Poster Presentation

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Puckering behaviours in phosphoric triamide structures containing aliphatic ring groups

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The conformational studies of non-rigid rings/segments are attracted interest not only in viewpoint of diversity of different topologies found but also due to pharmacological considerations in biological systems. Different techniques were applied for determining ring conformations including X-ray crystallography, computational calculation and NMR experiment. Among these considerations, puckering parameters, obtained from single crystal X-ray experiments, were defined for determination of any ring conformation for the rings of the sizes from three to the bigger rings of eight- and nine-membered sizes with more than degree of freedom. With this background in mind we investigated the conformations of puckered six- and seven-membered aliphatic rings in six new C(O)NHP(O)-based phosphoric triamide structures. The new compounds include the rings with the C6, NC5, C7 and NC6 heavy atom skeletons and the following factors are considered: (i) geometrical deviations caused by changing from C atom in C6 and C7 rings with the N heteroatom in C5N and C6N rings, (ii) steric effects, and (iii) crystal packing effect. In the structures with a P-NC5 and P-NC6 segment, the nitrogen atom bonded to the phosphorus show the angle confirming to the nearly sp2 angle and the amount of changes in different nitrogen containing aliphatic rings were discussed through a survey of analogous structures deposited in the Cambridge Structural Database (CSD). Hirshfeld surface analysis was screened when an interaction influences on the conformation observed in the solid state in order to detail inspection of contacts involving the ring. In the new structures, the six-membered ring merely shows the near-chair conformation, while the seven-membered ring was found in different conformations as near-chair, twist-chair and twist-sofa. The newly synthesized XC(O)NHP(O)Y2 phosphoric triamides (X = 4-CH3-C6H4 or CF3, Y = NHC7H13; X = 4-CH3-C6H4, Y = NC6H12, X = CCl3, Y = NC5H9-4-CH3, X = 2-Cl,5-F-C6H3, Y = NC5H10 and X = 2-Cl,5-F-C6H3, Y = N(CH3)(C6H11)) were characterized by 1H, 13C, 31P NMR and IR spectroscopies, mass spectrometry and single crystal X-ray diffraction analysis for all compounds, besides 19F NMR for fluorine containing compounds.

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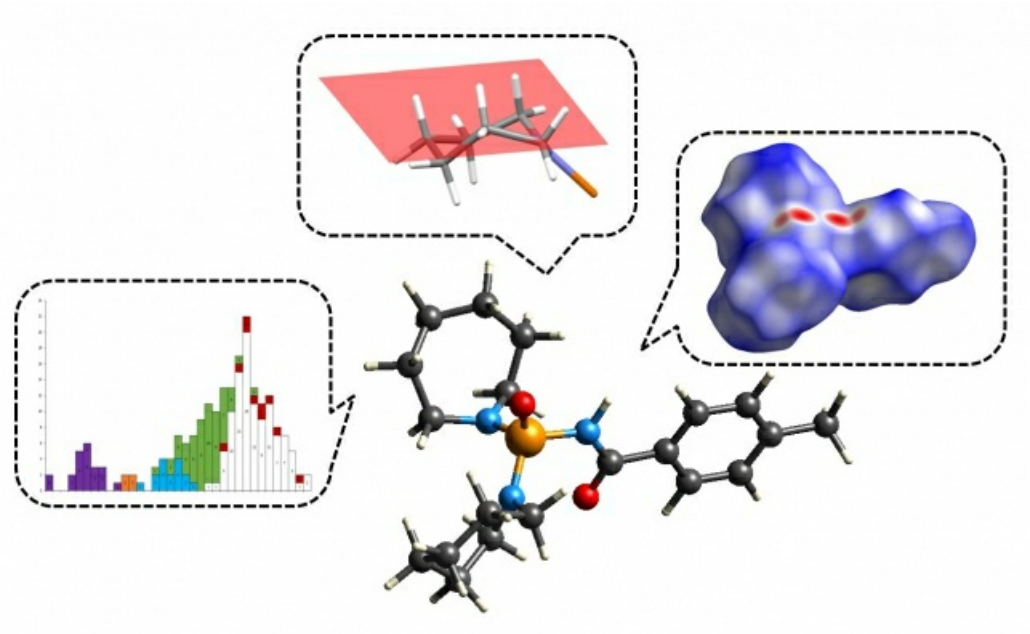

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