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*Original Citation:*

*Availability:*

This version is available <http://hdl.handle.net/2318/1800625> since 2021-09-10T10:20:55Z

*Published version:*

DOI:10.1007/s00269-020-01110-w

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# Ab initio compressibility of metastable low-albite

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(Dated: September 10, 2014)

TABLE I. Calculated unit cell parameters of albite

| $P$<br>(GPa) | $a$<br>(Å) | $b$<br>(Å) | $c$<br>(Å) | $\alpha$<br>(°) | $\beta$<br>(°) | $\gamma$<br>(°) | $V$<br>(Å <sup>3</sup> ) |
|--------------|------------|------------|------------|-----------------|----------------|-----------------|--------------------------|
| 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 <sub>1o</sub> | O <sub>a1</sub> | 1.7563 | 1.7461 | 1.7405 | 1.7344 | 1.7306 | 1.7216 |
| Al <sub>1o</sub> | O <sub>bo</sub> | 1.7511 | 1.7380 | 1.7336 | 1.7323 | 1.7340 | 1.7314 |
| Al <sub>1o</sub> | O <sub>co</sub> | 1.7377 | 1.7291 | 1.7276 | 1.7291 | 1.7319 | 1.7308 |
| Al <sub>1o</sub> | O <sub>do</sub> | 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 <sub>1m</sub> | O <sub>a1</sub> | 1.6112 | 1.6057 | 1.6028 | 1.5995 | 1.5964 | 1.5898 |
| Si <sub>1m</sub> | O <sub>bm</sub> | 1.6111 | 1.6058 | 1.6047 | 1.6067 | 1.6109 | 1.6138 |
| Si <sub>1m</sub> | O <sub>cm</sub> | 1.6314 | 1.6242 | 1.6198 | 1.6127 | 1.6056 | 1.5986 |
| Si <sub>1m</sub> | O <sub>dm</sub> | 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 <sub>2o</sub> | O <sub>a2</sub> | 1.6425 | 1.6331 | 1.6282 | 1.6234 | 1.6210 | 1.6155 |
| Si <sub>2o</sub> | O <sub>bo</sub> | 1.6041 | 1.5976 | 1.5949 | 1.5932 | 1.5934 | 1.5920 |
| Si <sub>2o</sub> | O <sub>cm</sub> | 1.6266 | 1.6179 | 1.6129 | 1.6064 | 1.6012 | 1.5963 |
| Si <sub>2o</sub> | O <sub>dm</sub> | 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 <sub>2m</sub> | O <sub>a2</sub> | 1.6564 | 1.6445 | 1.6385 | 1.6332 | 1.6324 | 1.6308 |
| Si <sub>2m</sub> | O <sub>bm</sub> | 1.6322 | 1.6254 | 1.6230 | 1.6227 | 1.6250 | 1.6253 |
| Si <sub>2m</sub> | O <sub>co</sub> | 1.6047 | 1.6021 | 1.6027 | 1.6049 | 1.6071 | 1.6082 |
| Si <sub>2m</sub> | O <sub>do</sub> | 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 |

<sup>1</sup> R. Downs, R. M. Hazen, and L. W. Finger, *Am. Mineral.* **79**, 1042 (1994).

