

MAE compared with
experimental CEBEs (eV)

Δ HF Δ MP2 Δ CCSD Δ CCSD(T)

2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0

cc-pCVDZ
/cc-pVDZ

cc-pCVTZ
/cc-pVTZ

cc-pCVQZ
/cc-pVQZ

cc-pCV5Z
/cc-pV5Z

Basis Set

