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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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) | 3.235a | **2.900** | **3.137** | **3.169** | **3.154** | **3.127** | **3.178** |
| 1A1(p-p\*) | (0,4,0,2) | (2,0,0,0) | 5.572b | **4.919** | **5.418** | **5.466** | **5.428** | **5.340** | **5.423** |
| 1A1(n,n-p\*,p\*) | (0,4,1,2) | (5,0,0,0) | 7.626a | **4.995** | **5.679** | **5.397** | **5.288** | **5.942** | **6.032** |
| 3B1(n,p-p\*,p\*) | (0,4,1,2) | (1,1,0,0) | 3.210a | **2.867** | **3.105** | **3.136** | **3.121** | **3.087** | **3.140** |

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