<sup>2</sup> 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 <sub>0</sub> |        |        |        |        |        |        |
|------------------|-----------------|------------------|------------------|--------|--------|--------|--------|--------|--------|
|                  |                 |                  | 1.00             | 0.95   | 0.91   | 0.88   | 0.86   | 0.82   | 0.80   |
| Al <sub>1o</sub> | O <sub>a1</sub> | Si <sub>1m</sub> | 140.41           | 138.57 | 137.97 | 140.27 | 142.26 | 143.90 | 144.22 |
| Si <sub>2o</sub> | O <sub>a2</sub> | Si <sub>2m</sub> | 129.45           | 128.60 | 128.64 | 128.26 | 127.46 | 126.50 | 126.10 |
| Al <sub>1o</sub> | O <sub>bo</sub> | Si <sub>2o</sub> | 140.74           | 136.01 | 130.26 | 123.94 | 121.25 | 118.19 | 116.98 |
| Si <sub>1m</sub> | O <sub>bm</sub> | Si <sub>2m</sub> | 161.86           | 160.13 | 155.48 | 145.59 | 139.22 | 132.66 | 130.27 |
| Al <sub>1o</sub> | O <sub>co</sub> | Si <sub>2m</sub> | 132.08           | 127.36 | 121.26 | 116.31 | 113.89 | 111.01 | 110.16 |
| Si <sub>1m</sub> | O <sub>cm</sub> | Si <sub>2o</sub> | 135.72           | 136.04 | 138.54 | 145.40 | 151.32 | 153.73 | 153.23 |
| Al <sub>1o</sub> | O <sub>do</sub> | Si <sub>2m</sub> | 133.89           | 135.06 | 137.89 | 143.28 | 147.11 | 152.17 | 154.78 |
| Si <sub>1m</sub> | O <sub>dm</sub> | Si <sub>2o</sub> | 151.17           | 153.97 | 157.15 | 156.53 | 148.94 | 140.64 | 138.34 |

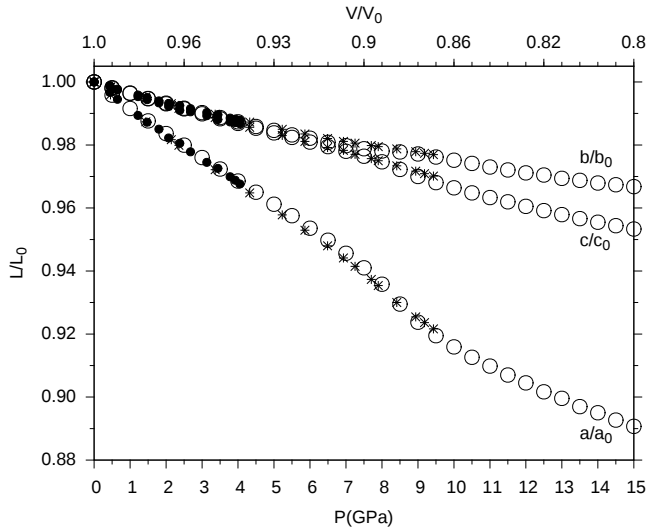


FIG. 1. Variation of the calculated cell parameters (normalized to their minimum energy values) as a function of pressure (empty circles). Full circles and asterisks represent experimental data by Downs *et al.*<sup>1</sup> and Benusa *et al.*,<sup>2</sup> respectively.

