Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: This file contains Cartesian coordinates for all optimized geometries, including **4c**, **H$_2$**, **4c-HH**, (*R*)**-4a**, **4a-HH**, **4c'**, **4c'-H**, **4c''**, **4a'**, **4a'-H**, **4a''**, **TS-rs**, (*S*)**-4a**.