**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of CH2O+.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 12B1(p,n) | (5,2,3,0) | (0,1,1,0) | 3.987 | **3.924** | **3.904** | **3.850** | **3.850** | **3.852** | **3.853** |
| 12A1(s,n) | (5,2,3,0) | (1,0,1,0) | 5.363 | **5.233** | **5.233** | **5.259** | **5.256** | **5.233** | **5.233** |
| 22B1(n,p\*) | (5,2,3,0) | (0,1,1,0) | 6.234 | **5.732** | **5.801** | **5.826** | **5.745** | **5.754** | **5.770** |
| 22B2(s,n) | (5,2,3,0) | (0,0,2,0) | 6.690 | **6.448** | **6.508** | **6.542** | **6.489** | **6.476** | **6.495** |
| 14B2(p,p\*) | (5,2,3,0) | (0,0,2,0) | 7.019 | **6.737** | **6.865** | **6.943** | **6.920** | **6.869** | **6.890** |
| 14A2(s,p\*) | (5,2,3,0) | (0,0,1,1) | 9.357 | **8.741** | **8.904** | **9.028** | **8.979** | **8.938** | **8.959** |

a Using reference (11e,10o) full valence active space.