**High-temperature behaviour of fedorite, Na2.5(Ca4.5Na2.5)[Si16O38]F2·2.8H2O, from Murun Alkaline Complex (Russia)**

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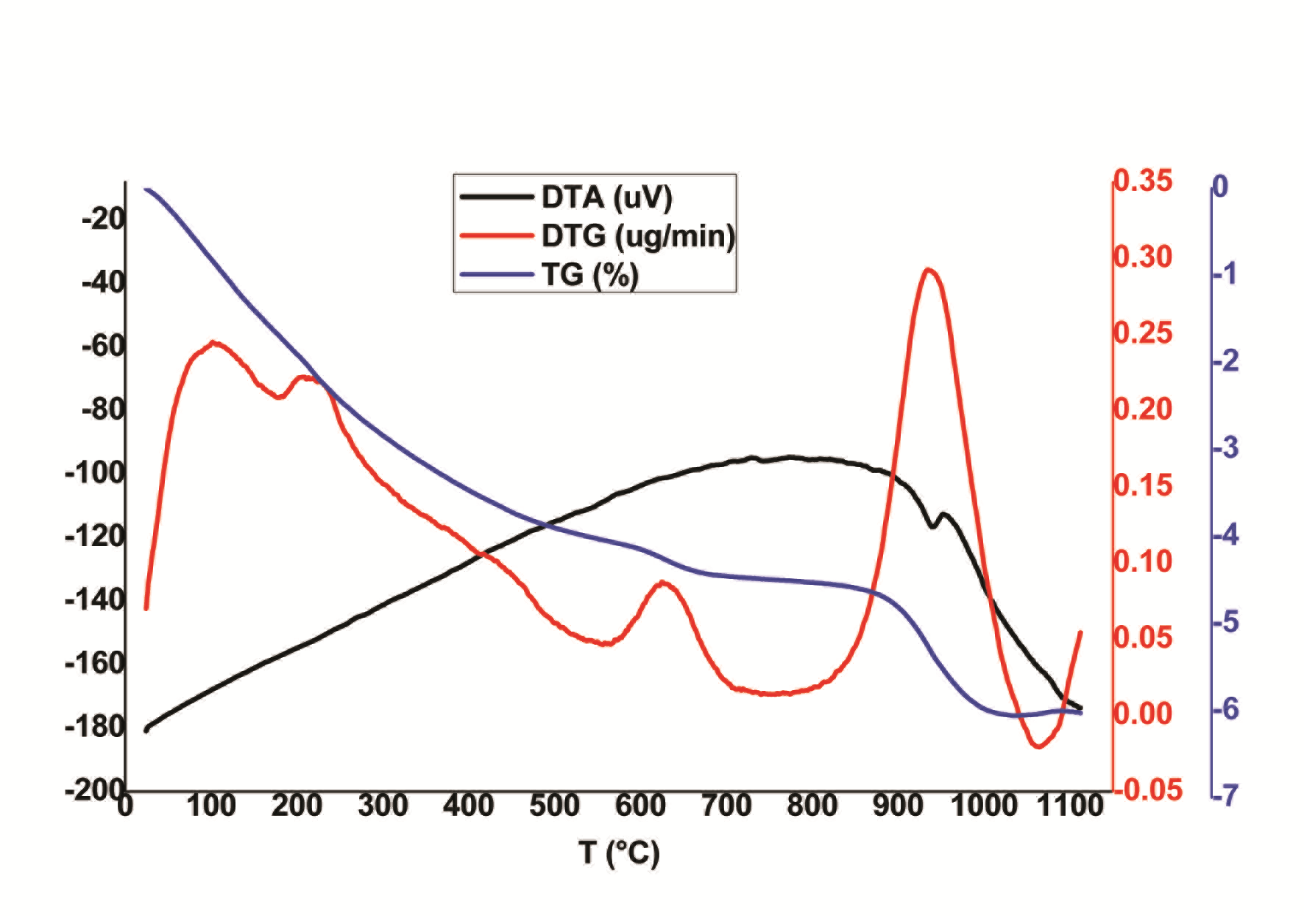
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**Fig. S1.** Sample of fedorite from the Gavrilovskaya zone (sample Gav-33): (a) unpolished sample; (b) polished sample.

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**Fig. S2.** Thin section image of sample Gav-33 in transmitted light. (a, d, e, g, i, l) polarizers are parallel; (b, c, f, h, j, k) polarizers are crossed. The interference color corresponds to a thickness of thin section (~ 30 μm). Fedorite occurs as elongated scaly subhedral grains up to 5.5 × 1.2 × 1.0 mm in size, showing perfect cleavage along {001}. Small euhedral crystals of aegirine (0.07 × 0.01−0.07 × 0.05 mm), amphibole (0.04 × 0.02−0.10 × 0.04 mm), and apatite (0.02 × 0.05−0.04 × 0.09 mm) were found as inclusions in fedorite (c, d, k, l) which indicates its earlier crystallization (Table S1). Fedorite grains are slightly cataclastic and can be replaced by secondary minerals (probably, pectolite) along the cleavage and the cracks of the cataclase. Needle-like aegirine grains are often located along the cleavage of the mineral (c). Larger subhedral aegirine grains (0.4 × 0.1 mm) are located at the boundary between fedorite and quartz grains. Aegirine grains exhibit pleochroism (from yellowish-green to blue-green).

Larger subhedral grains of amphibole (0.2 × 0.15−0.07 × 0.05 mm) and apatite (0.4 × 0.3−0.1 × 0.15 mm) also occur in xenomorphic relation to fedorite (g, j, l). Amphibole grains are pleochroic from light green to gray, and the interference colors have an unusual ink color. Microcline grains up to 0.4 × 0.3 mm in size and anhedral quartz grains are also xenomorphic in relation to fedorite (a, b, d-g, i). In turn, quartz is xenomorphic with respect to the microcline. The grain sizes of quartz vary from 0.1 × 0.15 to 0.5 × 0.2 mm. Quartz contains inclusions of apatite and fedorite crystals up to 0.1 × 0.25 mm and 0.15 × 0.1 mm in size, respectively. At the grain boundary of quartz, single elongated small grains of rutile up to 0.02 × 0.05 mm in size were found. Calcite is rare. Its grains are quite small and do not exceed 0.05 × 0.05 mm. They are xenomorphic in relation to fedorite. Fibrous grains of pectolite form fan-shaped aggregates and, possibly, were formed as a result of hypergene processes.

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**Figure S3.** Differential thermal analysis (DTA, black line), thermogravimetric analysis (TG, blue line), and the TG first derivative (DTG, red line) of Gav-33 sample measured in He and mass analysis of the evolved gases as a function of temperature recorded for fluorine (m/z = 19).

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**Figure S4.** Normalized distances of the Na interlayer cations versus temperature.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Minerals** | **Mineral formation order** | | | | | | | |
| Aegirine |  |  |  | |  |  |  |  |
|  |  | |  |  |  |  |  |
| Apatite |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |
| Amphibole |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |
| Fedorite |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |
| Microcline |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |
| Rutile |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |
| Quartz |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |
| Pectolite |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |
| Calcite |  |  | |  |  |  |  |  |
|  |  | |  |  |  |  |  |

**Table S1**. The order and relative duration of crystallization of the minerals in sample Gav-33.

**Table S2.** Crystallographic coordinates, occupancies, equivalent isotropic (Å2) and anisotropic displacement parameters of the studied fedorite from 100 to 300 °C, 500 and 600 °C.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | ***x/a*** | ***y/b*** | ***z/c*** | **Occupancy** | **Uiso/equivalent** | ***U*11** | ***U*22** | ***U*33** | ***U*12** | ***U*13** | ***U*23** |
| **100 °C** |  |  |  |  |  |  |  |  |  |  |  |  |
| *Na*1 | Na | 0.0000 | 0.0000 | 0.5000 | 0.7236 | 0.01550(12) | 0.0135 (3) | 0.0149 (3) | 0.0183 (3) | 0.0077 (2) | 0.0033 (2) | 0.0052 (2) |
| *Ca*1 | Ca | 0.0000 | 0.0000 | 0.5000 | 0.2765 | 0.01550(12) | 0.0135 (3) | 0.0149 (3) | 0.0183 (3) | 0.0077 (2) | 0.0033 (2) | 0.0052 (2) |
| *Na*2 | Na | 0.42236 (5) | 0.28460 (5) | 0.50945 (3) | 0.4298 | 0.01280(6) | 0.01190 (13) | 0.01125 (13) | 0.01520 (14) | 0.00638 (11) | 0.00331 (11) | 0.00360 (11) |
| *Ca*2 | Ca | 0.42236 (5) | 0.28460 (5) | 0.50945 (3) | 0.5702 | 0.01280(6) | 0.01190 (13) | 0.01125 (13) | 0.01520 (14) | 0.00638 (11) | 0.00331 (11) | 0.00360 (11) |
| *Na*3 | Na | 0.71135 (4) | 0.14789 (4) | 0.50088 (3) | 0.1593 | 0.01180(4) | 0.01137 (10) | 0.01082 (10) | 0.01382 (11) | 0.00590 (9) | 0.00368 (9) | 0.00472 (9) |
| *Ca*3 | Ca | 0.71135 (4) | 0.14789 (4) | 0.50088 (3) | 0.8407 | 0.01180(4) | 0.01137 (10) | 0.01082 (10) | 0.01382 (11) | 0.00590 (9) | 0.00368 (9) | 0.00472 (9) |
| *Na*4 | Na | 0.14933 (4) | 0.43385 (4) | 0.51660 (3) | 0.2482 | 0.01220(5) | 0.01094 (11) | 0.01126 (11) | 0.01445 (13) | 0.00591 (9) | 0.00343 (9) | 0.00444 (10) |
| *Ca*4 | Ca | 0.14933 (4) | 0.43385 (4) | 0.51660 (3) | 0.7518 | 0.01220(5) | 0.01094 (11) | 0.01126 (11) | 0.01445 (13) | 0.00591 (9) | 0.00343 (9) | 0.00444 (10) |
| *Si*1 | Si | 0.28400 (5) | 0.60139 (5) | 0.86973 (3) | 1 | 0.00900(6) | 0.00869 (13) | 0.00858 (13) | 0.00968 (14) | 0.00459 (11) | 0.00212 (11) | 0.00282 (11) |
| *Si*2 | Si | 0.13860 (5) | 0.74215 (5) | 0.72986 (3) | 1 | 0.00900(6) | 0.00811 (13) | 0.00799 (13) | 0.01177 (15) | 0.00425 (11) | 0.00289 (11) | 0.00446 (11) |
| *Si*3 | Si | 0.76839 (5) | 0.49686 (5) | 0.72737 (3) | 1 | 0.00960(6) | 0.00795 (13) | 0.00891 (13) | 0.01334 (15) | 0.00479 (11) | 0.00398 (11) | 0.00492 (11) |
| *Si*4 | Si | 0.26363 (5) | 0.10862 (5) | 0.72994 (3) | 1 | 0.00990(6) | 0.00812 (13) | 0.00835 (13) | 0.01373 (15) | 0.00483 (11) | 0.00185 (11) | 0.00367 (11) |
| *Si*5 | Si | 0.02044 (5) | 0.24077 (5) | 0.73382 (3) | 1 | 0.00960(6) | 0.00715 (13) | 0.00817 (13) | 0.01304 (15) | 0.00397 (11) | 0.00227 (11) | 0.00328 (11) |
