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05. PHYSICAL PROPERTIES AND STRUCTURE

05.2–24 CRYSTAL AND ELECTRONIC STRUCTURE OF (μ−H)₃
(CO)₉Os₃BCO. By Leh-Teh Hsu, Deng-Tang Jan and Sheldon
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The title compound (I) has been prepared and characterized
by single-crystal X-ray diffraction as well as spectroscopic methods
(1H, 13C, and 1H NMR). The compound is a carboxyl borylidyne
capped O₃ triangle as shown in the figure.

The electronic structure of I has also been studied by using the
Fenek-Hall quantum chemical approach with a fragment analysis
in terms of the metal cluster H₃(CO)₉Os³⁺ and capped ligand BCO.
The calculation suggests that the sp-hybridized boron forms a dative bond to the
metal triangle and the remaining p orbitals form multi-centered v bonds to the O₃ group.

The BCO unit in I has B=01.469(15)Å and C-O=1.31Å, while in H₃BCO (II) has B=0.14.54Å and C-O=1.31Å. The CO stretching frequency is 2120 cm⁻¹ in I and 2140 cm⁻¹ in II. To explain this difference, nonparameterized Fenek-Hall molecular orbital calculations are carried out on both I and II with a fragment analysis in terms of H₃(CO)₉Os⁺ and CO for the former, H₂Os and CO for the latter. The calculation suggests that the back v bonding in I is more significant, due to the predominant movement of the electron density of the main O₃B bonding orbitals to the CO π anti-bonding orbitals.

05.2–25 THE EFFECT OF CRYSTAL STRUCTURE AND PHASE
STABILITY ON THE SUPERCONDUCTIVITY OF EQUATOMIC TERNARY
FIFICIDE COMPOUNDS† By C. F. Meisner, Los Alamos
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The equatomic ternary compounds MX₃ with M = Ti, Zr, or
Hf, X = Ru or Os, and X = P or As typically crystallize at high temperatures in the ZrRuP₃-type hexagonal structure (P6/mm, M in 3g), X in 3f(c) and X in 2(c) and 1(u) and exhibit superconductivity at temperatures as high as 13.3 K for ZrRuB (Barz, Ku, Meisner, Tkak, and Mattias, Proc. Natl. Acad. Sci. USA (1980) 77, 3132; Meisner, Ku, and Barz, Mater. Res. Bull. (1983) 18, 983). These compounds are metastable and crystallize at low temperature structures have been useful in extracting atomic thermal motion information from the somewhat disordered crystal structure of the triclinic polymorph.

The room temperature structures (22°C) of three crystal polymorphs of the compound 4,4'-bis(ethoxy)-
azoxybenzenzenes (also called p,p'-azoxydiphenolene), a compound exhibiting a nematic liquid crystalline phase from 137 to 168°C, as well as a low-temperature structure of the triclinic polymorph, have been determined. These structures represent the initial phase of a systematic variable temperature X-ray crystallographic study of several members of a homologous series (4,4'-bis(methoxy)-, 4,4'-bis(ethoxy)-, and 4,4'-bis(propoxy)-azoxybenzenzenes) in an attempt to obtain information regarding the inter- and intermolecular interactions which must account for the liquid crystalline behavior of this series of compounds. The isolation of three crystal polymorphs at room temperature presents an opportunity to compare the intra- and intermolecular interactions for this nematicogenic molecule in three different packing arrangements. A comparison of the low- and room-temperature structures has been useful in extracting atomic thermal motion information from the somewhat disordered crystal structure of the triclinic polymorph.

The study by electron microscopy of virgin crystals shows that Pyroelectric phase does not transform into the ferroelectric phase when the virgin crystal is cooled to 168°C, while it is obtained to higher temperatures. The study also shows that Pyroelectric phase can be induced in the virgin crystals by applying a field of 1000 V cm⁻¹ for 20 min. The study also shows that Pyroelectric phase can be induced in the virgin crystals by applying a field of 1000 V cm⁻¹ for 20 min.

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In order to determine some of the differences in the phase transitions, a study by Hartsugh-Roodock theory has been carried out. A first result has been that the crystallization energy of the ferroelectric phase is less than the pyroelectric one. This suggests that the method of crystallization is where the pyroelectric phase is not obtained. Experimental results show that pyroelectic phase does not growth in low supersaturation, while it is obtained to higher values of supersaturation.