

Cs ₂ [S ₂ O ₆]	<i>hP20</i>	(186) <i>P6₃mc</i> – c ² b ³ a
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Cs₂S₂O₆ [1], Strukturbericht notation K1₂

Structural features: Cs atoms and O₃S-SO₃ units in a Ni₂In-type (ht-Co₂Ge) arrangement.

Liminda R. et al. (1980) [1]

Cs₂O₆S₂

a = 0.63566, *c* = 1.15391 nm, *c/a* = 1.815, *V* = 0.4038 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>c</i>	. <i>m</i> .	0.2056	0.7944	0.3104		single atom S
O2	6 <i>c</i>	. <i>m</i> .	0.4606	0.5394	0.0635		single atom S
S3	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.09394		non-coplanar triangle O ₃
S4	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.27654		non-coplanar triangle O ₃
Cs5	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.76131		9-vertex polyhedron O ₉
Cs6	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		9-vertex polyhedron O ₉

Transformation from published data: -*x*, -*y*, -*z*

Experimental: single crystal, diffractometer, X-rays, *R* = 0.066, *T* = 298 K

Remarks: Supersedes a structure proposal in space group (190) *P*-62*c* in [2]. Strukturbericht notation K1₂ was defined on the superseded structure proposal.

References: [1] Liminda R., Abrahams S.C., Bernstein J.L. (1980), J. Chem. Phys. 73, 1432-1438. [2] Hägg G. (1937), Strukturbericht 2, 107, 508.