| *Si*6 | Si | 0.39058 (5) | 0.73803 (5) | 0.13745 (3) | 1 | 0.00870(5) | 0.00841 (13) | 0.00823 (13) | 0.00903 (14) | 0.00428 (11) | 0.00202 (11) | 0.00262 (11) |
| *Si*7 | Si | 0.65203 (5) | −0.00510 (5) | 0.73017 (3) | 1 | 0.00940(6) | 0.00878 (13) | 0.00707 (13) | 0.01235 (15) | 0.00412 (11) | 0.00372 (11) | 0.00307 (11) |
| *Si*8 | Si | 0.52874 (5) | 0.62667 (5) | 0.73365 (3) | 1 | 0.00970(6) | 0.00930 (13) | 0.00803 (13) | 0.01291 (15) | 0.00539 (11) | 0.00337 (11) | 0.00320 (11) |
| O1 | O | 0.70361 (16) | 0.38750 (16) | 0.59851 (11) | 1 | 0.0201(2) | 0.0218 (5) | 0.0198 (5) | 0.0159 (5) | 0.0122 (4) | 0.0000 (4) | 0.0001 (4) |
| O2 | O | 0.12833 (17) | 0.66945 (16) | 0.60116 (10) | 1 | 0.0188(2) | 0.0258 (5) | 0.0176 (5) | 0.0145 (5) | 0.0121 (4) | 0.0081 (4) | 0.0049 (4) |
| O3 | O | 0.27650 (18) | 0.08220 (17) | 0.60360 (11) | 1 | 0.0217(2) | 0.0285 (6) | 0.0223 (5) | 0.0144 (5) | 0.0132 (5) | 0.0062 (4) | 0.0067 (4) |
| O4 | O | 0.42252 (19) | 0.5282 (2) | 0.60723 (12) | 1 | 0.0292(3) | 0.0260 (6) | 0.0355 (7) | 0.0191 (6) | 0.0205 (6) | −0.0069 (5) | −0.0085 (5) |
| O5 | O | 0.01449 (17) | 0.75423 (19) | 0.39078 (11) | 1 | 0.0246(3) | 0.0203 (5) | 0.0314 (7) | 0.0170 (5) | 0.0088 (5) | 0.0038 (4) | 0.0126 (5) |
| O6 | O | 0.57132 (16) | 0.95490 (16) | 0.60176 (10) | 1 | 0.0194(2) | 0.0191 (5) | 0.0211 (5) | 0.0136 (5) | 0.0085 (4) | 0.0033 (4) | 0.0042 (4) |
| O7 | O | 0.85286 (13) | 0.11945 (14) | 0.76726 (11) | 1 | 0.01680(19) | 0.0093 (4) | 0.0141 (4) | 0.0235 (5) | 0.0033 (3) | 0.0059 (4) | 0.0064 (4) |
| O8 | O | 0.67689 (15) | 0.59595 (15) | 0.76349 (11) | 1 | 0.01700(19) | 0.0164 (4) | 0.0206 (5) | 0.0231 (5) | 0.0150 (4) | 0.0081 (4) | 0.0089 (4) |
| O9 | O | 0.19319 (14) | 0.93756 (13) | 0.76582 (10) | 1 | 0.01580(19) | 0.0173 (4) | 0.0089 (4) | 0.0209 (5) | 0.0065 (3) | 0.0038 (4) | 0.0059 (3) |
| O10 | O | 0.62560 (16) | 0.82925 (14) | 0.76021 (12) | 1 | 0.0196(2) | 0.0209 (5) | 0.0104 (4) | 0.0325 (6) | 0.0096 (4) | 0.0112 (5) | 0.0110 (4) |
| O11 | O | 0.43824 (13) | 0.24978 (14) | 0.82227 (11) | 1 | 0.0170(2) | 0.0094 (4) | 0.0113 (4) | 0.0250 (5) | 0.0048 (3) | −0.0015 (4) | 0.0012 (4) |
| O12 | O | 0.58285 (15) | 0.07885 (14) | 0.81792 (11) | 1 | 0.01610(19) | 0.0175 (4) | 0.0116 (4) | 0.0231 (5) | 0.0092 (4) | 0.0113 (4) | 0.0055 (4) |
| O13 | O | 0.42569 (17) | 0.58047 (18) | 0.82757 (13) | 1 | 0.0225(3) | 0.0236 (5) | 0.0287 (6) | 0.0357 (7) | 0.0207 (5) | 0.0221 (5) | 0.0226 (6) |
| O14 | O | 0.26557 (15) | 0.73098 (16) | 0.81755 (12) | 1 | 0.0203(2) | 0.0143 (4) | 0.0173 (5) | 0.0303 (6) | 0.0082 (4) | −0.0002 (4) | 0.0131 (4) |
| O15 | O | 0.03927 (13) | 0.35132 (15) | 0.24033 (11) | 1 | 0.0180(2) | 0.0091 (4) | 0.0163 (4) | 0.0265 (6) | 0.0039 (3) | 0.0072 (4) | 0.0092 (4) |
| O16 | O | 0.11215 (15) | 0.42226 (14) | 0.83039 (12) | 1 | 0.0198(2) | 0.0135 (4) | 0.0093 (4) | 0.0274 (6) | 0.0020 (3) | 0.0055 (4) | −0.0008 (4) |
| O17 | O | 0.13129 (15) | 0.16094 (16) | 0.75331 (13) | 1 | 0.0221(3) | 0.0133 (4) | 0.0176 (5) | 0.0396 (7) | 0.0118 (4) | 0.0058 (4) | 0.0082 (5) |
| O18 | O | 0.75155 (15) | 0.39027 (16) | 0.81430 (12) | 1 | 0.0189(2) | 0.0154 (4) | 0.0206 (5) | 0.0293 (6) | 0.0104 (4) | 0.0111 (4) | 0.0189 (5) |
| O19 | O | 0.3333 (2) | 0.6731 (2) | 0.00353 (11) | 1 | 0.0267(3) | 0.0332 (7) | 0.0305 (7) | 0.0101 (4) | 0.0156 (6) | 0.0012 (4) | 0.0009 (4) |
| F | F | 0.15980 (15) | 0.20617 (15) | 0.41736 (10) | 1 | 0.0237(2) | 0.0228 (5) | 0.0251 (5) | 0.0211 (5) | 0.0127 (4) | 0.0035 (4) | 0.0048 (4) |
| *Na*5 | Na | 0.0850 (7) | 0.1068 (7) | 0.2173 (3) | 0.5686 | 0.0220(4) | 0.0162 (8) | 0.0170 (8) | 0.0350 (11) | 0.0095 (6) | 0.0085 (8) | 0.0097 (8) |
| *K* | K | 0.0747 (15) | 0.0975 (15) | 0.1912 (8) | 0.2162 | 0.0548(19) | 0.038 (3) | 0.044 (3) | 0.093 (6) | 0.024 (2) | 0.024 (4) | 0.032 (4) |
| *Na*6 | Na | 0.6605 (13) | −0.0211 (10) | 0.0006 (5) | 0.2673 | 0.111(2) | 0.158 (6) | 0.065 (4) | 0.033 (3) | 0.012 (4) | 0.003 (4) | 0.011 (3) |
| *Na*7 | Na | 0.6930 (17) | 0.6649 (15) | 0.0021 (6) | 0.2946 | 0.144(3) | 0.263 (7) | 0.196 (6) | 0.044 (3) | 0.185 (5) | 0.017 (5) | 0.015 (4) |
| *Na*8 | Na | 0.9845 (7) | 0.3362 (11) | 0.0038 (4) | 0.2575 | 0.0794(17) | 0.038 (2) | 0.148 (5) | 0.0175 (17) | 0.033 (3) | 0.0075 (16) | 0.007 (3) |
| O20w | O | 0.0000 | 0.0000 | 0.0000 | 0.172(9) | 0.029(3) | - | - | - | - | - | - |
| O21w | O | 0.118 (5) | −0.075 (5) | 0.002 (3) | 0.177(8) | 0.199(9) | - | - | - | - | - | - |
| O22w | O | 0.071 (4) | 0.178 (4) | −0.001 (3) | 0.188(8) | 0.159(8) | - | - | - | - | - | - |
| O23w | O | −0.024 (3) | 0.050 (3) | 0.0020 (19) | 0.173(8) | 0.087(6) | - | - | - | - | - | - |
| O24w | O | 0.108 (3) | 0.079 (3) | −0.0002 (18) | 0.292(8) | 0.152(6) | - | - | - | - | - | - |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| **200 °C** |  |  |  |  |  |  |  |  |  |  |  |  |
| *Na*1 | Na | 0.0000 | 0.0000 | 0.5000 | 0.7236 | 0.01880(12) | 0.0168 (3) | 0.0184 (3) | 0.0210 (3) | 0.0095 (2) | 0.0039 (2) | 0.0059 (2) |
| *Ca*1 | Ca | 0.0000 | 0.0000 | 0.5000 | 0.2765 | 0.01880(12) | 0.0168 (3) | 0.0184 (3) | 0.0210 (3) | 0.0095 (2) | 0.0039 (2) | 0.0059 (2) |
| *Na*2 | Na | 0.42284 (5) | 0.28498 (5) | 0.50994 (4) | 0.4298 | 0.01550(6) | 0.01462 (14) | 0.01380 (14) | 0.01794 (16) | 0.00785 (12) | 0.00391 (12) | 0.00412 (12) |
| *Ca*2 | Ca | 0.42284 (5) | 0.28498 (5) | 0.50994 (4) | 0.5702 | 0.01550(6) | 0.01462 (14) | 0.01380 (14) | 0.01794 (16) | 0.00785 (12) | 0.00391 (12) | 0.00412 (12) |
| *Na*3 | Na | 0.71163 (4) | 0.14807 (4) | 0.50109 (3) | 0.1593 | 0.01420(5) | 0.01384 (11) | 0.01290 (11) | 0.01668 (13) | 0.00717 (9) | 0.00464 (9) | 0.00561 (9) |
| *Ca*3 | Ca | 0.71163 (4) | 0.14807 (4) | 0.50109 (3) | 0.8408 | 0.01420(5) | 0.01384 (11) | 0.01290 (11) | 0.01668 (13) | 0.00717 (9) | 0.00464 (9) | 0.00561 (9) |
| *Na*4 | Na | 0.14970 (4) | 0.43445 (4) | 0.51742 (3) | 0.2482 | 0.01460(5) | 0.01338 (12) | 0.01368 (12) | 0.01720 (14) | 0.00731 (10) | 0.00416 (10) | 0.00538 (10) |
| *Ca*4 | Ca | 0.14970 (4) | 0.43445 (4) | 0.51742 (3) | 0.7518 | 0.01460(5) | 0.01338 (12) | 0.01368 (12) | 0.01720 (14) | 0.00731 (10) | 0.00416 (10) | 0.00538 (10) |
| *Si*1 | Si | 0.28398 (5) | 0.60088 (5) | 0.86982 (3) | 1 | 0.01070(6) | 0.01044 (14) | 0.00995 (14) | 0.01121 (15) | 0.00544 (12) | 0.00253 (12) | 0.00287 (11) |
| *Si*2 | Si | 0.13830 (5) | 0.74191 (5) | 0.73020 (3) | 1 | 0.01060(6) | 0.00946 (13) | 0.00909 (14) | 0.01370 (16) | 0.00477 (11) | 0.00334 (12) | 0.00486 (12) |
