determine the effect of the dopant atom on the thermoelectric Figure of Merit.

[1] Calliat et al., *High-Performance Thermoelectric Materials Based on β-Zn4Sb3*, NASA Jet Propulsion Laboratory, Nasatech Briefs, Vol. 23. No. 2

Keywords: thermoelectric materials, physical properties, Zn_4Sb_3

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Atomic Displacement Parameters and Specific Heat of *p*-Dichlorobenzene Polymorphs between 10 and 230 K

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Synchrotron data for the α- and β-polymorphs of *p*-dichlorobenzene (*p*-DCB) between 10 and 230 K were collected to 0.5 Å resolution at the ESRF and refined with a multipole model in order to deconvolute thermal motion from valence bonding density. Sealed tube data of the γ-polymorph were collected between 100 and 180 K to 0.7 Å resolution and refined with a spherical atom model. The multi-temperature atomic displacement parameters (ADPs) were analyzed in terms of libration and translation frequencies [1]. From the six external vibration frequencies and the intramolecular vibration frequencies from high-level DFT calculations heat capacities C_v were calculated with molecular Einstein and Debye models and found to be in fair agreement with C_p from calorimetric measurements [2].

[1] Bürgi H.-B., Capelli S.C., Birkedal H., *Acta Cryst*., 2000, A**56**, 425. [2] Dworkin A., Figuière P., Ghelfenstein M., Szwarc H., *J. Chem. Thermodyn.* 1976, **8**, 835.

Keywords: atomic displacement parameters, specific heat, polymorphs

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Anisotropic Displacement Parameters for Normal Mode Analysis: Which Refinement is Needed?

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Information on low-frequency modes of molecular motion in the crystal[1] can be extracted from Anisotropic Displacement Parameters (ADPs) measured over a wide range of temperatures. Here we investigate the bias on the ADPs due to effects of deformation density and its influence on the model of motion.

Four models were refined with a data set on (*E*)-2,2'-dimethylstilbene measured at 90 K to the high resolution of 0.41 Å[2]: 1) Spherical form factors 2) Multipole Parameters (MPPs) from a library[3] 3) MPPs fitted to a calculated charge density[4] 4) MPPs fitted to the experimental charge density. The ADPs from the different refinements differ by 0.00006 - 0.0017 A^2, corresponding to 1 to 20 s.u.. The U11 and U22 components lying in the molecular plane decrease for models 2, 3 and 4 as compared to model 1. The decrease is largest for model 4. In model 2 the U33-out of plane components are becoming clearly bigger whereas they become smaller with model 4 compared to a spherical model. In the Normal Mode Analysis these differences are reflected primarily in a decrease of the temperature independent part of the model of motion [1].

[1] Bürgi H.B., Capelli S.C., *Acta Cryst*., 2000, A**56**, 403-412. [2] Ogawa K., Harada J., *unpublished results*. [3] Pichon-Pesme V., et al., *J. Phys. Chem*., 1995, **99**, 6242-6250. [4] Courtesy of T. Koritsansky, Middle Tennessee State University.

Keywords: normal mode analysis, charge density analysis, anisotropic displacement parameters

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Intermolecular Interaction and Molecular Dynamics in Carboxylic Acid Crystals

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In this work we report about investigation of Davydov splitting value temperature changes for CH_2 rocking vibrations of pure crystalline carboxylic acids $CH_3(CH)_{n-2}COOH$ with odd (n=15,17,19) and even (n=10,14,16,22) number n of carbon atoms in the temperature region from 100K to the crystal melting temperature by FTIR spectra.

A statistic and dynamic model is proposed which provides adequate description of the observed effect. In the framework of this model the damping of vibrational excitons on orientational defects of different nature takes place. Genesis of such defects is connected with excitation of conformational, librational and rotational degrees of freedom of H-bonded molecular dimers at the different temperatures.

Theoretical analysis of the effect of resonance dynamical intermolecular interaction on the spectra of intramolecular vibrations of the crystals was performed in terms of stochastic equations with account of mentioned mechanisms. Computer simulation of such dependence was performed for crystalline normal chain carboxylic acids. Good agreement between the experimental and computer simulation results was obtained.

Keywords: intermolecular interactions, computer simulation, carboxylic acids

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Synthesis, Crystal Structures and Dielectric Properties of the Novel Linear High k Molecular Materials

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The crystal structures of the novel copper and iron complexes: dinitrate-aquadi-μ-hydroxobis-μ-(isonicotinato)copper(II) 'C12 H18 Cu N4 O14', **1**, and dinitrate-di-μ-hydroxobis-μ-(nicotinato)copper(II) 'C12 H14 Cu N4 O12', **2**, nitrate-diaquadi-μ-hydroxobis-μ-(nicotinato)copper(II),**3**, μ-(nicotinato)copper(II)hexafluoroacetylacetonate **4**, tetranitrate-diaquadi-μ-oxobis-μ-(isonicotinato) iron(III),**6**, and tetranitrate-diaquadi-μ-oxobis-μ-(nicotinato)iron(III) (C24 H40 Fe4 N4 O20·8(NO_3)·2(H_2O)) **,7**, and dielectric properties for **1**, **2, 4, 6** and 7 are reported. **1, 4, 6** and **7** crystallize in the monoclinic crystal system in space group $P2_1/c$. **2** crystallizes in the triclinic crystal system in space group $P\bar{1}$. **3** crystallizes in orthorhombic system, space group Pbca. The molecules of **1** and **2** are arranged in quasi-1D chains perpendicular to the *a*-axis. **3** and **4** are 2-D polymers lying perpendicular to the *c*- and *a*-axis respectively. The molecules **6** and **7** are arranged in layers along the a-axis. The studied samples show a linear dielectric behavior characterized by a high dielectric permittivity, which is attributed to displacements of ionic bonds in the molecules. The ionic-bonds show characteristic dielectric resonance in the range of few kHz. The high dielectric permittivity and low ac conductivity make these materials attractive for high-k dielectric applications.

Keywords: high k linear molecular materials, cf and cv measurements, dielectro-structural correlation