Integrated intensities of Bragg reflections from a clear natural quartz with five temperatures below and above the α-β transition (Tc°), using Mo Kα radiation. All symmetry independent reflections up to 2θ = 80° were used in least-squares refinement, which was based on the Gren-Carlier expansion. The atomic positions for 3 quartz were constrained on the sites with symmetry 222 for Si and with 2 for O. The Rw values in the refinements of the model including terms up to the fourth-order were improved as shown below with those of the second-order refinements in parentheses: 0.0377 (0.0350) at Tc-10 K, 0.0366 (0.0321) at Tc+4 K, 0.0413 (0.0252) at Tc+10 K, 0.0374 (0.0478) at Tc+60 K and 0.0302 (0.0356) at room temperature. Of the 38 third- and fourth-order coefficients, 13 were nearly zero for the room temperature data, while only a few were zero for the high temperature data. Atomic probability density functions (pdf) obtained from the high-order calculations were almost unimodal at the five temperatures. A split-atom model for 3 quartz, where 0 and Si respectively split into two sets of positions corresponding to a quarter and a half by the Baumgardt two law, was also fitted to the (Tc+K) data. This calculation converged at Rw=0.0459 for the positional parameters in good agreement with those obtained by neutron diffraction data at Tc+60 K (Wright & Lehmann, 1981). The solid state Chem., 52, 3697 have found an incommensurate phase in the ambient range of 1.8 K between α and γ phases. Although Gohara et al. (1983) (J. Phys. Soc. Japan, 52, 3697) have found an incommensurate phase in the range of 1.8 K between α and γ phases, we will continue our discussion, for the present, on the basis of the transition scheme traditionally adopted.

08.4-4 COMPUTATIONAL MODEL OF THE STRUCTURAL AND ELASTIC PROPERTIES OF THE HIGH-PRESSURE PHASES OF MgSiO3. GAUSSIAN, LILMENITE AND PEROVSKITE. By H. Natsui, Chemical laboratory, Kanazawa Medical University, Japan; M. Akaogi and T. Matsumoto, Department of Earth Sciences, Faculty of Science, Kanazawa University, Japan.

The three high-pressure phases of MgSiO3, garnet(majorite), ilmenite and perovskite, are considered to be the major constituents of the deep mantle. The purpose of this investigation is to develop a realistic potential energy model which is applicable to characterizing and predicting the structural and elastic properties of these three high-pressure phases, as a function of pressure. The continuum models are based on energy minimization with respect to the structural variables. The potential energy of the crystal is approximated to be the sum of Coulomb interaction, van der Waals attraction and short-range repulsive interaction between atoms. The energy parameters required to model the three phases are determined from a best fitting of the parameters to the observed zero-pressure structures of the ilmenite and perovskite phases as well as to the measured single-crystal elastic constants of the ilmenite phase. The resulting potential model is applied to simulating (1) the zero-pressure structure and elasticity of the garnet phase, (2) the zero-pressure elasticity of the perovskite phase, and (3) the high-pressure behaviors of the structures and elastic constants of the three phases.

08.4-6 OH=F SUBSTITUTION IN THE AMBLYGONITE-MONTEBRASITE SERIES: A CRYSTAL STRUCTURE AND SPECTROSCOPIC STUDY. By L.A. Grant, M. Raudsepp, F.C. Hawthorne, Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba, R3T 2N2; B.L. Sherriff, Department of Geology, McMaster University, Hamilton, Ontario, L8S 4M1; J.S. Hartman, Department of Chemistry, Brock University, St. Catharines, Ontario, L2S 3A1.

We have used single-crystal structure refinement, infrared and MAS NMR spectroscopies to investigate OH=F substitution in the amblygonite-montebasite series (L1A1PO4(OH,F)). The structures of compositions with F/(F+OH) = 0.04, 0.15, 0.30, 0.44, 0.54, 0.70 and 0.80 were refined from MoKα X-ray data. R indices were approximately 2-3% except for the 0.70 composition, for which four different refinements gave R indices of 5-8%. The <F-O> distance was constant across the series, and the <Al=0-OH,F> distances were a linear function of the F/(OH+F) ratio. The Li position had an unusually high anisotropic temperature factor that increased with increasing F content; a split atom model was used and the splitting was a maximum at the 0.70 composition. The infrared spectrum of the near OH end-member showed a sharp peak at ~3390 cm⁻¹, corresponding to the principal (O-H) stretching band. With progressive F=OH substitution, this peak rapidly broadened and shifted to lower wave-numbers, reaching ~3355 cm⁻¹ for F/(F+OH) = 0.70. All samples had a reasonably smooth envelope in this region, except for the 0.70 F/(F+OH) sample, which had a distinct shoulder on the high energy side of this band. The 27Al MAS NMR spectra gave a broad 3J peak at ~15.75 ppm that was insensitive to F/(F+OH) ratio. The 27Al spectrum gave a broad peak that decreased in width and shifted to slightly lower field with increasing F content. A TEM study is in progress to investigate the possibility of a variable domain structure across the series.