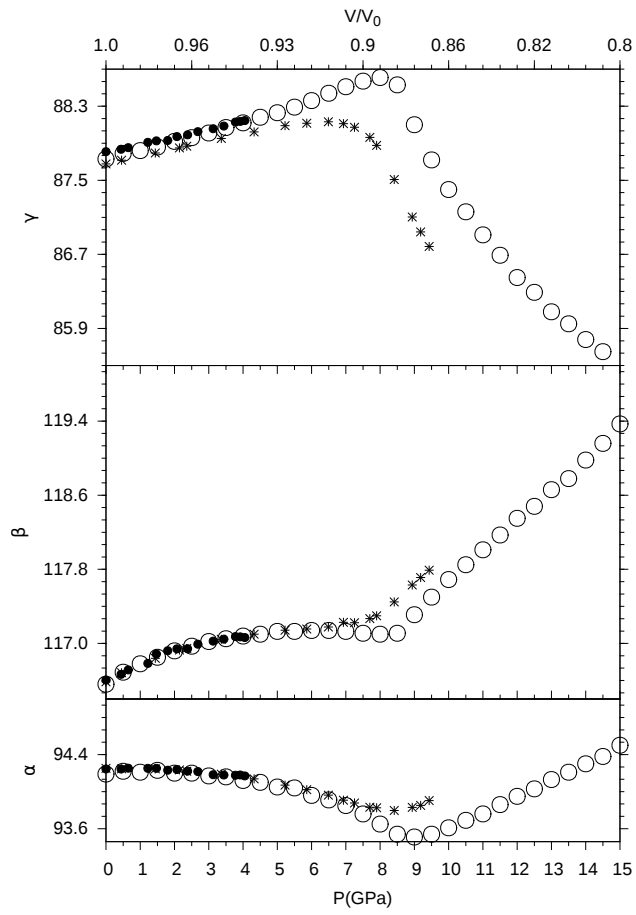


FIG. 2. Variation of the calculated cell angles (degrees) as a function of pressure (empty circles). Full circles and asterisks represent experimental data by Downs *et al.*<sup>1</sup> and by Benusa *et al.*,<sup>2</sup> respectively.

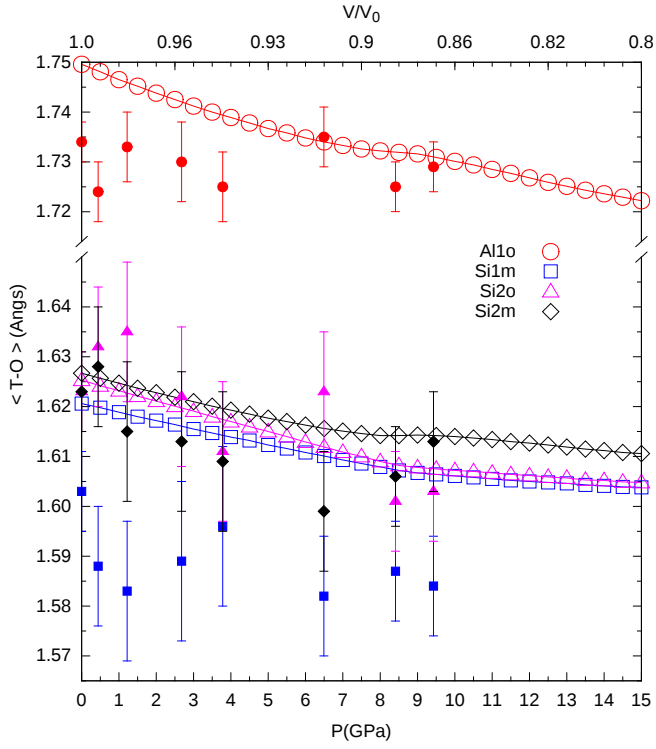


FIG. 3. Calculated averaged tetrahedral bond lengths  $\langle T-O \rangle$  as functions of pressure  $P$  (empty symbols). Full symbols represent the corresponding experimental data. Data below 4 GPa is from Downs *et al.*<sup>1</sup>; data above 4 GPa is from Benusa *et al.*<sup>2</sup>

