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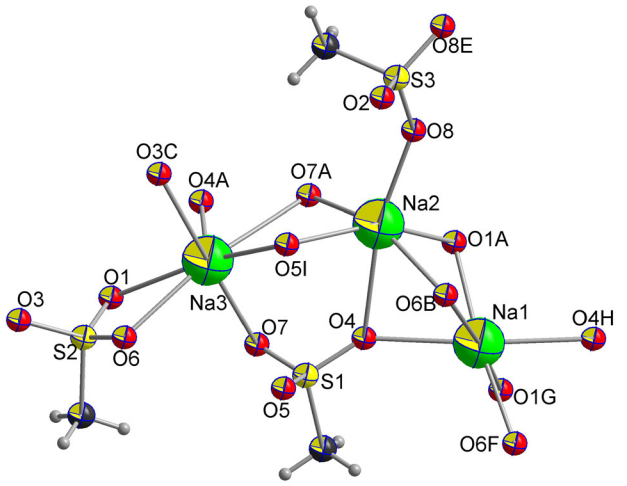
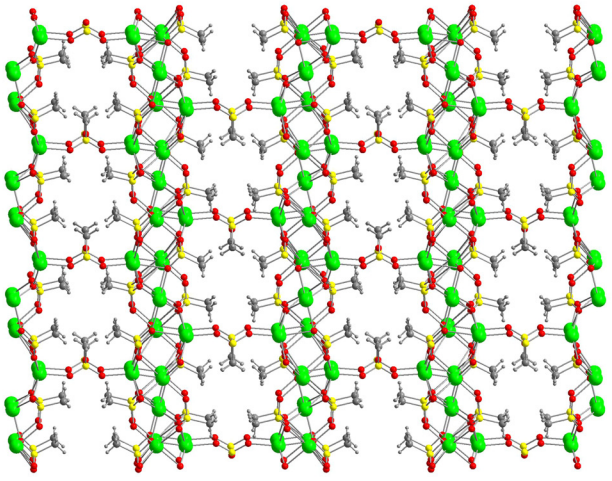
The crystal structure of sodium methylsulfonate





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Abstract
$C_5H_{15}Na_5O_{15}S_5$, orthorhombic, *Pbcm* (no. 53), a = 5.58810(10) Å, b = 16.9774(5) Å, c = 21.904 (5) Å, V = 2078.06(9) Å^3, Z = 4, $R_{gt}(F)$ = 0.0275, $wR_{ref}(F^2)$ = 0.0658, T = 125.80 K.

CCDC no.: 2430326

1 Source of materials

Put 9 mL DMF (N, N–Dimethylformamide), 21 mL ethanol, 0.4 g (10 mmol) NaOH, 0.96 g (10 mmol) methanesulfonic acid (MsA) into a beaker and stir for 1 h. Subsequently, the solution was naturally evaporated, and after about a week, large colorless crystals were obtained with a yield of almost 100 %.

2 Experimental details

The data were collected and processed using CrysAlis^{pro}.[1] The structure was solved by Direct Methods using Olex2 software[2] and refined with the SHELXL.[3] The hydrogen atom positions were fixed geometrically at the calculated distances and allowed to ride on the parent atoms. The U_{iso} of the H-atoms were set to 1.5 times U_{eq} of the parent atoms with C–H = 0.96 Å (aliphatic).

3 Comment

Over the past few decades, the design and preparation of coordination polymers (CPs) has attracted widespread attention due to their potential applications in fields such as gas storage/separation, catalyst, etc.[4,5,6] Many CPs constructed

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.30 × 0.30 × 0.25 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.73 mm^{-1}
Diffractometer, scan mode:	Rigaku SuperNova, ω scans
θ_{max}, completeness:	25.0°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4750, 1884, 0.023
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 $\sigma(I_{obs})$, 1,652
$N(param)_{refined}$:	144
Programs:	Rigaku,[1] Olex2,[2] SHELX[3]

from aromatic carboxylate linkers have been extensively studied,[7,8] however, coordination polymers constructed with sulfonic acid groups are still relatively rare.[9,10]

The title compound is a three network structure and crystallizes in the orthorhombic *Pbcm* space group. There are 2.5 Na(I) ions and 2.5 MsA ligands in the asymmetric unit. The Na1 and Na2 ions are in a similar coordination environment, both located at the slightly twisted octahedral center, with six vertices composed of six oxygen atoms from six methylsulfonyl groups. However, the Na3 ion is located in a slightly twisted seven coordinated pentagonal bipyramidal coordination environment, of which vertex composed of seven oxygen atoms from five methylsulfonic acid groups. And the Na–O bond distances range from 2.3151(17) to 2.8676(17) Å, which are within the normal range.[11,12] Methylsulfonate ions exhibit three different coordination modes, the first is the seven coordination mode (k^2–O, k^3–O, k^4–O)-u_7, the second is the six coordination mode (k^1–O, k^3–O, k^3–O)-u_6, and the third is the (k^1–O, k^1–O)-u_2 bridge mode. The methylsulfonate group connects sodium ions to form a two-dimensional layered structure using the first and second coordination modes mentioned above. The methyl sulphonate group uses the third bridging mode to link adjacent two-dimensional layers to form a three-dimensional structure (see lower part of the figure). Geometric parameters are all in the expected ranges.[13]

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