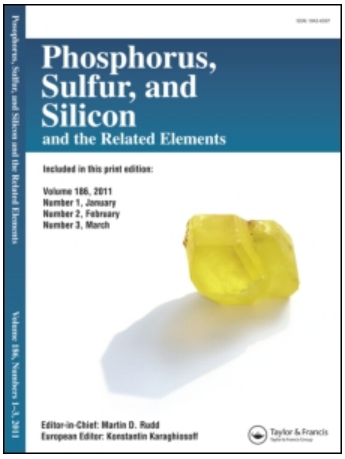

Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

Elgctron Density Distribution and Intramolecular Dynayics in Phosphorane $(Cl_3C)_2PCl_3$

M. Yu. Antipin[a]; A. N. Chernega[a]; Yu. T. Struchkov[a]; A. N. Nesmeyanov[a]
[a] Institute 02 Organoelement Compounds, Academy of Sciences of the USSR, Moscow, USSR

To cite this Article Antipin, M. Yu. , Chernega, A. N. , Struchkov, Yu. T. and Nesmeyanov, A. N.(1990) 'Elgctron Density Distribution and Intramolecular Dynayics in Phosphorane $(Cl_3C)_2PCl_3$', Phosphorus, Sulfur, and Silicon and the Related Elements, 51: 1, 223
To link to this Article: DOI: 10.1080/10426509008040757
URL: http://dx.doi.org/10.1080/10426509008040757

Phosphorus, Sulfur, and Silicon, 1990, Vols. 51/52, p. 223
Reprints available directly from the publisher
Photocopying permitted by license only

ELECTRON DENSITY DISTRIBUTION AND INTRAMOLECULAR DYNAMICS IN PHOSPHORANE $(Cl_3C)_2PCl_3$

M.Yu.ANTIPIN, A.N.CHERNEGA, and Yu.T.STRUCHKOV
A.N.Nesmeyanov Institute of Organoelement Compounds, Academy of Sciences of the USSR, 28 Vavilov Str., Moscow, USSR

The trigonal-bipyramidal structure of phosphorane $(Cl_3C)_2PCl_3$ (I) with two non-equivalent axial Cl_3C-groups at the P atom was established by the X-ray diffraction method. At 293°K these groups are involved in independent libration around the longest molecular axis and some characteristics of these motions were estimated from diffraction data. Electron density distribution in I was studied at 153°K (λMo, ca. 7000 reflections, "high-angle" refinement to R=0.027 using 1310 reflections with $\sin\theta/\lambda \geqslant 0.70$ $Å^{-1}$). At low temperature the above-mentioned independent librations of the Cl_3C-groups become frozen, which is proved by the rigid-body analysis of the anisotropic thermal parameters of I, and also by the NQR ^{35}Cl spectral data. All chemical bonds in I are characterized by peaks of positive deformation electron density (DED). Positive DED peaks are also found near Cl-atoms and attributed to the lone pairs of Cl-atoms. Elongation of the P-C bonds (2.000 (2) and 1.992 (2) Å) is caused by electrostatic repulsion of the positively charged P and C atoms, whose charges were estimated from diffraction data. The character of the electron density distribution in I is in accordance with the generally accepted notion on the nature of chemical bonds in pentacovalent phosphoranes.