Description of Additional Supplementary Files

File Name: Supplementary Data 1
Description: cif file 3a

File Name: Supplementary Data 2
Description: cif file 8

File Name: Supplementary Data 3
Description: cif file 9

File Name: Supplementary Data 4
Description: cif file 11

File Name: Supplementary Data 5
Description: DFT geometry-optimized coordinates