A Theoretician’s View of Crystallography
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Whether thinking qualitatively or quantitatively, molecular structure, most often determined by crystallography, is central to the aims of quantum chemists. This long-time consumer and observer of crystal structures will talk about the conceptual terrain between theorists and crystallographers. Among the topics broached will be the complex problem of what is a chemical bond, experimental and “chemical” standard deviations, and the working out of secondary, donor-acceptor interactions in the solid state.

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