An updated model of Rietveld structure refinement of Na/K–feldspar

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List of abbreviations used in this paper:

XRPD: X–ray powder diffraction
SC–XRD: single–crystal X–ray diffraction.
BB–XRPD: Bragg–Brentano XRPD
ALBITE: Albite sample from Jiaodong peninsula, Shandong Province, China.
PERTHITE: a perthite sample from Bayan Obo, Inner Mongolia, China.
GSAS: Rietveld refinement by General Structure Analysis System.
SDC: a soft distance constraint for Al/Si–O bond lengths.
T–O: Al/ Si–O bond length.
Albite–N: a model that did not apply SDCs during refining of the albite sample.
Albite: a model that applied SDCs during refining of the albite sample.
R-LPA: average value of lattice parameters of albite from the references.
R-BLA: average value of T–O bond lengths in one tetrahedron of albite from the references.
R-MAA: mean of six O–T–O angles in one tetrahedron of albite from the references
R-LPM: average value of lattice parameters of microcline from the references.
R-BLM: average value of T–O bond lengths in one tetrahedron of microcline from the references.
R-MAM: mean of six O–T–O angles in one tetrahedron of microcline from the references.
PERTHITE–a: the albite phase in the perthite sample.
PERTHITE–m: the microcline phase in the perthite sample.

Table S1. Structure parameters of albite in the ALBITE sample.

Atom type	*x*	*y*	*z*	O_{cc}	U_{iso}
Na	0.2754(5)	0.98926(24)	0.15465(6)	1.00	0.0688(9)
T_1o	0.0110(5)	0.16752(24)	0.20811(6)	1.00/0.00[a]	0.0204(9)
T_1m	0.0063(5)	0.81852(24)	0.23752(6)	0.00/1.00	0.0198(9)
T_2o	0.6941(5)	0.10852(24)	0.31482(6)	0.00/1.00	0.0202(9)
T_2m	0.6835(5)	0.88032(24)	0.36042(6)	0.00/1.00	0.0199(9)
O_A1	0.0077(5)	0.12901(24)	0.96608(6)	1.00	0.0105(9)
O_A2	0.5951(5)	0.99561(24)	0.28048(6)	1.00	0.0077(9)
O_Bo	0.8146(5)	0.10831(24)	0.19018(6)	1.00	0.0113(9)
O_Bm	0.8222(5)	0.84941(24)	0.25838(6)	1.00	0.0138(9)
O_Co	0.0154(5)	0.30171(24)	0.26868(6)	1.00	0.0100(9)
O_Cm	0.0261(5)	0.69171(24)	0.22878(6)	1.00	0.0102(9)
O_Do	0.2097(5)	0.10731(24)	0.38868(6)	1.00	0.0105(9)
O_Dm	0.1862(5)	0.86631(24)	0.43448(6)	1.00	0.0124(9)

Note: Estimated standard deviations, given in parentheses, refer to the last decimal place.
a. Al/Si site occupancies.

Table S2. Structure parameters of albite in the PERTHITE sample.

Atom type	*x*	*y*	*z*	O_{cc}	U_{iso}
Na	0.3400(10)	0.9773(7)	0.14685(15)	1.00	0.1059(34)
T_1o	0.0057(10)	0.1709(7)	0.20851(15)	1.00/0.00[a]	0.0460(34)
T_1m	0.0010(10)	0.8219(7)	0.23791(15)	0.00/1.00	0.0418(34)
T_2o	0.6888(10)	0.1119(7)	0.31521(15)	0.00/1.00	0.0419(34)
T_2m	0.6782(10)	0.8837(7)	0.36081(15)	0.00/1.00	0.0425(34)
O_A1	0.0025(10)	0.1324(7)	0.96657(15)	1.00	0.0576(34)
O_A2	0.5899(10)	0.9990(7)	0.28097(15)	1.00	0.0472(34)
O_Bo	0.8094(10)	0.1117(7)	0.19067(15)	1.00	0.0574(34)
O_Bm	0.8170(10)	0.8528(7)	0.25887(15)	1.00	0.0670(34)
O_Co	0.0102(10)	0.3051(7)	0.26917(15)	1.00	0.0531(34)
O_Cm	0.0209(10)	0.6951(7)	0.22927(15)	1.00	0.0483(34)
O_Do	0.2045(10)	0.1107(7)	0.38917(15)	1.00	0.0475(34)
O_Dm	0.1810(10)	0.8697(7)	0.43497(15)	1.00	0.0623(34)

Note: Estimated standard deviations, given in parentheses, refer to the last decimal place.
a. Al/Si site occupancies.

Table S3. Structure parameters of microcline in the PERTHITE sample.

Atom type	*x*	*y*	*Z*	O_{cc}	U_{iso}
K	0.28332(35)	0.99806(30)	0.14688(7)	1.00	0.0362(8)
T_1o	0.00899(35)	0.18666(30)	0.21789(7)	0.96/0.04[a]	0.0222(8)

T_1m	0.00856(35)	0.81906(30)	0.23200(7)	0.02/0.98	0.0219(8)
T_2o	0.70917(35)	0.11954(30)	0.34078(7)	0.01/0.99	0.0226(8)
T_2m	0.70415(35)	0.88488(30)	0.35040(7)	0.01/0.99	0.0140(8)
O_A1	0.99983(35)	0.14387(30)	0.98408(7)	1.00	0.0341(8)
O_A2	0.63394(35)	0.00437(30)	0.28637(7)	1.00	0.0330(8)
O_Bo	0.82034(35)	0.14607(30)	0.22038(7)	1.00	0.0369(8)
O_Bm	0.83024(35)	0.85687(30)	0.23978(7)	1.00	0.0379(8)
O_Co	0.03353(35)	0.31817(30)	0.25247(7)	1.00	0.0325(8)
O_Cm	0.03653(35)	0.69467(30)	0.26917(7)	1.00	0.0307(8)
O_Do	0.18944(35)	0.12277(30)	0.40518(7)	1.00	0.0322(8)
O_Dm	0.17573(35)	0.87387(30)	0.41148(7)	1.00	0.0326(8)

Note: Estimated standard deviations, given in parentheses, refer to the last decimal place.

a. Al/Si site occupancies.

