Quantum-Chemical Study of the Structure of Cyanophosphines and Their Oxides

E. A. Ishmaeva, V. E. Kataev, Ya. A. Vereshchagina, G. R. Fattakhova, Z. G. Bazhanova, and A. V. Kataev

Kazan State University, Kazan, Tatarstan, Russia
Arbuzov Institute of Organic and Physical Chemistry, Russian Academy of Sciences, Kazan, Tatarstan, Russia
Kazan State Technological University, Kazan, Tatarstan, Russia

Received June 7, 2001

Abstract - The structure of cyanophosphines and their oxides was studied by ab initio (RHF/6-31G**) and semiempirical (PM3) methods. Both methods predict that $MeOP(CN)_2$, $(MeO)_2PCN$, and $(MeO)_2P(O)CN$ exist in noneclipsed antiperiplanar and synclinal conformations. The calculation results nicely agree with measured dipole moments and Kerr constants of these compounds. The phenyl and diphenyl derivatives $PhP(CN)_2$, Ph_2PCN, Ph(Et)PCN, and $Ph_2P(O)CN$ prefer forms in which the phenyl ring plane is eclipsing the phosphorus lone electron pair or the phosphoryl bond. The interactions of the phosphorus lone electron pair with the phenyl ring and with the cyano group are lacking in the title compounds.