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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1Σ–(,\*) | (0,4,4,0) | (1,0,0,1) | 6.538 | **5.470** | **5.855** | **5.830** | **5.777** | **5.807** | **5.892** |
| 1Δ(,\*) | (0,4,4,0) | (2,0,0,1) | 6.796 | **5.779** | **6.130** | **6.144** | **6.095** | **6.087** | **6.169** |
| 3Σ+(,\*) | (0,4,4,0) | (2,0,0,0) | 4.857 | **4.040** | **4.449** | **4.492** | **4.445** | **4.448** | **4.517** |
| 3Δ(,\*) | (0,4,4,0) | (2,0,0,1) | 5.637 | **4.864** | **5.211** | **5.228** | **5.194** | **5.190** | **5.260** |
| 1A"[F](,\*) | (a’:4,a":4) | (A’:1,A":1) | 4.295 | **3.470** | **3.673** | **3.547** | **3.498** | **3.584** | **3.644** |

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