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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’’(n,\*) | (3,2) | (1,1) | 4.616 | **4.129** | **4.354** | **4.418** | **4.392** | **4.405** | **4.444** |
| 3A’’(n,\*) | (3,2) | (1,1) | 4.280 | **3.707** | **3.941** | **4.028** | **3.999** | **4.031** | **4.063** |

a Using reference (6e,5o) active space including valence nO, CO, σCO and \*CO, σ\*CO orbitals.