Crystallography in Inorganic Solid-State Chemistry

James A. Ibers, *Department of Chemistry, Northwestern University, Evanston, IL 60208-3113, U.S.A.* E-mail: ibers@chem.northwestern.edu

The pervasive importance of crystallography, particularly results obtained from single-crystal studies, in inorganic solid-state chemistry will be explored through a number of examples of metal chalcogenide systems. These examples will also illustrate the importance of other physical measurements in the characterization of such compounds. Among such examples, the $AMM'Q_3$ system (A=alkali metal; M=f-element; M' = d-element; Q=S, Se, or Te) will be used to emphasize the importance of concomitant optical and magnetic measurements and the compound $RbVSe_2$ will serve to illustrate the importance of theoretical calculations.

There are also pitfalls and difficulties in the applications of crystallography to solid-state systems. The determination of chemical composition through the refinement of site occupancies is one of the most highly abused areas. Some aspects of the refinement of site occupancies will be explored through the $NaLiM'S_2$ series and the $Er_{2-x}Sm_xSe_3$ system. Comparisons will be made with quantitative chemical analyses obtained through the use of inductively coupled plasma (ICP) analyses.

Finally, the compound $Ba_4Fe_2I_5S_4$ will be used to illustrate the structural challenges posed by the unexpected in solid-state syntheses.

Keywords: metal chalcogenides, chemical crystallography, physical properties structure relationships