

U₅Re₅Si₉

*hP*76

(176) $P6_3/m - i^2h^7gcd$

U₅Re₅Si₉ [1]

Structural features: Distorted ReSi₆ trigonal prisms, ReSi₆ octahedra and ReSi₅ square pyramids share atoms to form a 3D-framework; infinite columns of face-linked U₆ octahedra in channels parallel to [001] and additional U in voids.

Yarmolyuk Y.P. et al. (1985) [1]

Re₅Si₉U₅

$a = 1.6308$, $c = 0.5642$ nm, $c/a = 0.346$, $V = 1.2995$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	12i	1	0.171	0.286	0.005		bicapped square antiprism Re ₃ Si ₂ U ₅
Si2	12i	1	0.171	0.53	0.026		pseudo Frank-Kasper Si ₄ Re ₃ U ₄
U3	6h	<i>m</i> ..	0.0094	0.1263	¹ / ₄		15-vertex Frank-Kasper Si ₄ Re ₄ U ₇
U4	6h	<i>m</i> ..	0.035	0.35	¹ / ₄		pseudo Frank-Kasper Si ₉ Re ₇ U ₄
Re5	6h	<i>m</i> ..	0.2412	0.2129	¹ / ₄		icosahedron Si ₅ ReU ₆
U6	6h	<i>m</i> ..	0.3107	0.4728	¹ / ₄		14-vertex Frank-Kasper Si ₉ Re ₅
Si7	6h	<i>m</i> ..	0.391	0.36	¹ / ₄		tricapped trigonal prism Re ₄ U ₃ Si ₂
Re8	6h	<i>m</i> ..	0.4239	0.2201	¹ / ₄		octahedron Si ₆
Si9	6h	<i>m</i> ..	0.501	0.129	¹ / ₄		tricapped trigonal prism Re ₃ Si ₂ U ₄
Re10	6g	-1	¹ / ₂	0	0		cuboctahedron Si ₆ Re ₂ U ₄
U11	2d	-6..	² / ₃	¹ / ₃	¹ / ₄		14-vertex Frank-Kasper Re ₅ Si ₉
Re12	2c	-6..	¹ / ₃	² / ₃	¹ / ₄		pseudo Frank-Kasper Si ₆ U ₅

Transformation from published data: *y*,*x*,*-z*

Experimental: single crystal, diffractometer, X-rays, R = 0.089

References: [1] Yarmolyuk Y.P., Aksel'rud L.G., Gladyshevskii E.I., Bruskov V.A. (1985), Sov. Phys. Crystallogr. 30, 380-382 (Kristallografiya 30, 654-657).