Engineering Inorganic Crystals

PS08.03.01 CONSIDERATION OF BRIDGING GEOMETRIES IN RATIONAL SYNTHESIS OF OXOVANADIUM PHOSPHATES. Marcus R. Bond and Tom Otero, Departments of Chemistry, Southeast Missouri State University, Cape Girardeau, MO 63901 and Eastern Kentucky University, Richmond, KY 40475

While the preparation of new oxovanadium phosphate structural frameworks still lies largely in the realm of serendipity, the significant accumulation of structural data for these systems provides a foundation for developing rational synthetic strategies. The diversity of bridge types found in oxovanadium phosphates undoubtedly leads to the complicated array of observed structural types. Within these systems both one-atom (mu-O) and three-atom (mu-O, mu-O) bridges are found in single, double, triple, or quadruple bridges between oxovanadium centers. Double three-atom bridges provide the most variety offering at least seven distinct bridge configurations each with a wide range of distorted conformers. Systematic analysis of known bridge types, their geometries, and structural environments provides insight into the factors that govern adoption of various bridging modes and geometries in oxovanadium phosphate clusters and extended solids.

PS08.03.02 FINDING COMPOUND PROPERTY PATTERNS IN EMPIRICAL DATA SETS USING DISCOVERY METHODS. A. G. Jackson, Wright Laboratory, WPAFB, OH, USA, N. Kiselyova, Baikov Institute of Metallurgy, Moscow, Russia.

The extension of performance of materials beyond the current limits for bulk or thin films has become imperative because of demands for high performance. Frequently this means new materials must be designed that build on existing compounds in ways not easily determined using first principles computational approaches. Methods for exploring data bases to identify patterns of behavior are useful because of the classification and prediction possibilities they offer. The pyTarnidal net method has been applied to the prediction of new compounds based on known data on the elements of the compounds. Compound types A3BC15, ABF6, AB03 have been considered using various forms of positional formulas for structural elements of the structures of compounds where known. A Table of predicted compounds resulted from the analysis.

PS08.03.03 MOLECULAR CHAINS, GRIDS AND CUBICLES: DESIGNING INORGANIC POROUS SOLIDS. Piere Losier, Department of Chemistry, Queen's University, Kingston, Ontario, Canada.

Crystal engineering has lead to the rational design of inorganic polymers containing one- (chains), two- (grids), and three-dimensional (boxes or cubicles) frameworks based upon the established coordination chemistry of the incorporated transition metals (e.g. Co, Ni, Cu, Cd, Zn). Few solids consisting of square planar grids (1) have been reported and the large cavities in these two-dimensional frameworks (>50% by volume) usually lead to interpenetration or entanglement of one grid into another which results in a reduction or elimination of effective pore size. Recently, we reported the synthesis and structural characterization of an octahedral poroid solid (2), [Zn(4,4'-dipyridyl)2]SF6 • DMF, which consists of overlapping grids of [Zn(4,4'-dipyridyl)2] linked by the counterion [SF6]2-. This neutral inorganic polymer eschews interpenetration and has its cavities filled with solvent molecules. We present herein several examples of non-interpenetrated square grid and octahedral inorganic polymers.

Exotic Molecules-Inorganic/Mineral

PS08.05.01 CRYSTAL STRUCTURES OF NEW DOUBLE HYDROGEN PHOSPHATES WITH ENORMOUS UNIT CELLS. N. Anisimova, A. Ilyukhin, and N. Chudinova, Institute of General and Inorganic Chemistry, Russian Academy of Science, Moscow 117907, Russia.

Recently published [1] the direct method for the synthesis of cyclododecaphosphates (the biggest inorganic phosphate ring) includes the consistent thermal condensation of double ccesium iron hydrogen monophosphate into cyclophosphosphate Cs3FeP2O7. In the work [1] the previously unknown substance CsFeH5(P04)3 was firstly obtained and used as a starting material. The present work reports its crystal structure as well as the previously unknown structure of NaFe(H2P04)3H2P04.H2O. Unit cells of both compounds are characterized by the large dimensions unusual for other known inorganic hydrogen phosphates. The main structural elements of the structures of CsFeH5(P04)3 (Z=6; Pna21, a=9.365(1) Å, b=9.402(1) Å, c=12.802(1) Å) and of NaFe(H2P04)3H2P04.H2O (R=0.06; Pbnm, Z=8, a=7.49(1) Å, b=12.49(1) Å, c=13.49(1) Å) are the channels formed by PO4-tetrahedra and FeO6-octahedra. Cs and Na atoms are placed inside the channels. Due to their specific structures both compounds are essential for the formation of new complex phosphate anions. Acknowledgments: RFBR, DFG.