



STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 76 (2020)

Supporting information for article:

The incommensurately modulated structures (IMS) of low-temperature *e*-labradorite feldspars: a single-crystal X-ray and neutron diffraction study

Shiyun Jin, Huifang Xu, Xiaoping Wang, Ryan Jacobs and Dane Morgan

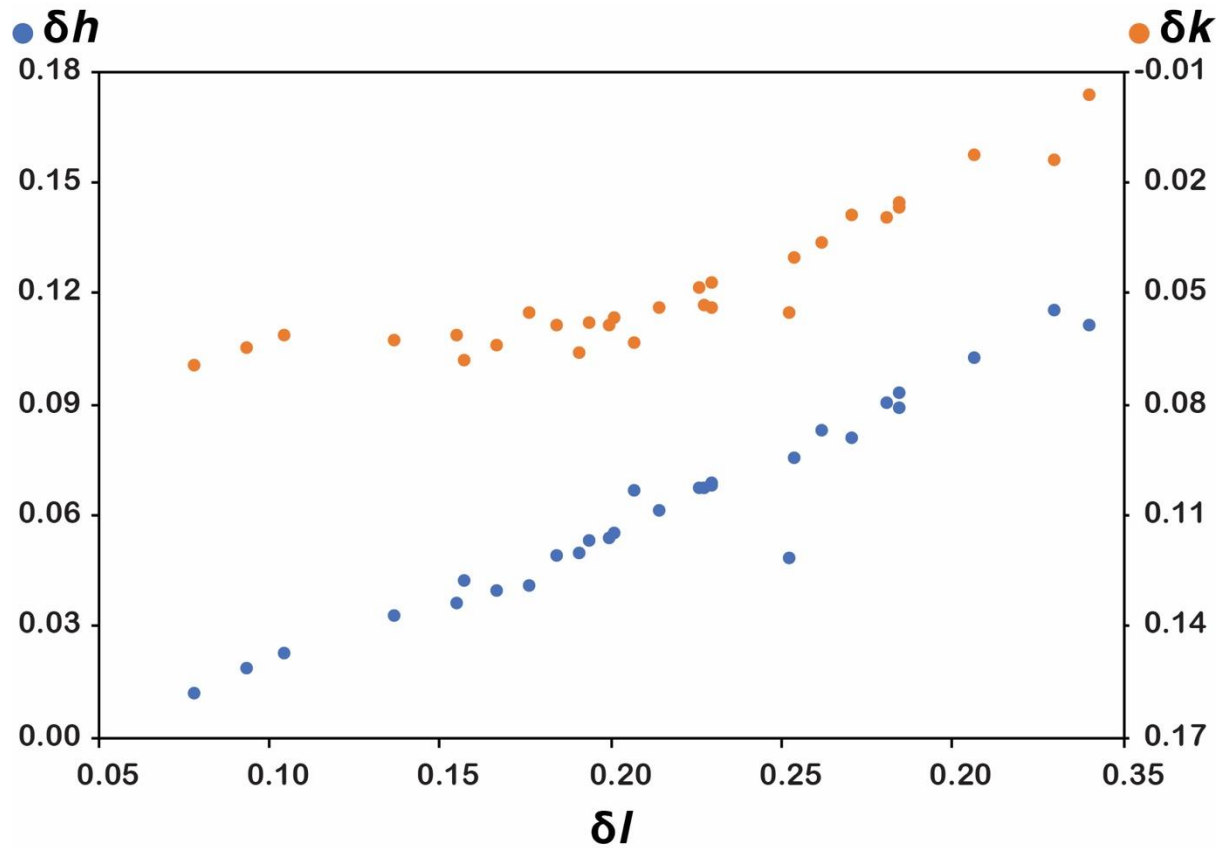


Figure S1 The δh and δk of the q -vector plotted against δl as in Smith & Brown (1988). This plot eliminates the error from the compositional analysis and shows strong correlation between the three components of the q -vectors. The points that obviously deviate from the trend are from volcanic samples with diffuse satellite reflections (Jin, Xu *et al.*, 2019).

