

Novel and Convenient Synthesis of 2,7-Dialkyl-1,8-dihydro-*As*-indacenes

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A novel and convenient synthetic route towards dialkyl *as*-indacenes was achieved by alkylation of malonic esters with *o*-xylylene dibromide, to give the corresponding tetraester, and related diacid. The alkyl groups on the central benzene ring induce intramolecular, regiospecific cycloeliminations leading selectively to the diketones, the precursors of the corresponding 1,8-dihydro-*As*-indacenes. The structure of the 2,7-dimethyl-1,8-dihydro-*As*-indacene was determined by X-ray diffraction. The compound 2,7-diethyl-1,8-dihydro-*As*-indacene was characterized by means of ¹H NMR, ¹³C NMR, FT-IR, UV/Vis measurements, electrochemistry, and elemental analysis. On the other hand, quantum chemical computations based on DFT methods were carried out to get insight into the molecular and electronic structures of the studied ligands. TDDFT approach was employed to calculate the vertical excitations and characterize the nature the UV/Vis absorption bands present in the experiments showing a very good agreement between experimental and calculated values. Finally, the reactivity of the compounds was assessed using the chemical potential (χ), chemical hardness (η), and electrophilicity (ω). Also, the electron-donating (σ^-), electron-accepting (σ^+), and the net electrophilicity powers (σ^\pm) indexes were studied. © Georg Thieme Verlag Stuttgart.

as-indacene

polycyclic bridge ligands

Regiospecific cycloeliminations

Electronic structure

Ketones

Quantum chemistry

Calculated values

Chemical hardness

Electron-accepting

Electron-donating

Quantum chemical computations

Regiospecific

Uv/vis absorptions

Vertical excitation

Ligands

article

carbon nuclear magnetic resonance

electrochemistry

electrophilicity

elemental analysis

excitation

hardness

proton nuclear magnetic resonance

synthesis