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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’(n,n-p\*,p\*) | (7,2) | (2,0) | 4.670 | **4.358** | **4.366** | **4.398** | **4.371** | **4.361** | **4.364** |

a Using reference (12e,9o) active space including full valence space.