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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,au,bu,bg) | State-average  (Ag,Au,Bu,Bg) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Ag(n,n-p\*,p\*) | (4,2,4,2) | (2,0,0,0) | 9.044 | **8.643** | **8.814** | **8.958** | **8.942** | **8.923** | **8.899** |

a Using reference (14e,12o) active space including valence , nO, σCC, σCO, σ\*CC, σ\*CO orbitals.