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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1A2(n,\*) | (0,3,1,1) | (1,0,0,1) | 3.436a | **3.144** | **3.433** | **3.536** | **3.525** | **3.404** | **3.460** |
| 1B1(n,\*) | (0,3,1,1) | (1,1,0,0) | 3.569a | **3.174** | **3.453** | **3.510** | **3.498** | **3.465** | **3.520** |
| 1B2(,\*) | (2,3,1,1) | (1,0,3,0) | 4.506b | **4.353** | **4.639** | **4.786** | **4.773** | **4.608** | **4.660** |
| 1B2(n,3s) | (2,3,1,1) | (1,0,3,0) | 4.594b | **5.150** | **5.253** | **5.338** | **5.346** | **5.225** | **5.250** |
| 1A1(,\*) | (0,3,0,1) | (2,0,0,0) | 6.464c | **5.317** | **5.844** | **5.721** | **5.537** | **5.746** | **5.878** |
| 1B2(n,3pz) | (2,3,1,1) | (1,0,3,0) | 5.272b | **5.862** | **5.931** | **5.981** | **5.991** | **5.899** | **5.918** |
| 3A2(n,\*) | (0,3,1,1) | (1,0,0,1) | 3.264a | **3.000** | **3.282** | **3.395** | **3.384** | **3.277** | **3.327** |
| 3B1(n,\*) | (0,3,1,1) | (1,1,0,0) | 3.514a | **3.067** | **3.355** | **3.409** | **3.396** | **3.362** | **3.421** |
| 3B2(,\*) | (2,3,1,1) | (1,0,3,0) | 3.797b | **3.754** | **3.971** | **4.166** | **4.169** | **3.946** | **3.988** |
| 3A1(,\*) | (0,3,0,1) | (2,0,0,0) | 3.830c | **3.772** | **4.010** | **4.145** | **4.133** | **3.952** | **4.002** |

a Using reference (6e,5o) active space including valence  and nS. b Using reference (6e,7o) active space including valence , nS, 3s and 3pz.

c Using reference (4e,4o) active space including valence .