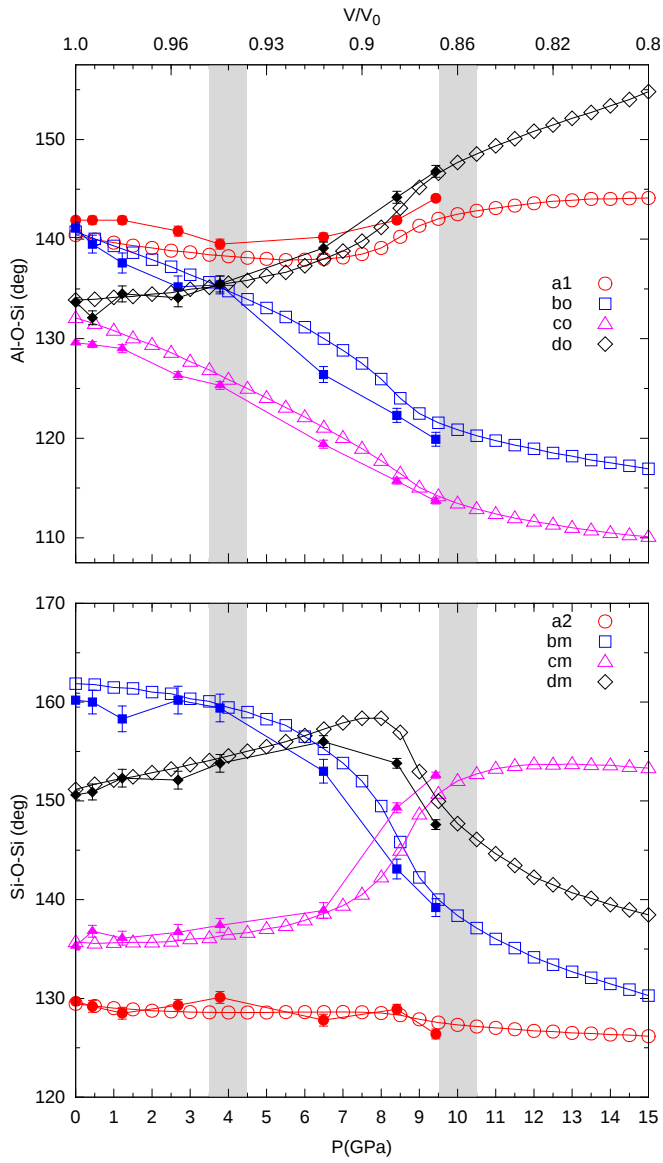


FIG. 4. Calculated T-O-T angles as functions of pressure  $P$  (empty symbols). Full symbols represent the corresponding experimental data. Data below 4 GPa is from Downs *et al.*<sup>1</sup>; data above 4 GPa is from Benusa *et al.*<sup>2</sup>

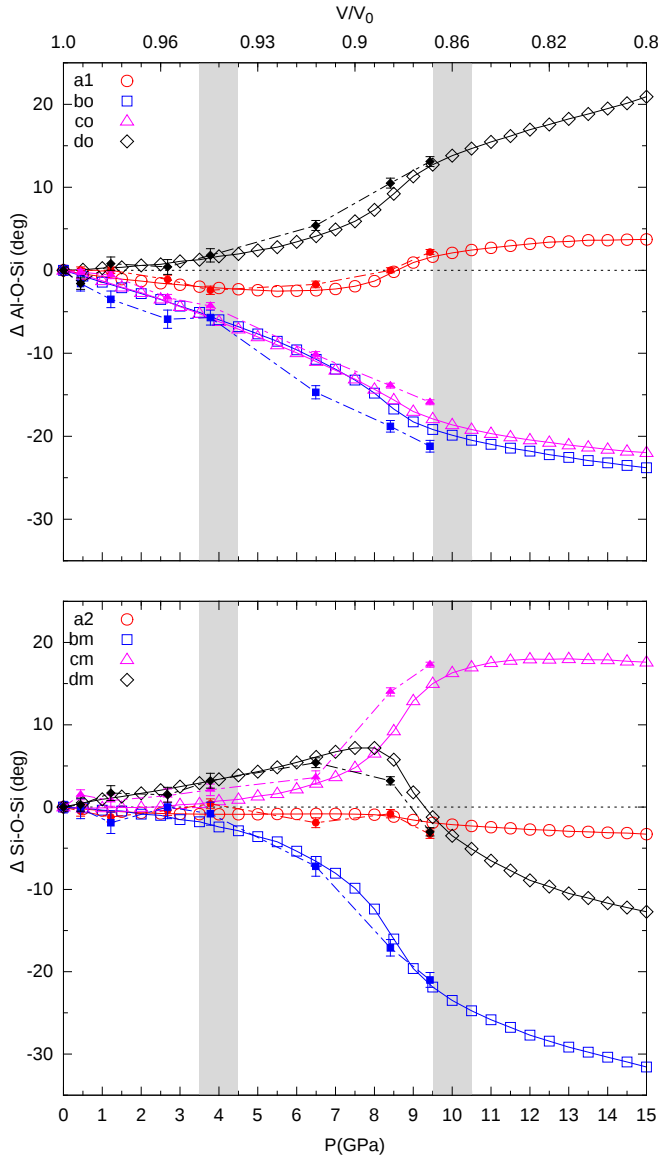


FIG. 5. Variation  $\Delta$  of the calculated T-O-T angles as a function of pressure  $P$  (empty symbols). Full symbols represent the corresponding experimental data. Data below 4 GPa is from Downs *et al.*<sup>1</sup>; data above 4 GPa is from Benusa *et al.*<sup>2</sup>

