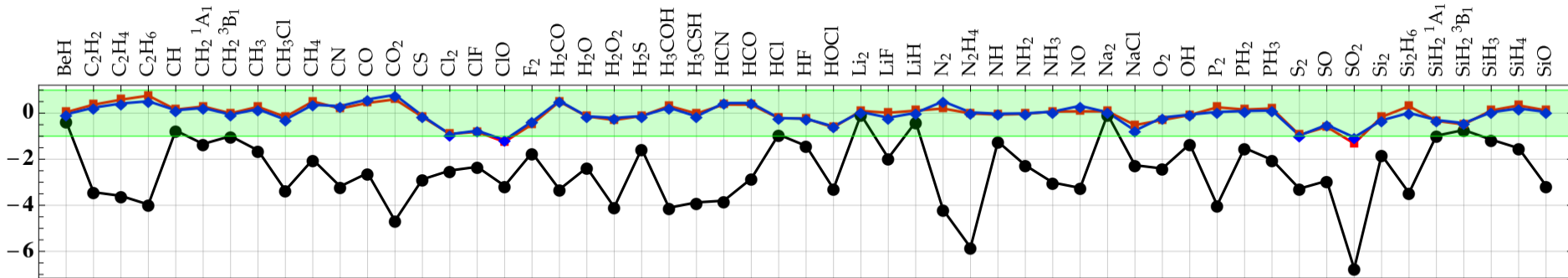


CBS deviation (kcal/mol)



● CCSD(T)/cc-pVQZ: MAD = 2.50 kcal.mol⁻¹

■ CCSD(T)+LDA/cc-pVQZ: MAD = 0.33 kcal.mol⁻¹

◆ CCSD(T)+PBE/cc-pVQZ: MAD = 0.31 kcal.mol⁻¹