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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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,\*) | (2,3,1,1) | (1,3,0,0) | 4.920a | **3.751** | **4.118** | **4.081** | **4.044** | **4.384** | **4.400** |
| 1A2(n,\*) | (0,4,2,1) | (1,0,0,3) | 5.638b | **5.311** | **5.618** | **5.859** | **5.852** | **5.637** | **5.667** |
| 1B2(n,3s) | (2,3,1,1) | (1,0,3,0) | 5.681a | **6.214** | **6.282** | **6.472** | **6.505** | **6.443** | **6.410** |
| 1B2(,\*) | (2,3,1,1) | (1,0,3,0) | 6.397a | **6.204** | **6.541** | **6.821** | **6.823** | **6.620** | **6.630** |
| 1B2(n,3pz) | (2,3,1,1) | (1,0,3,0) | 6.345a | **6.699** | **6.836** | **7.054** | **7.074** | **7.013** | **6.985** |
| 1A1(n,3py) | (0,4,2,1) | (4,0,0,0) | 6.840b | **7.032** | **7.269** | **7.294** | **7.281** | **7.242** | **7.255** |
| 1A1(,\*) | (0,4,2,1) | (4,0,0,0) | 10.420b | **8.115** | **8.959** | **8.807** | **8.185** | **9.065** | **9.213** |
| 3B1(n,\*) | (2,3,1,1) | (1,3,0,0) | 4.724a | **3.279** | **3.649** | **3.554** | **3.512** | **3.980** | **3.998** |
| 3B2(,\*) | (2,3,1,1) | (1,0,3,0) | 4.394a | **4.595** | **4.757** | **5.070** | **5.097** | **4.737** | **4.756** |
| 3A2(n,\*) | (0,4,2,1) | (1,0,0,3) | 5.404b | **5.056** | **5.358** | **5.599** | **5.596** | **5.419** | **5.438** |
| 3A1(,\*) | (0,4,2,1) | (4,0,0,0) | 6.587b | **6.614** | **6.928** | **7.168** | **7.162** | **6.818** | **6.864** |

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