$K_2ZrSi_3O_9$	*hP*30	(174) *P*-6 – $l^2k^2j^2ihg$

$K_2ZrSi_3O_9$ [1], wadeite
Structural features: Rings of three vertex-linked SiO_4 tetrahedra share vertices with ZrO_6 octahedra to form a 3D-framework.

Blinov V.A. et al. (1977) [1]
$K_2O_9Si_3Zr$
a = 0.6926, c = 1.0177 nm, c/a = 1.469, V = 0.4228 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6*l*	1	0.41167	0.31133	0.133		non-colinear SiZr
O2	6*l*	1	0.42967	0.07633	0.367		single atom Si
Si3	3*k*	*m*..	0.05267	0.46033	$^1/_2$		tetrahedron O_4
O4	3*k*	*m*..	0.26867	0.42333	$^1/_2$		non-colinear Si_2
O5	3*j*	*m*..	0.06367	0.24433	0		non-colinear Si_2
Si6	3*j*	*m*..	0.28067	0.20633	0		tetrahedron O_4
Zr7	2*i*	3..	$^2/_3$	$^1/_3$	0.2495		octahedron O_6
K8	2*h*	3..	$^1/_3$	$^2/_3$	0.193		non-coplanar triangle O_3
K9	2*g*	3..	0	0	0.306		non-coplanar triangle O_3

Transformation from published data: -*y*,-*x*,-*z*; origin shift $^1/_3$ $^2/_3$ 0
Experimental: single crystal, diffractometer, X-rays, R = 0.030
Remarks: Natural specimen of unknown origin. The structure was refined in space group (143) *P*3, but the authors state that true symmetry is space group (174) *P*-6 and report averaged coordinates. Space group (176) $P6_3/m$, generally considered for wadeite (see [2], [3]), was tested and rejected (R = 0.066).

References: [1] Blinov V.A., Shumyatskaya N.G., Voronkov A.A., Iliukhin V.V., Belov N.V. (1977), Sov. Phys. Crystallogr. 22, 31-35 (Kristallografiya 22, 59-65). [2] Henshaw D.E. (1955), Mineral. Mag. J. Mineral. Soc. 30, 585-595. [3] Ferreira P., Ferreira A., Rocha J., Soares M.R. (2001), Chem. Mater. 13, 355-363.