

**Synthesis and crystal structure of New rac-XP(O)(OC<sub>6</sub>H<sub>5</sub>)(NHC<sub>6</sub>H<sub>4</sub>-*p*-CH<sub>3</sub>) mixed-amidophosphinates [X = NHCH(CH<sub>3</sub>)<sub>2</sub>, NH(*cyclo*-C<sub>7</sub>H<sub>13</sub>) and NHCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>(2-Cl)]**

Mehrdad Pourayoubi<sup>a</sup>, **Fatemeh Karimi Ahmadabad<sup>a</sup>**, James A. Golen<sup>b</sup>, Arnold L. Rheingold<sup>b</sup> and Chao Chen<sup>b</sup>

<sup>a</sup> Department of Chemistry, Ferdowsi University of Mashhad, Mashhad, Iran.

<sup>b</sup> Department of Chemistry, University of California, San Diego, USA. (e-mail: pourayoubi@um.ac.ir)

Recently, the structures of some racemate mixed-amidophosphinates, with an (N<sup>2</sup>)P(O)(O)(N<sup>1</sup>) skeleton, were reported in which two different amido groups are bonded to P atom [1]. The systematic studies on such molecules may be useful according to the following reasons: i) to achieve an insight on which amido segment makes a stronger/weaker P-N bond, ii) preparation of racemate compounds [2], iii) study of the hydrogen-bond patterns, and a try to find some empirical rules benefit in prediction of hydrogen-bond pattern based on the molecular structure [3]. The title mixed-amidophosphinates, rac-phenyl (*iso*-propylamido)(*p*-tolylamido)phosphinate, (I), rac-phenyl (*cyclo*-heptylamido)(*p*-tolylamido)phosphinate, (II), and rac-phenyl (2-chlorobenzylamido)(*p*-tolylamido) phosphinate, (III), were synthesized from initial phosphorus-chlorine compound (R,S)-(Cl)P(O)(OC<sub>6</sub>H<sub>5</sub>)(NHC<sub>6</sub>H<sub>4</sub>-*p*-CH<sub>3</sub>) [3]. For each of (I) and (II), the asymmetric unit consists of two symmetrically independent molecules, and the asymmetric unit of (III) contains four molecules. The P atom in each molecule is in a distorted tetrahedral environment. The P-N (*p*-tolylamido) bond is slightly longer than the P-N (*iso*-propylamido), P-N (*cyclo*-heptylamido) and P-N (2-chlorobenzylamido) in (I), (II) and (III), respectively. In all structures, the oxygen atom of C<sub>6</sub>H<sub>5</sub>O group and the nitrogen atoms bonded to P atom do not take part in hydrogen bonding as an acceptor; whereas, the oxygen atom of phosphoryl acts as a double H-bond acceptor to form (N-H)(N-H)...OP grouping. In the crystal structures of (I), (II) and (III), adjacent molecules are hydrogen-bonded into linear arrangements, along [010] for (I) and [010] for both (II) and (III).

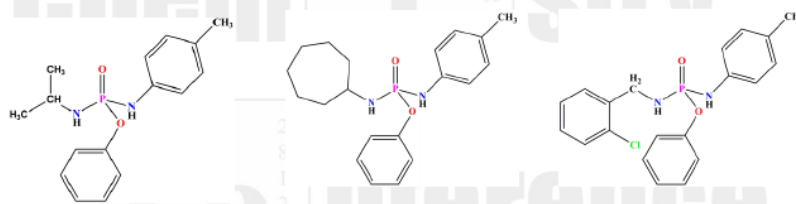


Fig. 1. The chemical structures of (I), (II) and (III) are shown (left to right, respectively).

**References**

- [1] M. Pourayoubi, F. Karimi Ahmadabad and M. Nečas, *Acta Cryst.E* 67 (2011) 2523.
- [2] M. Pourayoubi, F. Karimi Ahmadabad, H. Eshtiagh-Hosseini, M. Kučeráková, V. Eigner and M. Dušek, *Acta Cryst. C* C69 (2013) 1181-1185.
- [3] M. Toghraee, M. Pourayoubi and V. Divjakovic, *Polyhedron* 30 (2011) 1680-1690.