

Ba ₃ CrS ₅	<i>hP</i> 18	(185) <i>P6₃cm – c²ba</i>
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Ba₃CrS₅ [1]

Structural features: Infinite columns of face-linked CrS₆ octahedra parallel to [001].

Fukuoka H. et al. (2003) [1]

Ba₃CrS₅

$a = 0.91208$, $c = 0.6193$ nm, $c/a = 0.679$, $V = 0.4462$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	6 <i>c</i>	.. <i>m</i>	0.2122	0	0.247		non-colinear Cr ₂
Ba2	6 <i>c</i>	.. <i>m</i>	0.616	0	0.259		pseudo Frank-Kasper S ₉ Ba ₂ Cr ₂
S3	4 <i>b</i>	3.. ¹ / ₃	¹ / ₃	² / ₃	0.064		trigonal bipyramid Ba ₃ S ₂
Cr4	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		octahedron S ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.897

Experimental: single crystal, diffractometer, X-rays, R = 0.022, T = 296 K

Remarks: In the abstract of [1] the number of formula units per cell *Z* is misprinted as 6 instead of 2 (given in table 1 and in the text).

References: [1] Fukuoka H., Miyaki Y., Yamanaka S. (2003), J. Solid State Chem. 176, 206-212.