$Ba_3Fe_3Se_7$	*hP*26	(186) $P6_3mc$ – c^4b

$Ba_3Fe_3Se_7$ [1]
Structural features: Units of three edge-linked $FeSe_4$ tetrahedra (a Fe_3 triangular cluster, one Se common to the three tetrahedra) in a Mg-type (h.c.p.) arrangement. See Fig. IV.28.

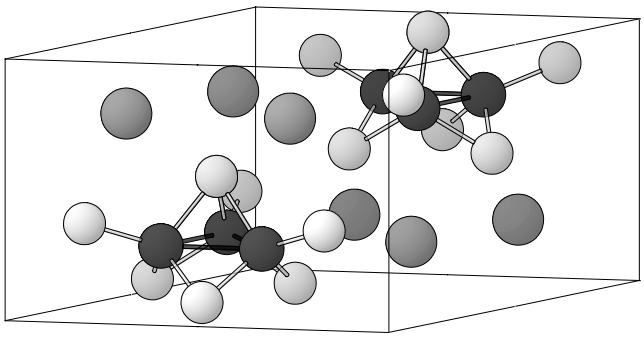

Fig. IV.28. **$Ba_3Fe_3Se_7$**

Arrangement of Fe_3Se_7 units (Fe atoms dark, Se atoms light) and Ba atoms (large).

Hong H.Y., Steinfink H. (1972) [1]
$Ba_3Fe_3Se_7$
a = 1.0843, c = 0.7384 nm, c/a = 0.681, V = 0.7518 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	6*c*	.*m*.	0.1911	0.8089	0.262		trigonal prism Se_6
Se2	6*c*	.*m*.	0.5427	0.4573	0.073		non-colinear Fe_2
Fe3	6*c*	.*m*.	0.7542	0.2458	0.248		tetrahedron Se_4
Se4	6*c*	.*m*.	0.8748	0.1252	0.3515		single atom Fe
Se5	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0		non-coplanar triangle Fe_3

Transformation from published data: origin shift 0 0 0.738
Experimental: single crystal, diffractometer, X-rays, R = 0.070, T = 298 K

Remarks: In [1] the *z*-coordinates of former sites Fe and Se(3) are misprinted as 0.0486 and 0.0738 instead of 0.486 and 0.738, respectively (see [2]).

References: [1] Hong H.Y., Steinfink H. (1972), J. Solid State Chem. 5, 93-104. [2] (1975), Structure Reports 39A, 23.