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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1B2(,\*) | (0,3,0,1) | (1,0,1,0) | 4.471a | **4.115** | **4.401** | **4.400** | **4.374** | **4.325** | **4.388** |
| 1B1(,3s) | (1,3,0,1) | (1,1,0,0) | 4.923b | **5.438** | **5.574** | **5.486** | **5.488** | **5.412** | **5.462** |
| 1A2(,3py) | (0,3,1,1) | (1,0,0,1) | 5.365c | **5.966** | **6.087** | **6.000** | **6.005** | **5.921** | **5.969** |
| 1A1(,3px) | (0,6,0,1) | (5,0,0,0) | 5.373d | **6.155** | **6.263** | **6.365** | **6.364** | **6.134** | **6.169** |
| 3B2(,\*) | (0,3,0,1) | (1,0,1,0) | 3.443a | **3.336** | **3.575** | **3.675** | **3.663** | **3.492** | **3.548** |
| 3A1(,\*) | (0,5,0,1) | (4,0,0,0) | 4.601e | **4.579** | **4.820** | **4.888** | **4.874** | **4.717** | **4.773** |

a Using reference (4e,4o) active space including valence . b Using reference (4e,5o) active space including valence  and 3s. c Using reference (4e,5o) active space including valence  and 3py.d Using reference (4e,7o) active space including valence , two 3px and one 3dxz. e Using reference (4e,6o) active space including valence , one 3px and one 3dxz.