as well by two O atoms from two different 5-hydroxyisophthalate anions with  $d(\text{Zn1}—\text{O1}) =$

$1.940(2) \text{ \AA}$  and  $d(\text{Zn1}—\text{O4A}) = 1.908(2) \text{ \AA}$ . Each 5-hydroxyisophthalate anion connects two  $\text{Zn}(\text{II})$  ions using its two carboxylate groups with  $\mu_1-\eta^1:\eta^0$  monodentate coordination modes to form a chain. The chains are further interlinked by 4,4'-bis(imidazol-1-ylmethyl)biphenyl molecules to a 2D wave-like layer.

**Table 1.** Data collection and handling.

|                                                         |                                                                 |
|---------------------------------------------------------|-----------------------------------------------------------------|
| Crystal:                                                | colorless block, size $0.16 \times 0.18 \times 0.21 \text{ mm}$ |
| Wavelength:                                             | Mo $K_{\alpha}$ radiation ( $0.71073 \text{ \AA}$ )             |
| $\mu$ :                                                 | $10.06 \text{ cm}^{-1}$                                         |
| Diffractionmeter, scan mode:                            | Oxford Diffraction Gemini R Ultra, $\omega$                     |
| $2\theta_{\text{max}}$ :                                | $58.36^\circ$                                                   |
| $N(hkl)_{\text{measured}}$ , $N(hkl)_{\text{unique}}$ : | 10252, 3157                                                     |
| Criterion for $I_{\text{obs}}$ , $N(hkl)_{\text{gt}}$ : | $I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$ , 1791              |
| $N(\text{param})_{\text{refined}}$ :                    | 193                                                             |
| Programs:                                               | SHELXS-97, SHELXL-97 [2]                                        |

**Table 2.** Atomic coordinates and displacement parameters (in  $\text{\AA}^2$ ).

| Atom   | Site | $x$    | $y$           | $z$    | $U_{\text{iso}}$ |
|--------|------|--------|---------------|--------|------------------|
| H(5)   | 4c   | 0.5795 | $\frac{1}{4}$ | 0.7416 | 0.105            |
| H(6)   | 4c   | 0.7487 | $\frac{1}{4}$ | 0.5116 | 0.048            |
| H(4)   | 4c   | 0.6800 | $\frac{1}{4}$ | 0.9197 | 0.052            |
| H(2)   | 4c   | 0.9405 | $\frac{1}{4}$ | 0.8119 | 0.047            |
| H(14)  | 8d   | 1.3120 | 0.3758        | 0.1498 | 0.074            |
| H(10)  | 8d   | 1.1161 | 0.4893        | 0.0903 | 0.112            |
| H(9)   | 8d   | 1.1469 | 0.3384        | 0.3814 | 0.068            |
| H(12A) | 8d   | 1.2502 | 0.4436        | 0.4088 | 0.102            |
| H(12B) | 8d   | 1.2088 | 0.5171        | 0.3516 | 0.102            |

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Table 2. Continued.

| Atom  | Site       | <i>x</i> | <i>y</i> | <i>z</i> | <i>U</i> <sub>iso</sub> |
|-------|------------|----------|----------|----------|-------------------------|
| H(17) | 8 <i>d</i> | 1.4582   | 0.5979   | 0.1281   | 0.077                   |
| H(18) | 8 <i>d</i> | 1.3347   | 0.5839   | 0.2720   | 0.086                   |

Table 2. Continued.

| Atom  | Site       | <i>x</i> | <i>y</i> | <i>z</i> | <i>U</i> <sub>iso</sub> |
|-------|------------|----------|----------|----------|-------------------------|
| H(15) | 8 <i>d</i> | 1.4338   | 0.3906   | 0.0038   | 0.067                   |
| H(11) | 8 <i>d</i> | 1.0081   | 0.3916   | 0.0490   | 0.110                   |

