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RESUMOS / ABSTRACTS
Thermodynamic and Theoretical Study of Diphenylpyridines


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The energetic and structural study of phenylpyridines has been a theme of research in our laboratory due to their interesting electronic correlation capabilities. This work focuses the thermodynamic study of some diphenylpyridine isomers (Figure 1), in order to understand the relationship between structure and energetics.

Figure 1. Schematic structural formulas of: (I) 2,6-diphenylpyridine; (II) 2,5-diphenylpyridine; (III) 3,5-diphenylpyridine.

Therefore, the compounds shown in figure 1, were synthesized using the Suzuki-Miyaura methodology. The standard molar enthalpies of formation for the three isomers on crystalline state will be derived, at \( T = 298.15 \text{ K} \) by static bomb combustion calorimetry. The vapour pressures of the three isomers will be determined by a static apparatus based on a MKS capacitance diaphragm manometer recently described in the literature. Through the standard molar enthalpies of formation in the condensed phase and the standard molar enthalpies of sublimation, the standard molar enthalpies of formation in the gaseous phase will be derived for the three isomers.

Computational chemistry (Density Functional Theory DFT) will be used in order to perform the geometry optimizations, energetic analysis and to derive the vibrational frequencies for the selected isomers.

References:


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Presentation: POSTER
Thermodynamic and Theoretical Study of Diphenylpyridines

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Aim

- Phenyl and polyphenylpyridines are promising compounds for the use in electronic material (organic light-emitting diodes (OLEDs), photovoltaic cells, sensors, thin film transistors (OTFTs)) because of the possibility of high electronic correlation.

Experimental

Synthesis
- The compounds were synthesized by Suzuki cross-coupling reactions based on a procedure optimized for an aqueous - organic solvent (1).

Results
- The vapour pressures of 2,5-diphenylpyridine were measured on a static apparatus based on a MKS capacitance diaphragm manometer.

Computational Chemistry
- Pyridine (Py), 2-phenylpyridine (2-PPy), 3-phenylpyridine (3-PPy), 4-phenylpyridine (4-PPy), 2,4-diphenylpyridine (2,4-DPPy), 2,3-diphenylpyridine (2,3-DPPy), 2,6-diphenylpyridine (2,6-DPPy) and 3,5-diphenylpyridine (3,5-DPPy) were studied by computational chemistry.

Discussion
- From the X-Ray structure of 2,6-diphenylpyridine, a weak C-H…π interaction was found. The X-ray data show the same plane of the phenyl ring and the plane of the pyridine ring.

References

Context:
- The static apparatus, based on a MKS capacitance diaphragm manometer, enables the measurement of vapour pressures for 2,5-diphenylpyridine. The vapour pressures were measured on a static apparatus described in the literature. The vapour pressures were measured for 2,5-diphenylpyridine in the pressure range (0.4 – 133) Pa and temperature range (243 to 473) K.

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The geometry optimizations and fundamental frequency calculations were performed by density functional theory (DFT) with the hybrid exchange correlation functional B3LYP at the level of theory B3LYP / 6-311G++

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