

**K<sub>2</sub>UF<sub>6</sub> β<sub>1</sub>** [2]; Zr<sub>6</sub>CoGa<sub>2</sub> [3]; Zr<sub>6</sub>FeAl<sub>2</sub> [4]

Structural features: Infinite columns of base-linked KF<sub>6</sub>F<sub>3</sub> and UF<sub>6</sub>F<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework (a framework of base- and edge-linked KF<sub>6</sub> trigonal prisms with single columns of UF<sub>6</sub> prisms shifted by *c*/2 in channels). Ordering variant of Fe<sub>2</sub>P. See Fig. IV.4.

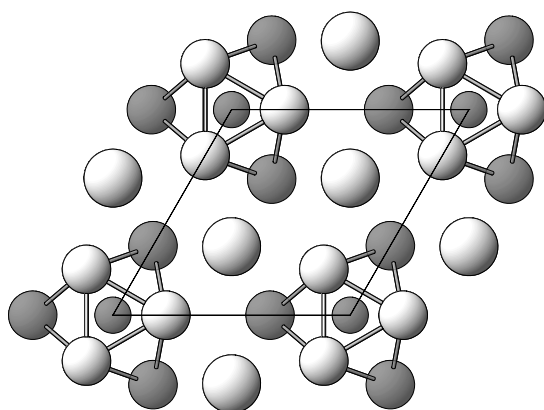


Fig. IV.4. **K<sub>2</sub>UF<sub>6</sub> β<sub>1</sub>**

Arrangement of UF<sub>6</sub>F<sub>3</sub> tricapped trigonal prisms (U atoms small, F atoms medium) and K atoms (large) viewed along [001]. Light and dark atoms are shifted by *c*/2.

Brunton G. (1969) [1]

F<sub>6</sub>K<sub>2</sub>U

*a* = 0.65528, *c* = 0.3749 nm, *c/a* = 0.572, *V* = 0.1394 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.223	0	1/2		non-colinear U <sub>2</sub>
F2	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.662	0	0		single atom U
K3	2 <i>d</i>	-6..	1/3	2/3	1/2		tricapped trigonal prism F <sub>9</sub>
U4	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism F <sub>9</sub>

Experimental: single crystal, diffractometer, X-rays, *R* = 0.061

References: [1] Brunton G. (1969), Acta Crystallogr. B 25, 2163-2164. [2] Zachariasen W.H. (1948), J. Am. Chem. Soc. 70, 2147-2151. [3] Belyavina N.N., Markiv V.Y. (1982), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1982(5), 39-42. [4] Gingl F., Yvon K., Zavalij I.Y., Yartys' V.A., Fischer P. (1995), J. Alloys Compd. 226, 1-4.