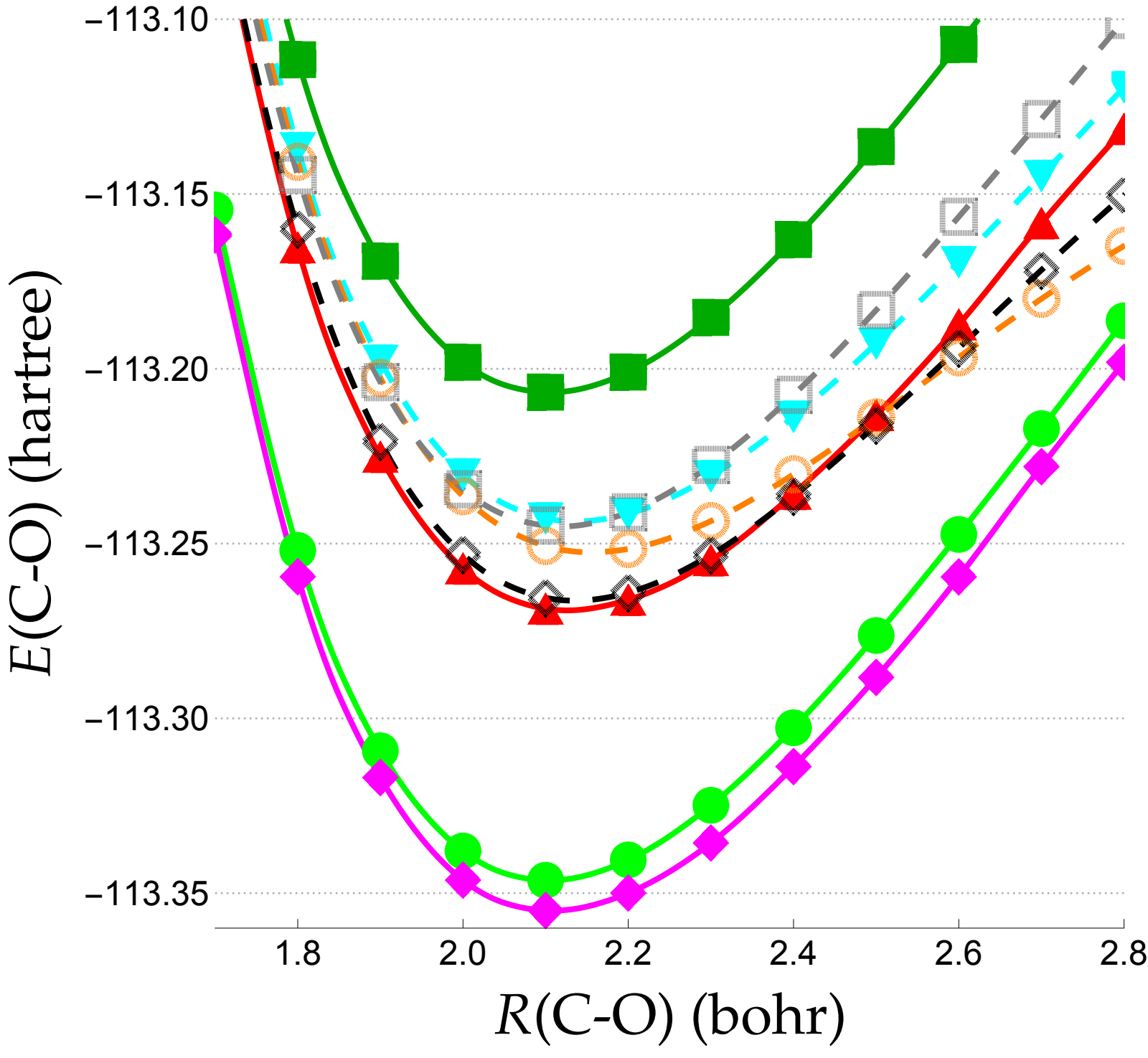
−113.10
−113.15
−113.20
−113.25
−113.30
−113.35
E(C-O) (hartree)
1.8
2.0
2.2
2.4
2.6
2.8
R(C-O) (bohr)