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(CH₂CN)₃ (Larsen, Retrup & Dahl, Acct. Cryst. (1981) A37, C-128) initiated further experimental investigations. A new set of X-ray diffraction data was collected at ILL, max. sin $\theta/\lambda = 1.25\text{Å}^{-1}$. Low temperature neutron data was collected at ILL, max. sin $\theta/\lambda = 0.95\text{Å}^{-1}$. The parameters for P, C and N from refinements using high order X-ray data agree well with those obtained from the neutron data. The deformation in P(CH₂CN)₃ was calculated using the former (X-ray) parameters except for hydrogen where the results from the neutron study was employed. P(CH₂CN)₃ crystallizes in the polar space group P3₂1c. Phases from multipole refinement were used in the calculation of $\rho(\text{obs})$. In the deformation density $\rho = \rho(\text{obs}) - \rho(\text{ph})$, 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 effects of anomalous scattering resulted in noticeable changes in the density around P, but did not affect the density in the CH₂CN region.

The related phosphine, P(CH₂CH₂CN), crystallizes in the centric space group P2₁/n and a similar study has been undertaken for this compound.

06.2-16 THE ELECTRON DEFORMATION DENSITY OF 1-P-DI-RUARYL-triazine. By K. Angelmum, R. Goldziher, and G. Krüger, MPI für Kohlenforschung, D-4330 Mülheim-Ruhr, FRG.

The crystal structure of 1,2,3-triazine has been determined at 100 K (space group P1, $a = 5.7688(4)$, $b = 6.6732(6)$, $c = 5.6725(4)$, $\alpha = 110.080(6)$, $\beta = 113.94(5)$, $\gamma = 95.302(6)$, $Z = 2$). The deformation density obtained by the X-X method is compared with the theoretical deformation density calculated for a free molecule. Anisotropy in the experimental electron distribution can be attributed to intermolecular interactions extending in several cases further than 3 Å.