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The crystal structure of hexaquazinc(II) poly(hexakis(μ₂-4-methylbenzenesulfinato-κ²O:O′) dizinc(II))

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Abstract

C_{42}H_{54}O_{18}S_{6}Zn_{3}, trigonal, P\text{\textsuperscript{3}1\text{\textsuperscript{m}}} (no. 162), a = 9.2916(13) Å, c = 18.121(4) Å, V = 1354.9(5) Å\text{\textsuperscript{3}}, Z = 0.99996, R_{gt}(F) = 0.0490, wR_{ref}(F^2) = 0.1330, T = 293(2) K.

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The molecular 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.

1 Source of materials

An amount of 0.1782 g sodium toluene-4-sulphinate (1.0 mmol and 0.1098 g) zinc acetate dihydrate (0.5 mmol) solids were solved to 15 ml ethanol-water (v:v = 2:1) solution under stirring. The mixture was kept at 68 °C and stirred for 5 h. After cooling to room temperature, the solution was filtered into a small flask. The block crystals were obtained in 21 days.

2 Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.96–0.98 Å, O–H = 0.86 Å). Their U_{eq} values were set to 1.2U_{eq} or 1.5U_{eq} of the parent atoms.

3 Comment

In the past decade, the studies on the structure and properties of zinc complexes have been one of the hotspots of coordination chemistry. Because they show novel structures and excellent properties such as fluorescent “off-on” probe [5], carbon dioxide cycloaddition catalyst [6], early diagnosis and treatment of infantile rickets [7], catalysis of ring-opening co-polymerization of ε-caprolactone and δ-valerolactone [8], and so on. We have also synthesized and structurally characterized some Zn(II) complexes [9–11].
The crystal structure of C42H54O18S6Zn3

The bond lengths of Zn1–O are 2.1166(18) Å, and Zn2–O are 2.075(2) Å. The [Zn(H2O)6]2+ unit and the [Zn(toluene-4-sulphinate)4]2+ unit are linked by hydrogen bonds, and further form 1D channeled structure.

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References


