Synthesis & crystallographic, spectroscopic and computational characterization of O-R substituents effects on the torsional angle of 3,3',4,4' substituted biphenyls

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In this work we synthesize, characterize and study by single crystal & powder X-ray diffraction, Raman scattering and quantum mechanics calculations, the structure of a series of biphenyls substituted in positions 3,3',4,4' - with a variety of R- groups connected to the biphenyl core through oxygen atoms (R: methyl, acetyl, hexyl).[1,2] The six member series split into two groups with striking differences in molecular conformation as well as in melting points (viz., in the solid state three members are strictly planar and present significantly lower m.p., while the remaining three are highly twisted, with larger m.p.). Thus, the aim of the work is to understand if any of the intervening molecular fragments exerts any decisive influence on the molecular planarity as well as on the thermal stability of the compounds.


Keywords: Substituted biphenyls; torsion angle; Raman spectroscopy; molecular conformation; rational synthesis.

We thank financial support from the University of Buenos Aires (grants UBACyT 20020130100776BA and20020170100512BA) and CONICET (grant number PIP20110101035 and fellowships to NV (PhD) and VEM (postdoc)).

Acta Cryst. (2021), A77, C896