

04.X-01 RECENT DEVELOPMENTS IN REACTION PATH STUDIES. By H.B. Bürgi, Laboratorium für Kristallographie, Universität Bern, Freiestr.3, CH-3012 Bern, Switzerland.

Reaction path studies are based on the following working hypothesis: If a correlation can be found between two or more independent parameters describing the structure of a given structural fragment in a variety of environments, then the correlation function maps a minimum energy path in the corresponding parameter space¹. This approach continues to be used by various groups for interpreting the results of series of crystal structure analyses. Recent results concern the nucleophilic substitution reactions, the Berry mechanism in phosphoranes and phase transitions of ionic compounds. In at least one case it has been possible to apply the working hypothesis to a single structure and to interpret the thermal motion parameters of an octahedral Cu(II) complex in terms of the energy surface for dynamic Jahn-Teller distortion.

1) P. Murray-Rust, H.B. Bürgi, J.D. Dunitz, J. Amer. Chem. Soc. 97, 921 (1975).

04.X-02 MOLECULAR INTERACTIONS IN HOST-GUEST COMPLEXES. By K. N. Trueblood, Department of Chemistry, University of California, Los Angeles, California 90024, USA.

Highly structured molecular complexes may be prepared from molecules or ions that possess stereoelectronically complementary binding sites. In the present context, the host is an organic molecule or ion whose binding sites converge in the complex. The guest is a molecule or ion whose binding sites diverge in the complex. Emphasis will be placed on the molecular interactions that permit and facilitate molecular recognition in complexation. The primary focus will be on complexes with synthetic hosts, with emphasis on hosts prepared by Cram and his colleagues (Accts. Chem. Res. 11 8-14 (1978)) and on the structural studies of them by Goldberg and in our laboratories, but some recent work by others in this area will also be mentioned.

Among the topics to be considered will be: planned variability in the degree of conformational reorganization of hosts upon complexation, factors affecting the extent to which the host envelops the guest (complexes classified as perching, nesting, or capsular), evidence of molecular deformation and molecular flexibility or rigidity in hosts and in their complexes, the energetics of complexation, and the geometry of hydrogen bonding and other ion-dipole or dipole-dipole interactions in complexes, especially at ether oxygen atoms. This work has been supported by National Science Foundation Grants CHE77-18748 and CHE80-22526.

04.X-03 HIGH RESOLUTION NMR STUDIES OF CRYSTALLINE ORGANIC SOLIDS. By C. A. Fyfe, Guelph-Waterloo Centre for Graduate Work in Chemistry, Guelph Campus, Department of Chemistry, University of Guelph, Guelph, Ontario Canada.

Techniques and equipment will be described which make possible the measurement of high-resolution NMR spectra of solid samples. The complementary nature of these measurements to X-ray crystallographic studies will be described and exemplified and results presented on several cases where chemical reactions occur in the solid state.

04.X-04 NEW SOLID STATE REACTIONS OF TRANSITION METAL COMPLEXES. By Bruce M. Foxman, Department of Chemistry, Brandeis University, Waltham, MA 02254, USA.

Three new types of reactions have been studied:

1. Octahedral coordination polymers of the type MX_2L_2 , where $M=Ni, Co$, $X=halide$, $L=P(CH_2CH_2CN)_3$, are produced by solid-state reaction and have been reported by us previously. Many of these polymers undergo a further solid-state reaction which involves cross-linking of the octahedral polymer strands. The complex chemistry and crystallography of the randomly oriented product will be reported.
2. The solid-state and solution decomposition of the well-known charge transfer complex ferrocene: tetracyanoethylene yield various ferricenium cyanocarbon anion complexes. Comparative studies of substituted ferrocene: TCNE complex reactivity will also be discussed.
3. New pathways for the generation of coordination polymers via solid-state reaction have been explored. "Crystal-engineering" of the monomer precursor complexes has been based upon familiar aspects of inorganic and organic solid-state chemistry. Crystal structure vs reactivity correlations obtained in the early stages of this work will be discussed.