Ab initio compressibility of metastable low albite: revealing a lambda-type singularity at pressures of the Earth's upper mantle

Ab initio compressibility of metastable low-albite

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TABLE I. Calculated unit cell parameters of albite

P (GPa)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å^3)
0	8.2051	12.854	7.2086	94.19	116.56	87.73	678.18
1	8.1359	12.807	7.1833	94.21	116.78	87.82	666.38
2	8.0707	12.768	7.1587	94.20	116.92	87.92	655.95
3	8.0084	12.729	7.1358	94.17	117.02	88.01	646.29
4	7.9471	12.691	7.1137	94.12	117.08	88.12	637.14
5	7.8867	12.657	7.0922	94.05	117.13	88.23	628.47
6	7.8243	12.624	7.0712	93.96	117.14	88.36	620.06
7	7.7590	12.594	7.0501	93.85	117.13	88.51	611.69
8	7.6785	12.572	7.0258	93.65	117.10	88.61	602.56
9	7.5795	12.560	6.9923	93.51	117.31	88.10	590.34
10	7.5153	12.534	6.9664	93.61	117.69	87.40	579.84
11	7.4652	12.507	6.9443	93.76	118.01	86.91	570.99
12	7.4214	12.483	6.9241	93.95	118.35	86.45	562.85
13	7.3811	12.461	6.9051	94.13	118.66	86.08	555.43
14	7.3437	12.442	6.8879	94.30	118.98	85.78	548.48
15	7.3083	12.427	6.8721	94.50	119.37	85.45	541.61

TABLE II. Calculated tetrahedral bond lengths in albite (Å)

		0 GPa	4 GPa	6 GPa	8 GPa	9 GPa	12 GPa
Al_{1o}	O_{a1}	1.7563	1.7461	1.7405	1.7344	1.7306	1.7216
Al_{1o}	O_{bo}	1.7511	1.7380	1.7336	1.7323	1.7340	1.7314
Al_{1o}	O_{co}	1.7377	1.7291	1.7276	1.7291	1.7319	1.7308
Al_{1o}	O_{do}	1.7535	1.7423	1.7375	1.7329	1.7300	1.7233
average		1.7497	1.7389	1.7348	1.7322	1.7316	1.7268
Si_{1m}	O_{a1}	1.6112	1.6057	1.6028	1.5995	1.5964	1.5898
Si_{1m}	O_{bm}	1.6111	1.6058	1.6047	1.6067	1.6109	1.6138
Si_{1m}	O_{cm}	1.6314	1.6242	1.6198	1.6127	1.6056	1.5986
Si_{1m}	O_{dm}	1.6288	1.6199	1.6160	1.6125	1.6139	1.6179
average		1.6206	1.6139	1.6108	1.6079	1.6067	1.6050
Si_{2o}	O_{a2}	1.6425	1.6331	1.6282	1.6234	1.6210	1.6155
Si_{2o}	O_{bo}	1.6041	1.5976	1.5949	1.5932	1.5934	1.5920
Si_{2o}	O_{cm}	1.6266	1.6179	1.6129	1.6064	1.6012	1.5963
Si_{2o}	O_{dm}	1.6280	1.6194	1.6157	1.6129	1.6156	1.6209
average		1.6253	1.6170	1.6129	1.6090	1.6078	1.6062
Si_{2m}	O_{a2}	1.6564	1.6445	1.6385	1.6332	1.6324	1.6308
Si_{2m}	O_{bm}	1.6322	1.6254	1.6230	1.6227	1.6250	1.6253
Si_{2m}	O_{co}	1.6047	1.6021	1.6027	1.6049	1.6071	1.6082
Si_{2m}	O_{do}	1.6135	1.6052	1.6008	1.5960	1.5928	1.5864
average		1.6267	1.6193	1.6163	1.6142	1.6143	1.6127

[1] R. Downs, R. M. Hazen, and L. W. Finger, Am. Mineral. **79**, 1042 (1994).

[2] M. D. Benusa, R. J. Angels, and N. L. Ross, Am. Mineral. **90**, 1115 (2005).

