Appendix C:

Na – O and K – O bond lengths of investigated cells of the study "First-principles investigation of the lattice vibrations in the alkali feldspar solid solution" published by Artur Benisek, Edgar Dachs, Michael Grodzicki in Physics and Chemistry of Minerals.

Due to structural details of low albite and low microcline, Na was coordinated fivefold, whereas K sevenfold. The coordination numbers are in accordance with Downs et al. (1996). The Na – O and K – O bond lengths are listed in ascending order for low albite and low microcline, respectively.

Na – O bond lengths (Å):

	X_{Or}				
	0	0.25	0.5	0.75	1
Na 001 – O 002	2.30366	2.37390	2.46171	-	-
Na 001 – O 007	2.36410	2.40196	2.48539	-	-
Na 001 – O 019	2.39039	2.42894	2.50759	-	-
Na 001 – O 017	2.43864	2.47843	2.45919	-	-
Na 001 – O 001	2.52181	2.71383	3.05038	-	-
				-	-
Na 001 – O 008	2.96423	2.87844	2.71608	-	-
Na 001 – O 013	3.02264	2.77850	2.54396	-	-

	X_{Or}				
	0	0.25	0.5	0.75	1
Na 002 – O 010	2.30366	-	-	2.54604	-
Na 002 – O 015	2.36410	-	-	2.63809	-
Na 002 – O 027	2.39039	-	-	2.67897	-
Na 002 – O 025	2.43864	-	-	2.51907	-
Na 002 – O 009	2.52181	-	-	2.94529	-
Na 002 – O 016	2.96423	-	-	2.69003	-
Na 002 – O 005	3.02264	-	-	2.59607	-

K – O bond lengths (Å):

	X_{Or}				
	0	0.25	0.5	0.75	1
K 004 – O 026	-	-	2.53224	2.58011	2.62928
K 004 – O 009	-	-	2.68684	2.69174	2.74256
K 004 – O 025		-	2.69508	2.77873	2.77215
K 004 – O 031	-	-	2.69791	2.72794	2.84334
K 004 – O 032	-	-	2.92272	2.87152	2.86497
K 004 – O 011	-	-	2.72119	2.73597	2.86849
K 004 – O 021	-		3.17610	2.86655	2.88142
K 004 – O 012	-	-	3.05123	3.16208	3.01696
K 004 – O 022	-	-	3.07804	3.33197	3.33606

	X_{Or}				
	0	0.25	0.5	0.75	1
K 002 – O 010	-	2.46050	-	-	2.62928
K 002 – O 025	-	2.62422	-	-	2.74256
K 002 – O 009		2.64322	-	-	2.77215
K 002 – O 015	-	2.60702	-	-	2.84334
K 002 – O 016	-	2.91023	-	-	2.86497
K 002 – O 027	-	2.63152	-	-	2.86849
K 002 – O 005	-	3.12253	-	-	2.88142
K 002 – O 028	-	3.11886	-	-	3.01696
K 002 – O 006	-	3.10240	-	-	3.33606