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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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+(s,) | (6,3,3,0) | (1,1,1,0) | 3.048a | **2.811** | **2.833** | **2.896** | **2.866** | **2.885** | **2.885** |
| 2Π(,) | (6,3,3,0) | (0,2,2,0) | 4.874a | **4.652** | **4.699** | **4.766** | **4.745** | **4.730** | **4.727** |
| 2Σ+(s,) | (6,3,3,0) | (2,1,1,0) | 7.397a | **7.020** | **7.058** | **7.119** | **7.075** | **7.062** | **7.067** |
| 2Σ–(,3s) | (7,3,3,0) | (0,1,1,1) | 7.055b | **7.166** | **7.416** | **7.569** | **7.590** | **7.560** | **7.535** |
| 2Π(,\*) | (6,3,3,0) | (0,3,3,0) | 8.058a | **7.128**c | **7.483** | **7.647** | **7.550** | **7.505**c | **7.537** |
| 2Φ(,\*) | (6,3,3,0) | (0,2,2,0) | 8.773a | **7.793** | **8.182** | **8.333** | **8.282** | **8.237** | **8.230** |
| 4Π(,\*) | (6,3,3,0) | (0,2,2,0) | 7.142a | **6.542** | **6.796** | **6.910** | **6.854** | **6.825** | **6.841** |
| 4Σ–(,3s) | (7,3,3,0) | (0,1,1,1) | 6.732b | **6.827** | **7.065** | **7.218** | **7.228** | **7.202** | **7.181** |

a Using reference (15e,12o) full valence active space. b Using reference (15e,13o) full valence active space plus one 3s orbital. c Using a level shift of 0.4 a.u.