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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1A1(n,n-p\*,p\*) | (2,2,1,0) | (3,0,0,0) | 12.225 | **10.400** | **10.420** | **10.296** | **10.265** | **10.718** | **10.713** |

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