

Supplementary Material for manuscript

The natural tiling approach to cation conductivity in KAlO_2 polymorphs

Vladimir I. Voronin,^a Georgi Sh. Shekhtman^b and Vladislav A. Blatov^{c*}

^aInstitute of Metal Physics Urals Branch RAS, S.Kovalevskoy Street 18, 620041 Ekaterinburg, Russia, ^bInstitute of High Temperature Electrochemistry Urals Branch RAS, S.Kovalevskoy Street 22, 620990 Ekaterinburg, Russia, and ^cSamara State University, Ac. Pavlov Street 1, 443011 Samara, Russia. E-mail: blatov@ssu.samara.ru

Parameters of a triclinic quasi-cubic subcell in KAlO_2 polymorphs^{*}

T, K	a , Å	b , Å	c , Å	α , deg.	β , deg.	γ , deg.	V , Å ³
300	7.731	7.645	7.770	91.34	90.50	89.65	924.13
400	7.738	7.670	7.775	91.27	90.57	89.70	926.65
500	7.747	7.683	7.79	91.23	90.4	89.72	929.88
600	7.759	7.703	7.796	91.15	90.36	89.75	934.21
700	7.772	7.727	7.792	90.77	90.27	89.77	938.91
773	7.782	7.766	7.797	90.54	90.21	89.82	942.54
833	7.805						950.93
923	7.816						955.22
1023	7.832						960.89

^{*} Above 813 K the subcell coincides with the cubic unit cell. E.s.d.'s do not exceed 0.001 Å for linear parameters, 0.01° for angular parameters, and 0.01 Å³ for the subcell volume.