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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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(n,p-p\*,p\*) | (0,4,1,2) | (1,1,0,0) | 5.136a | **4.649** | **4.914** | **5.041** | **5.025** | **5.008** | **5.018** |
| 1A1(p,p-p\*,p\*) | (0,4,0,2) | (2,0,0,0) | 6.146b | **5.612** | **5.983** | **6.057** | **6.022** | **5.910** | **5.979** |
| 1A1(p-p\*) | (0,4,1,2) | (5,0,0,0) | 9.160a | **6.244** | **7.172** | **6.872** | **6.662** | **7.468** | **7.548** |
| 3B1(n,p-p\*,p\*) | (0,4,1,2) | (1,1,0,0) | 5.075a | **4.542** | **4.814** | **4.933** | **4.913** | **4.897** | **4.913** |

a Using reference (8e,7o) active space including valence  and nO orbitals. b Using reference (6e,6o) active space including valence  orbitals.