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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’’(n,\*) | (3,4) | (1,2) | 4.021a | **3.674** | **3.977** | **4.012** | **3.981** | **3.893** | **3.940** |
| 1A’’(,\*) | (3,4) | (1,2) | 7.610a | **6.426** | **6.790** | **6.524** | **6.436** | **6.673** | **6.773** |
| 3A’’(n,\*) | (3,4) | (1,1) | 3.524a | **3.251** | **3.459** | **3.588** | **3.577** | **3.497** | **3.509** |
| 3A’(,\*) | (2,4) | (2,0) | 4.979b | **5.030** | **5.246** | **5.372** | **5.350** | **5.117** | **5.159** |

a Using reference (8e,7o) active space including valence  and nO orbitals. b Using reference (6e,6o) active space including valence  orbitals.