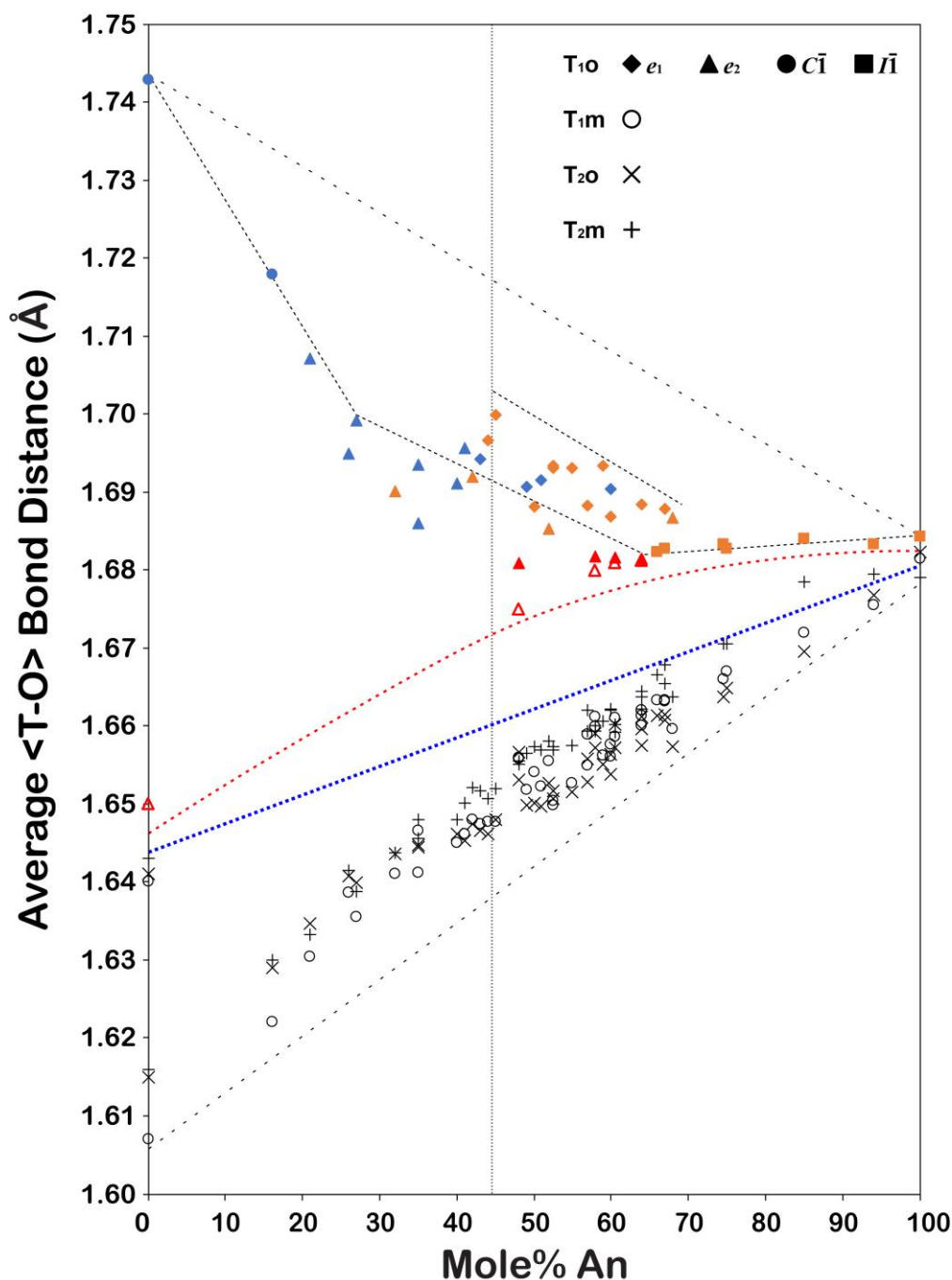


Figure S2 Average $\langle T-O \rangle$ bond distances of samples in this paper and several previously published papers (Jin & Xu, 2017a,b,c; Jin, Wang *et al.*, 2018; Jin, Xu *et al.*, 2019). Data points less calcic than An₂₀ or more calcic than An₇₅ are from Kroll & Ribbe (1983). The points for $\langle T_{1o}-O \rangle$ are color and shape coded based on their structure and origin. For two samples with the same composition, the one with less ordered structure is shifted slightly to the left to be discernible. The blue dotted line shows the regression of the total average $\langle T-O \rangle$ distance in each structure. The black dash lines outline the boundaries of the e_1 and e_2 structures. The red dotted line shows the trend for volcanic and heated plagioclase structures.