TABLE III. Calculated T-O-T angles in albite (degrees)

			V/V$_0$						
			1.00	0.95	0.91	0.88	0.86	0.82	0.80
Al_{1o}	O_{a1}	Si_{1m}	140.41	138.57	137.97	140.27	142.26	143.90	144.22
Si_{2o}	O_{a2}	Si_{2m}	129.45	128.60	128.64	128.26	127.46	126.50	126.10
Al_{1o}	O_{bo}	Si_{2o}	140.74	136.01	130.26	123.94	121.25	118.19	116.98
Si_{1m}	O_{bm}	Si_{2m}	161.86	160.13	155.48	145.59	139.22	132.66	130.27
Al_{1o}	O_{co}	Si_{2m}	132.08	127.36	121.26	116.31	113.89	111.01	110.16
Si_{1m}	O_{cm}	Si_{2o}	135.72	136.04	138.54	145.40	151.32	153.73	153.23
Al_{1o}	O_{do}	Si_{2m}	133.89	135.06	137.89	143.28	147.11	152.17	154.78
Si_{1m}	O_{dm}	Si_{2o}	151.17	153.97	157.15	156.53	148.94	140.64	138.34

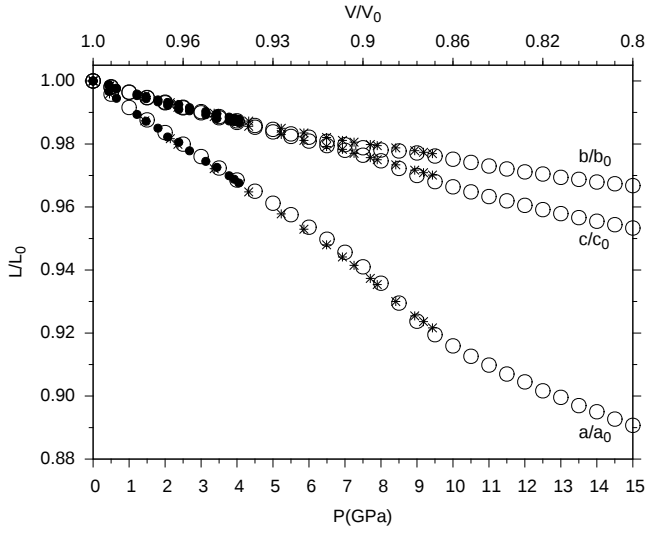

FIG. 1. Variation of the calculated cell parameters (normalized to their minimum energy values) as a function of pressure (empty circles). Full circles and asterisks represent experimental data by Downs *et al.*[1] and Benusa *et al.*,[2] respectively.