Figure S1. Representation of a four-tetrahedron ring in monoclinic and triclinic alkali feldspar structures.

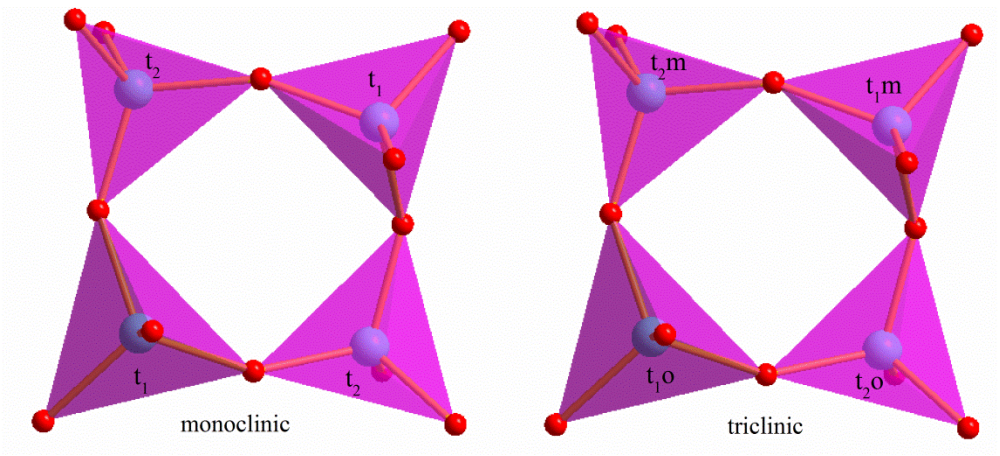


Fig. S2 Plots of Al/Si–O bond length vs. Al/(Al+Si) ratio for albite and microcline in published papers.