| *Si*3 | Si | 0.76861 (5) | 0.49721 (5) | 0.72786 (4) | 1 | 0.01120(6) | 0.00952 (14) | 0.01030 (14) | 0.01543 (16) | 0.00563 (12) | 0.00462 (12) | 0.00569 (12) |
| *Si*4 | Si | 0.26358 (5) | 0.10819 (5) | 0.73051 (4) | 1 | 0.01150(6) | 0.00959 (14) | 0.00968 (14) | 0.01571 (16) | 0.00558 (12) | 0.00224 (12) | 0.00406 (12) |
| *Si*5 | Si | 0.02088 (5) | 0.24046 (5) | 0.73466 (4) | 1 | 0.01110(6) | 0.00859 (13) | 0.00935 (14) | 0.01478 (16) | 0.00467 (11) | 0.00254 (12) | 0.00344 (12) |
| *Si*6 | Si | 0.39066 (5) | 0.73840 (5) | 0.13751 (3) | 1 | 0.01020(6) | 0.01021 (13) | 0.00969 (14) | 0.01035 (14) | 0.00518 (11) | 0.00238 (11) | 0.00281 (11) |
| *Si*7 | Si | 0.65248 (5) | −0.00507 (5) | 0.73069 (3) | 1 | 0.01090(6) | 0.01039 (14) | 0.00810 (13) | 0.01437 (16) | 0.00478 (12) | 0.00429 (12) | 0.00345 (11) |
| *Si*8 | Si | 0.52921 (5) | 0.62704 (5) | 0.73433 (4) | 1 | 0.01140(6) | 0.01111 (14) | 0.00942 (14) | 0.01514 (16) | 0.00641 (12) | 0.00429 (12) | 0.00395 (12) |
| O1 | O | 0.70399 (17) | 0.38802 (17) | 0.59878 (11) | 1 | 0.0233(2) | 0.0247 (6) | 0.0229 (6) | 0.0188 (5) | 0.0137 (5) | 0.0007 (4) | 0.0005 (4) |
| O2 | O | 0.12798 (18) | 0.66950 (16) | 0.60119 (11) | 1 | 0.0219(2) | 0.0301 (6) | 0.0203 (5) | 0.0172 (5) | 0.0142 (5) | 0.0101 (5) | 0.0055 (4) |
| O3 | O | 0.27596 (19) | 0.08185 (18) | 0.60404 (12) | 1 | 0.0256(3) | 0.0328 (7) | 0.0260 (6) | 0.0176 (5) | 0.0152 (5) | 0.0076 (5) | 0.0073 (5) |
| O4 | O | 0.42316 (19) | 0.5286 (2) | 0.60788 (13) | 1 | 0.0318(3) | 0.0286 (7) | 0.0374 (8) | 0.0214 (6) | 0.0216 (6) | −0.0072 (5) | −0.0084 (5) |
| O5 | O | 0.01406 (18) | 0.7543 (2) | 0.39009 (12) | 1 | 0.0278(3) | 0.0242 (6) | 0.0351 (7) | 0.0193 (6) | 0.0107 (5) | 0.0048 (5) | 0.0141 (5) |
| O6 | O | 0.57164 (17) | 0.95482 (17) | 0.60194 (11) | 1 | 0.0223(2) | 0.0221 (5) | 0.0243 (6) | 0.0155 (5) | 0.0099 (5) | 0.0031 (4) | 0.0049 (4) |
| O7 | O | 0.85303 (14) | 0.11888 (15) | 0.76759 (12) | 1 | 0.0200(2) | 0.0107 (4) | 0.0168 (5) | 0.0280 (6) | 0.0036 (4) | 0.0072 (4) | 0.0077 (4) |
| O8 | O | 0.67732 (15) | 0.59639 (16) | 0.76400 (12) | 1 | 0.0199(2) | 0.0191 (5) | 0.0232 (5) | 0.0277 (6) | 0.0169 (4) | 0.0095 (4) | 0.0101 (4) |
| O9 | O | 0.19326 (15) | 0.93719 (14) | 0.76631 (11) | 1 | 0.0189(3) | 0.0208 (5) | 0.0103 (4) | 0.0252 (6) | 0.0078 (4) | 0.0048 (4) | 0.0072 (4) |
| O10 | O | 0.62607 (17) | 0.82935 (15) | 0.76072 (13) | 1 | 0.0227(2) | 0.0241 (5) | 0.0119 (4) | 0.0367 (7) | 0.0109 (4) | 0.0116 (5) | 0.0113 (4) |
| O11 | O | 0.43815 (14) | 0.24918 (15) | 0.82242 (12) | 1 | 0.0203(2) | 0.0109 (4) | 0.0141 (4) | 0.0296 (6) | 0.0060 (3) | −0.0024 (4) | 0.0008 (4) |
| O12 | O | 0.58357 (16) | 0.07902 (14) | 0.81830 (11) | 1 | 0.0194(3) | 0.0215 (5) | 0.0133 (4) | 0.0277 (6) | 0.0110 (4) | 0.0141 (4) | 0.0064 (4) |
| O13 | O | 0.42603 (18) | 0.58092 (19) | 0.82814 (14) | 1 | 0.0264(3) | 0.0280 (6) | 0.0340 (7) | 0.0409 (8) | 0.0245 (6) | 0.0255 (6) | 0.0260 (6) |
| O14 | O | 0.26468 (16) | 0.72961 (17) | 0.81735 (13) | 1 | 0.0242(2) | 0.0173 (5) | 0.0213 (5) | 0.0358 (7) | 0.0102 (4) | −0.0003 (5) | 0.0161 (5) |
| O15 | O | 0.03923 (14) | 0.35109 (16) | 0.23987 (12) | 1 | 0.0211(3) | 0.0109 (4) | 0.0185 (5) | 0.0307 (6) | 0.0043 (4) | 0.0085 (4) | 0.0101 (4) |
| O16 | O | 0.11299 (15) | 0.42164 (15) | 0.83131 (12) | 1 | 0.0237(3) | 0.0164 (5) | 0.0108 (4) | 0.0321 (7) | 0.0023 (4) | 0.0064 (4) | −0.0016 (4) |
| O17 | O | 0.13114 (16) | 0.16019 (17) | 0.75392 (14) | 1 | 0.0254(3) | 0.0157 (5) | 0.0216 (5) | 0.0450 (8) | 0.0146 (4) | 0.0075 (5) | 0.0097 (5) |
| O18 | O | 0.75115 (15) | 0.38989 (17) | 0.81429 (13) | 1 | 0.0223(3) | 0.0183 (5) | 0.0240 (6) | 0.0352 (7) | 0.0126 (4) | 0.0130 (5) | 0.0222 (5) |
| O19 | O | 0.3330 (2) | 0.6732 (2) | 0.00348 (11) | 1 | 0.0306(3) | 0.0377 (8) | 0.0355 (7) | 0.0108 (5) | 0.0175 (6) | 0.0015 (5) | 0.0014 (5) |
| F | F | 0.16032 (16) | 0.20669 (16) | 0.41758 (11) | 1 | 0.0274(2) | 0.0266 (5) | 0.0288 (6) | 0.0238 (5) | 0.0145 (5) | 0.0039 (4) | 0.0050 (4) |
| *Na*5 | Na | 0.0871 (11) | 0.1103 (10) | 0.2214 (5) | 0.5686 | 0.0245(6) | 0.0189 (11) | 0.0192 (11) | 0.0359 (19) | 0.0103 (9) | 0.0078 (13) | 0.0095 (12) |
| *K* | K | 0.076 (2) | 0.099 (2) | 0.1977 (10) | 0.2162 | 0.0451(16) | 0.036 (3) | 0.039 (3) | 0.062 (5) | 0.020 (2) | 0.014 (4) | 0.017 (4) |
| *Na*6 | Na | 0.649 (2) | −0.0216 (13) | 0.0009 (7) | 0.2673 | 0.189(3) | 0.287 (8) | 0.090 (5) | 0.042 (4) | 0.007 (6) | 0.004 (5) | 0.017 (4) |
| *Na*7 | Na | 0.676 (3) | 0.650 (2) | 0.0020 (9) | 0.2946 | 0.282(4) | 0.608 (9) | 0.346 (8) | 0.064 (5) | 0.405 (6) | 0.022 (7) | 0.020 (6) |
| *Na*8 | Na | 0.9824 (9) | 0.3523 (19) | 0.0042 (6) | 0.2575 | 0.184(3) | 0.047 (3) | 0.371 (8) | 0.031 (3) | 0.062 (5) | 0.013 (2) | 0.008 (5) |
| O20w | O | 0.0000 | 0.0000 | 0.0000 | 0.222(8) | 0.040(3) | - | - | - | - | - | - |
| O21w | O | 0.067 (4) | −0.043 (4) | −0.001 (2) | 0.183(8) | 0.117(7) | - | - | - | - | - | - |
| O23w | O | 0.043 (4) | 0.111 (4) | −0.001 (2) | 0.165(8) | 0.104(7) | - | - | - | - | - | - |
| O24w | O | 0.109 (4) | 0.077 (4) | −0.002 (2) | 0.163(8) | 0.107(7) | - | - | - | - | - | - |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| **300 °C** |  |  |  |  |  |  |  |  |  |  |  |  |
| *Na*1 | Na | 0.0000 | 0.0000 | 0.5000 | 0.7236 | 0.02260(15) | 0.0204 (3) | 0.0218 (4) | 0.0252 (4) | 0.0114 (3) | 0.0046 (3) | 0.0071 (3) |
| *Ca*1 | Ca | 0.0000 | 0.0000 | 0.5000 | 0.2765 | 0.02260(15) | 0.0204 (3) | 0.0218 (4) | 0.0252 (4) | 0.0114 (3) | 0.0046 (3) | 0.0071 (3) |
| *Na*2 | Na | 0.42351 (6) | 0.28528 (6) | 0.51055 (4) | 0.4298 | 0.01820(7) | 0.01719 (16) | 0.01630 (16) | 0.02084 (19) | 0.00925 (14) | 0.00464 (14) | 0.00500 (14) |
| *Ca*2 | Ca | 0.42351 (6) | 0.28528 (6) | 0.51055 (4) | 0.5702 | 0.01820(7) | 0.01719 (16) | 0.01630 (16) | 0.02084 (19) | 0.00925 (14) | 0.00464 (14) | 0.00500 (14) |
| *Na*3 | Na | 0.71176 (4) | 0.14808 (5) | 0.50102 (3) | 0.1593 | 0.01660(6) | 0.01640 (13) | 0.01516 (13) | 0.01933 (15) | 0.00857 (11) | 0.00550 (11) | 0.00654 (11) |
| *Ca*3 | Ca | 0.71176 (4) | 0.14808 (5) | 0.50102 (3) | 0.8408 | 0.01660(6) | 0.01640 (13) | 0.01516 (13) | 0.01933 (15) | 0.00857 (11) | 0.00550 (11) | 0.00654 (11) |
| *Na*4 | Na | 0.14990 (5) | 0.43502 (5) | 0.51783 (3) | 0.2482 | 0.01730(6) | 0.01601 (14) | 0.01654 (14) | 0.02012 (16) | 0.00893 (12) | 0.00508 (12) | 0.00663 (12) |
