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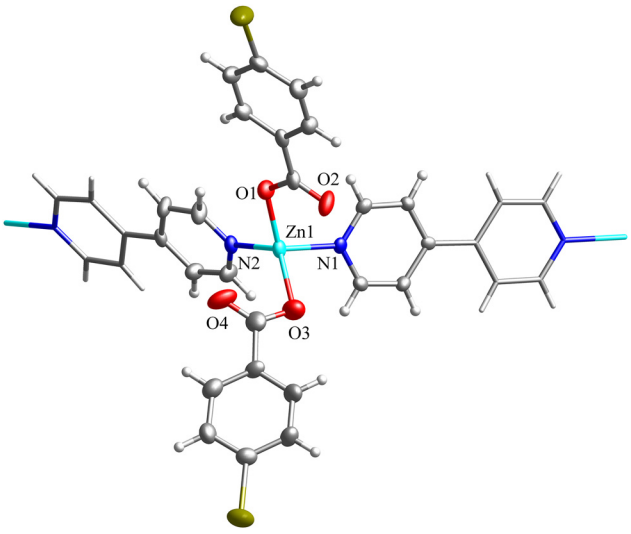
# Crystal structure of *catena*-poly[($\mu_2$-4,4′-bipyridine-$\kappa^2N$:$N'$)-bis(4-bromobenzoato-$\kappa^1O$)zinc(II)], $C_{24}H_{16}Br_2N_2O_4Zn$

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**Abstract**

$C_{24}H_{16}Br_2N_2O_4Zn$, monoclinic, *I*2/*a* (no. 15), $a$ = 7.4191(9) Å, $b$ = 24.458(3) Å, $c$ = 25.810(3) Å, $\beta$ = 92.426(3)°, $V$ = 4679.2(10) Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.0514, $wR_{ref}(F^2)$ = 0.1710, T = 296(2) K.

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A part of the title polymeric structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

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

| | |
|---|---|
| Crystal: | Colorless block |
| Size: | 0.18 × 0.16 × 0.15 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 4.50 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$-scans |
| $\theta_{max}$, completeness: | 25°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 11890, 4132, 0.040 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs}$ > 2 σ($I_{obs}$), 2752 |
| $N(param)_{refined}$: | 298 |
| Programs: | Bruker programs [1], SHELX [2] |

## Source of material

A mixture of $Zn(NO_3)_2 \cdot 6H_2O$ (1 mmol, 297.5 mg), 4,4′-bipyridine (1 mmol, 156.2 mg), and 4-bromobenzoic acid (2 mmol, 402.0 mg) was dissolved in 1 mL dimethylformamide and 3 mL $H_2O$ and heated in a 15 mL autoclave under autogenous pressure at 413 K for 72 h. After cooling to room temperature, colourless block crystals formed.

## Experimental details

Hydrogen atoms were positioned using a riding model, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Discussion

The design and construction of coordination polymers are of great interest because of their fascinating architectures and interesting properties [3–8]. Using the carboxylic acid and nitrogen containing mixed ligands is the common synthetic strategy for the synthesis of coordination polymers [5, 9–11]. In this study, we selected 4-bromobenzoate and 4,4′-bipyridine as ligands to react with $Zn(NO_3)_2 \cdot 6H_2O$

In the title compound, there are one Zn(II) cation, two 4-bromobenzoate ligands, and two half of the 4,4′-bipyridine ligand in the asymmetric unit. The atom Zn1 is four coordinated with a distorted tetrahedral geometry by two N atoms from two symmetry 4,4′-bipyridine ligands and two

