



● CCSD(T)/cc-pVTZ: MAD = 6.06 kcal.mol⁻¹ ■ CCSD(T)+LDA/cc-pVTZ: MAD = 1.19 kcal.mol⁻¹ ◆ CCSD(T)+PBE/cc-pVTZ: MAD = 0.85 kcal.mol⁻¹