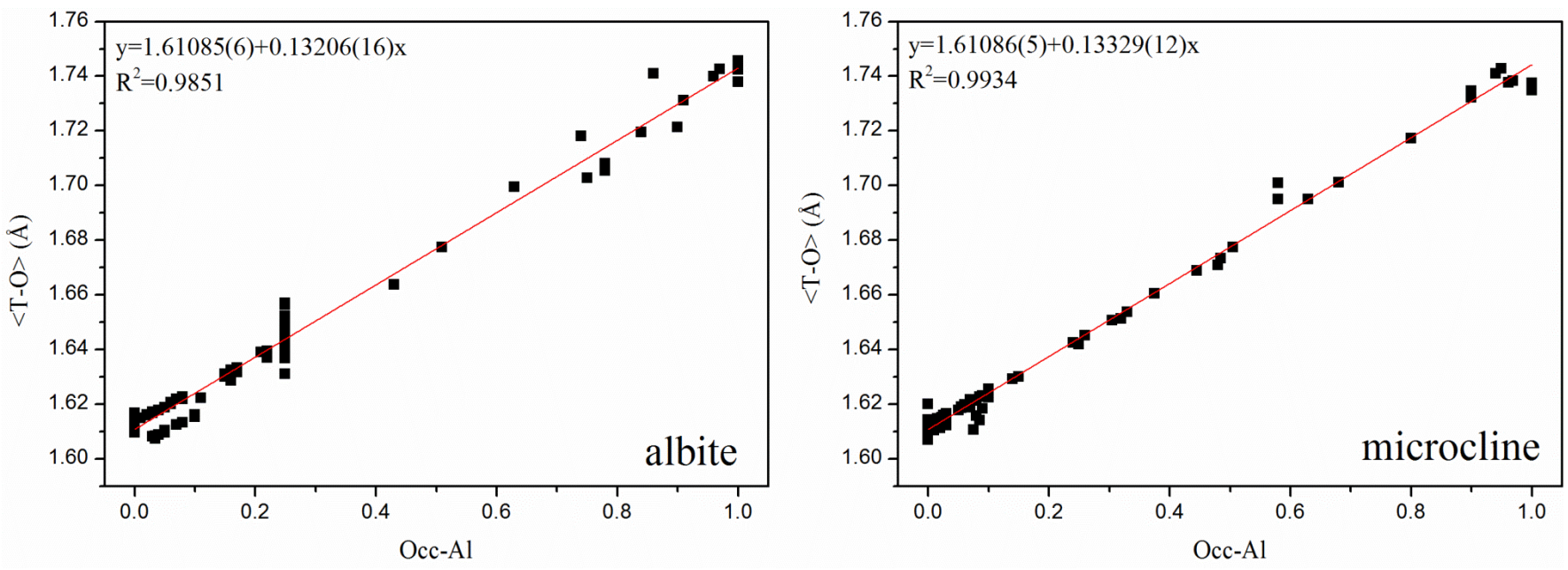
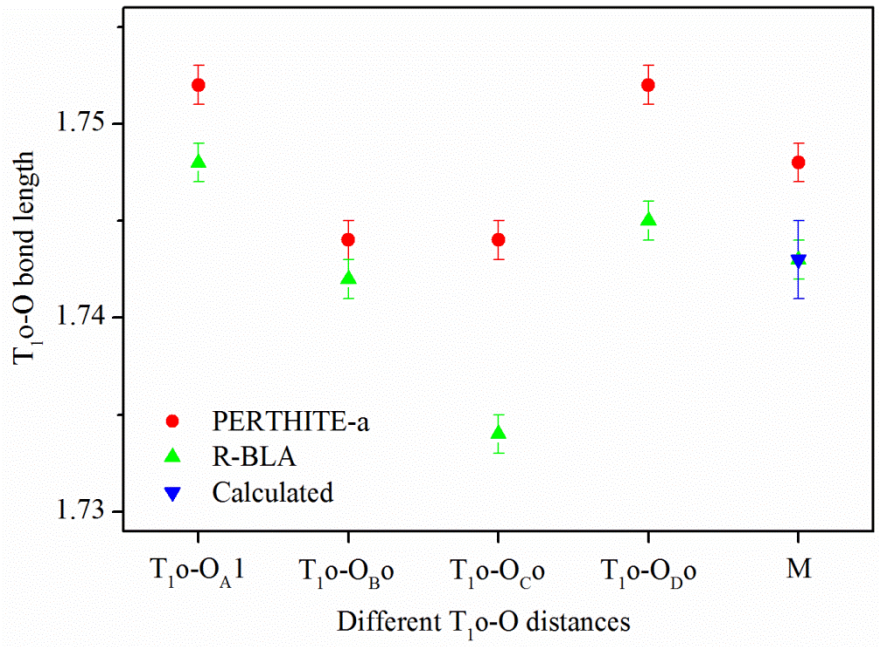
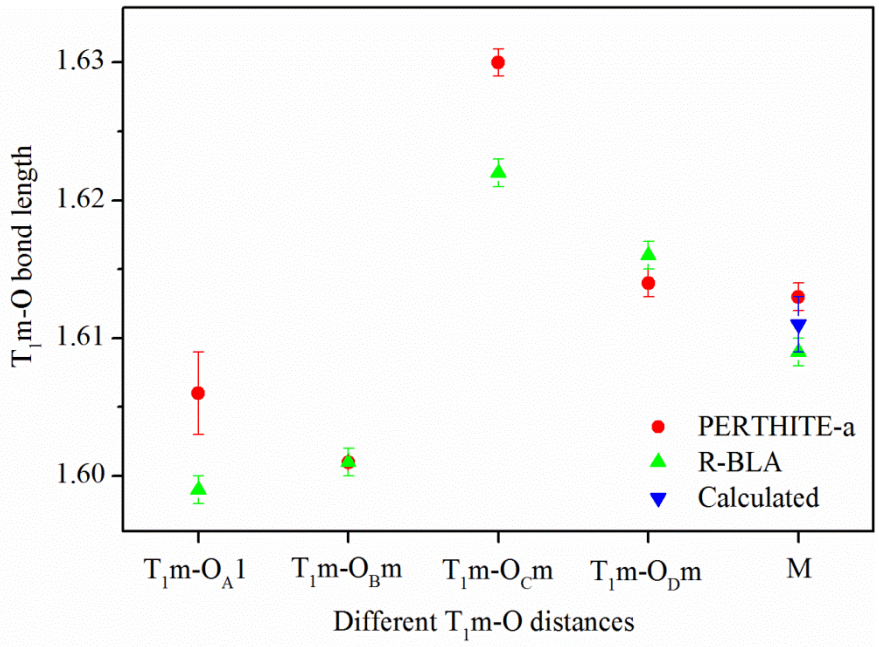
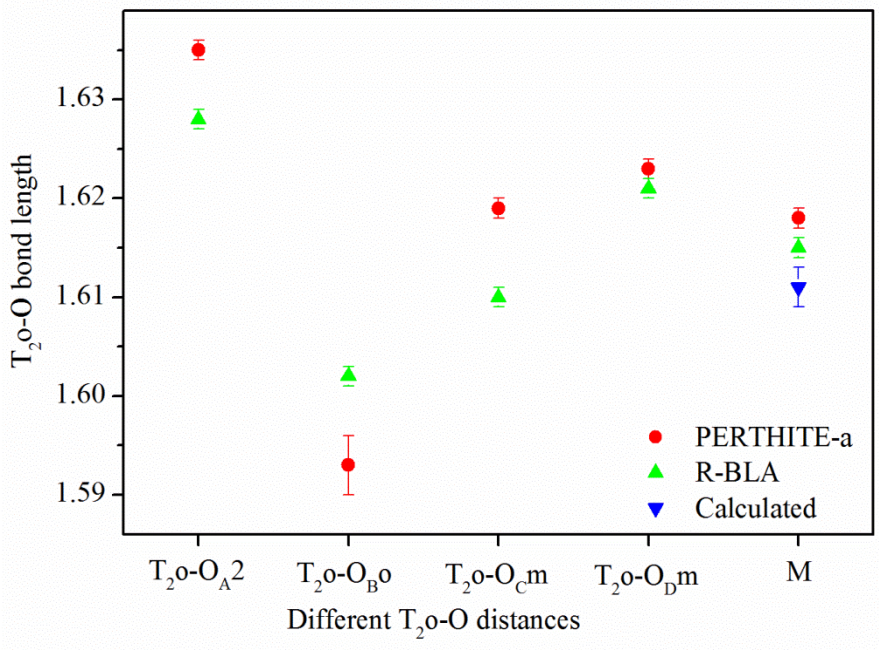


Figure S3. T–O distances in four tetrahedrons of albite in the PERTHITE sample (PERTHITE–a) and those from the albite references (R-BLA). M denotes the mean for PERTHITE–a, R-BLA, and calculated value from Equation (1); ●PERTHITE–a; ▲R-BLA; ▼Calculated. The vertical bars represent errors. If no bar is given, then the error is contained within the area of the symbol.