| *Ca*4 | Ca | 0.14990 (5) | 0.43502 (5) | 0.51783 (3) | 0.7518 | 0.01730(6) | 0.01601 (14) | 0.01654 (14) | 0.02012 (16) | 0.00893 (12) | 0.00508 (12) | 0.00663 (12) |
| *Si*1 | Si | 0.28407 (5) | 0.60116 (5) | 0.86981 (4) | 1 | 0.01210(6) | 0.01219 (15) | 0.01148 (16) | 0.01238 (17) | 0.00634 (13) | 0.00303 (13) | 0.00344 (13) |
| *Si*2 | Si | 0.13807 (5) | 0.74197 (5) | 0.73047 (4) | 1 | 0.01210(7) | 0.01107 (15) | 0.01080 (15) | 0.01538 (17) | 0.00578 (13) | 0.00387 (13) | 0.00568 (13) |
| *Si*3 | Si | 0.76858 (5) | 0.49767 (5) | 0.72813 (4) | 1 | 0.01270(7) | 0.01098 (15) | 0.01185 (16) | 0.01710 (18) | 0.00650 (13) | 0.00522 (13) | 0.00625 (14) |
| *Si*4 | Si | 0.26376 (5) | 0.10818 (5) | 0.73072 (4) | 1 | 0.01310(7) | 0.01129 (15) | 0.01102 (16) | 0.01767 (19) | 0.00659 (13) | 0.00270 (14) | 0.00457 (14) |
| *Si*5 | Si | 0.02142 (5) | 0.24080 (5) | 0.73465 (4) | 1 | 0.01270(7) | 0.01003 (15) | 0.01069 (15) | 0.01667 (18) | 0.00540 (13) | 0.00305 (13) | 0.00386 (13) |
| *Si*6 | Si | 0.39040 (5) | 0.73782 (5) | 0.13722 (4) | 1 | 0.01170(7) | 0.01196 (15) | 0.01126 (15) | 0.01139 (16) | 0.00605 (13) | 0.00267 (12) | 0.00317 (12) |
| *Si*7 | Si | 0.65307 (5) | −0.00431 (5) | 0.73076 (4) | 1 | 0.01250(7) | 0.01202 (15) | 0.00941 (15) | 0.01625 (18) | 0.00569 (13) | 0.00495 (13) | 0.00407 (13) |
| *Si*8 | Si | 0.52940 (5) | 0.62789 (5) | 0.73424 (4) | 1 | 0.01280(7) | 0.01277 (16) | 0.01093 (16) | 0.01651 (18) | 0.00732 (13) | 0.00498 (14) | 0.00462 (13) |
| O1 | O | 0.7042 (2) | 0.3881 (2) | 0.59932 (13) | 1 | 0.0261(3) | 0.0282 (7) | 0.0259 (6) | 0.0203 (6) | 0.0154 (6) | 0.0012 (5) | 0.0006 (5) |
| O2 | O | 0.1281 (2) | 0.66987 (19) | 0.60181 (12) | 1 | 0.0245(3) | 0.0336 (7) | 0.0227 (6) | 0.0186 (6) | 0.0156 (6) | 0.0106 (5) | 0.0059 (5) |
| O3 | O | 0.2763 (2) | 0.0819 (2) | 0.60432 (13) | 1 | 0.0284(3) | 0.0376 (8) | 0.0293 (7) | 0.0190 (6) | 0.0180 (6) | 0.0094 (6) | 0.0079 (5) |
| O4 | O | 0.4234 (2) | 0.5294 (2) | 0.60790 (14) | 1 | 0.0343(3) | 0.0313 (8) | 0.0403 (9) | 0.0226 (7) | 0.0223 (7) | −0.0065 (6) | −0.0073 (6) |
| O5 | O | 0.0136 (2) | 0.7540 (2) | 0.38999 (14) | 1 | 0.0313(3) | 0.0277 (7) | 0.0392 (9) | 0.0219 (7) | 0.0122 (6) | 0.0060 (5) | 0.0153 (6) |
| O6 | O | 0.57185 (19) | 0.9551 (2) | 0.60202 (12) | 1 | 0.0250(3) | 0.0256 (6) | 0.0269 (7) | 0.0169 (6) | 0.0113 (5) | 0.0033 (5) | 0.0048 (5) |
| O7 | O | 0.85357 (16) | 0.11891 (18) | 0.76703 (13) | 1 | 0.0229(3) | 0.0123 (5) | 0.0195 (5) | 0.0307 (7) | 0.0040 (4) | 0.0074 (5) | 0.0079 (5) |
| O8 | O | 0.67727 (18) | 0.59695 (19) | 0.76361 (14) | 1 | 0.0231(3) | 0.0224 (6) | 0.0267 (6) | 0.0328 (7) | 0.0199 (5) | 0.0117 (5) | 0.0122 (5) |
| O9 | O | 0.19313 (18) | 0.93715 (16) | 0.76640 (13) | 1 | 0.0215(2) | 0.0248 (6) | 0.0119 (4) | 0.0281 (6) | 0.0094 (4) | 0.0061 (5) | 0.0085 (4) |
| O10 | O | 0.62667 (19) | 0.83012 (17) | 0.76063 (15) | 1 | 0.0257(3) | 0.0275 (6) | 0.0138 (5) | 0.0417 (8) | 0.0125 (5) | 0.0130 (6) | 0.0134 (5) |
| O11 | O | 0.43814 (16) | 0.24883 (17) | 0.82261 (14) | 1 | 0.0232(3) | 0.0124 (4) | 0.0165 (5) | 0.0336 (7) | 0.0070 (4) | −0.0026 (4) | 0.0013 (5) |
| O12 | O | 0.58474 (18) | 0.08023 (17) | 0.81842 (13) | 1 | 0.0225(3) | 0.0254 (6) | 0.0155 (5) | 0.0316 (7) | 0.0129 (5) | 0.0160 (5) | 0.0070 (5) |
| O13 | O | 0.4264 (2) | 0.5823 (2) | 0.82809 (16) | 1 | 0.0293(3) | 0.0305 (7) | 0.0385 (8) | 0.0443 (9) | 0.0269 (7) | 0.0274 (7) | 0.0282 (7) |
| O14 | O | 0.26397 (18) | 0.7295 (2) | 0.81761 (15) | 1 | 0.0279(3) | 0.0203 (6) | 0.0246 (6) | 0.0409 (9) | 0.0121 (5) | 0.0000 (6) | 0.0180 (6) |
| O15 | O | 0.03960 (16) | 0.35063 (18) | 0.24019 (14) | 1 | 0.0245(3) | 0.0127 (5) | 0.0217 (6) | 0.0358 (8) | 0.0051 (4) | 0.0100 (5) | 0.0119 (5) |
| O16 | O | 0.11368 (18) | 0.42187 (17) | 0.83125 (14) | 1 | 0.0269(3) | 0.0190 (5) | 0.0127 (5) | 0.0355 (8) | 0.0028 (4) | 0.0069 (5) | −0.0021 (5) |
| O17 | O | 0.13140 (18) | 0.1603 (2) | 0.75368 (17) | 1 | 0.0292(4) | 0.0182 (6) | 0.0253 (6) | 0.0513 (10) | 0.0169 (5) | 0.0082 (6) | 0.0115 (6) |
| O18 | O | 0.75114 (18) | 0.3912 (2) | 0.81484 (14) | 1 | 0.0253(3) | 0.0204 (6) | 0.0280 (7) | 0.0382 (8) | 0.0137 (5) | 0.0137 (5) | 0.0247 (6) |
| O19 | O | 0.3332 (2) | 0.6726 (2) | 0.00328 (13) | 1 | 0.0333(4) | 0.0404 (9) | 0.0392 (9) | 0.0124 (5) | 0.0192 (8) | 0.0018 (6) | 0.0019 (5) |
| F | F | 0.16108 (18) | 0.20736 (19) | 0.41847 (12) | 1 | 0.0315(3) | 0.0314 (6) | 0.0338 (7) | 0.0270 (6) | 0.0178 (6) | 0.0048 (5) | 0.0057 (5) |
| *Na*5 | Na | 0.0870 (10) | 0.1092 (10) | 0.2259 (6) | 0.5686 | 0.0274(6) | 0.0216 (11) | 0.0232 (12) | 0.0396 (16) | 0.0130 (10) | 0.0097 (10) | 0.0105 (12) |
| *K* | K | 0.082 (2) | 0.107 (2) | 0.2057 (12) | 0.2162 | 0.0536(18) | 0.044 (3) | 0.049 (3) | 0.081 (6) | 0.027 (3) | 0.025 (4) | 0.036 (4) |
| *Na*6 | Na | 0.638 (2) | −0.0203 (16) | 0.0028 (9) | 0.2673 | 0.237(4) | 0.331 (9) | 0.098 (6) | 0.058 (5) | −0.027 (7) | −0.009 (7) | 0.022 (5) |
| *Na*7 | Na | 0.667 (4) | 0.644 (3) | 0.0033 (13) | 0.2946 | 0.342(4) | 0.732 (9) | 0.442 (8) | 0.107 (7) | 0.505 (7) | 0.059 (8) | 0.073 (7) |
| *Na*8 | Na | 0.9813 (12) | 0.356 (2) | 0.0026 (7) | 0.2575 | 0.217(3) | 0.063 (4) | 0.410 (9) | 0.040 (4) | 0.065 (7) | 0.016 (3) | −0.018 (7) |
| O20w | O | 0.0000 | 0.0000 | 0.0000 | 0.181(8) | 0.044(4) | - | - | - | - | - | - |
| O21w | O | 0.058 (5) | −0.048 (5) | 0.000 (3) | 0.131(8) | 0.118(8) | - | - | - | - | - | - |
| O23w | O | 0.047 (5) | 0.098 (5) | −0.006 (3) | 0.083(7) | 0.073(8) | - | - | - | - | - | - |
| O24w | O | 0.114 (5) | 0.077 (5) | −0.002 (3) | 0.090(7) | 0.081(8) | - | - | - | - | - | - |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| **500 °C** |  |  |  |  |  |  |  |  |  |  |  |  |
| *Na*1 | Na | 0.0000 | 0.0000 | 0.5000 | 0.7236 | 0.03540(19) | 0.0328 (4) | 0.0346 (5) | 0.0379 (5) | 0.0185 (4) | 0.0068 (4) | 0.0097 (4) |
| *Ca*1 | Ca | 0.0000 | 0.0000 | 0.5000 | 0.2765 | 0.03540(19) | 0.0328 (4) | 0.0346 (5) | 0.0379 (5) | 0.0185 (4) | 0.0068 (4) | 0.0097 (4) |
| *Na*2 | Na | 0.42435 (6) | 0.28616 (6) | 0.51162 (4) | 0.4298 | 0.02460(8) | 0.02327 (18) | 0.02241 (18) | 0.0285 (2) | 0.01291 (15) | 0.00656 (15) | 0.00709 (15) |
| *Ca*2 | Ca | 0.42435 (6) | 0.28616 (6) | 0.51162 (4) | 0.5702 | 0.02460(8) | 0.02327 (18) | 0.02241 (18) | 0.0285 (2) | 0.01291 (15) | 0.00656 (15) | 0.00709 (15) |
