ML. 14–H 2 FROM CRYSTAL STATICS TOWARDS MO-
LECULAR DYNAMICS. By Jack D. Dunitz, Organic
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Although X-ray (and neutron) diffraction can provide
information about atomic vibrations as well as about
atomic positions, the results of crystal structure anal-
yses are still usually considered in an essentially static
sense. Here we discuss two ways in which information
about molecular motions may be extracted from crys-
tallographic 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 pa-
rameter space. The connection with molecular motion
comes about if we assume that the distribution of sam-
ple 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 am-
plitudes estimated in this way for internal motions
(mostly torsional) are reasonable. Internal molecular
motions are more readily detectable from low-temper-
ature data. However, the bad reputation associated with
AVPs from routine room-temperature crystal structure
analyses is not always entirely justified. Interesting in-
dications about internal molecular motions can some-
times be derived even from AVPs of only moderate ac-
curacy.

ML. 14–H 4 STRUCTURAL STUDIES OF PHASE TRANSITIONS IN
ONE DIMENSIONAL CONDUCTORS AND SUPERCONDUCTORS. By
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One important structural feature of one dimensional con-
ductors is a particular lattice distorsion predicted by
theories of an ideal one dimensional metal(*Peierls, Quantum
Theory of Solids, Clarendon* (1964). In the models, this
distorsion takes place at $0°$ K , with precursor fluc-
tuations 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 distorsion
takes place and results in a new type of phase tran-
sition. (*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 distorsion,
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 $(TMTSF)_2 X^-$, supercon-
ductivity 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 modi-
fications.

ML. 16–H 2 SYMMETRY AND ASSEMBLY OF VIRUS STRUCTURES.

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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 ident-
ical subunits arranged with cubic symmetry (for spheri-
cal 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 sub-
units 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 Struc-
tural 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 con-
sidering protein oligomers, likely with "variable bonding
potentials", as the sub-assembly units of spherical vi-
ruses. 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–H 4 STRUCTURAL CHEMISTRY OF METAL CLUSTER
COMPOUNDS By R. Mattes, Institute of Inorganic
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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 re-
semble fragments of metallic lattices with lim-
iting triangular faces. Typical examples of
halide type clusters are Mo_6Cl_{12} or Mo_6Se_8.
Halides of low-valent Sc, Y and lanthanoides
will be reviewed as well. Their structures can
be described by the principle of 'cluster con-
densation' (A. Simon, Angew.Chem. (1981) 93,
23). Using cryptands or macrocycles as chela-
ting 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 bond-
ing, and correlating or predicting cluster geo-
metry 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 appli-
cation as superconductors.