

ML.14-H2 FROM CRYSTAL STATICS TOWARDS MOLECULAR DYNAMICS. By Jack D. Dunitz, Organic Chemistry Laboratory, Swiss Federal Institute of Technology, ETH-Zentrum, CH-8092 Zürich, Switzerland.

Although X-ray (and neutron) diffraction can provide information about atomic vibrations as well as about atomic positions, the results of crystal structure analyses are still usually considered in an essentially static sense. Here we discuss two ways in which information about molecular motions may be extracted from crystallographic data. In the structure correlation method we search for correlations among structural parameters from many individual structures, each structure being regarded as a sample point in a many-dimensional parameter space. The connection with molecular motion comes about if we assume that the distribution of sample points maps the low-lying regions of the molecular potential energy surface. The second approach involves the analysis of anisotropic vibration parameters (AVPs). For many molecules the rigid-body model behind the usual T, L, S analysis is clearly inadequate. Improved agreement between observed and calculated AVPs can often be achieved by introducing appropriate internal molecular motions into the analysis. Mean-square amplitudes estimated in this way for internal motions (mostly torsional) are reasonable. Internal molecular motions are more readily detectable from low-temperature data. However, the bad reputation associated with AVPs from routine room-temperature crystal structure analyses is not always entirely justified. Interesting indications about internal molecular motions can sometimes be derived even from AVPs of only moderate accuracy.

ML.14-H4 STRUCTURAL STUDIES OF PHASE TRANSITIONS IN ONE DIMENSIONAL CONDUCTORS AND SUPERCONDUCTORS. By R. Comès, Université Paris Sud, Bâtiment 510, 91405 ORSAY, France

One important structural feature of one dimensional conductors is a particular lattice distortion predicted by theories of an ideal one dimensional metal (Peierls, *Quantum Theory of Solids*, Clarendon (1964)). In the models, this distortion takes place at 0° K, with precursor fluctuations in a wide temperature range and a giant anomaly in the phonon dispersion at twice the Fermi wave vector ($2k_F$) (Afanasev and Kagan, *Sov. Phys. JETP* 16, 1030, (1963)). Real systems retain the main feature of the earlier models (Comès et al., *Phys. Rev.* B8, 571, (1973); Renker et al., *Phys. Rev. Lett.* 30, 1144, (1973); Shirane et al., *Phys. Rev.* B14, 2325, (1976)), but weak coupling between conducting chains raises to a finite value the temperature at which the lattice distortion takes place and results in a new type of phase transition. (Renker et al., *Phys. Rev. Lett.* 32, 836, (1974); Comès et al., *Phys. Rev. Lett.* 35, 1518, (1975); Kagoshima et al., *J. Phys. Soc. Jpn* 39, 1143, (1975)). Competing effects have further considerably enriched the original picture. Such effects include transverse as well as longitudinal polarizations of the distortion, different instabilities on different molecular chains, $2k_F$ but also $4k_F$ instabilities (Pouget et al., *Phys. Rev. Lett.* 37, 437, (1976)), and commensurability effects (Friend et al., *Phys. Rev. Lett.* 40, (1978); Megtert et al., *Sol. St. Comm.* 37, 875, (1981)). In the recent class of organic superconductors (TMTSF)₂X⁺, superconductivity is not only in competition with the Peierls instability, but also width order-disorder transitions involving the counter ions X (Moret et al., *Phys. Rev. Lett.* 49, 1008, (1982)). Further complications arise from quenching effects and X-ray radiation induced modifications.

ML.16-H2 SYMMETRY AND ASSEMBLY OF VIRUS STRUCTURES. By Bror Strandberg, Department of Molecular Biology, University of Uppsala, Box 562, S-751 22 Uppsala, SWEDEN

Already in 1956 Crick and Watson predicted (Nature 177, 473-475, 1956) that the nucleic acid of simple viruses is protected by a protein shell constructed from identical subunits arranged with cubic symmetry (for spherical viruses) or helical symmetry (for rod shaped viruses). For the spherical viruses genomic economy and optimal covering favoured icosahedral symmetry. The problem of how to incorporate more than 60 identical protein subunits in spherical viruses was in 1962 tackled by Caspar and Klug (Cold Spring Harbor Symp. Quant. Biol., 27, 1-24, 1962) who showed how multiple sets of 60 two-dimensional objects could cover the surface of an icosahedron while maintaining quasi-symmetrical environments.

In recent years detailed structural analysis have been done on three spherical plant viruses, namely of TBSV (Harrison et al., Nature 276, 368-373, 1978) of SBMV (Abad-Zapatero et al., Nature 286, 33-39, 1980) and of STNV (Liljas et al., J. Mol. Biol. 159, 93-108, 1982) as well as of the adenovirus hexon (R.M. Burnett, in Structural Biology, McPherson and Jurnak eds., vol. II, The Viruses, Wiley New York, in press) and a low resolution structure of the polyoma virus capsid (Rayment et al., Nature 295, 110-115, 1982). These studies point to that the icosahedral surface lattices predicted by Caspar and Klug are correct while the quasi-equivalence theory has to be modified. Many arguments point to the need for considering protein oligomers, likely with "variable bonding potentials", as the sub-assembly units of spherical viruses. These possibilities will be discussed as well as the forces which contribute to the stability of the assembled virus particles.

The assembly of a helical virus particle (TMV) will be discussed with emphasis on the comparison with assembly of spherical viruses.

ML.16-H4 STRUCTURAL CHEMISTRY OF METAL CLUSTER COMPOUNDS By R. Mattes, Institute of Inorganic Chemistry, University of Münster, Corrensstr. 36, 4400 Münster, Bundesrepublik Deutschland

Three types of metal cluster compounds can be defined: (1) the 'carbonyl' type, (2) the 'halide' type of the transition metals and the lanthanoids, and (3) the 'naked' metal cluster type of main group metals. The most extensive group are the carbonyl clusters with the metals in zero or negative oxidation states. They may contain 20 and more metal atoms per cluster unit. The arrangements of the metal atoms resemble fragments of metallic lattices with limiting triangular faces. Typical examples of halide type clusters are Mo₆Cl₁₂ or Mo₆Se₈. Halides of low-valent Sc, Y and lanthanoids will be reviewed as well. Their structures can be described by the principle of 'cluster condensation' (A. Simon, *Angew. Chem.* (1981) 93, 23). Using cryptands or macrocycles as chelating agents for the counterions, new types of 'naked' clusters were obtained (J.D. Corbett, *J. Am. Chem. Soc.* (1983) 105, 5715).

Theories and rules concerning the type of bonding, and correlating or predicting cluster geometry will be discussed, as well as clusters with encapsulated non-metal atoms. Some metal atom clusters show fluxional behaviour. Clusters may provide simple models of catalysts in heterogeneous catalysis and may find application as superconductors.