| *Na*3 | Na | 0.71250 (4) | 0.14813 (4) | 0.50100 (3) | 0.1593 | 0.02060(6) | 0.02035 (13) | 0.01872 (13) | 0.02407 (15) | 0.01063 (11) | 0.00708 (11) | 0.00806 (11) |
| *Ca*3 | Ca | 0.71250 (4) | 0.14813 (4) | 0.50100 (3) | 0.8408 | 0.02060(6) | 0.02035 (13) | 0.01872 (13) | 0.02407 (15) | 0.01063 (11) | 0.00708 (11) | 0.00806 (11) |
| *Na*4 | Na | 0.15024 (5) | 0.43576 (5) | 0.51825 (4) | 0.2482 | 0.02310(7) | 0.02117 (15) | 0.02192 (15) | 0.02734 (18) | 0.01189 (13) | 0.00685 (13) | 0.00881 (13) |
| *Ca*4 | Ca | 0.15024 (5) | 0.43576 (5) | 0.51825 (4) | 0.7518 | 0.02310(7) | 0.02117 (15) | 0.02192 (15) | 0.02734 (18) | 0.01189 (13) | 0.00685 (13) | 0.00881 (13) |
| *Si*1 | Si | 0.28409 (5) | 0.60143 (5) | 0.86975 (3) | 1 | 0.01500(6) | 0.01532 (15) | 0.01494 (15) | 0.01443 (16) | 0.00811 (13) | 0.00345 (12) | 0.00424 (12) |
| *Si*2 | Si | 0.13723 (5) | 0.74211 (5) | 0.73097 (4) | 1 | 0.01570(7) | 0.01421 (15) | 0.01422 (15) | 0.01994 (17) | 0.00754 (13) | 0.00494 (13) | 0.00772 (13) |
| *Si*3 | Si | 0.76843 (5) | 0.49823 (5) | 0.72845 (4) | 1 | 0.01580(7) | 0.01384 (15) | 0.01520 (15) | 0.02067 (18) | 0.00832 (13) | 0.00636 (13) | 0.00766 (13) |
| *Si*4 | Si | 0.26382 (5) | 0.10769 (5) | 0.73094 (4) | 1 | 0.01660(7) | 0.01431 (15) | 0.01421 (15) | 0.02215 (18) | 0.00844 (13) | 0.00356 (13) | 0.00585 (13) |
| *Si*5 | Si | 0.02222 (5) | 0.24115 (5) | 0.73446 (4) | 1 | 0.01630(7) | 0.01263 (14) | 0.01378 (15) | 0.02160 (18) | 0.00681 (13) | 0.00363 (13) | 0.00505 (13) |
| *Si*6 | Si | 0.39030 (5) | 0.73728 (5) | 0.13684 (3) | 1 | 0.01480(6) | 0.01521 (15) | 0.01435 (15) | 0.01416 (15) | 0.00775 (13) | 0.00331 (12) | 0.00394 (12) |
| *Si*7 | Si | 0.65412 (5) | −0.00327 (5) | 0.73084 (4) | 1 | 0.01590(7) | 0.01497 (15) | 0.01203 (14) | 0.02066 (18) | 0.00707 (13) | 0.00600 (13) | 0.00490 (13) |
| *Si*8 | Si | 0.52974 (5) | 0.62943 (5) | 0.73404 (4) | 1 | 0.01640(7) | 0.01594 (16) | 0.01439 (15) | 0.02163 (18) | 0.00941 (13) | 0.00679 (13) | 0.00625 (13) |
| O1 | O | 0.70512 (19) | 0.38774 (19) | 0.59987 (12) | 1 | 0.0318(3) | 0.0349 (7) | 0.0310 (7) | 0.0246 (6) | 0.0180 (6) | 0.0039 (5) | 0.0012 (5) |
| O2 | O | 0.1277 (2) | 0.67027 (19) | 0.60218 (12) | 1 | 0.0308(3) | 0.0411 (8) | 0.0295 (6) | 0.0238 (6) | 0.0194 (6) | 0.0129 (5) | 0.0085 (5) |
| O3 | O | 0.2777 (2) | 0.0816 (2) | 0.60476 (13) | 1 | 0.0342(3) | 0.0451 (8) | 0.0368 (7) | 0.0255 (6) | 0.0239 (7) | 0.0130 (6) | 0.0112 (6) |
| O4 | O | 0.4234 (2) | 0.5310 (2) | 0.60794 (14) | 1 | 0.0401(3) | 0.0366 (8) | 0.0451 (9) | 0.0291 (7) | 0.0242 (7) | −0.0050 (6) | −0.0049 (6) |
| O5 | O | 0.0133 (2) | 0.7529 (2) | 0.38975 (13) | 1 | 0.0366(3) | 0.0326 (7) | 0.0461 (9) | 0.0280 (7) | 0.0166 (7) | 0.0066 (5) | 0.0184 (6) |
| O6 | O | 0.57237 (18) | 0.95614 (19) | 0.60230 (12) | 1 | 0.0307(3) | 0.0315 (6) | 0.0336 (7) | 0.0214 (6) | 0.0147 (6) | 0.0039 (5) | 0.0073 (5) |
| O7 | O | 0.85425 (15) | 0.11985 (17) | 0.76660 (13) | 1 | 0.0295(3) | 0.0153 (5) | 0.0257 (6) | 0.0406 (7) | 0.0055 (4) | 0.0096 (5) | 0.0109 (5) |
| O8 | O | 0.67606 (18) | 0.59628 (19) | 0.76253 (14) | 1 | 0.0303(3) | 0.0290 (6) | 0.0354 (7) | 0.0424 (8) | 0.0262 (6) | 0.0146 (6) | 0.0151 (6) |
| O9 | O | 0.19285 (18) | 0.93716 (16) | 0.76666 (13) | 1 | 0.0286(3) | 0.0313 (6) | 0.0167 (5) | 0.0389 (7) | 0.0122 (5) | 0.0090 (5) | 0.0124 (5) |
| O10 | O | 0.62699 (19) | 0.83097 (16) | 0.76055 (15) | 1 | 0.0324(3) | 0.0343 (7) | 0.0165 (5) | 0.0509 (9) | 0.0144 (5) | 0.0148 (6) | 0.0151 (5) |
| O11 | O | 0.43761 (15) | 0.24756 (17) | 0.82329 (13) | 1 | 0.0295(3) | 0.0165 (5) | 0.0211 (5) | 0.0421 (8) | 0.0095 (4) | −0.0034 (5) | 0.0010 (5) |
| O12 | O | 0.58665 (18) | 0.08171 (16) | 0.81855 (13) | 1 | 0.0285(3) | 0.0325 (6) | 0.0200 (5) | 0.0405 (7) | 0.0171 (5) | 0.0204 (6) | 0.0094 (5) |
| O13 | O | 0.4272 (2) | 0.5844 (2) | 0.82795 (15) | 1 | 0.0362(3) | 0.0388 (8) | 0.0470 (9) | 0.0522 (9) | 0.0329 (7) | 0.0334 (7) | 0.0321 (8) |
| O14 | O | 0.26237 (18) | 0.72911 (19) | 0.81825 (15) | 1 | 0.0347(3) | 0.0272 (6) | 0.0313 (7) | 0.0492 (9) | 0.0164 (5) | 0.0003 (6) | 0.0222 (6) |
| O15 | O | 0.04020 (16) | 0.35048 (18) | 0.23978 (14) | 1 | 0.0316(3) | 0.0165 (5) | 0.0271 (6) | 0.0465 (8) | 0.0063 (5) | 0.0130 (5) | 0.0145 (6) |
| O16 | O | 0.11489 (17) | 0.42160 (16) | 0.83138 (14) | 1 | 0.0340(3) | 0.0238 (6) | 0.0161 (5) | 0.0446 (8) | 0.0035 (4) | 0.0074 (6) | −0.0024 (5) |
| O17 | O | 0.13167 (18) | 0.16030 (19) | 0.75261 (15) | 1 | 0.0345(3) | 0.0247 (6) | 0.0328 (7) | 0.0571 (10) | 0.0229 (6) | 0.0108 (6) | 0.0149 (7) |
| O18 | O | 0.75043 (17) | 0.39291 (19) | 0.81586 (14) | 1 | 0.0309(3) | 0.0264 (6) | 0.0342 (7) | 0.0446 (8) | 0.0171 (5) | 0.0165 (6) | 0.0291 (6) |
| O19 | O | 0.3337 (2) | 0.6733 (2) | 0.00323 (12) | 1 | 0.0403(3) | 0.0481 (9) | 0.0489 (9) | 0.0125 (5) | 0.0225 (8) | 0.0020 (5) | 0.0013 (5) |
| F | F | 0.16303 (19) | 0.2099 (2) | 0.42012 (13) | 1 | 0.0427(3) | 0.0422 (7) | 0.0444 (8) | 0.0390 (7) | 0.0240 (7) | 0.0071 (6) | 0.0083 (6) |
| *Na*5 | Na | 0.0875 (4) | 0.1107 (4) | 0.2252 (2) | 0.5686 | 0.0330(4) | 0.0261 (9) | 0.0291 (10) | 0.0472 (10) | 0.0166 (8) | 0.0109 (7) | 0.0127 (7) |
| *K* | K | 0.0818 (13) | 0.1032 (14) | 0.2083 (12) | 0.2162 | 0.134(3) | 0.081 (4) | 0.089 (5) | 0.266 (7) | 0.050 (4) | 0.072 (5) | 0.090 (5) |
| *Na*6 | Na | 0.642 (3) | −0.0223 (18) | 0.0014 (10) | 0.2673 | 0.301(4) | 0.453 (9) | 0.128 (7) | 0.070 (5) | −0.003 (8) | −0.003 (8) | 0.023 (5) |
| *Na*7 | Na | 0.664 (4) | 0.640 (3) | 0.0010 (12) | 0.2946 | 0.400(4) | 0.838 (9) | 0.473 (8) | 0.101 (6) | 0.561 (7) | −0.015 (8) | −0.003 (7) |
| *Na*8 | Na | 0.9830 (16) | 0.363 (3) | 0.0048 (9) | 0.2575 | 0.338(4) | 0.097 (5) | 0.714 (10) | 0.057 (4) | 0.149 (8) | 0.028 (4) | 0.033 (8) |
| O20w | O | 0.0000 | 0.0000 | 0.0000 | 0.353(9) | 0.195(7) | - | - | - | - | - | - |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| **600 °C** |  |  |  |  |  |  |  |  |  |  |  |  |
| *Na*1 | Na | 0.0000 | 0.0000 | 0.5000 | 0.7236 | 0.0377(2) | 0.0346 (5) | 0.0362 (5) | 0.0406 (5) | 0.0194 (4) | 0.0065 (4) | 0.0093 (4) |
| *Ca*1 | Ca | 0.0000 | 0.0000 | 0.5000 | 0.2765 | 0.0377(2) | 0.0346 (5) | 0.0362 (5) | 0.0406 (5) | 0.0194 (4) | 0.0065 (4) | 0.0093 (4) |
| *Na*2 | Na | 0.42473 (6) | 0.28645 (6) | 0.51209 (5) | 0.4298 | 0.02740(8) | 0.0258 (2) | 0.0249 (2) | 0.0319 (2) | 0.01436 (17) | 0.00744 (17) | 0.00809 (17) |
