**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of CO+.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 2Π(p,s) | (4,2,2,0) | (1,1,1,0) | 3.535 | **3.419** | **3.381** | **3.320** | **3.293** | **3.313** | **3.312** |
| 2Σ+(s,s\*) | (4,2,2,0) | (2,0,0,0) | 6.158 | **5.880** | **5.891** | **5.942** | **5.887** | **5.869** | **5.873** |
| 2Π(s,p\*) | (4,2,2,0) | (1,1,1,0) | 9.777 | **9.180** | **9.301** | **9.392** | **9.344** | **9.322** | **9.328** |
| 4Σ+(p,p\*) | (4,2,2,0) | (2,0,0,0) | 7.393 | **7.048** | **7.246** | **7.359** | **7.320** | **7.255** | **7.284** |
| 4Δ(p,p\*) | (4,2,2,0) | (2,0,0,1) | 8.648 | **8.189** | **8.364** | **8.446** | **8.416** | **8.341** | **8.376** |
| 4Σ–(p,p\*) | (4,2,2,0) | (1,0,0,1) | 9.467 | **8.970** | **9.168** | **9.291** | **9.230** | **9.135** | **9.176** |

a Using reference (9e,8o) full valence active space.