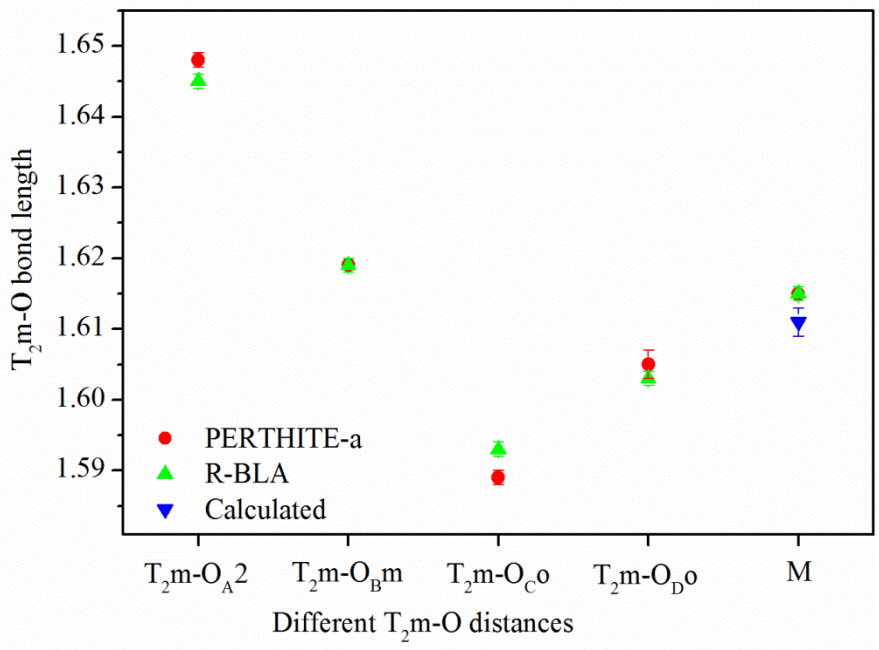
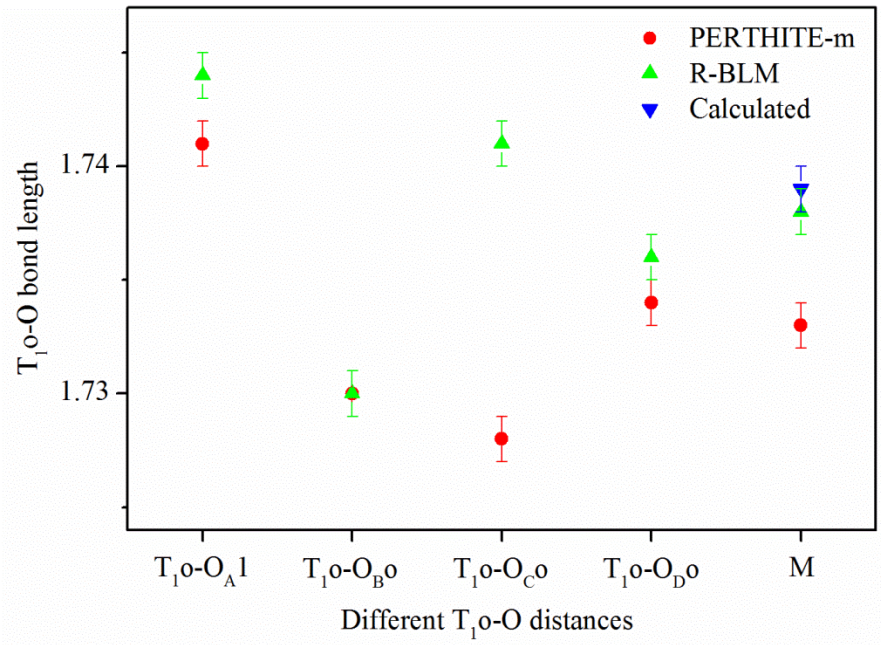
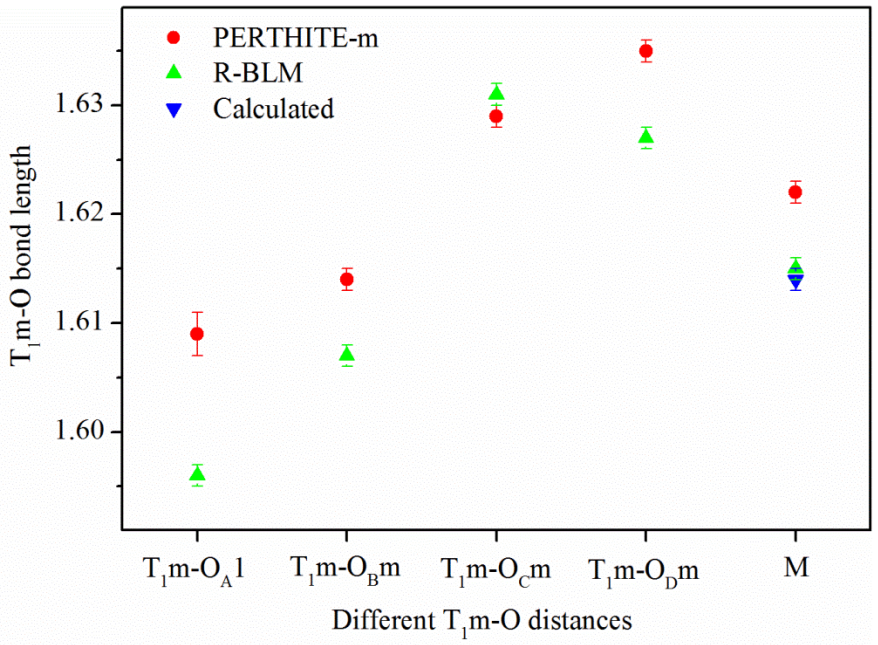
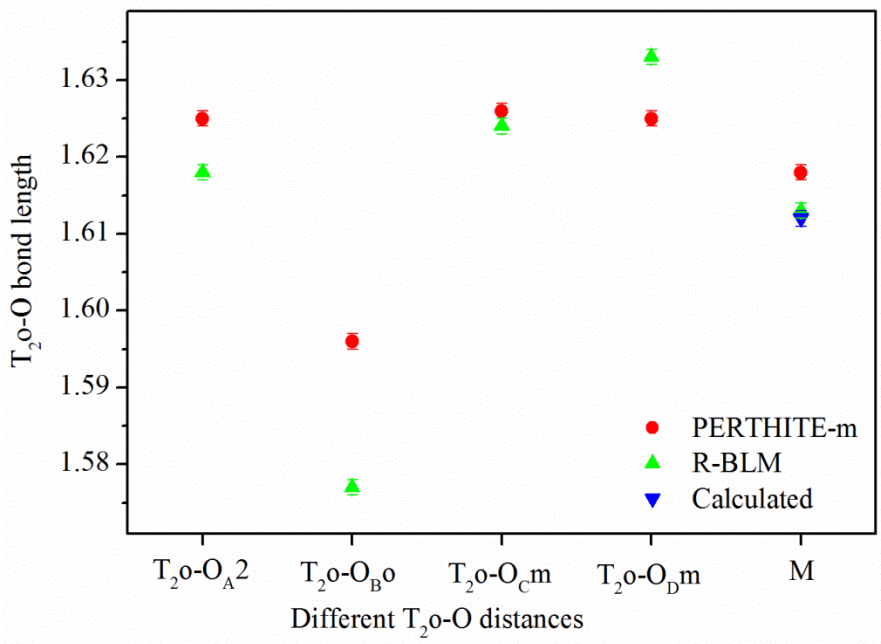


