

Er<sub>4.8</sub>Si<sub>2.7</sub>C<sub>0.5</sub>

hP54

(187) *P*-6*m*2 – ok<sup>6</sup>j<sup>6</sup>ihg**Er<sub>5</sub>Si<sub>3</sub>C<sub>0.5</sub>** [1]

Structural features: SiEr<sub>8</sub>Er monocapped square antiprisms (SiEr<sub>6</sub>Er<sub>3</sub> tricapped trigonal prisms; partial vacancies ignored) share atoms to form a 3D-framework; C in octahedral voids. Infinite columns of face-sharing CEr<sub>6</sub> octahedra and infinite linear -Er- chains. Filled-up derivative of Mn<sub>5</sub>Si<sub>3</sub> with C in octahedral voids.

Al Shahery G.M.Y. et al. (1982) [1]

C<sub>0.54</sub>Er<sub>4.76</sub>Si<sub>2.66</sub>*a* = 1.441, *c* = 0.6322 nm, *c/a* = 0.439, *V* = 1.1369 nm<sup>3</sup>, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Er1	12 <i>o</i>	1	0.00107	0.33373	0.2475		14-vertex Frank-Kasper Si <sub>6</sub> Er <sub>8</sub>
Si2	3 <i>k</i>	<i>mm</i> 2	0.08017	0.91983	<sup>1</sup> / <sub>2</sub>	0.92	
Er3	3 <i>k</i>	<i>mm</i> 2	0.25577	0.74423	<sup>1</sup> / <sub>2</sub>		non-colinear C <sub>2</sub>
Si4	3 <i>k</i>	<i>mm</i> 2	0.45907	0.54093	<sup>1</sup> / <sub>2</sub>		pseudo Frank-Kasper Er <sub>9</sub> C <sub>2</sub> Si <sub>2</sub>
Er5	3 <i>k</i>	<i>mm</i> 2	0.58267	0.41733	<sup>1</sup> / <sub>2</sub>		7-capped pentagonal prism C <sub>2</sub> Si <sub>5</sub> Er <sub>10</sub>
Si6	3 <i>k</i>	<i>mm</i> 2	0.81177	0.18823	<sup>1</sup> / <sub>2</sub>		pseudo Frank-Kasper Er <sub>9</sub> Si <sub>2</sub>
Er7	3 <i>k</i>	<i>mm</i> 2	0.91977	0.08023	<sup>1</sup> / <sub>2</sub>	0.8	
Er8	3 <i>j</i>	<i>mm</i> 2	0.07247	0.92753	0		non-colinear C <sub>2</sub>
Si9	3 <i>j</i>	<i>mm</i> 2	0.23797	0.76203	0	0.4	non-colinear Er <sub>2</sub>
Er10	3 <i>j</i>	<i>mm</i> 2	0.41147	0.58853	0	0.72	non-colinear Si <sub>2</sub>
Si11	3 <i>j</i>	<i>mm</i> 2	0.53607	0.46393	0		pseudo Frank-Kasper Er <sub>9</sub> C <sub>2</sub> Si <sub>2</sub>
Er12	3 <i>j</i>	<i>mm</i> 2	0.74477	0.25523	0		non-colinear C <sub>2</sub>
Si13	3 <i>j</i>	<i>mm</i> 2	0.87197	0.12803	0		pseudo Frank-Kasper Er <sub>9</sub> C <sub>2</sub> Si <sub>2</sub>
C14	2 <i>i</i>	3 <i>m</i> .	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0.21	0.66	7-vertex polyhedron Er <sub>6</sub> C
C15	2 <i>h</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.29	0.48	7-vertex polyhedron Er <sub>6</sub> C
C16	2 <i>g</i>	3 <i>m</i> .	0	0	0.16	0.48	4-vertex polyhedron CEr <sub>3</sub>

Transformation from published data: origin shift <sup>1</sup>/<sub>3</sub> <sup>2</sup>/<sub>3</sub> <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.110

Remarks: Short interatomic distances: d(Er7-Si2) = 0.200 nm, d(Er10-Si9) = 0.220 nm. We assume that in table 2 of [1] the occupancy of former Er(3*k*)<sub>1</sub> is misprinted as 0.35 instead of 0.25 (maximum value for Wyckoff position 3*k*).

References: [1] Al Shahery G.M.Y., Jones D.W., McColm I.J., Steadman R. (1982), J. Less-Common Met. 87, 99-108.