Table 3. Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

| Atom  | Site       | <i>x</i>   | <i>y</i>  | <i>z</i>   | <i>U</i> <sub>11</sub> | <i>U</i> <sub>22</sub> | <i>U</i> <sub>33</sub> | <i>U</i> <sub>12</sub> | <i>U</i> <sub>13</sub> | <i>U</i> <sub>23</sub> |
|-------|------------|------------|-----------|------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| Zn(1) | 4 <i>c</i> | 0.98206(2) | ¼         | 0.24482(4) | 0.0293(2)              | 0.0770(3)              | 0.0286(2)              | 0                      | 0.0018(1)              | 0                      |
| O(1)  | 4 <i>c</i> | 0.9026(1)  | ¼         | 0.4072(2)  | 0.036(1)               | 0.050(1)               | 0.027(1)               | 0                      | 0.0054(8)              | 0                      |
| O(2)  | 4 <i>c</i> | 1.0104(1)  | ¼         | 0.5696(2)  | 0.028(1)               | 0.074(2)               | 0.040(1)               | 0                      | 0.0031(9)              | 0                      |
| O(5)  | 4 <i>c</i> | 0.6115(1)  | ¼         | 0.6713(2)  | 0.022(1)               | 0.145(2)               | 0.044(1)               | 0                      | −0.0027(9)             | 0                      |
| C(6)  | 4 <i>c</i> | 0.7654(2)  | ¼         | 0.6060(3)  | 0.033(2)               | 0.058(2)               | 0.028(2)               | 0                      | −0.005(1)              | 0                      |
| N(2)  | 8 <i>d</i> | 1.1570(1)  | 0.4276(1) | 0.2594(2)  | 0.047(1)               | 0.078(1)               | 0.063(1)               | −0.013(1)              | 0.018(1)               | 0.002(1)               |
| C(4)  | 4 <i>c</i> | 0.7244(2)  | ¼         | 0.8505(3)  | 0.028(2)               | 0.069(2)               | 0.033(2)               | 0                      | 0.004(1)               | 0                      |
| C(1)  | 4 <i>c</i> | 0.8568(2)  | ¼         | 0.6441(3)  | 0.025(1)               | 0.038(2)               | 0.035(2)               | 0                      | 0.003(1)               | 0                      |
| C(7)  | 4 <i>c</i> | 0.9299(2)  | ¼         | 0.5343(3)  | 0.033(2)               | 0.034(2)               | 0.029(2)               | 0                      | 0.000(1)               | 0                      |
| C(2)  | 4 <i>c</i> | 0.8801(2)  | ¼         | 0.7860(3)  | 0.022(1)               | 0.063(2)               | 0.032(2)               | 0                      | −0.003(1)              | 0                      |
| C(3)  | 4 <i>c</i> | 0.8140(2)  | ¼         | 0.8889(3)  | 0.028(2)               | 0.065(2)               | 0.031(2)               | 0                      | −0.003(1)              | 0                      |
| N(1)  | 8 <i>d</i> | 1.0589(1)  | 0.3403(1) | 0.2236(2)  | 0.039(1)               | 0.081(1)               | 0.048(1)               | −0.005(1)              | 0.0059(9)              | 0.013(1)               |
| C(5)  | 4 <i>c</i> | 0.7001(2)  | ¼         | 0.7109(3)  | 0.021(1)               | 0.066(2)               | 0.040(2)               | 0.0                    | −0.003(1)              | 0                      |
| C(14) | 8 <i>d</i> | 1.3411(2)  | 0.4210(1) | 0.1457(3)  | 0.049(1)               | 0.049(2)               | 0.088(2)               | −0.014(1)              | 0.012(1)               | 0.004(1)               |
| C(13) | 8 <i>d</i> | 1.3108(2)  | 0.4782(2) | 0.2265(3)  | 0.048(1)               | 0.065(2)               | 0.061(2)               | −0.014(1)              | 0.013(1)               | −0.004(1)              |
| C(10) | 8 <i>d</i> | 1.1090(2)  | 0.4469(2) | 0.1440(4)  | 0.079(2)               | 0.103(3)               | 0.099(3)               | −0.025(2)              | 0.006(2)               | 0.050(2)               |
| C(9)  | 8 <i>d</i> | 1.1251(2)  | 0.3637(2) | 0.3034(3)  | 0.043(1)               | 0.079(2)               | 0.048(1)               | −0.005(1)              | 0.006(1)               | 0.007(1)               |
| C(12) | 8 <i>d</i> | 1.2307(2)  | 0.4690(2) | 0.3242(3)  | 0.077(2)               | 0.100(2)               | 0.079(2)               | −0.036(2)              | 0.032(2)               | −0.025(2)              |
| C(16) | 8 <i>d</i> | 1.4607(1)  | 0.4960(1) | 0.0483(3)  | 0.037(1)               | 0.041(1)               | 0.054(1)               | −0.004(1)              | −0.002(1)              | 0.005(1)               |
| O(3)  | 4 <i>c</i> | 0.7812(2)  | ¼         | 1.1317(3)  | 0.049(2)               | 0.324(6)               | 0.037(2)               | 0                      | 0.000(1)               | 0                      |
| C(8)  | 4 <i>c</i> | 0.8395(2)  | ¼         | 1.0429(3)  | 0.029(2)               | 0.114(3)               | 0.030(2)               | 0                      | 0.004(1)               | 0                      |
| C(17) | 8 <i>d</i> | 1.4289(2)  | 0.5527(1) | 0.1311(3)  | 0.070(2)               | 0.051(2)               | 0.071(2)               | −0.025(1)              | 0.017(1)               | −0.009(1)              |
| C(18) | 8 <i>d</i> | 1.3548(2)  | 0.5444(2) | 0.2185(3)  | 0.081(2)               | 0.063(2)               | 0.072(2)               | −0.021(2)              | 0.027(2)               | −0.023(1)              |
| C(15) | 8 <i>d</i> | 1.4146(2)  | 0.4301(1) | 0.0581(3)  | 0.043(1)               | 0.041(1)               | 0.084(2)               | −0.001(1)              | 0.015(1)               | −0.002(1)              |
| C(11) | 8 <i>d</i> | 1.0497(2)  | 0.3930(2) | 0.1223(3)  | 0.062(2)               | 0.138(3)               | 0.075(2)               | −0.020(2)              | −0.010(2)              | 0.053(2)               |
| O(4)  | 4 <i>c</i> | 0.9199(2)  | ¼         | 1.0688(2)  | 0.035(1)               | 0.190(3)               | 0.031(1)               | 0                      | −0.006(1)              | 0                      |

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## References

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