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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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(,\*) | (0,4,0,2) | (1,0,2,0) | 6.708a | **5.616** | **5.955** | **5.714** | **5.654** | **5.988** | **6.061** |
| 1A2(,3s) | (2,2,0,2) | (1,0,0,2) | 5.213b | **5.775** | **5.878** | **5.921** | **5.921** | **5.770** | **5.808** |
| 1B1(,3py) | (0,2,1,2) | (1,1,0,0) | 6.078c | **6.440** | **6.594** | **6.428** | **6.417** | **6.409** | **6.470** |
| 1A2(,3pz) | (2,2,0,2) | (1,0,0,2) | 5.779b | **6.462** | **6.547** | **6.591** | **6.591** | **6.413** | **6.451** |
| 1B2(,3px) | (0,4,0,2) | (1,0,2,0) | 6.157a | **6.561** | **6.723** | **6.616** | **6.596** | **6.545** | **6.606** |
| 1A1(,\*) | (0,2,0,2)  (0,2,0,2) | (2,0,0,0)  (3,0,0,0) | 6.609d,e  6.488d,e | **6.249**  **6.130** | **6.686**  **6.627** | **6.848**  **6.781** | **6.817**  **6.751** | **6.558**  **6.501** | **6.650**  **6.589** |
| 3B2(,\*) | (0,2,0,2) | (1,0,1,0) | 3.260d | **3.095** | **3.336** | **3.420** | **3.408** | **3.262** | **3.314** |
| 3A1(,\*) | (0,2,0,2) | (3,0,0,0) | 4.921d | **4.779** | **5.143** | **5.312** | **5.296** | **5.031** | **5.097** |
| 3A2(,3s) | (1,2,0,2) | (1,0,0,1) | 5.534f | **5.740** | **5.909** | **5.743** | **5.732** | **5.747** | **5.808** |
| 3B1(,3py) | (0,2,1,2) | (1,1,0,0) | 6.047c | **6.402** | **6.557** | **6.414** | **6.401** | **6.371** | **6.433** |

a Using reference (4e,6o) active space including valence  and two 3px orbitals. b Using reference (4e,6o) active space including valence , 3s and 3pz orbitals. c Using reference (4e,5o) active space including valence  and 3py orbitals. d Using reference (4e,4o) active space including valence  orbitals. e Strong double-excitation character. f Using reference (4e,5o) active space including valence  and 3s orbitals.