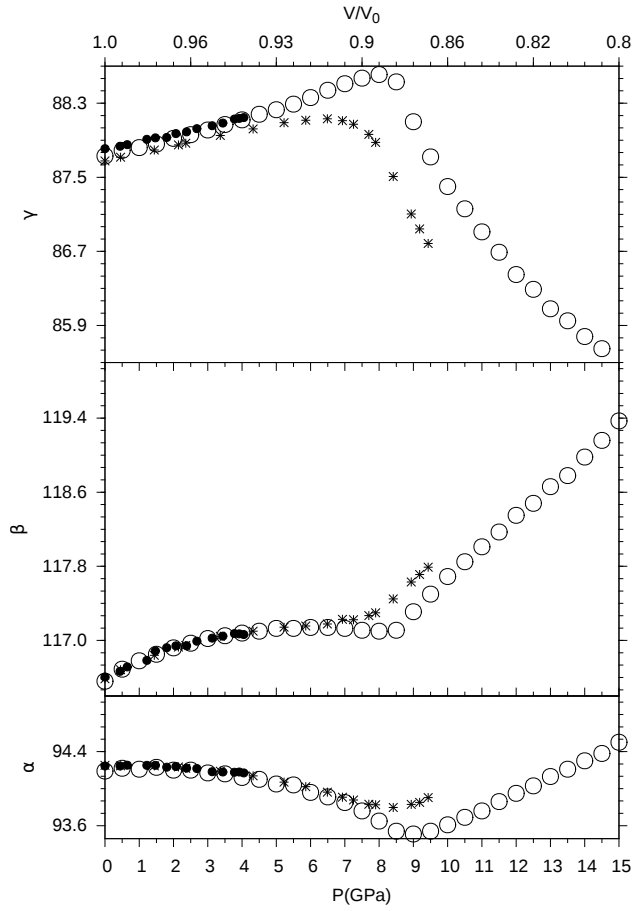

FIG. 2. Variation of the calculated cell angles (degrees) as a function of pressure (empty circles). Full circles and asterisks represent experimental data by Downs *et al.*[1] and by Benusa *et al.*,[2] respectively.

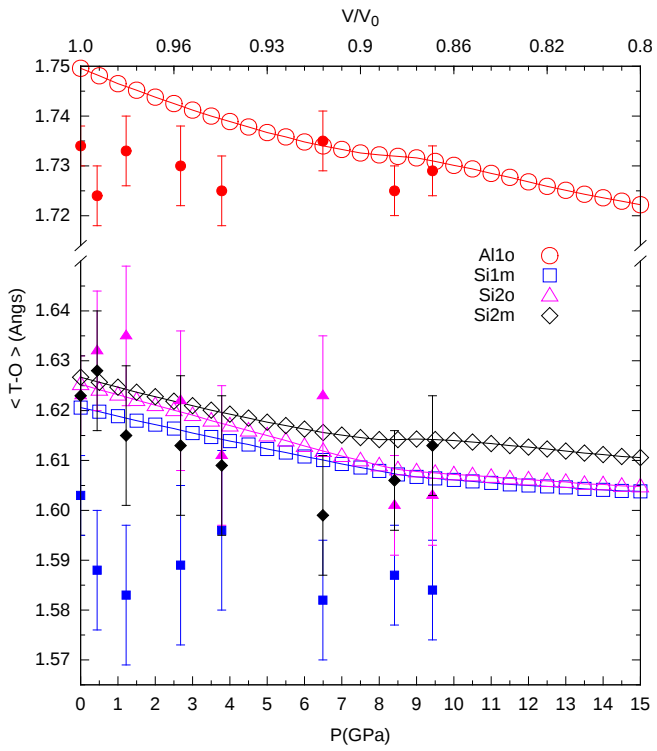

FIG. 3. Calculated averaged tetrahedral bond lengths < T-O > as functions of pressure P (empty symbols). Full symbols represent the corresponding experimental data. Data below 4 GPa is from Downs *et al.*[1]; data above 4 GPa is from Benusa *et al.*[2]

