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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,au,bu,bg) | State-average  (Ag,Au,Bu,Bg) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Au(n,\*) | (4,2,4,2) | (1,1,0,0) | 3.421a | **2.515** | **2.818** | **2.994** | **2.904** | **2.937** | **2.965** |
| 1Bg(n,\*) | (4,2,4,3) | (1,0,0,2) | 4.685b | **3.886**c | **4.212** | **4.377** | **4.300** | **4.312**c | **4.360** |
| 1Ag(n,\*2) | (4,2,4,2) | (2,0,0,0) | 5.924a | **5.211** | **5.372** | **5.546** | **5.518** | **5.549** | **5.535** |
| 1Bg(n,\*) | (4,2,4,3) | (1,0,0,2) | 7.352b,d | **5.984**c | **6.522** | **6.800** | **6.639** | **6.722**c | **6.764** |
| 1Bu(n,3px) | (4,2,5,2) | (1,0,1,0) | 7.039e | **7.342** | **7.608** | **7.808** | **7.838** | **7.812** | **7.782** |
| 3Au(n,\*) | (4,2,4,2) | (1,1,0,0) | 3.058a | **2.118** | **2.414** | **2.588** | **2.495** | **2.551** | **2.573** |
| 3Bg(n,\*) | (4,2,4,2) | (1,0,0,1) | 4.608a | **3.528** | **3.899** | **4.101** | **3.991** | **4.007** | **4.041** |
| 3Bu(,\*) | (4,2,4,2) | (1,0,1,0) | 5.457a | **4.912** | **5.136** | **5.210** | **5.168** | **5.137** | **5.173** |
| 3Ag(,\*) | (4,2,4,2) | (2,0,0,0) | 6.694a | **6.024** | **6.317** | **6.407** | **6.335** | **6.274** | **6.335** |

a Using reference (14e,12o) active space including valence , two nO, σCC, σCO, σ\*CC and σ\*CO orbitals. b Using reference (14e,13o) active space including valence , two nO, σCC, σCO, σ\*CC, σ\*CO and 3pz orbitals. c Level shift = 0.4 au. d Non-negligible doubly-excited and Rydberg character. e Using reference (14e,13o) active space including valence , two nO, σCC, σCO, σ\*CC, σ\*CO and 3px orbitals.