Figure S4. T–O distances in four tetrahedrons of microcline in the PERTHITE sample (PERTHITE–m) and those from the microcline references (R-BLM). M denotes the mean for PERTHITE–m, R-BLM, and calculated value from the equation (2); ●PERTHITE–m; ▲R-BLM; ▼Calculated. The vertical bars represent errors. If no bar is given, then the error is contained within the area of the symbol.







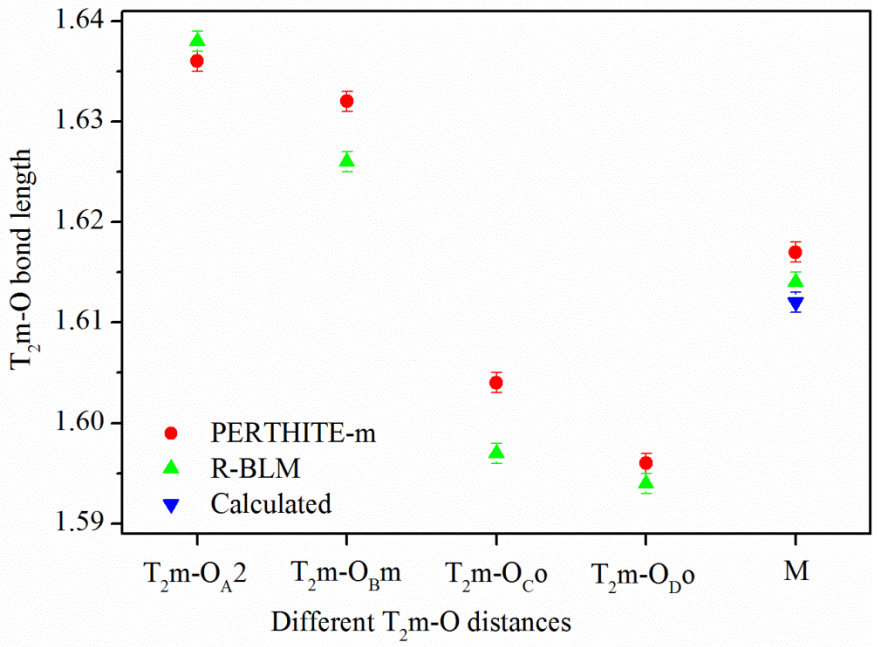
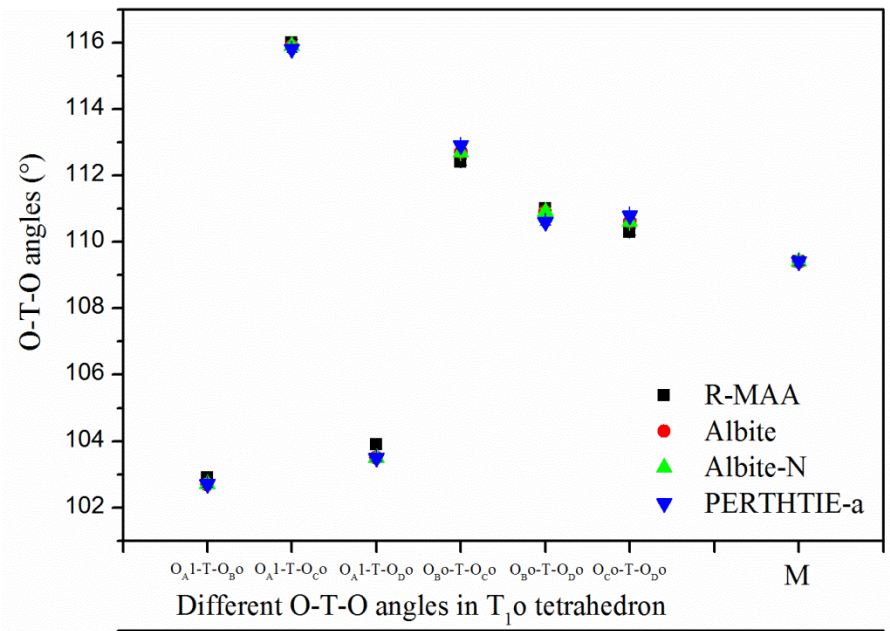
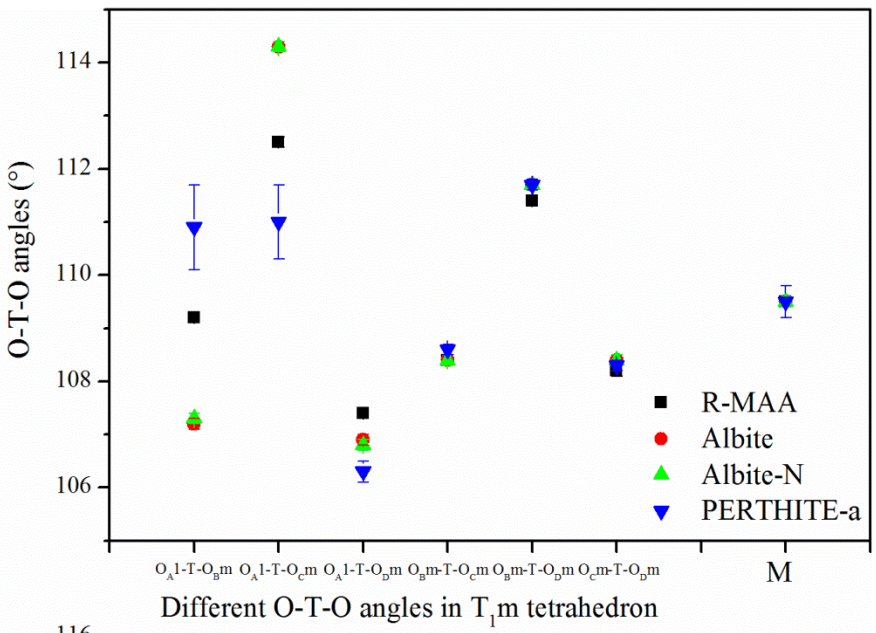
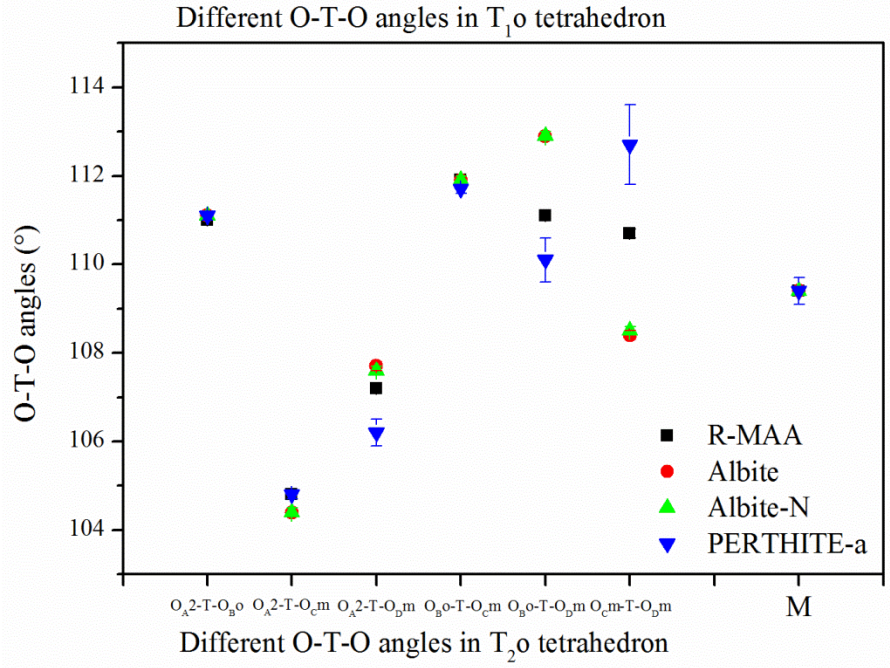


Figure S5. O–T–O angles in four tetrahedrons of albite from the albite references (R-MAA), the model Albite, the model Albite–N, and albite in PERTHITE sample (PERTHITE–a). M denotes the mean for R-MAA, Albite, Albite–N, and PERTHITE–a; ■R-MAA; ●Albite; ▲Albite–N; ▼PERTHITE–a. The vertical bars represent errors. If no bar is given, then the error is contained within the area of the symbol.







