

Pressure-induced structural transformations in the low-cristobalite form of AlPO_4

H.K. POSWAL,^{1,*} NANDINI GARG,¹ MADDURY SOMAYAZULU,² AND SURINDER M. SHARMA

Fig. S1 Evolution of lattice parameters at 13 GPa during equilibration of the structure obtained at 12 GPa .

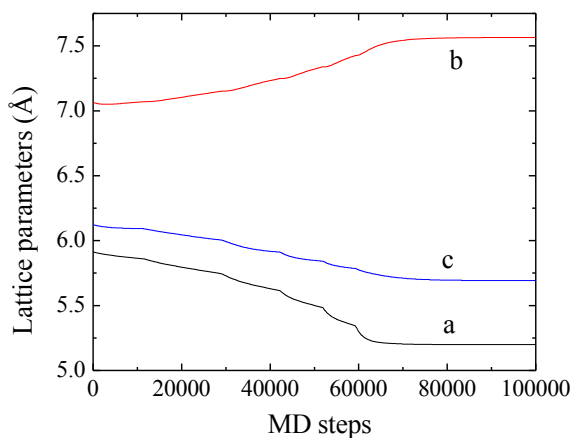


Fig. S2 Calculated partial radial distribution functions of Al-O, P-O and O-O at various pressures after equilibrating structures for 2000 MD time steps. The onset of the phase transition can be seen at ~ 13 GPa.

