

Russian Journal of General Chemistry 2003 vol.73 N6, pages 921-927

Quantum-chemical estimation of the stability and reactivity of diphosponium salts

Zagumennov V., Vedernikov A., Nikitin E., Solomonov B.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

For a series of diphosponium salts containing two positively charged covalently bonded phosphorus atoms, $X_nY_{3-n}P^+ + X_nY_{3-n}P^+$ (X = alkyl substituent, Y = amino group, $n = 0-3$), the stability, reactivity, and P-P bond strength were evaluated by various physicochemical methods. The P-P bond energy is appreciably influenced by both steric factors and donor properties of the substituents. The calculations confirmed that transformations of diphosponium salts can involve cleavage of both P-P and P-N (or P-C) bonds.

<http://dx.doi.org/10.1023/A:1026304918818>
