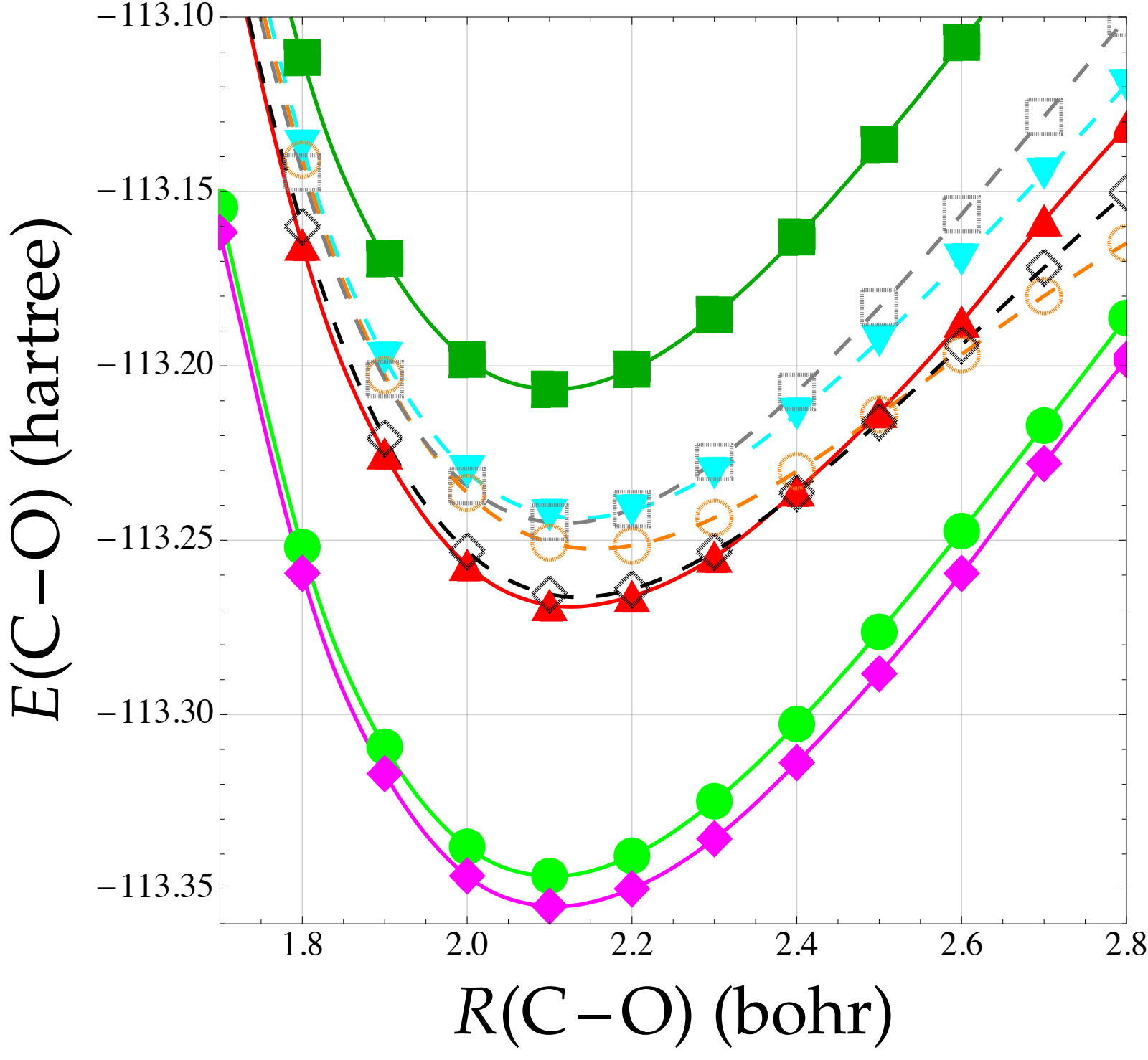
−113.10
−113.15
−113.20
−113.25
−113.30
−113.35
1.8
2.0
2.2
2.4
2.6
2.8
E(C−O) (hartree)
R(C−O) (bohr)