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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’’(n,\*) | (3,4) | (1,1) | 2.064 | **1.838** | **2.054** | **2.067** | **2.054** | **1.998** | **2.054** |
| 3A’’(n,\*) | (3,4) | (1,1) | 1.853 | **1.595** | **1.812** | **1.821** | **1.806** | **1.787** | **1.839** |

a Using reference (8e,7o) active space including valence  and nO orbitals.