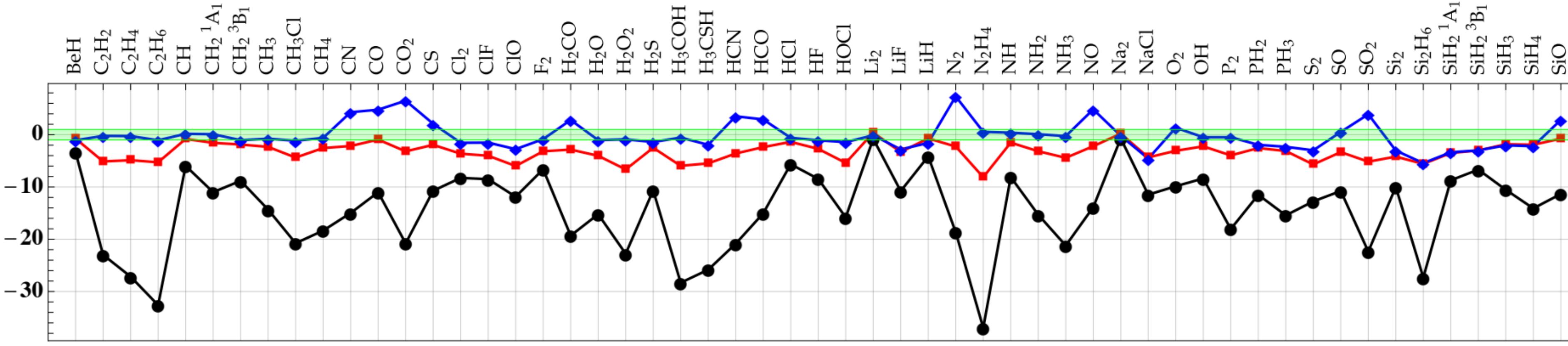


CBS deviation (kcal/mol)



● CCSD(T)/cc-pVDZ: MAD = 14.29 kcal.mol<sup>-1</sup>

■ CCSD(T)+LDA/cc-pVDZ: MAD = 3.24 kcal.mol<sup>-1</sup>

◆ CCSD(T)+PBE/cc-pVDZ: MAD = 1.96 kcal.mol<sup>-1</sup>