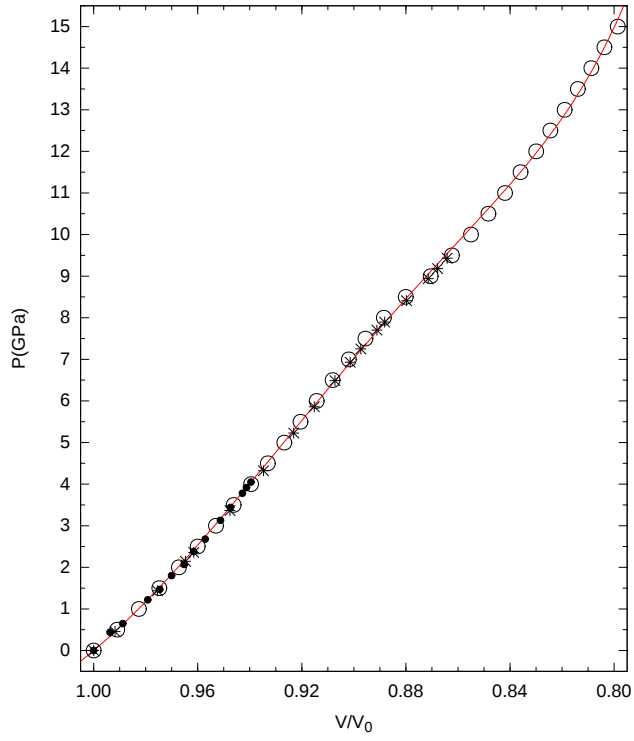


FIG. 6. Variation of pressure  $P$  (GPa) as a function of the unit cell volume  $V$  (normalized to its minimum energy value  $V_0$ ). Calculated data (empty circles) fitted to the 5<sup>th</sup> order Birch-Murnaghan equation (red line). Full circles and asterisks represent experimental data by Downs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



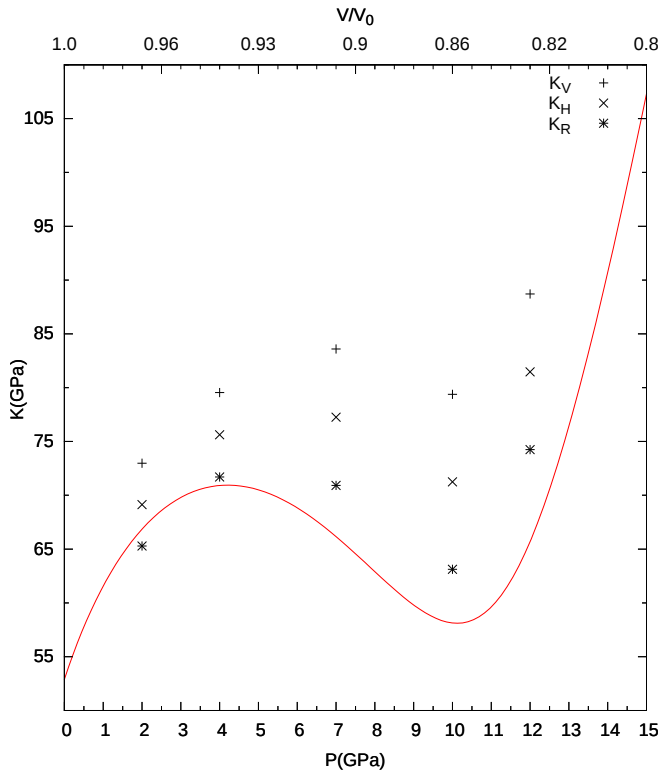


FIG. 7. Variation of the calculated bulk modulus  $K$  as a function of pressure  $P$ . The solid red line shows the bulk modulus  $K$  fitted to the 5th order Birch-Murnaghan equation of state. Analytical bulk moduli obtained *via* elastic constant calculations at different pressures,  $K_V$ ,  $K_H$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