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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1A2(n,\*) | (2,3,1,0) | (1,0,0,2) | 4.768a | **4.189** | **4.443** | **4.497** | **4.480** | **4.549** | **4.574** |
| 1B2(n,3s) | (4,2,1,0) | (1,0,2,0) | 5.502b | **6.354** | **6.460** | **6.697** | **6.810** | **6.669** | **6.644** |
| 1A2(n,3px) | (2,3,1,0) | (1,0,0,2) | 7.459a | **7.551** | **7.803** | **7.706** | **7.650** | **7.678** | **7.757** |
| 1A1(n,3py) | (2,2,2,0) | (2,0,0,0) | 7.030c | **7.464** | **7.670** | **7.752** | **7.749** | **7.746** | **7.759** |
| 1B2(n,3pz) | (4,2,1,0) | (1,0,2,0) | 6.438b | **7.473** | **7.567** | **7.800** | **7.914** | **7.758** | **7.727** |
| 3A2(n,\*) | (2,2,1,0) | (1,0,0,1) | 4.466d | **3.886** | **4.133** | **4.217** | **4.199** | **4.235** | **4.265** |
| 3A1(,\*) | (2,2,0,0) | (2,0,0,0) | 6.218e | **6.071** | **6.241** | **6.277** | **6.284** | **6.218** | **6.256** |

a Using reference (6e,6o) active space including valence , nO, σCO, σ\*CO and 3px orbitals. b Using reference (6e,7o) active space including valence , nO, σCO, σ\*CO, 3s and 3pz orbitals. c Using reference (6e,6o) active space including valence , nO, σCO, σ\*CO and 3py orbitals. d Using reference (6e,5o) active space including valence , nO, σCO and σ\*CO orbitals. e Using reference (4e,4o) active space including valence , σCO and σ\*CO orbitals.