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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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) | 1.427 | **1.484** | **1.433** | **1.362** | **1.356** | **1.356** | **1.355** |
| 2Σ+(s,s\*) | (4,2,2,0) | (2,0,0,0) | 3.277 | **3.208** | **3.244** | **3.319** | **3.270** | **3.240** | **3.248** |
| 2Π(s,p\*) | (4,2,2,0) | (1,1,1,0) | 8.242 | **7.745** | **7.921** | **8.038** | **7.982** | **7.946** | **7.957** |
| 2Σ+(sp,p\*s) | (4,2,2,0) | (2,0,0,0) | 8.976 | **8.113** | **8.482** | **8.598** | **8.505** | **8.403** | **8.476** |
| 2Σ–(p,p\*) | (4,2,2,0) | (1,0,0,1) | 9.439 | **8.319** | **8.672** | **8.759** | **8.641** | **8.529** | **8.626** |
| 2Δ(p,p\*) | (4,2,2,0) | (2,0,0,1) | 9.379 | **8.468** | **8.772** | **8.875** | **8.790** | **8.681** | **8.756** |
| 4Σ+(p,p\*) | (4,2,2,0) | (2,0,0,0) | 6.103 | **5.785** | **6.056** | **6.143** | **6.098** | **6.030** | **6.075** |
| 4Δ(p,p\*) | (4,2,2,0) | (2,0,0,1) | 7.483 | **6.914** | **7.169** | **7.244** | **7.189** | **7.099** | **7.161** |
| 4Σ–(p,p\*) | (4,2,2,0) | (1,0,0,1) | 8.291 | **7.647** | **7.964** | **8.106** | **8.010** | **7.879** | **7.956** |

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