

$\text{H}_3\text{Cs}_2\text{Na}[\text{SO}_4]_3$ *hP48*(176) $P6_3/m - i^2h^3fb$ **Cs₂Na(HSO₄)₃** [1]

Structural features: NaO₆ octahedra share vertices with three SO₄ tetrahedra on each side to form infinite chains parallel to [001].

Chisholm C.R.I. et al. (2001) [1]

 $\text{Cs}_2\text{H}_3\text{NaO}_{12}\text{S}_3$ $a = 0.85712$, $c = 0.998$ nm, $c/a = 1.164$, $V = 0.6350$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.2459	0.1098	0.1547	0.5	
O2	12 <i>i</i>	1	0.2771	0.065	0.1107	0.5	
O3	6 <i>h</i>	<i>m</i> ..	0.1815	0.3706	$\frac{1}{4}$		single atom S
S4	6 <i>h</i>	<i>m</i> ..	0.307	0.0272	$\frac{1}{4}$		
O5	6 <i>h</i>	<i>m</i> ..	0.4879	0.0641	$\frac{1}{4}$		single atom S
Cs6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.00613		9-vertex polyhedron O ₉
Na7	2 <i>b</i>	-3..	0	0	0		
H8	12 <i>i</i>	1	0.217	0.294	0.208	0.5	

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.029

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Chisholm C.R.I., Cowan L.A., Haile S.M., Klooster W.T. (2001), Chem. Mater. 13, 2574-2583.