**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of NO.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 2Σ+(p\*,3s) | (5,2,2,0) | (1,1,1,0) | 5.287a | **6.058** | **6.057** | **6.057** | **6.083** | **6.065** | **6.052** |
| 2Π(p\*,3px,y) | (4,3,3,0) | (0,2,2,0) | 5.920b | **7.180** | **7.085** | **7.139** | **7.288** | **7.169** | **7.130** |
| 2Σ+(p\*,3pz) | (6,2,2,0) | (2,1,1,0) | 5.921c | **7.245** | **7.130** | **7.153** | **7.293** | **7.176** | **7.146** |
| 2Π(p,p\*) | (4,3,3,0) | (0,3,3,0) | 7.944b,d | **7.604**e | **7.752** | **7.838** | **7.811** | **7.705**e | **7.744** |
| 4Σ–(s,p\*) | (4,2,2,0) | (0,1,1,1) | 6.725f | **6.093** | **6.280** | **6.417** | **6.368** | **6.376** | **6.396** |
| 4Π(p,p\*) | (4,2,2,0) | (0,2,2,0) | 6.802f | **6.667** | **6.773** | **6.813** | **6.812** | **6.745** | **6.769** |

a Using reference (11e,9o) full valence active space plus one 3s orbital. b Using reference (11e,10o) full valence active space plus one 3px and one 3py orbitals. c Using reference (11e,10o) full valence active space plus one 3s and one 3pz orbitals. d Partial (36%) double excitation character. e Using a level shift of 0.4 a.u. f Using reference (11e,8o) full valence active space.