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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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) | 3.999a | **3.640** | **3.917** | **3.983** | **3.951** | **3.863** | **3.899** |
| 1A’’(,\*) | (3,4) | (1,2) | 6.624a | **5.487** | **5.817** | **5.577** | **5.495** | **5.715** | **5.813** |
| 3A’’(n,\*) | (3,4) | (1,1) | 3.521a | **3.259** | **3.483** | **3.606** | **3.595** | **3.500** | **3.520** |
| 3A’(,\*) | (2,4) | (2,0) | 4.686b | **4.302** | **4.585** | **4.658** | **4.630** | **4.538** | **4.589** |

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