| *Ca*2 | Ca | 0.42473 (6) | 0.28645 (6) | 0.51209 (5) | 0.5702 | 0.02740(8) | 0.0258 (2) | 0.0249 (2) | 0.0319 (2) | 0.01436 (17) | 0.00744 (17) | 0.00809 (17) |
| *Na*3 | Na | 0.71280 (5) | 0.14829 (5) | 0.50099 (3) | 0.1593 | 0.02330(6) | 0.02323 (15) | 0.02129 (15) | 0.02746 (17) | 0.01235 (13) | 0.00841 (13) | 0.00931 (13) |
| *Ca*3 | Ca | 0.71280 (5) | 0.14829 (5) | 0.50099 (3) | 0.8408 | 0.02330(6) | 0.02323 (15) | 0.02129 (15) | 0.02746 (17) | 0.01235 (13) | 0.00841 (13) | 0.00931 (13) |
| *Na*4 | Na | 0.15053 (5) | 0.43629 (6) | 0.51864 (4) | 0.2482 | 0.02610(8) | 0.02408 (17) | 0.02507 (18) | 0.0309 (2) | 0.01358 (15) | 0.00781 (15) | 0.01033 (15) |
| *Ca*4 | Ca | 0.15053 (5) | 0.43629 (6) | 0.51864 (4) | 0.7518 | 0.02610(8) | 0.02408 (17) | 0.02507 (18) | 0.0309 (2) | 0.01358 (15) | 0.00781 (15) | 0.01033 (15) |
| *Si*1 | Si | 0.28411 (5) | 0.60164 (5) | 0.86962 (4) | 1 | 0.01650(7) | 0.01692 (16) | 0.01638 (17) | 0.01533 (17) | 0.00874 (14) | 0.00359 (13) | 0.00436 (13) |
| *Si*2 | Si | 0.13662 (5) | 0.74206 (5) | 0.73121 (4) | 1 | 0.01730(7) | 0.01566 (16) | 0.01563 (17) | 0.02201 (19) | 0.00827 (14) | 0.00534 (14) | 0.00837 (14) |
| *Si*3 | Si | 0.76849 (5) | 0.49893 (6) | 0.72892 (4) | 1 | 0.01740(7) | 0.01558 (16) | 0.01688 (17) | 0.02274 (19) | 0.00942 (14) | 0.00733 (14) | 0.00879 (15) |
| *Si*4 | Si | 0.26358 (5) | 0.10745 (6) | 0.73141 (4) | 1 | 0.01830(7)4 | 0.01566 (16) | 0.01571 (17) | 0.0243 (2) | 0.00918 (14) | 0.00395 (15) | 0.00647 (15) |
| *Si*5 | Si | 0.02260 (5) | 0.24103 (5) | 0.73471 (4) | 1 | 0.01800(8) | 0.01383 (16) | 0.01515 (17) | 0.0241 (2) | 0.00749 (14) | 0.00397 (14) | 0.00554 (15) |
| *Si*6 | Si | 0.39024 (5) | 0.73707 (5) | 0.13672 (4) | 1 | 0.01630(7) | 0.01669 (16) | 0.01605 (16) | 0.01535 (17) | 0.00861 (14) | 0.00365 (13) | 0.00424 (13) |
| *Si*7 | Si | 0.65488 (5) | −0.00285 (5) | 0.73094 (4) | 1 | 0.01760(7) | 0.01665 (17) | 0.01336 (16) | 0.0228 (2) | 0.00782 (14) | 0.00675 (14) | 0.00545 (14) |
| *Si*8 | Si | 0.53035 (6) | 0.63045 (6) | 0.73419 (4) | 1 | 0.01810(8) | 0.01775 (17) | 0.01597 (17) | 0.0236 (2) | 0.01044 (14) | 0.00752 (15) | 0.00688 (15) |
| O1 | O | 0.7053 (2) | 0.3879 (2) | 0.60040 (13) | 1 | 0.0349(3) | 0.0382 (8) | 0.0353 (8) | 0.0270 (7) | 0.0207 (7) | 0.0049 (6) | 0.0014 (6) |
| O2 | O | 0.1274 (2) | 0.6706 (2) | 0.60237 (13) | 1 | 0.0338(3) | 0.0449 (9) | 0.0326 (7) | 0.0259 (7) | 0.0214 (7) | 0.0137 (6) | 0.0089 (6) |
| O3 | O | 0.2775 (2) | 0.0811 (2) | 0.60520 (14) | 1 | 0.0382(4) | 0.0498 (10) | 0.0414 (9) | 0.0290 (7) | 0.0267 (8) | 0.0151 (7) | 0.0131 (6) |
| O4 | O | 0.4242 (2) | 0.5320 (2) | 0.60806 (15) | 1 | 0.0427(4) | 0.0399 (9) | 0.0471 (10) | 0.0319 (8) | 0.0261 (8) | −0.0052 (7) | −0.0042 (7) |
| O5 | O | 0.0126 (2) | 0.7534 (2) | 0.38958 (15) | 1 | 0.0399(4) | 0.0364 (8) | 0.0497 (10) | 0.0311 (8) | 0.0189 (7) | 0.0071 (6) | 0.0200 (7) |
| O6 | O | 0.5729 (2) | 0.9563 (2) | 0.60236 (13) | 1 | 0.0335(3) | 0.0345 (7) | 0.0372 (8) | 0.0237 (6) | 0.0166 (6) | 0.0044 (5) | 0.0086 (6) |
| O7 | O | 0.85487 (17) | 0.12078 (19) | 0.76701 (15) | 1 | 0.0331(3) | 0.0170 (5) | 0.0284 (7) | 0.0460 (9) | 0.0059 (5) | 0.0112 (5) | 0.0123 (6) |
| O8 | O | 0.6757 (2) | 0.5962 (2) | 0.76285 (15) | 1 | 0.0338(3) | 0.0331 (7) | 0.0384 (8) | 0.0470 (9) | 0.0290 (7) | 0.0161 (6) | 0.0161 (7) |
| O9 | O | 0.1933 (2) | 0.93727 (17) | 0.76739 (15) | 1 | 0.0319(3) | 0.0353 (7) | 0.0179 (5) | 0.0440 (8) | 0.0139 (5) | 0.0101 (6) | 0.0137 (5) |
| O10 | O | 0.6275 (2) | 0.83196 (18) | 0.76109 (16) | 1 | 0.0358(4) | 0.0378 (8) | 0.0188 (6) | 0.0563 (10) | 0.0162 (6) | 0.0157 (7) | 0.0174 (6) |
| O11 | O | 0.43743 (17) | 0.24715 (18) | 0.82393 (15) | 1 | 0.0329(3) | 0.0175 (5) | 0.0239 (6) | 0.0472 (9) | 0.0104 (5) | −0.0039 (5) | 0.0009 (6) |
| O12 | O | 0.5875 (2) | 0.08237 (18) | 0.81851 (14) | 1 | 0.0315(3) | 0.0360 (7) | 0.0226 (6) | 0.0441 (8) | 0.0191 (6) | 0.0221 (6) | 0.0102 (6) |
| O13 | O | 0.4274 (2) | 0.5851 (2) | 0.82804 (17) | 1 | 0.0396(4) | 0.0431 (9) | 0.0509 (10) | 0.0577 (10) | 0.0362 (8) | 0.0372 (8) | 0.0356 (9) |
| O14 | O | 0.2617 (2) | 0.7290 (2) | 0.81850 (16) | 1 | 0.0382(4) | 0.0306 (7) | 0.0339 (7) | 0.0534 (10) | 0.0178 (6) | −0.0003 (7) | 0.0240 (7) |
| O15 | O | 0.04013 (17) | 0.3502 (2) | 0.23907 (16) | 1 | 0.0354(3) | 0.0181 (5) | 0.0304 (7) | 0.0518 (9) | 0.0066 (5) | 0.0148 (6) | 0.0157 (7) |
| O16 | O | 0.11541 (19) | 0.42163 (18) | 0.83163 (16) | 1 | 0.0370(3) | 0.0264 (6) | 0.0184 (6) | 0.0481 (9) | 0.0046 (5) | 0.0081 (6) | −0.0023 (6) |
| O17 | O | 0.13228 (19) | 0.1607 (2) | 0.75340 (17) | 1 | 0.0385(4) | 0.0273 (7) | 0.0371 (8) | 0.0635 (11) | 0.0254 (6) | 0.0120 (7) | 0.0170 (8) |
| O18 | O | 0.75038 (19) | 0.3939 (2) | 0.81634 (15) | 1 | 0.0345(3) | 0.0294 (7) | 0.0378 (8) | 0.0495 (9) | 0.0185 (6) | 0.0184 (6) | 0.0322 (7) |
| O19 | O | 0.3338 (3) | 0.6736 (3) | 0.00314 (13) | 1 | 0.0444(4) | 0.0539 (11) | 0.0534 (11) | 0.0139 (6) | 0.0249 (9) | 0.0022 (6) | 0.0024 (6) |
| F | F | 0.1637 (2) | 0.2104 (2) | 0.42086 (15) | 1 | 0.0486(4) | 0.0482 (9) | 0.0496 (9) | 0.0458 (9) | 0.0272 (8) | 0.0089 (7) | 0.0099 (7) |
| *Na*5 | Na | 0.0867 (3) | 0.1093 (3) | 0.2231 (2) | 0.5686 | 0.0394(5) | 0.0299 (9) | 0.0321 (9) | 0.0621 (12) | 0.0186 (7) | 0.0158 (8) | 0.0184 (8) |
| *K* | K | 0.0783 (16) | 0.0983 (17) | 0.1959 (17) | 0.2162 | 0.212(3) | 0.124 (6) | 0.152 (6) | 0.424 (9) | 0.087 (5) | 0.116 (7) | 0.150 (7) |
| *Na*6 | Na | 0.640 (3) | −0.0225 (19) | 0.0010 (12) | 0.2673 | 0.319(4) | 0.468 (9) | 0.124 (7) | 0.092 (6) | −0.019 (8) | 0.042 (8) | 0.020 (6) |
| *Na*7 | Na | 0.664 (4) | 0.641 (3) | 0.0022 (13) | 0.2946 | 0.467(4) | 0.986 (9) | 0.611 (9) | 0.096 (6) | 0.701 (7) | −0.007 (8) | 0.006 (7) |
| *Na*8 | Na | 0.9834 (19) | 0.366 (4) | 0.0055 (10) | 0.2575 | 0.401(4) | 0.128 (5) | 0.915 (10) | 0.060 (5) | 0.238 (8) | 0.038 (4) | 0.076 (8) |
| O20w | O | 0.0000 | 0.0000 | 0.0000 | 0.349(9) | 0.212(8) | - | - | - | - | - | - |

**Table S3.** Selected bond distances (Å) derived from the structure refinement of the studied fedorite from 100 to 300, 500 and 600 °C.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **100 °C** | **200°C** | **300 °C** | **500 °C** | **600 °C** |  |  | **100 °C** | **200°C** | **300 °C** | **500 °C** | **600 °C** |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| *Si*1-O13 | 1.6083(12) | 1.6041(13) | 1.6024(14) | 1.6035(14) | 1.6029(15) |  | *Si*5-O5 | 1.5820(14) | 1.5830(14) | 1.5828(16) | 1.5804(15) | 1.5795(17) |
| *Si*1-O14 | 1.6057(12) | 1.6040(12) | 1.6037(14) | 1.6019(14) | 1.5997(15) |  | *Si*5-O7 | 1.6230(11) | 1.6239(12) | 1.6226(13) | 1.6229(13) | 1.6204(14) |
