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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1B1(s,\*) | (3,1,3,1) | (1,1,0,0) | 7.484 | **6.584** | **6.861** | **6.909** | **6.796** | **6.770** | **6.853** |
| 1B2(p,\*) | (3,1,3,1) | (1,0,1,0) | 7.471 | **6.474** | **6.892** | **6.955** | **6.827** | **6.870** | **6.957** |
| 3B2(p,\*) | (3,1,3,1) | (1,0,1,0) | 4.598 | **4.274** | **4.469** | **4.527** | **4.506** | **4.396** | **4.460** |
| 3B1(s,\*) | (3,1,3,1) | (1,1,0,0) | 7.078 | **6.320** | **6.564** | **6.612** | **6.519** | **6.472** | **6.547** |

a Reference (8e,8o) active space including valence CC, σCC and \*CC, σ\*CC orbitals.