The p-conjugated P-flowers C16(PH)8 and C16(PF)8 are potential materials for organic n-type semiconductors

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Following the theme of this special issue, two new compounds, the P-flowers C16(PH)8 and C16(PF)8, are designed by us and subsequently characterized by quantum chemical computations. Their geometries and infrared signatures are analyzed and compared to those of the well-known sulflower C16S8. Their electronic structure and aromaticity are examined using the electron localization function (ELF) and also by the total and partial densities of state (DOS). Both C16(PF)6 and C16(PH)8 molecules exhibit small energy barrier of electron injection (Fe = 0.33 eV for the gold electrode for the former, and Fe = 0.1 eV for the calcium electrode for the latter), remarkably low reorganization energy and high rate of electron hopping. Thus, both theoretically designed P-flower molecules are predicted to be excellent candidates for organic n-type