

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description:

Cartesian coordinates (in Tinker format) of the FC, FS, Coln and TIDIR geometries of the QM/MM models calculated at the SA2-CASSCF(12,12)/6-31G*/AMBER level of theory. The models correspond to the Arch set (Arch2, Arch3, QuasAr1, Archon2, QuasAr2, Arch7, Arch5).

File Name: Supplementary Data 2

Description:

Cartesian coordinates (in Tinker format) of the FC, FS and TIDIR geometries of the QM/MM models calculated at the XMS-CASPT2/SA3-CASSCF(12,12)/ANO-L-vDZP/AMBER level of theory. The models correspond to the Arch set (Arch2, Arch3, QuasAr1, Archon2, QuasAr2, Arch7, Arch5).