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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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(p,p-p\*,p\*) | (4,2,4,2) | (3,0,0,0) | 7.081 | **6.584** | **6.699** | **6.732** | **6.649** | **6.672** | **6.684** |

a Using reference (12e,12o) active space including valence , σCN, σ\*CN orbitals.