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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’(n,n-p\*,p\*) | (10,3) | (3,0) | 8.185a | **7.970** | **7.967** | **7.992** | **8.001** | **7.945** | **7.939** |
|  | (11,3) | (4,0) | 8.337b | **7.978** | **8.005** | **8.025** | **8.009** | **7.968** | **7.969** |

a Using reference (18e,13o) active space including full valence space. b Using reference (18e,14o) active space including full valence space and one Rydberg 3s orbital.