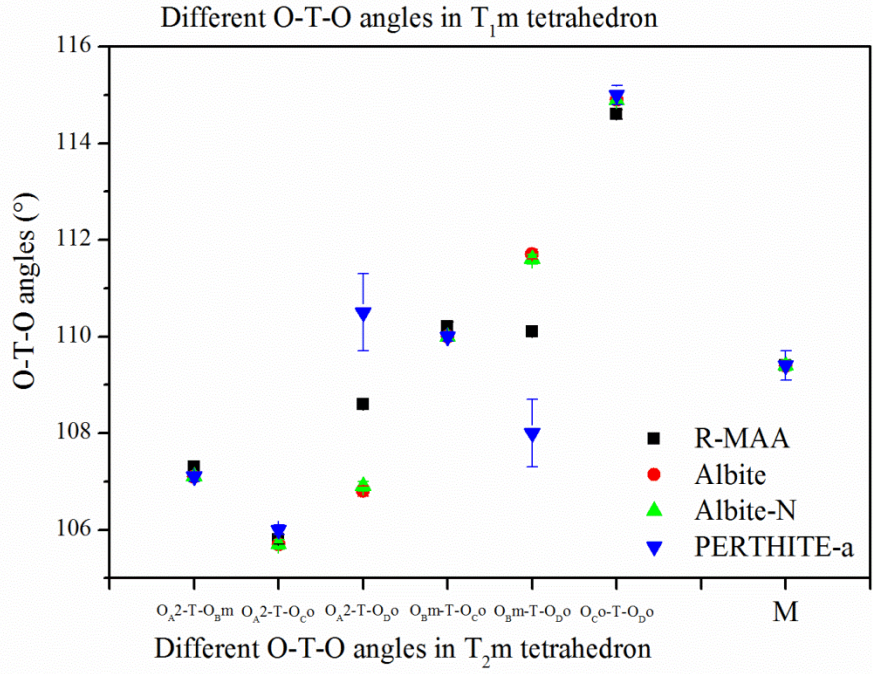
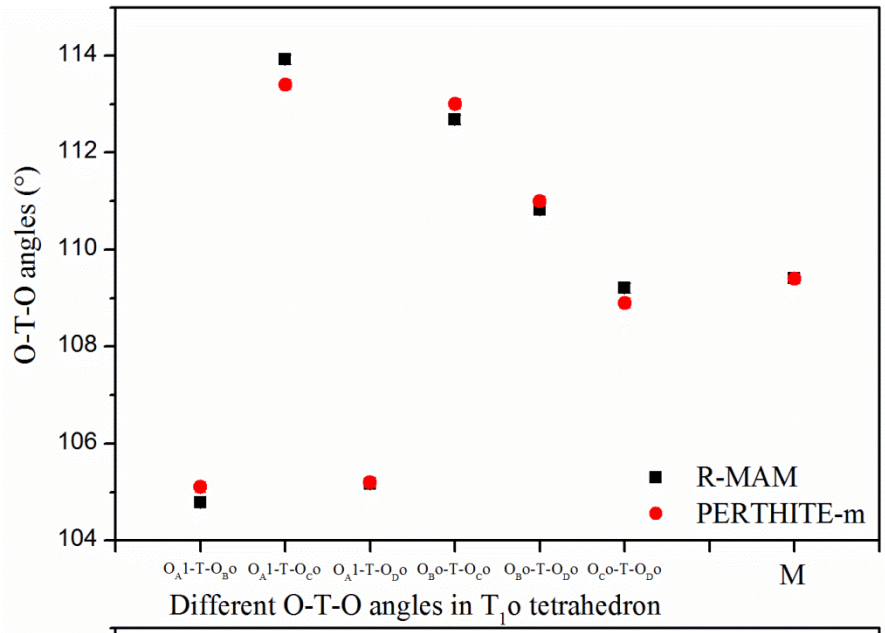
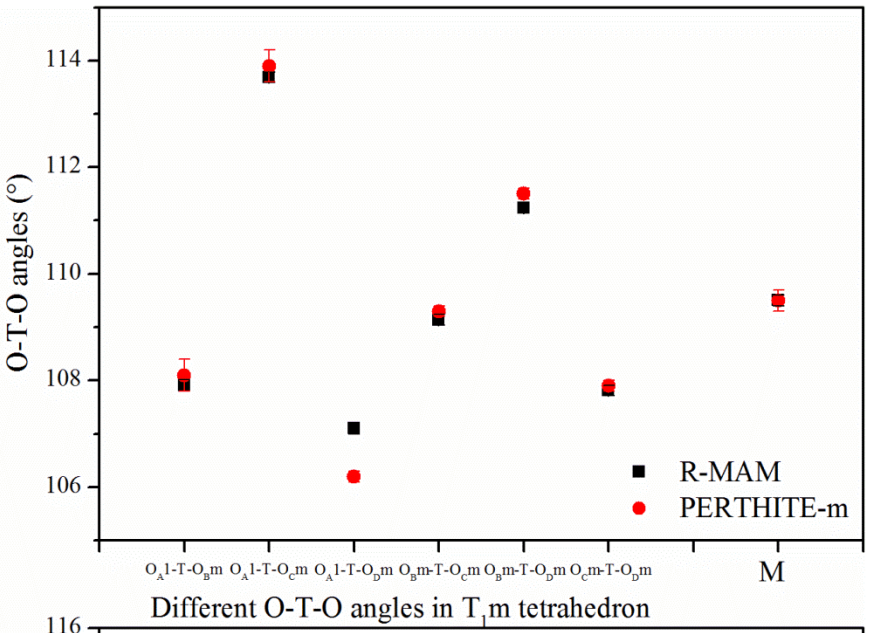
