

$\text{CrSi}_3\text{B}_{14.67}\text{Se}_{16}$  $hP112$  $(182) P6_322 - i^8g^2ca$ **CrSi<sub>3</sub>(B<sub>12</sub>)Se<sub>12</sub>(B<sub>2</sub>Se<sub>3</sub>)<sub>1.33</sub> [1]**

Structural features: B<sub>12</sub>Se<sub>12</sub> units (a B<sub>12</sub> icosahedron surrounded by a larger Se<sub>12</sub> icosahedron) share atoms with CrSe<sub>6</sub> octahedra and SiSe<sub>4</sub> tetrahedra to form a 3D-framework; infinite B<sub>2</sub>Se<sub>3</sub> chains with B<sub>2</sub>Se<sub>2</sub> rings in large channels parallel to [001] (partial disorder).

Sugimori M. et al. (2000) [1]

 $\text{B}_{12}\text{CrSe}_{15.98}\text{Si}_3$  $a = 1.29772$ ,  $c = 0.95322$  nm,  $c/a = 0.735$ ,  $V = 1.3902$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	12 <i>i</i>	1	0.0149	0.1586	0.0703	0.112	
Se2	12 <i>i</i>	1	0.035	0.1602	0.1399	0.098	
Se3	12 <i>i</i>	1	0.0513	0.1408	0.2119	0.075	
Se4	12 <i>i</i>	1	0.113	0.012	0.204	0.225	
Se5	12 <i>i</i>	1	0.15902	0.50565	0.06124		non-colinear BSi
Se6	12 <i>i</i>	1	0.38759	0.05727	0.32604		non-colinear BSi
B7	12 <i>i</i>	1	0.5381	0.2061	0.2838		pentagonal pyramid B <sub>5</sub> Se
B8	12 <i>i</i>	1	0.589	0.2539	0.1099		pentagonal pyramid B <sub>5</sub> Se
Se9	6 <i>g</i>	.2.	0.1522	0	0	0.13	
Si10	6 <i>g</i>	.2.	0.53476	0	0		tetrahedron Se <sub>4</sub>
Cr11	2 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron Se <sub>6</sub>
Se12	2 <i>a</i>	32.	0	0	0	0.53	

Transformation from published data:  $-x, -y, -z$ ; origin shift  $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.048$ 

Remarks: Part of B not located. Short interatomic distances for partly occupied site(s).

References: [1] Sugimori M., Fukuoka H., Imoto H., Saito T. (2000), J. Organomet. Chem. 611, 547-550.