Table S1 Electron microprobe analyses results

SAMPLE	Oxide Weight Percentage							Formula per 8 oxygen							
	SiO ₂	Al ₂ O ₃	FeO	CaO	Na ₂ O	K ₂ O	TOTAL	Si	Al	Fe	Ca	Na	K	Totals	
7147A	55.025	28.731	0.172	10.778	5.315	0.441	100.462	2.473	1.522	0.006	0.519	0.463	0.025	13.010	An _{51.5} Ab _{46.0} Or _{2.5}
	54.034	28.812	0.179	10.909	5.093	0.414	99.442	2.455	1.543	0.007	0.531	0.449	0.024	13.009	An _{52.9} Ab _{44.7} Or _{2.4}
	54.505	28.548	0.225	10.960	5.144	0.412	99.795	2.468	1.524	0.009	0.532	0.452	0.024	13.008	An _{52.8} Ab _{44.8} Or _{2.4}
	54.860	28.607	0.284	11.082	5.252	0.392	100.476	2.469	1.517	0.011	0.534	0.458	0.022	13.013	An _{52.6} Ab _{45.1} Or _{2.2}
	54.491	28.550	0.229	10.784	5.164	0.406	99.624	2.470	1.525	0.009	0.524	0.454	0.023	13.006	An _{52.3} Ab _{45.3} Or _{2.3}
	55.210	28.800	0.245	10.795	5.112	0.403	100.566	2.477	1.523	0.009	0.519	0.445	0.023	12.996	An _{52.6} Ab _{45.1} Or _{2.3}
Volga Blue yellow	53.905	29.147	0.445	11.014	4.895	0.484	99.890	2.441	1.556	0.017	0.534	0.430	0.028	13.006	An _{53.9} Ab _{43.3} Or _{2.8}
	54.115	28.896	0.211	11.330	4.866	0.470	99.887	2.450	1.542	0.008	0.550	0.427	0.027	13.005	An _{54.7} Ab _{42.5} Or _{2.7}
	53.773	29.156	0.472	11.255	4.783	0.459	99.899	2.435	1.556	0.018	0.546	0.420	0.027	13.002	An _{55.0} Ab _{42.3} Or _{2.7}
	54.324	28.802	0.223	11.299	4.814	0.429	99.891	2.458	1.536	0.008	0.548	0.422	0.025	12.996	An _{55.1} Ab _{42.5} Or _{2.5}
	53.485	29.280	0.334	11.529	4.632	0.424	99.684	2.429	1.567	0.013	0.561	0.408	0.025	13.003	An _{56.5} Ab _{41.1} Or _{2.5}
	54.076	29.059	0.172	11.171	4.754	0.539	99.770	2.449	1.551	0.007	0.542	0.417	0.031	12.998	An _{54.7} Ab _{42.1} Or _{3.1}
	53.892	28.896	0.277	11.403	4.692	0.481	99.641	2.447	1.546	0.011	0.555	0.413	0.028	12.999	An _{55.7} Ab _{41.5} Or _{2.8}
	53.503	29.211	0.512	11.305	4.649	0.545	99.726	2.428	1.563	0.019	0.550	0.409	0.032	13.001	An _{55.5} Ab _{41.3} Or _{3.2}
89GM97	53.903	29.048	0.337	11.312	4.795	0.437	99.831	2.443	1.552	0.013	0.549	0.421	0.025	13.003	An _{55.2} Ab _{42.3} Or _{2.5}
	52.935	29.150	0.485	11.581	4.544	0.428	99.122	2.419	1.570	0.019	0.567	0.403	0.025	13.001	An _{57.0} Ab _{40.5} Or _{2.5}
	51.720	28.366	0.505	11.385	4.235	0.428	96.639	2.424	1.567	0.020	0.572	0.385	0.026	12.993	An _{58.2} Ab _{39.2} Or _{2.6}
	53.273	28.723	0.472	11.154	4.908	0.475	99.005	2.433	1.546	0.018	0.546	0.435	0.028	13.005	An _{54.1} Ab _{43.1} Or _{2.7}
	53.772	29.259	0.462	11.386	4.722	0.462	100.062	2.433	1.560	0.017	0.552	0.414	0.027	13.004	An _{55.6} Ab _{41.7} Or _{2.7}
	52.837	29.528	0.723	11.892	4.439	0.403	99.823	2.404	1.583	0.027	0.580	0.392	0.023	13.010	An _{58.3} Ab _{39.4} Or _{2.4}
52.264	29.601	0.592	11.762	4.545	0.426	99.191	2.392	1.597	0.023	0.577	0.403	0.025	13.016	An _{57.4} Ab _{40.1} Or _{2.5}	