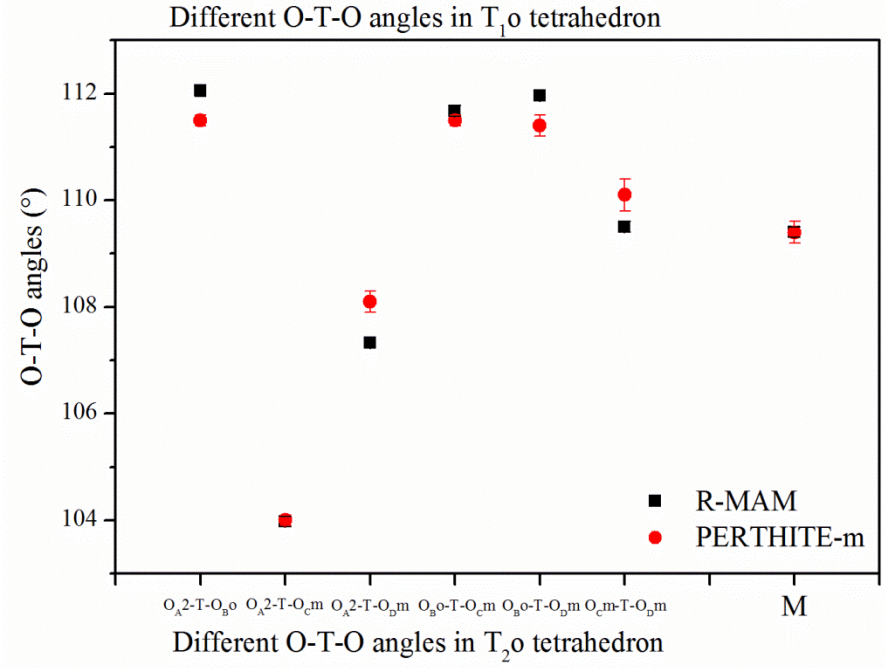
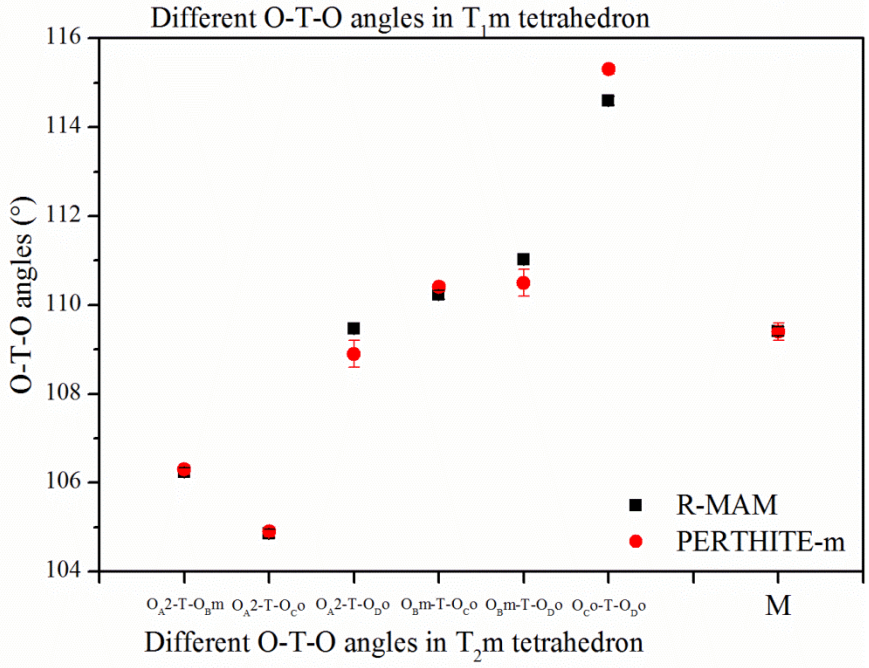


