

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Cartesian coordinates (O3LYP) for DtBuCzB (S_0)

File Name: Supplementary Data 2

Description: Cartesian coordinates (O3LYP) for [DtBuCzB·p-BQ]²⁻ (S_0)

File Name: Supplementary Data 3

Description: Cartesian coordinates (O3LYP) for [(DtBuCzB)₂·p-BQ]²⁻ (S_0)