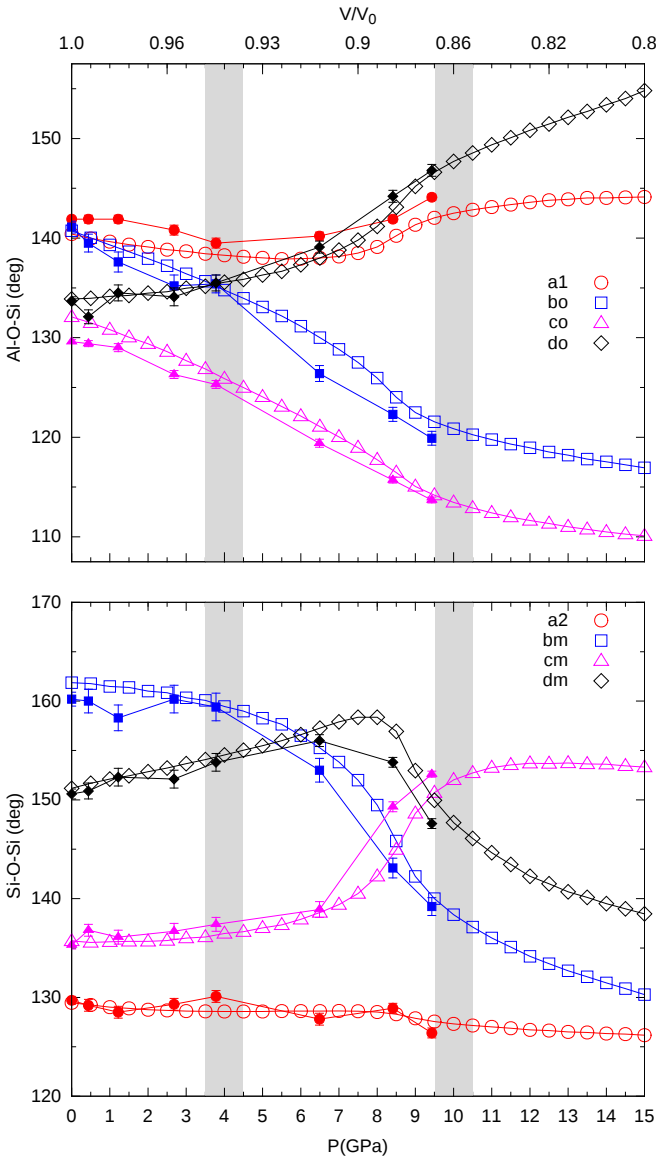

FIG. 4. Calculated T-O-T angles as functions of pressure P (empty symbols). Full symbols represent the corresponding experimental data. Data below 4 GPa is from Downs *et al.*[1]; data above 4 GPa is from Benusa *et al.*[2]

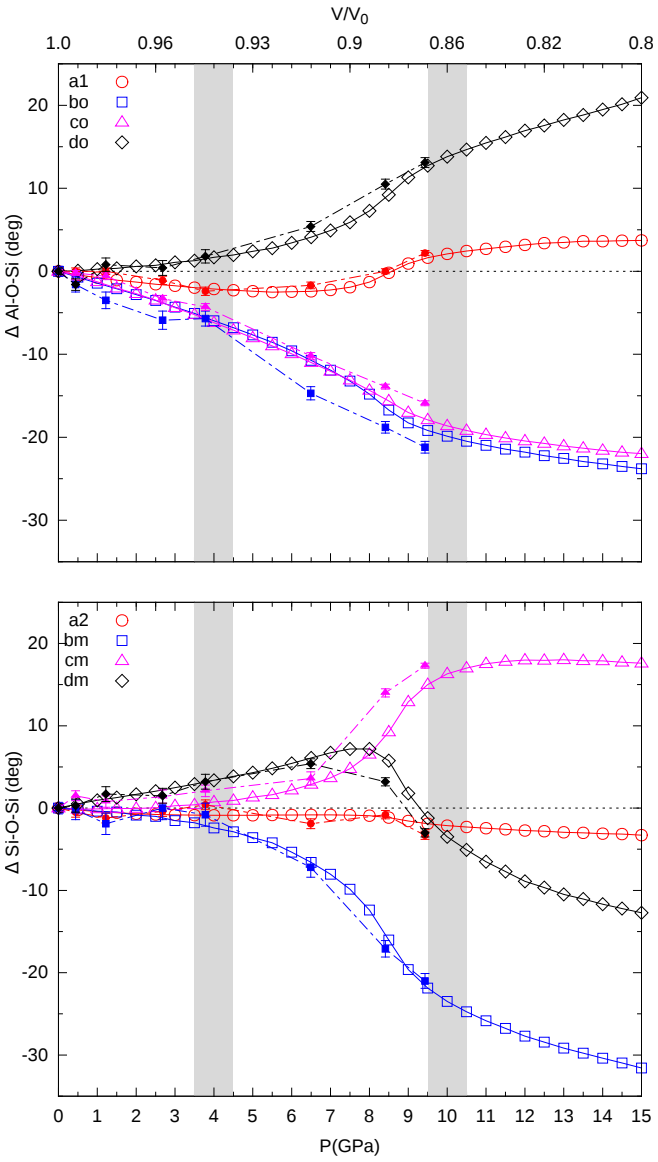

FIG. 5. Variation Δ of the calculated T-O-T angles as a function of pressure P (empty symbols). Full symbols represent the corresponding experimental data. Data below 4 GPa is from Downs *et al.*[1]; data above 4 GPa is from Benusa *et al.*[2]

