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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,b3u,b2u,b1g,b1u,b2g,b3g,au) | State-average  (Ag,B3u,B2u,B1g,B1u,B2g,B3g,Au) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Σ–u(,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,0,0,0,1) | 7.141 | **6.031** | **6.399** | **6.370** | **6.318** | **6.390** | **6.463** |
| 1Δu(,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,1,0,0,1) | 7.464 | **6.348** | **6.696** | **6.713** | **6.663** | **6.677** | **6.754** |
| 3Σ+u(,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,1,0,0,0) | 5.276 | **4.463** | **4.855** | **4.923** | **4.879** | **4.891** | **4.948** |
| 1Σ–u[F](,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,0,0,0,1) | 5.678 | **4.745** | **5.066** | **5.008** | **4.968** | **5.044** | **5.113** |

a All calculations using a full valence (8e,8o)  active space.