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Crystal structure of \textit{catena}-poly[aqua-(\(\mu_4\)-4,4\textsuperscript{′}-pyridine-3,5-diyl)dibenzoato-\(\kappa^4\)O,O\textsuperscript{′}:O\textsuperscript{′′}:O\textsuperscript{′′′}) zinc(II)], C\textsubscript{19}H\textsubscript{13}NO\textsubscript{5}Zn

![Structure diagram]

https://doi.org/10.1515/ncrs-2020-0197
Received April 22, 2020; accepted June 2, 2020; available online June 17, 2020

\textbf{Abstract}
C\textsubscript{19}H\textsubscript{13}NO\textsubscript{5}Zn, monoclinic, \(P2_1/c\) (no. 13), \(a = 16.7294(5)\) Å, \(b = 6.4986(2)\) Å, \(c = 7.1414(2)\) Å, \(\beta = 100.449(3)\) °, \(V = 763.51(4)\) Å\(^3\), \(Z = 2\), \(R_{\text{gt}}(F) = 0.0297\), \(wR_{\text{ref}} (F^2) = 0.0732\), \(T = 293(2)\) K.

\textbf{CCDC no.:} 2007140

A part of the coordination polymer title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

\textbf{Source of material}
A mixture of 4,4\textsuperscript{′}-pyridine-3,5-diyl dibenzoic acid (0.0319 g, 0.1 mmol), zinc nitrate hexahydrate (0.0298 g, 0.1 mmol) and deionized water (10 mL) was added to a 25 mL Teflon-lined stainless steel autoclave, heated at 393 K in an oven for 72 h, then cooled to room temperature automatically. Colorless block crystals were obtained, filtered, washed with deionized water, and dried in air (yield 35.2%, based on 4,4\textsuperscript{′}-pyridine-3,5-diyl dibenzoic acid).

\begin{table}[h]
\centering
\caption{Data collection and handling.}
\begin{tabular}{lll}
\hline
\textbf{Crystal:} & Colorless needle \\
\textbf{Size:} & 0.12 × 0.09 × 0.08 mm \\
\textbf{Wavelength:} & Mo Ka radiation (0.71073 Å) \\
\textbf{\(\mu\)} & 1.64 mm\(^{-1}\) \\
\textbf{Diffractometer, scan mode:} & Xcalibur, \(\omega\) \\
\textbf{\(\theta_{\text{max}}\), completeness:} & 26.4°, >99% \\
\textbf{\(N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}, R_{\text{int}}:\)} & 3268, 1553, 0.026 \\
\textbf{Criterion for \(I_{\text{obs}}\), \(N(hkl)_{\text{gt}}:\)} & \(I_{\text{obs}} > 2 \sigma(I_{\text{obs}}), 1342\) \\
\textbf{Programs:} & Crysalis\textsuperscript{PRO} [1], Olex2 [2], SHELX [3, 4] \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å\(^2\)).}
\begin{tabular}{cccccc}
\hline
\textbf{Atom} & \textbf{x} & \textbf{y} & \textbf{z} & \textbf{U_{iso}} & \textbf{U_{eq}} \\
\hline
Zn1 & 0.500000 & 0.68318(6) & 0.750000 & 0.02041(14) & \\
O1 & 0.45174(9) & 0.3049(3) & 0.5156(2) & 0.0215(4) & \\
O2 & 0.39483(10) & 0.5794(3) & 0.6225(2) & 0.0269(4) & \\
O3 & 0.500000 & 0.9896(4) & 0.750000 & 0.0333(7) & \\
H3 & 0.484(2) & 1.067(5) & 0.659(4) & 0.049(10)* & \\
N1 & 0.000000 & −0.2777(5) & 0.250000 & 0.0269(4) & \\
C1 & 0.22312(14) & 0.0447(4) & 0.3040(3) & 0.0235(5) & \\
C2 & 0.15305(13) & 0.1467(4) & 0.3558(3) & 0.0229(5) & \\
C3 & 0.16155(14) & 0.3390(4) & 0.4429(3) & 0.0209(5) & \\
H5 & 0.115557 & 0.410662 & 0.461875 & 0.025(2)* & \\
C4 & 0.11155(14) & 0.3198(4) & 0.5404(3) & 0.0229(5) & \\
C5 & 0.07251(13) & 0.0450(4) & 0.3011(3) & 0.0191(5) & \\
C6 & 0.15305(13) & 0.1301(4) & 0.3842(3) & 0.0229(6) & \\
C7 & 0.345102 & 0.059639 & 0.363490 & 0.027(2)* & \\
C8 & 0.23772(13) & 0.4249(4) & 0.5017(3) & 0.0270(5) & \\
C9 & 0.116031 & −0.240975 & 0.342866 & 0.029(2)* & \\
\hline
\end{tabular}
\end{table}
Experimental details

The structure was solved by direct methods with the SHELXS-2018 program. All H-atoms from C-atoms were positioned with idealized geometry and refined using a riding model with C–H = 0.93 Å with $U_{iso}(H) = 1.2U_{eq}(C)$. The H-atom from O was located with O-peak and refined freely.

Comment

Known as a famous N-heterocyclic aromatic dicarboxylic acid ligand, 4,4′-pyridine-3,5-diylbenzoic acid and its deprotonated forms have been used to build various metal coordination polymers or metal-organic frameworks. Due to variable coordination numbers (usually 4, 5 or 6) of zinc cations and the flexible coordination modes of 4,4′-pyridine-3,5-diylbenzoic acid, some examples of 4,4′-pyridine-3,5-diylbenzoate- or its N-oxide-based Zn(II) complexes have been reported [5–9]. We herein report a new two-dimensional Zn(II) complex based on this ligand.

As shown in the figure, the asymmetric unit of the title complex consists of a half five-coordinated Zn(II) cation, a half 4,4′-pyridine-3,5-diylbenzoate and a half coordination water molecule. The N atom from the ligand is not involved in coordination, which is different from similar complexes [5–9]. The bond lengths of Zn(II)—O in the complex are 1.991, 1.949, and 2.193 Å, respectively, all of which are comparable with similar complexes [5–9].

Acknowledgements: Key scientific research projects of general colleges and universities in Hunan Province (18A458), Natural Science Foundation of Hunan Province (2016JJ6141), Key R & D and technological innovation projects of science and Technology Bureau of Chenzhou (zdyf201916).

References