**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of ClO2.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 12B2(n,p\*) | (5,2,4,1) | (0,1,1,0) | 2.731a | **3.093** | **3.009** | **2.992** | **3.078** | **2.964** | **2.940** |
| 12A1(n,p\*) | (5,2,4,1) | (1,1,0,0) | 2.908a | **3.136** | **3.076** | **3.055** | **3.124** | **3.027** | **3.012** |
| 12A2(p,p\*) | (5,2,4,1) | (0,1,0,1) | 3.225a | **3.308** | **3.319** | **3.416** | **3.448** | **3.337** | **3.315** |
| 22A1(p\*,s\*) | (5,2,4,1) | (2,1,0,0) | 4.743a | **4.330** | **4.524** | **4.647** | **4.568** | **4.515** | **4.548** |
| 22B2(p\*,s\*) | (5,2,4,1) | (0,1,2,0) | 5.564a | **5.192** | **5.313** | **5.433** | **5.364** | **5.357** | **5.358** |
| 32A1(p\*,3s) | (6,2,4,1) | (3,1,0,0) | 6.728b | **7.061** | **7.243** | **7.297** | **7.293** | **7.204** | **7.183** |
| 14B2(p,s\*) | (5,2,4,1) | (0,1,1,0) | 5.907a | **6.025** | **6.184** | **6.288** | **6.358** | **6.108** | **6.133** |
| 14A2(n,s\*) | (5,2,4,1) | (0,1,0,1) | 6.265a | **5.954** | **6.222** | **6.417** | **6.440** | **6.259** | **6.278** |
| 14B1(n,s\*) | (5,2,4,1) | (0,2,0,0) | 6.517a | **6.149** | **6.448** | **6.637** | **6.657** | **6.462** | **6.489** |

a Using reference (19e,12o) full valence active space. b Using reference (19e,13o) full valence active space plus one 3s orbital.