| *Si*1-O16 | 1.6075(12) | 1.6053(12) | 1.6043(14) | 1.6048(14) | 1.6043(15) |  | *Si*5-O16 | 1.6302(12) | 1.6218(13) | 1.6219(14) | 1.6210(14) | 1.6212(15) |
| *Si*1-O19 | 1.5946(14) | 1.5885(14) | 1.5869(16) | 1.5865(14) | 1.5861(16) |  | *Si*5-O17 | 1.6269(12) | 1.6260(12) | 1.6261(14) | 1.6244(13) | 1.6238(15) |
| <*Si*1-O> | 1.604(3) | 1.600(3) | 1.599(3) | 1.600(3) | 1.598(3) |  | <*Si*5-O> | 1.616(3) | 1.614(3) | 1.614(3) | 1.612(3) | 1.611(3) |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| *Si*2-O2 | 1.5955(12) | 1.5918(13) | 1.5887(15) | 1.5908(14) | 1.5906(16) |  | *Si*6-O11 | 1.6088(11) | 1.6116(12) | 1.6114(14) | 1.6097(13) | 1.6086(14) |
| *Si*2-O9 | 1.6293(11) | 1.6221(12) | 1.6220(13) | 1.6218(13) | 1.6207(14) |  | *Si*6-O12 | 1.6193(11) | 1.6113(12) | 1.6104(13) | 1.6120(13) | 1.6114(14) |
| *Si*2-O14 | 1.6141(12) | 1.6158(13) | 1.6151(15) | 1.6148(14) | 1.6153(15) |  | *Si*6-O18 | 1.6107(11) | 1.6095(12) | 1.6107(14) | 1.6089(13) | 1.6095(14) |
| *Si*2-O15 | 1.6249(11) | 1.6248(12) | 1.6236(15) | 1.6237(13) | 1.6219(14) |  | *Si*6-O19 | 1.5935(14) | 1.5908(14) | 1.5905(16) | 1.5861(14) | 1.5850(16) |
| <*Si*2-O> | 1.617(2) | 1.614(3) | 1.613(3) | 1.613(3) | 1.612(3) |  | <*Si*6-O> | 1.608(2) | 1.606(3) | 1.606(3) | 1.604(3) | 1.604(3) |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| *Si*3-O1 | 1.5912(13) | 1.5873(14) | 1.5864(16) | 1.5868(15) | 1.5869(16) |  | *Si*7-O6 | 1.5871(13) | 1.5899(13) | 1.5910(15) | 1.5897(15) | 1.5897(16) |
| *Si*3-O8 | 1.6313(11) | 1.6271(12) | 1.6269(13) | 1.6246(13) | 1.6224(14) |  | *Si*7-O7 | 1.6282(11) | 1.6295(12) | 1.6303(13) | 1.6302(13) | 1.6302(14) |
| *Si*3-O15 | 1.6196(11) | 1.6210(12) | 1.6239(15) | 1.6197(13) | 1.6190(14) |  | *Si*7-O10 | 1.6270(12) | 1.6251(12) | 1.6257(14) | 1.6265(13) | 1.6235(14) |
| *Si*3-O18 | 1.6227(12) | 1.6219(12) | 1.6204(14) | 1.6200(13) | 1.6183(15) |  | *Si*7-O12 | 1.6306(11) | 1.6221(12) | 1.6212(13) | 1.6189(13) | 1.6189(14) |
| <*Si*3-O> | 1.616(2) | 1.614(3) | 1.614(3) | 1.613(3) | 1.612(3) |  | <*Si*7-O> | 1.618(2) | 1.617(3) | 1.617(3) | 1.617(3) | 1.616(3) |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| *Si*4-O3 | 1.5858(13) | 1.5811(14) | 1.5818(16) | 1.5823(15) | 1.5821(17) |  | *Si*8-O4 | 1.5842(14) | 1.5815(15) | 1.5815(16) | 1.5798(16) | 1.5790(17) |
| *Si*4-O9 | 1.6330(11) | 1.6313(12) | 1.6322(13) | 1.6305(13) | 1.6302(14) |  | *Si*8-O8 | 1.6192(11) | 1.6210(12) | 1.6215(14) | 1.6217(13) | 1.6211(15) |
| *Si*4-O11 | 1.6272(12) | 1.6255(12) | 1.6252(14) | 1.6251(13) | 1.6260(14) |  | *Si*8-O10 | 1.6298(12) | 1.6245(12) | 1.6248(14) | 1.6218(13) | 1.6213(14) |
| *Si*4-O17 | 1.6254(12) | 1.6239(12) | 1.6235(14) | 1.6236(13) | 1.6216(15) |  | *Si*8-O13 | 1.6212(12) | 1.6184(13) | 1.6185(15) | 1.6169(14) | 1.6193(15) |
| <*Si*4-O> | 1.618(2) | 1.616(3) | 1.618(3) | 1.616(3) | 1.615(3) |  | <*Si*8-O> | 1.614(3) | 1.612(3) | 1.612(3) | 1.610(3) | 1.610(3) |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | *M*1 position (*Na*1*Ca*1) | |  |  |  |  |  | *M*3 position (*Na*3*Ca*3) | |  |  |  |
| *M*1-O3 (x2) | 2.4708(14) | 2.4767(15) | 2.4830(18) | 2.5005(17) | 2.5028(19) |  | *M*3-O1 | 2.4290(13) | 2.4171(13) | 2.4243(16) | 2.4247(15) | 2.4268(16) |
| *M*1-O5 (x2) | 2.5652(17) | 2.5533(17) | 2.555(2) | 2.5654(19) | 2.558(2) |  | *M*3-O2 | 2.4156(13) | 2.4209(14) | 2.4219(15) | 2.4243(15) | 2.4246(16) |
| *M*1-F (x2) | 2.3664(12) | 2.3692(13) | 2.3697(16) | 2.3795(16) | 2.3789(15) |  | *M*3-O3 | 2.4035(14) | 2.3956(15) | 2.3953(17) | 2.3855(16) | 2.3840(18) |
| <*M*1-O, F> | 2.467(4) | 2.466(4) | 2.469(4) | 2.482(4) | 2.480(4) |  | *M*3-O5 | 2.4269(14) | 2.4379(15) | 2.4432(18) | 2.4407(16) | 2.4471(18) |
|  |  |  |  |  |  |  | *M*3-O6 | 2.4055(13) | 2.4064(14) | 2.4086(16) | 2.4088(15) | 2.4097(17) |
|  |  |  |  |  |  |  | *M*3-O6' | 2.4592(13) | 2.4725(14) | 2.4773(16) | 2.4885(15) | 2.4954(17) |
|  |  |  |  |  |  |  | <*M*3-O> | 2.433(3) | 2.437(4) | 2.442(4) | 2.445(4) | 2.449(4) |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | *M*2 position (*Na*2*Ca*2) | |  |  |  |  |  | *M*4 position (*Na*4*Ca*4) | |  |  |  |
| *M*2-O1 | 2.3986(13) | 2.4040(14) | 2.4029(16) | 2.4077(16) | 2.4078(18) |  | *M*4-O1 | 2.4828(14) | 2.4855(15) | 2.4929(17) | 2.4996(17) | 2.5050(18) |
| *M*2-O3 | 2.4121(14) | 2.4183(15) | 2.4198(17) | 2.4229(16) | 2.4300(18) |  | *M*4-O2 | 2.4849(14) | 2.4944(15) | 2.5019(17) | 2.5056(17) | 2.5066(19) |
| *M*2-O4 | 2.4210(15) | 2.4104(16) | 2.4159(18) | 2.4244(18) | 2.4269(19) |  | *M*4-O2' | 2.4234(13) | 2.4108(13) | 2.4114(15) | 2.4149(15) | 2.4164(16) |
| *M*2-O4' | 2.5652(19) | 2.569(2) | 2.569(2) | 2.568(2) | 2.565(2) |  | *M*4-O4 | 2.3576(14) | 2.3667(15) | 2.3675(17) | 2.3642(17) | 2.3669(18) |
| *M*2-O6 | 2.4787(14) | 2.4683(15) | 2.4726(17) | 2.4894(16) | 2.4906(18) |  | *M*4-O5 | 2.3668(14) | 2.3693(14) | 2.3693(17) | 2.3688(16) | 2.3715(18) |
| *M*2-F | 2.3194(12) | 2.3275(13) | 2.3292(15) | 2.3255(16) | 2.3236(18) |  | *M*4-F | 2.3516(13) | 2.3450(13) | 2.3463(15) | 2.3374(16) | 2.3381(18) |
| <*M*2-O, F> | 2.469(4) | 2.466(4) | 2.470(4) | 2.476(4) | 2.478(4) |  | <*M*4-*O*, F> | 2.440(3) | 2.440(4) | 2.444(4) | 2.448(4) | 2.450(4) |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| *Na*5-O7 | 2.581(6) | 2.578(9) | 2.558(9) | 2.580(3) | 2.582(3) |  | *Na*7-O8 | 2.904(8) | 2.926(12) | 2.967(17) | 2.957(17) | 2.968(19) |
| *Na*5-O8 | 2.568(6) | 2.550(8) | 2.571(9) | 2.566(3) | 2.574(3) |  | *Na*7-O9 | 3.861(9) | 3.897(12) | 3.913(19) | 3.941(15) | 3.920(18) |
| *Na*5-O9 | 2.539(6) | 2.541(10) | 2.532(9) | 2.534(3) | 2.540(3) |  | *Na*7-O10 | 3.851(9) | 3.894(12) | 3.938(15) | 3.937(17) | 3.941(19) |
| *Na*5-O10 | 2.506(6) | 2.502(10) | 2.505(9) | 2.507(3) | 2.509(3) |  | *Na*7-O11 | 2.844(9) | 2.770(15) | 2.73(2) | 2.75(2) | 2.72(2) |
| *Na*5-O15 | 2.582(6) | 2.560(9) | 2.569(8) | 2.555(3) | 2.561(3) |  | *Na*7-O11' | 3.519(11) | 3.403(16) | 3.37(2) | 3.352(18) | 3.36(2) |
| *Na*5-O17 | 2.527(6) | 2.524(9) | 2.498(9) | 2.524(3) | 2.525(3) |  | *Na*7-O13 | 2.828(10) | 2.757(15) | 2.75(2) | 2.731(18) | 2.73(2) |