	52.902	29.045	0.505	11.841	4.530	0.433	99.255	2.416	1.563	0.019	0.579	0.401	0.025	13.004	An _{57.6} Ab _{39.9} Or _{2.5}
	52.713	29.719	0.492	11.712	4.393	0.400	99.429	2.403	1.597	0.019	0.572	0.388	0.023	13.002	An _{58.2} Ab _{39.5} Or _{2.4}
Volga Blue colourless	52.836	29.439	0.263	12.122	4.352	0.329	99.340	2.410	1.583	0.010	0.592	0.385	0.019	12.999	An _{59.5} Ab _{38.6} Or _{1.9}
	53.135	29.423	0.257	11.942	4.451	0.353	99.561	2.417	1.577	0.010	0.582	0.393	0.020	12.999	An _{58.5} Ab _{39.5} Or _{2.1}
	52.573	29.148	0.317	12.033	4.676	0.389	99.135	2.408	1.573	0.012	0.590	0.415	0.023	13.022	An _{57.4} Ab _{40.4} Or _{2.2}
	53.773	29.493	0.364	12.114	4.450	0.306	100.499	2.424	1.567	0.014	0.585	0.389	0.018	12.996	An _{59.0} Ab _{39.2} Or _{1.8}
	52.097	29.398	0.504	12.153	4.419	0.391	98.962	2.393	1.592	0.019	0.598	0.394	0.023	13.019	An _{59.0} Ab _{38.8} Or _{2.3}
	51.743	29.352	0.279	11.996	4.445	0.350	98.164	2.393	1.600	0.011	0.594	0.399	0.021	13.017	An _{58.6} Ab _{39.3} Or _{2.0}
Dul-15-6A	52.849	30.752	0.487	13.412	3.976	0.135	101.612	2.363	1.621	0.018	0.643	0.345	0.008	12.997	An _{64.6} Ab _{34.6} Or _{0.8}
	52.293	30.742	0.438	13.232	3.930	0.140	100.773	2.357	1.633	0.017	0.639	0.343	0.008	12.997	An _{64.5} Ab _{34.7} Or _{0.8}
	52.722	30.726	0.469	13.379	4.057	0.156	101.510	2.361	1.622	0.018	0.642	0.352	0.009	13.004	An _{64.0} Ab _{35.1} Or _{0.9}
	51.579	30.537	0.475	13.244	3.928	0.149	99.911	2.348	1.638	0.018	0.646	0.347	0.009	13.006	An _{64.5} Ab _{34.6} Or _{0.9}

Table S2 Lattice parameters and average $\langle T - O \rangle$ bond distances of samples that are plotted in Figure S2.

Sample	%An	a	b	c	alpha	beta	gamma	T ₁₀	T _{1m}	T ₂₀	T _{2m}	$\langle T-O \rangle$
Amelia	0	8.1420	12.7850	7.1590	94.190	116.610	87.680	1.7430	1.6070	1.6150	1.6160	1.6453
Tiburon	0	8.1520	12.8580	7.1080	93.589	116.455	90.115	1.6500	1.6400	1.6410	1.6430	1.6435
Camedo	16	8.1553	12.8206	7.1397	93.965	116.475	88.632	1.7180	1.6220	1.6290	1.6300	1.6498
7133	21	8.1434	12.8240	7.1289	93.921	116.517	89.036	1.7073	1.6305	1.6347	1.6333	1.6514
Gem29	26	8.1447	12.8379	7.1193	93.792	116.434	89.510	1.6949	1.6387	1.6408	1.6414	1.6540
97490	27	8.1529	12.8330	7.1211	93.798	116.443	89.302	1.6993	1.6355	1.6399	1.6388	1.6534
1974	32	8.1512	12.8452	14.2252	93.720	116.389	89.615	1.6901	1.6410	1.6436	1.6438	1.6546
91315c	35	8.1464	12.8460	14.2216	93.708	116.372	89.871	1.6859	1.6466	1.6447	1.6480	1.6563
91315c_2	35	8.1498	12.8446	14.2276	93.764	116.399	89.591	1.6935	1.6412	1.6444	1.6455	1.6562
T-12-22a	40	8.1535	12.8468	14.2222	93.682	116.344	89.719	1.6911	1.6450	1.6461	1.6480	1.6576
89GM69	41	8.1461	12.8414	14.2192	93.732	116.322	89.647	1.6958	1.6461	1.6453	1.6501	1.6593
SK90-49.1	42	8.1575	12.8532	14.2184	93.663	116.303	89.778	1.6920	1.6480	1.6475	1.6521	1.6599
7144	43	8.1521	12.8420	14.2160	93.712	116.320	89.706	1.6942	1.6474	1.6465	1.6517	1.6600
H4-04-2	44	8.1635	12.8484	14.2250	93.630	116.324	89.641	1.6968	1.6477	1.6461	1.6506	1.6603
H4-04	45	8.1659	12.8546	14.2354	93.580	116.311	89.594	1.7001	1.6477	1.6481	1.6520	1.6620
Hogarth Range	48	8.1594	12.8639	14.2076	93.538	116.206	90.280	1.6808	1.6558	1.6531	1.6551	1.6612
Hogarth Range(H)	48	8.1627	12.8630	14.2006	93.539	116.150	90.385	1.6749	1.6559	1.6567	1.6555	1.6608
91413b	49	8.1571	12.8473	14.2116	93.671	116.252	89.913	1.6907	1.6518	1.6498	1.6565	1.6622

