06.7-4 SUBERIC ACID CHARGE DENSITY FROM X-RAY AND NEUTRON DIFFRACTION. By B. M. Craven, Q. Gao, H. P. Weber and R. K. McMullan*, Crystallography Department, University of Pittsburgh, Pittsburgh, PA 15260 USA, and *Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973 USA.

The structure of suberic acid $HOOC(CH_2)_6COOH$ (Housty & Hospital, Acta Cryst. 18, 753; 1965) has been redetermined by neutron diffraction at 18, 75 and 123 K and by X-ray diffraction at 123 K. Bond lengths for methylene C-C [1.526(2) Å] and C-H groups [1.086(4) Å] have been corrected for thermal motion, including internal and anharmonic vibrations. (These are mean and r.m.s. errors for the combined distribution of bond lengths at three temperatures.) Due to internal vibrations, nuclear m.s. amplitudes are greater at the center of the $(CH_2)_6$ chain than at the carboxylic acid groups. The charge density in the crystal structure is being analyzed using the rigid pseudoatom model of Stewart (Acta Cryst. A32, 565; 1976). Multipole electron population parameters from the X-ray data will be used to map the electrostatic potential (Stewart, God. Jugosl. cent. Krist. 17, 1; 1982) and to estimate the energy of the carboxylic acid H-bonding interaction (Spackman, J. Chem. Phys. 85, 6587; 1986).

Work supported by NIH Grant HL-20350, and carried out in part at Brookhaven National Laboratory under contract from the U.S. Department of Energy.

06.7-5 COMPARISON OF EXPERIMENTAL AND THEORETICAL ELECTROSTATIC POTENTIALS OF CARCINOGENIC NITROSOMINES. By J.F. Noonan, R. Bar-Adon, L.I. Foss, and E.D. Stevens, Department of Chemistry, University of New Orleans, New Orleans, LA, 70148, U.S.A.

Experimental electrostatic potentials have been calculated from multipole refinement parameters obtained from low temperature, high resolution x-ray diffraction measurements of N-nitroso- diphenylamine (NDPhA) and 4-(N-methyl-N-nitrosamino)-1-(3- pyridyl)-1-butanone (NNK). NNK is a carcinogenic derivative of nicotine found in cigarette smoke. NDPhA is a weak carcinogen used in the rubber industry. Since little is known regarding the mechanisms of carcinogenesis of nitrosamines, we have begun the study of the electron distributions and electrostatic potentials to aid in understanding the initial steps of activation.

For NDPhA, a total of 17,001 x-ray intensity measurements were collected at 100 K and averaged to yield 7372 independent reflections. The data were refined with a multipole deformation model including terms through the hexadecapole level yielding $R_w = 0.056$ with 214 parameters. For NNK, a total of 19,072 intensity measurements were made at 100 K and averaged to yield 7316 independent reflections. Multipole refinement converged at $R_w = 0.044$ with 288 parameters.

Experimental electrostatic potentials have been calculated by a modified Fourier series summation using structure factors representing the total charge density (both electron and proton contributions) calculated from the multipole refinement parameters. Potentials of isolated molecules are approximated by expanding the unit cell until the overlap between molecules is negligible. The experimental results show regions of negative potential located at the oxygen and nitrogen lone-pairs of the -NO group.

Theoretical electrostatic potentials have also been calculated for NDPhA by ab initio methods using a STO-5G basis set with atomic coordinates taken from the x-ray study. The theoretical potential is in qualitative agreement in the region surrounding the nitroso-group, showing negative potentials near the oxygen and nitrogen lone-pairs of about -50 kcal/mole. The influence of the crystal lattice on the electrostatic potential has been investigated by theoretical calculations on water clusters.

06.7-6 THE ELECTRON DENSITY DISTRIBUTION AND CRYSTAL PROPERTIES. By R.P. Ozerov, V.G. Tsirelśon, V.A. Strelt́sov, M. Kapphan, Mendeleev Institute of Chemical Technology, Miusskaja Sq. 9, Moscow 125820, USSR.

1. The electric field gradient (EFG) at the iron nucleus site in Hematite, α-Fe_2O_3(H) and Sodium Nitroprusside, $Na_2Fe(CN)_5NO.2H_2O$(SNP) was calculated from X-ray diffraction data.

Two sets of experimental intensities measured at room temperature and 153K were used. All necessary corrections including TDS, anomalous scattering and others were applied. The Schwarzenbach approach in EFG calculations was used. The EFG tensor has only one independent term eq_{zz} at the iron nucleus site in both compounds (the slight symmetry distortion in SNP had been neglected). The results are as follows: eq_{zz}=0,33(5)(H), eq_{zz}=1,17(14) (SNP).10^{22} V/m^2, the H:SNP ratio (which is free of the iron nucleus excited on 14,4 kev level quadrupole moment value Q) was found to be 0,282(20). The same value from Mössbauer experiment is 0,28(2). The Q value derived is 0,14(2).10^{-28}m^2.

2. Quantum topology approach to the X-ray diffraction experiment interpretation.

Bader's approach was applied to the X-ray electron density analysis in crystalline ethane. The experimental set of X-ray reflections has been taken from van Nes and Vos (Acta Cryst., B34, 1947, 1978). Critical point of rank 3 and signature 1 was found on C - C bond line.