| *Na*5-O20w | 2.584(4) | 2.627(6) | 2.681(7) | 2.672(2) | 2.646(3) |  | *Na*7-O13' | 3.394(11) | 3.285(16) | 3.24(2) | 3.26(2) | 3.26(2) |
| *Na*5-O21w | - | 2.77(3) | - | - | - |  | *Na*7-O16 | 3.181(9) | 3.189(13) | 3.190(17) | 3.194(17) | 3.190(19) |
| *Na*5-O21w' | - | 2.80(3) | - | - | - |  | *Na*7-O17 | 2.997(8) | 3.033(12) | 3.045(18) | 3.084(15) | 3.061(17) |
| *Na*5-O23w | 2.63(2) | 2.78(3) | 2.75(4) | - | - |  | *Na*7-O18 | 3.486(8) | 3.478(12) | 3.484(19) | 3.445(17) | 3.453(19) |
| *Na*5-O23w' | 2.69(2) | 2.80(3) | 2.87(4) | - | - |  | *Na*7-O19 | 3.139(10) | 3.069(13) | 3.040(17) | 3.037(16) | 3.049(19) |
| *Na*5-O24w | 2.74(2) | 2.79(3) | 2.84(4) | - | - |  | *Na*7-O19' | 3.512(12) | 3.420(19) | 3.37(3) | 3.37(2) | 3.36(3) |
| *Na*5-O24w' | 2.76(2) | 2.80(3) | 2.86(4) | - | - |  | *Na*7-O20w | 3.123(14) | 3.29(2) | 3.36(3) | 3.38(3) | 3.39(3) |
| *Na*5-F | 2.380(4) | 2.327(6) | 2.286(7) | 2.314(3) | 2.346(3) |  | *Na*7-O21w | 3.46(4) | 3.35(4) | 3.46(5) | - | - |
|  |  |  |  |  |  |  | *Na*7-O21w' | 3.58(4) | 3.46(4) | 3.48(5) | - | - |
| *K*1-O7 | 2.649(13) | 2.618(19) | 2.632(18) | 2.595(11) | 2.621(13) |  | *Na*7-O23w | 3.02(3) | 2.54(4) | 2.64(5) | - | - |
| *K*1-O8 | 2.599(12) | 2.596(16) | 2.542(17) | 2.581(11) | 2.599(13) |  | *Na*7-O23w' | 3.34(3) | - | - | - | - |
| *K*1-O9 | 2.570(13) | 2.552(19) | 2.550(18) | 2.554(11) | 2.586(13) |  | *Na*7-O24w | - | 2.41(4) | - | - | - |
| *K*1-O10 | 2.570(13) | 2.563(18) | 2.534(18) | 2.525(11) | 2.542(13) |  |  |  |  |  |  |  |
| *K*1-O15 | 2.606(13) | 2.590(18) | 2.538(18) | 2.577(11) | 2.601(13) |  | *Na*8-O7 | 2.957(5) | 2.997(9) | 3.002(10) | 3.047(15) | 3.058(19) |
| *K*1-O17 | 2.603(12) | 2.561(17) | 2.585(18) | 2.557(11) | 2.596(13) |  | *Na*8-O8 | 3.816(6) | 3.90(1) | 3.942(13) | 3.961(14) | 3.969(15) |
| *K*1-O20w | 2.275(9) | 2.345(12) | 2.441(14) | 2.472(14) | 2.32(2) |  | *Na*8-O12 | 3.543(5) | 3.537(8) | 3.521(10) | 3.537(14) | 3.541(17) |
| *K*1-O21w | 2.79(4) | 2.50(3) | 2.58(4) | - | - |  | *Na*8-O14 | 3.401(5) | 3.376(7) | 3.380(10) | 3.358(12) | 3.350(14) |
| *K*1-O21w' | 2.81(5) | 2.55(3) | 2.61(4) | - | - |  | *Na*8-O15 | 2.923(5) | 2.954(9) | 2.989(12) | 2.982(13) | 2.977(14) |
| *K*1-O22w | 2.69(4) | 3.09(7) | - | - | - |  | *Na*8-O16 | 2.705(6) | 2.671(8) | 2.658(11) | 2.669(12) | 2.670(13) |
| *K*1-O22w' | 2.76(4) | 3.31(9) | - | - | - |  | *Na*8-O16' | 3.357(7) | 3.218(12) | 3.207(14) | 3.169(18) | 3.15(2) |
| *K*1-O23w | 2.32(3) | 2.51(3) | 2.55(4) | - | - |  | *Na*8-O18 | 2.854(6) | 2.814(9) | 2.815(10) | 2.774(15) | 2.755(18) |
| *K*1-O23w' | 2.40(3) | 2.54(3) | 2.62(4) | - | - |  | *Na*8-O18' | 3.390(7) | 3.286(11) | 3.257(15) | 3.253(16) | 3.242(17) |
| *K*1-O24w | 2.45(2) | 2.52(3) | 2.63(4) | - | - |  | *Na*8-O19 | 3.012(6) | 2.921(9) | 2.905(12) | 2.895(14) | 2.886(14) |
| *K*1-O24w' | 2.47(2) | 2.54(3) | 2.63(4) | - | - |  | *Na*8-O19' | 3.318(7) | 3.260(11) | 3.250(14) | 3.233(18) | 3.22(2) |
| *K*1-F | 2.690(9) | 2.608(12) | 2.528(14) | 2.514(14) | 2.67(2) |  | *Na*8-O20w | 3.324(9) | 3.488(17) | 3.53(2) | 3.59(3) | 3.62(3) |
|  |  |  |  |  |  |  | *Na*8-O21w | 2.18(4) | 2.77(4) | 2.81(5) | - | - |
| *Na*6-O7 | 3.781(8) | 3.823(11) | 3.900(14) | 3.883(15) | 3.890(16) |  | *Na*8-O23w | 2.73(3) | 2.66(4) | 2.86(5) | - | - |
| *Na*6-O9 | 2.865(7) | 2.880(9) | 2.892(12) | 2.893(13) | 2.893(17) |  | *Na*8-O24w | 3.25(3) | 3.43(4) | 3.51(5) | - | - |
| *Na*6-O10 | 2.969(7) | 2.981(10) | 3.044(14) | 3.008(14) | 3.001(15) |  | *Na*8-O24w' | 3.65(3) | 3.78(4) | 3.80(5) | - | - |
| *Na*6-O11 | 3.349(7) | 3.335(9) | 3.325(12) | 3.312(13) | 3.307(16) |  |  |  |  |  |  |  |
| *Na*6-O12 | 2.837(8) | 2.805(11) | 2.792(13) | 2.800(14) | 2.793(18) |  |  |  |  |  |  |  |
| *Na*6-O12' | 3.388(10) | 3.307(14) | 3.223(18) | 3.276(19) | 3.271(19) |  |  |  |  |  |  |  |
| *Na*6-O13 | 3.376(7) | 3.353(10) | 3.371(13) | 3.337(14) | 3.329(15) |  |  |  |  |  |  |  |
| *Na*6-O14 | 2.929(8) | 2.892(11) | 2.833(15) | 2.866(15) | 2.860(16) |  |  |  |  |  |  |  |
| *Na*6-O14' | 3.485(9) | 3.426(13) | 3.377(16) | 3.400(18) | 3.39(2) |  |  |  |  |  |  |  |
| *Na*6-O15 | 3.904(7) | 3.943(10) | 3.971(13) | 3.980(14) | 3.988(16) |  |  |  |  |  |  |  |
| *Na*6-O19 | 3.077(9) | 3.02(1) | 2.968(14) | 2.981(16) | 2.969(16) |  |  |  |  |  |  |  |
| *Na*6-O19' | 3.351(10) | 3.301(14) | 3.250(18) | 3.283(19) | 3.27(2) |  |  |  |  |  |  |  |
| *Na*6-O20w | 3.179(12) | 3.291(19) | 3.41(2) | 3.37(3) | 3.39(3) |  |  |  |  |  |  |  |
| *Na*6-O21w | - | 2.49(4) | 2.68(5) | - | - |  |  |  |  |  |  |  |
| *Na*6-O22w | 3.43(4) | - | - | - | - |  |  |  |  |  |  |  |
| *Na*6-O22w' | 3.60(4) | - | - | - | - |  |  |  |  |  |  |  |
| *Na*6-O23w | 2.77(3) | 3.36(4) | 3.47(6) | - | - |  |  |  |  |  |  |  |
| *Na*6-O23w' | 3.65(3) | 3.49(4) | 3.56(5) | - | - |  |  |  |  |  |  |  |
| *Na*6-O24w | 2.56(3) | 2.65(4) | 2.71(5) | - | - |  |  |  |  |  |  |  |

**Table S4.** Bond valence balance (in vu) for interlayer cations of fedorite at T = 25 °C.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | O7 | O8 | O9 | O10 | O11 | O12 | O13 | O14 | O15 | O16 | O17 | O18 | O19 | O20w | O21w | O22w | O23w | O24w | F | **cations\*** |
| *Na*5 | 0.119 | 0.123 | 0.136 | 0.143 |  |  |  |  | 0.122 |  | 0.135 |  |  | 0.134 | **0.042 0.037** |  | 0.056 **0.050** | **0.040 0.040** | 0.129 | 1.097 |
| *K* | 0.207 | 0.220 | 0.243 | 0.241 |  |  |  |  | 0.215 |  | 0.215 |  |  |  |  | **0.033 0.026** |  |  | 0.065 | 1.406 |
| *Na*6 | **0.005** |  | 0.052 **0.004** | **0.043 0.003** | **0.014 0.011** | 0.059 **0.013** | **0.015** | 0.051 **0.014** | **0.003** |  |  | **0.015 0.012** | **0.031 0.009** | **0.025** |  | **0.039** | **0.030 0.05** | 0.116 |  | 0.278 |
| *Na*7 |  | 0.050 |  |  | 0.059 |  | 0.057 **0.014** |  |  |  | **0.037** |  | **0.031** | **0.027** | **0.034** | **0.049** | **0.023** |  |  | 0.166 |
| *Na*8 | **0.046** | **0.004** |  |  |  | **0.009** |  | **0.013** | **0.048** | 0.078 **0.016** | **0.012** | 0.057 | **0.036 0.015** | **0.02** | 0.129 |  |  | **0.045** |  | 0.264 |
| Bond valence, s*ij* = Σ*j* exp [(*R*O-*Rij*)/B], where *Rij* is the bond length between ions *i* and *j*, *R*O and B are the bond-valence parameters (Brown and Altermatt 1985; Brese and O'Keeffe 1991).  \*Bond-valence sums have been calculated excluding the contributions ≤ 0.05 vu (reported in bold), see text. | | | | | | | | | | | | | | | | | | | | |