

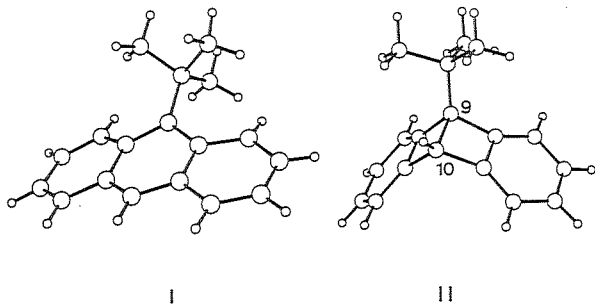
## 06.2-15 THE DEFORMATION DENSITY IN STABLE

ALIPHATIC PHOSPHINES. By Sine Larsen, Department of Physical Chemistry, University of Copenhagen, DK-2100 Copenhagen, Denmark.

Earlier theoretical and experimental studies of the deformation density in  $P(CH_2CN)_3$  (Larsen, Rettrup & Dahl, Acta Cryst. (1981) **A37**, C-128) initiated further experimental investigations. A new set of X-ray diffraction data was collected at 105K, max.  $\sin \theta/\lambda = 1.25\text{\AA}^{-1}$ . Low temperature neutron data was collected at ILL, max.  $\sin \theta/\lambda = 0.95\text{\AA}^{-1}$ . The parameters for P, C and N from refinements using high order X-ray data agree well with those obtained from the neutron data.  $\rho(\text{sph})$  was calculated using the former (X-ray) parameters except for hydrogen where the results from the neutron study was employed.  $P(CH_2CN)_3$  crystallize in the polar space group  $R3c$ . Phases from multipole refinement were used in the calculation of  $\rho(\text{obs})$ . In the deformation density  $\Delta\rho = \rho(\text{obs}) - \rho(\text{sph})$  the phosphorous lone pair has significant "s-character". This is consistent with other experimental observations, e.g. lone pair ionization potential and molecular geometry. During this analysis it was observed that the different approaches employed to correct for the effects of anomalous scattering resulted in noticeable changes in the density around P, but did not affect the density in the  $CH_2CN$  region. The related phosphine,  $P(CH_2CH_2CN)_3$ , crystallize in the centric space group  $P2_1/m$  and a similar study has been undertaken for this compound.

06.2-16 THE ELECTRON DEFORMATION DENSITY OF 9-T-BUTYL-9,10-DEWAR-ANTHRACENE AND ITS PRECURSOR, 9-T-BUTYL-ANTHRACENE. By K. Angermund, R. Goddard, and C. Krüger, MPI für Kohlenforschung, D-4330 Mülheim-Ruhr, FRG.

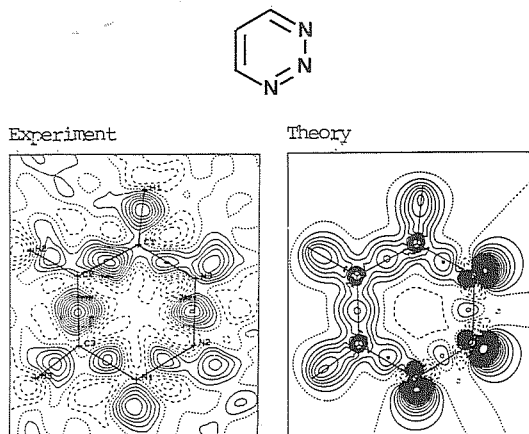
The crystal structures and the deformation densities (X-X) of 9-t-butyl-anthracene(I) and 9-t-butyl-9,10-Dewar-anthracene(II) (H. Dreeskamp, B. Jahn, and J. Pabst, Z. Naturforsch. (1981) **36a**, 665), have been determined (100 K, I:  $P2_1/c$ ,  $a = 11.137(1)$ ,  $b = 6.8927(8)$ ,  $c = 17.792(1)$  Å,  $\beta = 107.681(5)^\circ$ ,  $Z = 4$ ; II:  $P2_1/c$ ,  $a = 6.080(1)$ ,  $b = 17.210(5)$ ,  $c = 13.221(2)$  Å,  $\beta = 104.69(1)^\circ$ ,  $Z = 4$ ). The "Dewar bond" between C9 and C10 in II (1.623(2) Å) is significantly longer than a normal C-C single bond, and the deformation density shows it to be bent. The build up of electron density between the carbon atoms in I correlates directly with the reduced overlap population calculated by Extended-Hückel methods (assuming ideal geometry).



The deformation densities are compared with those obtained from ab initio calculations on Dewar-benzene and 1-methyl-Dewar-benzene.

06.2-17 THE ELECTRON DEFORMATION DENSITY OF 1,2,3-TRIAZINE. ASYMMETRY AS A CONSEQUENCE OF INTERMOLECULAR INTERACTIONS IN THE SOLID STATE. By K. Angermund, R. Goddard, C. Krüger and H. Neunhoeffer, MPI für Kohlenforschung, D-4330 Mülheim-Ruhr, FRG; \*Technische Hochschule Darmstadt, D-6100 Darmstadt, FRG.

The crystal structure of 1,2,3-triazine has been determined at 100 K (space group  $P\bar{1}$ ,  $a = 5.7688(4)$ ,  $b = 6.8732(6)$ ,  $c = 5.6725(4)$  Å,  $\alpha = 110.080(6)$ ,  $\beta = 113.947(5)$ ,  $\gamma = 95.302(6)^\circ$ ,  $Z = 2$ ). The deformation density obtained by the X-X method is compared with the theoretical deformation density calculated for a free molecule. Asymmetry in the experimental electron distribution can be attributed to intermolecular interactions extending in several cases further than 3 Å.

06.2-18 CRYSTAL STRUCTURE AND ELECTRON DENSITY STUDIES OF PYRIDINE DERIVATIVES: By U. Ohms, H. Guth and E. Hellner, Institut für Mineralogie, H. Dannöhl and A. Schweig, Fachbereich Physikalische Chemie, Sonderforschungsbereich 127 "Kristallstruktur und chemische Bindung", Universität Marburg, D-3550 Marburg, FRG

Electron density studies of pyridine derivatives are part of a project on experimental and theoretical investigations of electron density distributions in crystals. Within this project we studied the crystal structure of 2-pyridone, which was first described by B. Penfold (Acta Crystallogr., **6**, 591, 1953). We confirmed this structure. Crystal data:  $a = 13.657(3)$ ,  $b = 5.912(2)$ ,  $c = 5.701(2)$  Å at 293K.  $a = 13.564(3)$ ,  $b = 5.792(2)$ ,  $c = 5.598(2)$  Å at 120K, space group  $P2_12_12_1$ ,  $Z = 4$ .

X-ray and neutron data sets were collected on automated four circle diffractometers at both temperatures, refinement agreement factors are 0.034 and 0.041 for the x-ray data and 0.041 and 0.041 for the neutron data at 293, 120 K, resp. Two different models, one based on a charge cloud model and one on a multipole expansion, were applied to the data. These results will be shown together with X-X and X-N syntheses. They will be compared with electron density maps of 4-methylpyridine.

4-31G+BF AHF dynamic deformation densities will be presented for both compounds (for the methods see: A. Schweig and coworkers in "Electron Distributions and the Chemical Bond", P. Coppens and M.B. Hall, eds., Plenum Press, 1982, p. 255 and Int. Rev. Phys. Chem. in press). The agreement between experimental and theoretical densities is good for 4-methylpyridine.