Figure S6. O–T–O angles in four tetrahedrons of microcline from the microcline references (R-MAM) and microcline in PERTHITE sample (PERTHITE–m). M denotes the mean for R-MAM and PERTHITE–m; ■ R-MAM; ●PERTHITE–m. The vertical bars represent errors. If no bar is given, then the error is contained within the area of the symbol.


O-T-O angles (°)
114
112
110
108
106
104
R-MAM
PERTHITE-m
O_A1-T-O_Bo
O_A1-T-O_Co
O_A1-T-O_Do
O_Bo-T-O_Co
O_Bo-T-O_Do
O_Co-T-O_Do
M
Different O-T-O angles in T_1o tetrahedron


O-T-O angles (°)
114
112
110
108
106
R-MAM
PERTHITE-m
O_A1-T-O_Bm
O_A1-T-O_Cm
O_A1-T-O_Dm
O_Bm-T-O_Cm
O_Bm-T-O_Dm
O_Cm-T-O_Dm
M
Different O-T-O angles in T_1m tetrahedron


O-T-O angles (°)
112
110
108
106
104
R-MAM
PERTHITE-m
O_A2-T-O_Bo
O_A2-T-O_Cm
O_A2-T-O_Dm
O_Bo-T-O_Cm
O_Bo-T-O_Dm
O_Cm-T-O_Dm
M
Different O-T-O angles in T_2o tetrahedron


O-T-O angles (°)
116
114
112
110
108
106
104
R-MAM
PERTHITE-m
O_A2-T-O_Bm
O_A2-T-O_Co
O_A2-T-O_Do
O_Bm-T-O_Co
O_Bm-T-O_Do
O_Co-T-O_Do
M
Different O-T-O angles in T_2m tetrahedron