SKGO-12	50	8.1614	12.8545	14.2112	93.590	116.250	90.008	1.6881	1.6541	1.6501	1.6574	1.6624
987L	51	8.1668	12.8509	14.2086	93.580	116.230	89.840	1.6916	1.6522	1.6497	1.6570	1.6626
Dul-15-8B	52	8.1625	12.8586	14.2038	93.554	116.216	90.159	1.6852	1.6555	1.6527	1.6581	1.6629
R2923	52.5	8.1658	12.8542	14.2096	93.609	116.273	89.809	1.6934	1.6505	1.6507	1.6574	1.6630
7147A	52.5	8.1640	12.8536	14.2096	93.620	116.253	89.780	1.6931	1.6498	1.6517	1.6570	1.6629
Volga Blue	55	8.1690	12.8537	14.2096	93.602	116.289	89.825	1.6931	1.6527	1.6515	1.6575	1.6637
89GM97	57	8.1742	12.8639	14.2056	93.485	116.183	90.086	1.6883	1.6589	1.6558	1.6620	1.6662
MXGC	58	8.1603	12.8612	14.1976	93.534	116.118	90.433	1.6818	1.6612	1.6573	1.6600	1.6650
MXGC(H)	58	8.1615	12.8620	14.1974	93.547	116.102	90.481	1.6800	1.6599	1.6590	1.6594	1.6646
Volga Blue	59	8.1729	12.8590	14.2110	93.572	116.232	89.933	1.6934	1.6562	1.6550	1.6606	1.6663
67796b	60	8.1674	12.8554	14.2106	93.593	116.239	90.032	1.6904	1.6561	1.6539	1.6622	1.6656
11044.p1	60	8.1719	12.8602	14.2016	93.514	116.198	90.172	1.6869	1.6576	1.6563	1.6620	1.6657
96GM1	60.5	8.1626	12.8622	14.1986	93.512	116.130	90.421	1.6816	1.6587	1.6572	1.6591	1.6641
96GM1(H)	60.5	8.1652	12.8647	14.1954	93.543	116.085	90.456	1.6809	1.6611	1.6602	1.6602	1.6656
Lake CO. e2	64	8.1617	12.8657	14.1946	93.523	116.105	90.509	1.6814	1.6613	1.6596	1.6637	1.6665
Lake CO. e2(H)	64	8.1628	12.8607	14.1988	93.569	116.075	90.534	1.6812	1.6621	1.6612	1.6622	1.6667
Dul-15-6A	64	8.1684	12.8620	14.2016	93.540	116.182	90.236	1.6884	1.6600	1.6575	1.6644	1.6676
28-88	66	8.1635	12.8615	14.1936	93.510	116.124	90.530	1.6823	1.6633	1.6613	1.6665	1.6683
SKHHM new	67	8.1705	12.8637	14.1986	93.548	116.207	90.376	1.6879	1.6632	1.6608	1.6679	1.6699
Lake CO. I $\bar{1}$	67	8.1618	12.8632	14.1898	93.521	116.117	90.575	1.6828	1.6633	1.6615	1.6655	1.6682
11044.p3	68	8.1719	12.8647	14.1954	93.527	116.187	90.275	1.6867	1.6596	1.6574	1.6637	1.6668

7155	74.5	8.1662	12.8680	14.1927	93.477	116.143	90.666	1.6832	1.6660	1.6637	1.6705	1.6709
55-88	75	8.1652	12.8633	14.1832	93.469	116.073	90.730	1.6827	1.6670	1.6649	1.6705	1.6713
Traversella	85	8.1830	12.8830	14.1860	93.380	115.870	90.820	1.6840	1.6720	1.6695	1.6785	1.6760
Grass Valley	94	8.1784	12.8736	14.1766	93.187	115.938	91.142	1.6833	1.6755	1.6768	1.6795	1.6788
Val Pesmeda	100	8.1730	12.8690	14.1650	93.113	115.913	91.261	1.6843	1.6815	1.6823	1.6790	1.6818