

06.2-05 CHARGE DENSITY STUDIES OF γ -AMINO-BUTYRIC ACID (GABA) AND PHOSPHORYLETHANOLAMINE (PEA). H.-P. Weber*, S. Swaminathan**, R. K. McMullan***, and B.M. Craven**.

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These molecules are of interest because GABA is a neurotransmitter and PEA represents most of the polar moiety of the phosphatidylethanolamine lipids. Both molecules are zwitterions and have a *gauche* conformation at one of the bonds in the backbone, (C-C-C-C in GABA and C-C-C-N⁺ in PEA). We will attempt to relate the observed charge density in the crystal structures with the conformations of these zwitterions.

Matching sets of neutron and X-ray diffraction data have been collected at low temperature (122 K for GABA; 126 K for PEA). The neutron data extend to $\sin\theta/\lambda \approx 0.8 \text{ \AA}^{-1}$ and the X-ray data to 1.2 \AA^{-1} (GABA) and 1.0 \AA^{-1} (PEA). Structure refinements using the neutron data are in agreement with the previous results of Steward, Player and Warner [Acta Cryst. B29, 2038 (1973)] for GABA and of Kraut [Acta Cryst. 14, 1146 (1961)] for PEA. Charge density refinements are in progress using the multipole model of Stewart [Acta Cryst. A32, 565 (1976)].

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06.2-06 CHARGE DENSITY IN CoLiPO_4 OLIVINE-TYPE STRUCTURE, by J. Vicat, J.C. Guitel and D. Tran Qui, Laboratoire de Cristallographie, C.N.R.S., 166 X, 38042 Grenoble Cedex, France.

The electron distribution in CoLiPO_4 has been determined from single X-ray diffraction measurements at room temperature. All reflections up to $\sin\theta/\lambda = 1.37 \text{ \AA}^{-1}$ were measured (AgK α radiation, check on multiple diffraction). Equivalent reflections were averaged and the structure was refined with the program MOLLY (Hansen and Coppens, Acta Cryst., A 34, 1978, 909), using 2654 independent reflections.

Parameters describing multipole deformation functions indicate a strong quadrupole on Co, P and O atoms. P shows also a significant octopole. The atomic charges are: - 0.12(6) for Co, 0.80(10) for Li, 0.98(12) for P and - 0.41(4) for O; corresponding κ values are 0.996(5), 1.79(36), 1.033(13), 0.976(3). For AlPO_4 , NgoThong and Schwarzenbach (Acta Cryst., A 35, 1979, 658) found 1.0(1) and - 0.60(4) for atomic charges of P and O (corresponding κ values are 1.03(1) and 0.975(4)).

No significant peaks are found in the residual density map with high order reflections ($\sin\theta/\lambda > 0.9 \text{ \AA}^{-1}$) indicating the absence of important anharmonic thermal vibration. Conventional X-X maps calculated with all reflections show two elongated peaks of 1.4 e\AA^{-3} around Co, comparable to those found by Johansen's theoretical calculations (Acta Cryst., A 32, 1976, 353). Within the phosphate group, P and O are covalently bonded: maps show local maxima of 0.6 e\AA^{-3} which lie slightly off P-O bond directions. In addition two higher peaks of 0.9 e\AA^{-3} are also found at a distance of 0.4 \AA from P, which are as yet unexplained. Lone pair peaks of the oxygen atoms are clearly separated.

06.2-07 AN ELECTRON DENSITY DISTRIBUTION STUDY OF $\text{NaHC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ at 120K. By R. Delaplane, R. Tellgren and I. Olovsson, Institute of Chemistry, University of Uppsala, Box 531, S-751 21 Uppsala, Sweden.

The deformation electron density of sodium hydrogen oxalate monohydrate has been studied previously at 295K using X-ray and neutron diffraction techniques (Tellgren R., Thomas J.O., and Olovsson I., Acta Cryst. (1977) B33, 3500). Due to increased resolution gained at reduced temperature, X-ray diffraction data consisting of 3981 reflections with $I > 3\sigma(I)$ have been measured at 120K for $0 < \sin\theta/\lambda < 1.35 \text{ \AA}^{-1}$. A set of neutron diffraction data consisting of about 1250 intensities was collected at 120K at the R2 Reactor at Studsvik, Sweden.

A high-order least-squares refinement included 1277 X-ray reflections for which $\sin\theta/\lambda > 1.00 \text{ \AA}^{-1}$. The structure model consisted of positional and anisotropic thermal parameters for Na, C and O. Parameters for H were derived from the neutron diffraction measurements. Maps of X-X μ O difference electron density were calculated. A second refinement based on 3981 reflections included variable multipole deformation parameters (Hirshfeld F.L., Isr.J.Chem. (1977) 16 226). Dynamic and static deformation density maps were calculated from these parameters. The main features appearing in the deformation density maps are an excess of electron density concentrated in the covalent bonds and a more diffuse density in the lone-pair regions around the oxygen atoms. Effects attributed to hydrogen bonding will be discussed.

06.2-08 CHARGE DENSITY STUDY OF METHYLIDYNE TRICOBALT NONACARBONYL - DIRECT AND RECIPROCAL SPACE ANALYSES.* By P. Leung, A. Holladay & P. Coppens, Department of Chemistry, State University of New York at Buffalo, New York, 14214 U.S.A.

A charge density study of $\text{Co}_3(\text{CO})_9\text{CH}$ has been performed with X-ray and neutron diffraction data collected at 100K. The objective of these experiments is to understand the bonding of the apical CH group with the three cobalt atoms which can be used as a model for an adsorbed hydrogen species on metal surface. The deformation densities were calculated with a X-N formalism at a resolution of 0.85 \AA^{-1} . The charge deformation density in the methylidyne region is consistent with a delocalized bonding model of the CH group to the Co_3 triangle. Charge accumulation was observed to be in a direction toward the basal plane, rather than toward the individual cobalts. The C-H bond, however, is strongly localized. The electron density distribution in the $\text{Co}(\text{CO})_3$ regions indicates the electrostatic nature of bonding between Co and CO. The Co deformation density is observed to be located in a region such as to avoid the carbonyl ligands.

An estimate of the net atomic charges were made with both the kappa refinement and a direct space polyhedral partitioning technique. All atoms appear to be very close to neutral, except for the apical CH group (net charges: C - .57(10) and H + .20(4)).

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