Description of Additional Supplementary Files

Supplementary Data 1: Energy and imaginary vibrational frequency of calculated structures using B3LYP-D3 method.

Supplementary Data 2: Energy and imaginary vibrational frequency of calculated structures using M062X method.

Supplementary Data 3: Energy and imaginary vibrational frequency of calculated structures using ωB97XD method.

Supplementary Data 4: B3LYP-D3 (SMD, chlorobenzene) for optimization, Cartesian Coordinates and Energies in Hartree