

Supplementary Information

Table1: Calculated and Experimental Structural properties from the Teter Potential Model Tests – references indicate source of the atomic positions for each structure. All structures optimised using the General Utility Lattice Program (GULP)¹.

Structure	a (Å)			b (Å)			c (Å)		
	Exp	Calc	% diff	Exp	Calc	% diff	Exp	Calc	% diff
Kyanite ²	7.1170	7.1521	0.49	7.8600	7.8888	0.37	5.5750	5.5788	0.07
Andalusite ³	7.7930	7.8462	0.68	7.8973	7.9541	0.72	5.5558	5.5615	0.10
Sillimanite ²	7.3717	7.4695	1.33	7.5243	7.5443	0.27	5.7242	5.8587	2.35
Quartz ⁴	4.9134	4.9353	0.45	4.9134	4.9353	0.45	5.4052	5.4451	0.74
Stishovite ⁵	4.1812	4.1725	0.21	4.1812	4.1725	0.21	2.6662	2.6649	0.05
Coesite ⁶	7.1400	7.0843	0.78	12.3710	12.4097	0.31	7.1750	7.2199	0.63
Cristobalite ⁷	4.9717	4.9438	0.56	4.9717	4.9438	0.56	6.9223	6.7058	3.13
Gibbsite ⁸	8.7420	8.9410	2.28	5.1120	5.1091	0.06	9.8010	9.9486	1.51
Corundum ⁹	4.7589	4.7681	0.19	4.7589	4.7681	0.19	12.9912	13.1647	1.34
		α (°)			β (°)			γ (°)	
Kyanite	90.02	89.98	0.05	101.02	101.03	0.01	106.06	105.99	0.07
Andalusite	90.00	90.00	0.00	90.00	90.00	0.00	90.00	90.00	0.00
Sillimanite	90.00	90.00	0.00	90.00	90.00	0.00	90.00	90.00	0.00
Quartz	90.00	90.00	0.00	90.00	90.00	0.00	120.00	120.00	0.00
Stishovite	90.00	90.00	0.00	90.00	90.00	0.00	90.00	90.00	0.00
Coesite	90.00	90.00	0.00	120.34	120.39	0.04	90.00	89.99	0.01
Cristobalite	90.00	90.00	0.00	90.00	90.00	0.00	90.00	90.00	0.00
Gibbsite	90.00	90.00	0.00	94.54	90.01	4.80	90.00	90.00	0.00
Corundum	90.00	90.00	0.00	90.00	90.00	0.00	120.00	120.00	0.00
		Density (g/cm ³) ¹⁰			Bulk Modulus (GPa) ¹⁰			Shear Modulus (GPa) ¹⁰	
Kyanite	3.6640	3.6298	0.93	-	202.2200	-	-	105.1070	-
Andalusite	3.1500	3.1259	0.77	162.0000	158.6768	2.05	99.1000	91.8329	7.33
Sillimanite	3.2410	3.2603	0.60	170.8000	181.4548	6.24	91.5000	92.3348	0.91
Quartz	2.6500	2.6062	1.65	36.4000	35.1301	3.49	-	38.4159	-
Stishovite	4.2900	4.3015	0.27	316.0000	345.4134	9.31	220.0000	207.0695	5.88
Coesite	2.9200	2.9160	0.14	113.7000	129.0052	13.46	61.6000	55.7952	9.42
Cristobalite	2.3350	2.4352	4.29	16.4000	12.5689	23.36	39.1000	38.9393	0.41
Gibbsite	2.4210	2.2756	6.01	-	58.2094	-	-	29.0147	-
Corundum	3.9800	3.9193	1.53	253.3000	268.6118	6.04	163.2000	135.8447	16.76

Table 2: Potential model cut-off tests. Some of the structures specified above were optimised with different maximum cut-off values. A successful result indicates the structure was optimised with no instability in the final structure and reproduced the structural properties within reasonable limits.

Structure	Formula	Cut-off values tested (Å)			
		10	12	14	15
Kaolinite	Al ₄ Si ₄ O ₁₈ H ₈	Fail	Fail	Pass	Pass
Andalusite	Al ₂ SiO ₅	Fail	Fail	Fail	Pass
Kyanite	Al ₂ SiO ₅	Fail	Pass	Fail	Pass
Sillimanite	Al ₂ SiO ₅	Pass	Pass	Pass	Pass
Quartz	SiO ₂	Fail	Pass	Pass	Pass
Stishovite	SiO ₂	Pass	Pass	Fail	Pass
Coesite	SiO ₂	Fail	Pass	Fail	Pass
Gibbsite	AlOH	Pass	Fail	Pass	Pass
Corundum	AlO ₃	Pass	Pass	Fail	Pass

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