

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>

Determination of Spin-Spin Coupling Constants J(PP) on the Basis of ^{13}C and ^{31}P NMR Data

E. G. Ilyin^a; M. v. Simonov^a; N. P. Nesterova^b; I. V. Leont-yeva^b; I. M. Aladzeva^b; T. Ja. Medved^b; T. A. Mastryukova^b; M. I. Kabatchnik^b; Yu. A. Buslaev^a

^a N.S. Kurnakov Institute of General and Inorganic Chemistry, Academy of Sciences of the USSR, MOSCOW, USSR ^b A.N. Nesmeyanov Institute of Organo-Element Compounds, Academy of Sciences of the USSR, MOSCOW, USSR

To cite this Article Ilyin, E. G. , Simonov, M. v. , Nesterova, N. P. , Leont-yeva, I. V. , Aladzeva, I. M. , Medved, T. Ja. , Mastryukova, T. A. , Kabatchnik, M. I. and Buslaev, Yu. A.(1990) 'Determination of Spin-Spin Coupling Constants J(PP) on the Basis of ^{13}C and ^{31}P NMR Data', Phosphorus, Sulfur, and Silicon and the Related Elements, 51: 1, 349

To link to this Article: DOI: 10.1080/10426509008040878

URL: <http://dx.doi.org/10.1080/10426509008040878>

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.

DETERMINATION OF SPIN-SPIN COUPLING CONSTANTS J(PP) ON THE BASIS OF ^{13}C AND ^{31}P NMR DATA

E.G.ILYIN., M.V.SIMONOV, N.P.NESTEROVA^a, I.V.LEONT-YEVAA^a, I.M.ALADZEVAA^a, T.JA.MEDVED^a, T.A.MASTRYUKOVA^a, M.I.KABATCHNIKA^a, and YU.A.BUSLAEV
N.S.Kurnakov Institute of General and Inorganic Chemistry, Academy of Sciences of the USSR, Leninskyi Prospect 31, 117907 Moscow, USSR
^aA.N.Nesmeyanov Institute of Organo-Element Compounds, Academy of Sciences of the USSR, Vavilov Str. 28, 117334 Moscow, USSR

The diphosphine dioxides $\text{Ph}_2\text{P}(\text{O})\text{CH}_2\text{P}(\text{O})\text{Ph}_2$ (I), $\text{Ph}_2\text{P}(\text{O})\text{CH}_2\text{CH}_2\text{P}(\text{O})\text{Ph}_2$ (II), $\text{Ph}_2\text{P}(\text{O})\text{CH}=\text{CHP}(\text{O})\text{Ph}_2$ -cis (III), -trans (IV), $[\text{Ph}_2\text{P}(\text{O})]\text{C}=\text{CH}$ (V), $[\text{Ph}_2\text{P}(\text{O})]_2\text{C}=\text{PPh}_3$ (VI), and also non-symmetric $\text{Ph}_2(\text{P})\text{OCH}=\text{CHP}(\text{O})\text{PhEt}$ -trans (VII), $\text{Et}_2\text{P}(\text{O})\text{CH}=\text{CHP}(\text{O})\text{PhEt}$ -trans (VIII), have been studied in CH_2Cl_2 and CHCl_3 solutions by means of ^{13}C and ^{31}P NMR.

The ^{13}C chemical shift values in ortho-, meta-, and para-positions of phenyl-groups and bridging carbon atoms are obtained. The spin-spin coupling constants J(CP) are found. On the basis of ^{13}C NMR spectra, the spin-spin coupling constants of compounds (I-V, VII) are calculated.

The J(PP) value for V is in good agreement with what was found from ^1H NMR spectra. The estimation of angle values between phosphoryl groups of dioxides is discussed.

Temperature dependence of ^{31}P relaxation times T_1 and T_2 of dioxides is studied.