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Crystallography of mineral phase transitions

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Phase transitions have been studied over the past 50 years by making use of evolving experimental techniques and theoretical approaches to understanding how and why they occur. This presentation reviews some crystallographic insights that have helped understand what is happening in a few different examples of phase transitions in minerals and related phases. An enormous amount of work has been done on the $(Mg,Fe)SiO_3$ perovskite to postperovskite transition since its discovery by Murakami et al. (2004). However, there are interesting crystallographic aspects to this transition based on the coordination of (Mg,Fe) in the eightfold site and how this is related to changes in structure with increasing pressure and temperature. In addition, substantial work has been done on (Mg,Fe)O phase transitions, but here again there are unanswered questions that can be resolved or at least partially answered by using a crystallographic approach. Shannon and Prewitt (1969) published a table of effective ionic radii that included radii values for Fe and other transition elements in both HS and LS states, but because these radii were derived using data obtained at ambient conditions, several questions arise as to how and/or whether they can be extrapolated for use under varying temperatures and pressures. These questions can be answered at least partially by examining the results from the experiments described above. Other examples of phases for which crystallographic data are available are based on FeS and Fe_2O_3 and a few other compositions with related, but different structural relationships that evolve as functions of pressure and temperature. FeS is now known to exist in at least six different crystal structures and a comparison of its properties in these structures along with its coordination and spin state provides important information about its physical character. The structures of the transition-metal sesquioxides are still not completely characterized, but the study of these phases also provides remarkable in-

sight to how different transition metals behave at elevated pressures and temperatures.