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.3343 (6) | 0.39270 (18) | 0.91798 (16) | 0.0347 (11) |
| N2 | 0.4173 (6) | 0.30300 (19) | 0.83117 (18) | 0.0389 (11) |
| O1 | 0.0591 (6) | 0.36148 (18) | 0.81889 (16) | 0.0540 (12) |
| O2 | −0.1100 (6) | 0.3944 (2) | 0.87963 (17) | 0.0686 (15) |
| O3 | 0.1359 (9) | 0.2886 (2) | 0.9383 (2) | 0.0899 (18) |
| O4 | 0.1074 (8) | 0.2340 (3) | 0.8745 (2) | 0.096 (2) |
| Zn1 | 0.20946 (9) | 0.33098 (3) | 0.87544 (3) | 0.0397 (2) |
| Br1 | −0.65849 (14) | 0.45154 (4) | 0.66781 (3) | 0.0930 (4) |
| Br2 | −0.06264 (13) | 0.05801 (4) | 1.07217 (4) | 0.0862 (3) |
| C1 | 0.3135 (7) | 0.4451 (2) | 0.9045 (2) | 0.0358 (13) |
| H1 | 0.252135 | 0.453118 | 0.873212 | 0.043* |
| C2 | 0.3793 (7) | 0.4882 (2) | 0.93497 (19) | 0.0314 (12) |
| H2 | 0.364100 | 0.524058 | 0.923595 | 0.038* |
| C3 | 0.4680 (6) | 0.4776 (2) | 0.98250 (19) | 0.0272 (11) |
| C4 | 0.4908 (7) | 0.4229 (2) | 0.9960 (2) | 0.0375 (13) |
| H4 | 0.551670 | 0.413641 | 1.026999 | 0.045* |
| C5 | 0.4243 (8) | 0.3827 (2) | 0.9640 (2) | 0.0397 (14) |
| H5 | 0.441381 | 0.346501 | 0.974098 | 0.048* |
| C6 | 0.5737 (9) | 0.2843 (3) | 0.8502 (2) | 0.0542 (17) |
| H6 | 0.595445 | 0.285745 | 0.885947 | 0.065* |
| C7 | 0.7069 (9) | 0.2627 (3) | 0.8204 (2) | 0.0491 (16) |
| H7 | 0.813937 | 0.249841 | 0.835930 | 0.059* |
| C8 | 0.6788 (8) | 0.2605 (2) | 0.7667 (2) | 0.0370 (14) |
| C9 | 0.5167 (8) | 0.2812 (3) | 0.7468 (2) | 0.0494 (16) |
| H9 | 0.492385 | 0.282006 | 0.711158 | 0.059* |
| C10 | 0.3914 (8) | 0.3008 (3) | 0.7803 (3) | 0.0529 (17) |
| H10 | 0.281561 | 0.313178 | 0.766047 | 0.063* |
| C11 | −0.0794 (8) | 0.3867 (2) | 0.8340 (2) | 0.0438 (15) |
| C12 | −0.2108 (8) | 0.4055 (2) | 0.7929 (2) | 0.0402 (14) |
| C13 | −0.1870 (9) | 0.3957 (3) | 0.7405 (2) | 0.0511 (16) |
| H13 | −0.081027 | 0.379184 | 0.730458 | 0.061* |
| C14 | −0.3169 (10) | 0.4099 (3) | 0.7030 (3) | 0.0596 (19) |
| H14 | −0.298974 | 0.402650 | 0.668205 | 0.072* |
| C15 | −0.4734 (10) | 0.4350 (3) | 0.7175 (3) | 0.0578 (18) |
| C16 | −0.4995 (10) | 0.4472 (3) | 0.7694 (3) | 0.0591 (19) |
| H16 | −0.603679 | 0.464874 | 0.779207 | 0.071* |
| C17 | −0.3674 (8) | 0.4324 (3) | 0.8060 (2) | 0.0486 (16) |
| H17 | −0.383750 | 0.440747 | 0.840604 | 0.058* |
| C18 | 0.0985 (10) | 0.2440 (4) | 0.9194 (3) | 0.066 (2) |
| C19 | 0.0427 (8) | 0.2004 (3) | 0.9586 (2) | 0.0483 (16) |
| C20 | 0.0497 (10) | 0.1480 (3) | 0.9417 (3) | 0.066 (2) |
| H20 | 0.075012 | 0.140893 | 0.907401 | 0.079* |
| C21 | 0.0191 (10) | 0.1046 (3) | 0.9755 (3) | 0.0623 (19) |
| H21 | 0.028166 | 0.068582 | 0.964477 | 0.075* |
| C22 | −0.0248 (9) | 0.1165 (3) | 1.0255 (3) | 0.0556 (18) |
| C23 | −0.0390 (10) | 0.1698 (3) | 1.0424 (3) | 0.061 (2) |
| H23 | −0.072667 | 0.177433 | 1.075961 | 0.073* |
| C24 | −0.0026 (10) | 0.2111 (3) | 1.0089 (3) | 0.064 (2) |
| H24 | −0.008435 | 0.247175 | 1.020185 | 0.076* |

O atoms from two different 4-bromobenzoate ligands (see the figure). The Zn—O bond lengths are in the range of 1.948(4)–2.019(5) Å, and the Zn—N bond lengths are 2.063(5), and 2.074(4) Å [9, 12]. Zn(II) cations are linked by 4,4′-bipyridine ligands to form a Zigzag chain structure with the Zn—Zn distances of 11.222 and 11.240 Å.

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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