

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: Atomic coordinates of the optimized geometries for the studied systems.

File name: Supplementary Data 2

Description: The single-crystal data of *E-2*, *E-3*, *E-4*, *Z-4*, *Z-5*, and *Z-6* are summarized in Supplementary Data 2 and archived at the Cambridge Crystallographic Data Centre under deposition no. CCDC 2249588 (*E-4*), 2249589 (*Z-4*), 2249590 (*Z-5*), 2249591 (*Z-6*), 2260917 (*E-2*), and 2260918 (*E-3*).