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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’’(n,\*) | (5,3) | (1,1) | 5.951a | **5.451** | **5.660** | **5.732** | **5.712** | **5.671** | **5.708** |
| 1A’(n,3s) | (7,3) | (4,0) | 6.165b | **6.640** | **6.795** | **6.916** | **6.978** | **6.810** | **6.816** |
| 1A’(n,3p) | (7,3) | (4,0) | 6.743b | **7.320** | **7.453** | **7.571** | **7.643** | **7.458** | **7.462** |
| 1A’(,\*) | (7,3) | (4,0) | 8.801b | **7.128** | **7.877** | **8.107** | **7.640** | **7.780** | **7.952** |
| 3A’’(n,\*) | (5,3) | (1,1) | 5.886a | **5.156** | **5.363** | **5.439** | **5.378** | **5.372** | **5.413** |
| 3A’(,\*) | (4,3) | (2,0) | 6.095c | **5.616** | **5.876** | **5.978** | **5.900** | **5.870** | **5.914** |

a Reference (10e,8o) active space including valence , nO, σCN, σCO and s\*CN, σ\*CO orbitals. b Reference (10e,10o) active space including valence , nO, σCN, σCO and s\*CN, σ\*CO, Rydberg 3s and 3p orbitals. c Reference (8e,7o) active space including valence , σCN, σCO and s\*CN, σ\*CO orbitals.