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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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(,\*) | (4,3,2,0) | (1,0,0,1) | 3.977a | **3.697** | **3.920** | **3.968** | **3.932** | **3.851** | **3.899** |
| 1B1(,3s) | (5,3,2,0) | (1,1,0,0) | 5.216b | **5.788** | **5.991** | **6.067** | **6.093** | **5.971** | **6.000** |
| 1A2(p,3p) | (4,3,3,0) | (1,0,0,2) | 6.381c | **7.055** | **7.248** | **7.262** | **7.280** | **7.151** | **7.191** |
| 3A2(,\*) | (4,3,2,0) | (1,0,0,1) | 3.922a | **3.586** | **3.810** | **3.850** | **3.803** | **3.742** | **3.789** |
| 3A1(p,\*) | (4,3,2,0) | (2,0,0,0) | 5.793a | **5.430** | **5.647** | **5.693** | **5.650** | **5.587** | **5.634** |
| 3B1(,3s) | (5,3,2,0) | (1,1,0,0) | 5.048b | **5.599** | **5.794** | **5.866** | **5.889** | **5.770** | **5.801** |
| 3A2(,3p) | (4,3,3,0) | (1,0,0,2) | 6.348c | **7.015** | **7.212** | **7.224** | **7.238** | **7.111** | **7.154** |
| 1A"[F](,\*) | (a’:6,a":3) | (A’:1,A":1) | 0.952a | **0.879** | **1.045** | **1.039** | **1.017** | **0.947** | **0.995** |

a Reference (10e,9o) active space including valence , σCC, σCO and σ\*CC, σ\*CO orbitals. b Reference (10e,10o) active space including valence , σCC, σCO and σ\*CC, σ\*CO, Rydberg 3s orbitals. c Reference (10e,10o) active space including valence , σCC, σCO and σ\*CC, σ\*CO, Rydberg 3p orbitals.