

Phase Transition Thermodynamics of Diphenylpyridines

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Polyphenylpyridines are fascinating systems due to their p electronic structure that makes them potential organic semiconductors. The research interest in this type of molecular systems is primarily motivated by the applications such as organic light emitting devices (OLEDs), organic field effect transistors (OFETs), and organic photovoltaic cells (OPVCs). Organic semiconductors can be classified as small molecules or oligomers and polymers. Oligomers can be deposited by physical vapour deposition techniques while conjugated polymers can be processed from solution, thus it is necessary the knowledge of thermodynamics properties. This work focuses the thermodynamic study of some diphenylpyridine isomers in order to understand the relationship between structure, energetics and electronic correlation. The present work is part of a more wide project dealing with the thermodynamic study of oligomers of conducting polymers.^[1] The three isomers were synthesized using the palladium catalysed Suzuki – Miyaura cross – coupling reaction.^[2] The vapour pressures of the considered compounds were determined by a static apparatus based on a MKS capacitance diaphragm manometer recently described in the literature.^[3] Based on the previous results the standard molar enthalpies, entropies and Gibbs functions of sublimation were derived at $T = 298.15$ K. The standard ($p^\circ = 0.1$ MPa) molar enthalpies of formation, in the condensed phase, at $T = 298.15$ K, for the three diphenylpyridines, were derived from the standard molar enthalpies of combustion, at the same reference temperature, determined by static bomb combustion calorimetry. The thermodynamic results obtained in the study of phase transition (fusion and sublimation) as well the vapour pressures at different temperatures, will be used to evaluate the energetics of solid-liquid and solid-gas equilibrium. A comparative and differential analysis between the three isomers was done based on the obtained results concerning the thermodynamic, structural, spectroscopic and computational chemistry (*ab-initio*, MP2 and B3LYP) studies.

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[1] “Thermodynamic Study of Conducting Polymers”, FCT project ref: POCI/QUI/61873/2004

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