**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of Criegee’s intermediate.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’’(n-p\*) | (5,3) | (1,1) | 2.387 | **2.234** | **2.318** | **2.388** | **2.440** | **2.339** | **2.348** |
| 1A’(p-p\*) | (5,3) | (2,0) | 4.201 | **3.645** | **3.881** | **3.866** | **3.746** | **3.825** | **3.870** |

a Using reference (10e,8o) active space including valence , σOO, σCO, σ\*OO, σ\*CO, and one nO orbitals.