ISSN 1070-3632, Russian Journal of General Chemistry, 2018, Vol. 88, No. 11, pp. 2251–2256. © Pleiades Publishing, Ltd., 2018.
Original Russian Text © R.R. Ismagilova, A.A. Kuznetsova, D.V. Chachkov, S.F. Malysheva, N.A. Belogorlova, Ya.A. Vereshchagina, 2018, published in Zhurnal Obshchei Khimii, 2018, Vol. 88, No. 11, pp. 1770–1775.

Dedicated to the 115th anniversary of B.A. Arbuzov's birth

Conformational Analysis of Tris(3-methylphenyl)phosphine and Its Chalcogenides

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Received September 13, 2018

Abstract—Conformational analysis of tris(3-methylphenyl)phosphine and its chalcogenides has been performed by methods of dipole moments, IR spectroscopy, and quantum chemistry [DFT B3PW91/6-31G(df,p)]. In solution, these compounds exist as an equilibrium of conformers with *gauche*- and *cis*-arrangement of the substituents at the phosphorus atom relative to the P=X bond (X = lone electron pair, O, S, Se).

Keywords: tris(3-methylphenyl)phosphine, phosphine chalcogenides, dipole moment, conformational analysis, DFT calculations

DOI: 10.1134/S1070363218110026

Organophosphorus compounds, in particular aryl-substituted phosphines, are widely used as ligands in the complex formation processes. Complexes of transition metals containing tolyl-substituted phosphine ligands are widely applied as catalysts of various industrial processes [1–7] and can act as mesoporous structures and zeolites [8]. Copper(I) complexes with *m*-tolylphosphine ligands are used in manufacturing of organic light-emitting diodes [9, 10]. Palladium complexes of tritolyl-substituted phosphines exhibit antibacterial and antitumor activity [11, 12] and are used as new polymeric materials [13]; the clusters with silver(I) exhibit luminescent properties [14].

Elucidation of the structure of substituted phosphines is essential for the rationalization of their physico-chemical properties, including complex formation, and prediction of their reactivity. The reference literature contains data on molecular structure of tris(*o*-tolyl)-substituted phosphine and its chalcogenides [15], tris(*m*-tolyl)-substituted phosphine, its sulfide, and its selenide [16], and tris(*p*-tolyl)-substituted phosphine selenide [17] in the solid state, yet the structure of these phosphines in the solution has been considered mainly from the viewpoint of their action as ligands in the complex formation with metals. Theoretical studies of spatial structure of the phosphines with bulky tolyl substituents at the phosphorus atom have been limited as well. For example, predominant conformations of tris(*o*-tolyl)phosphine and its chalcogenides have been identified by means of the semiempirical PM3 method [18]; complexes of triphenylphosphine with zeolite Y have been calculated [8] and stability of the tris(*m*-tolyl)phosphine complexes with Cu(I) has been evaluated [9] by means of the DFT methods.

In view of the scarcity of the data on the structure of tolyl-substituted phosphines in solution, we investigated spatial structure of tris(3-tolyl)phosphine and its chalcogenides (potential ligands) by means the dipole moments and quantum chemistry [DFT B3PW91/6-31G(df,p)] methods.

Polarity of tris(3-methylphenyl)phosphine **1**, tris(3-methylphenyl)phosphine oxide **2**, tris(3-methylphenyl)-