

This article was downloaded by:

On: 29 January 2011

Access details: Access Details: Free Access

Publisher Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



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 (Cl₃C)₂PCl₃

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 (Cl₃C)₂PCl₃', 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>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

ELECTRON DENSITY DISTRIBUTION AND INTRAMOLECULAR DYNAMICS IN PHOSPHORANE $(\text{Cl}_3\text{C})_2\text{PCl}_3$

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 $(\text{Cl}_3\text{C})_2\text{PCl}_3$ (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 $\sin\theta/\lambda \geq 0.70 \text{ \AA}^{-1}$). 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 pentavalent phosphoranes.