

CsAs	<i>hP36</i>	(189) <i>P-62m</i> – kji ² hgfe
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CsAs [1]

Structural features: As₃ rings.

Emmerling F., Röhr C. (2002) [1]

AsCs

$a = 1.2197$, $c = 1.0463$ nm, $c/a = 0.858$, $V = 1.3480$ nm³, $Z = 18$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	<i>6k</i>	<i>m..</i>	0.3222	0.5452	$\frac{1}{2}$		non-colinear As ₂
As2	<i>6j</i>	<i>m..</i>	0.1166	0.3459	0		non-colinear As ₂
Cs3	<i>6i</i>	<i>..m</i>	0.36649	0	0.31618		15-vertex Frank-Kasper As ₈ Cs ₇
Cs4	<i>6i</i>	<i>..m</i>	0.69441	0	0.26449		pseudo Frank-Kasper As ₇ Cs ₆
Cs5	<i>4h</i>	<i>3..</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.17888		16-vertex Frank-Kasper As ₉ Cs ₇
As6	<i>3g</i>	<i>m2m</i>	0.115	0	$\frac{1}{2}$		non-colinear As ₂
As7	<i>3f</i>	<i>m2m</i>	0.4631	0	0		non-colinear As ₂
Cs8	<i>2e</i>	<i>3.m</i>	0	0	0.1792		16-vertex Frank-Kasper As ₉ Cs ₇

Experimental: single crystal, diffractometer, X-rays, R = 0.061, T = 215 K

References: [1] Emmerling F., Röhr C. (2002), Z. Naturforsch. B 57, 963-975.