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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1B1(,3s) | (3,2,0,0) | (1,1,0,0) | 6.213a | **6.585** | **6.743** | **6.664** | **6.633** | **6.571** | **6.636** |
| 1A1(,3px) | (2,3,0,0) | (2,0,0,0) | 6.898b | **7.140** | **7.321** | **7.249** | **7.203** | **7.181** | **7.244** |
| 3A1(,\*) | (2,2,0,0) | (2,0,0,0) | 4.655c | **4.408** | **4.595** | **4.614** | **4.614** | **4.530** | **4.584** |

a Using reference (4e,5o) active space including valence , σCC, σ\*CC and 3s orbitals. b Using reference (4e,5o) active space including valence , σCC, σ\*CC and 3px orbitals. c Using reference (4e,4o) active space including valence , σCC and σ\*CC orbitals.