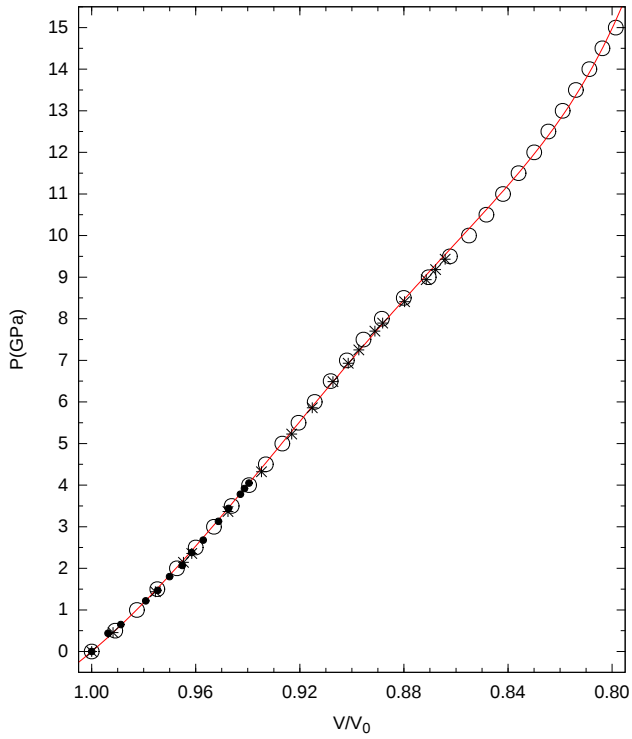

FIG. 6. Variation of pressure P (GPa) as a function of the unit cell volume V (normalized to its minimum energy value V_0). Calculated data (empty circles) fitted to the $5th$ order Birch-Murnaghan equation (red line). Full circles and asterisks represent experimental data by Downs *et al.*[1] and by Benusa *et al.*,[2] respectively.

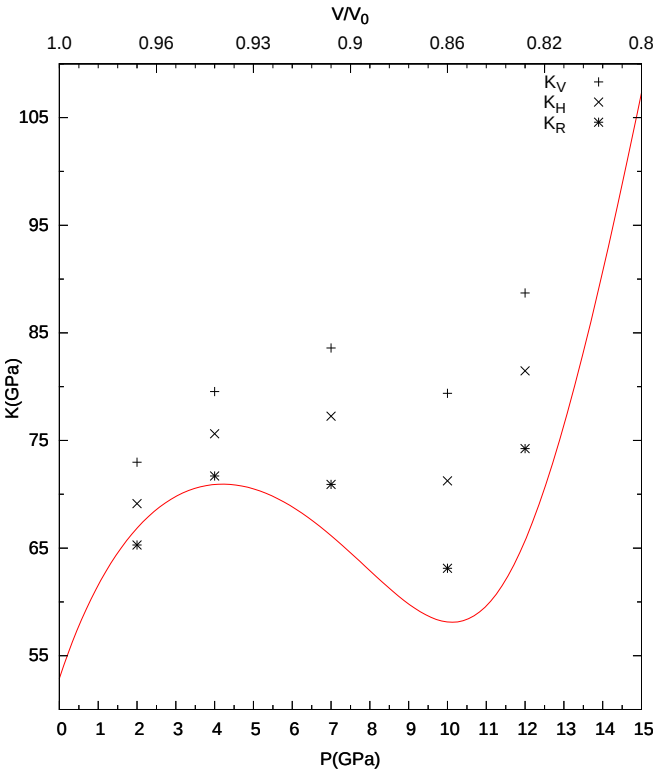

FIG. 7. Variation of the calculated bulk modulus K as a function of pressure P. The solid red line shows the bulk modulus K fitted to the $5th$ order Birch-Murnaghan equation of state. Analytical bulk moduli obtained *via* elastic constant calculations at different pressures, K_V, K_H and K_R, are also reported.