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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’’(n,\*) | (4,2) | (1,1) | 2.117a | **1.600** | **1.839** | **1.945** | **1.905** | **1.906** | **1.942** |
| 1A’(n2,\*2) | (4,2) | (2,0) | 4.740a | **4.666** | **4.686** | **4.734** | **4.728** | **4.706** | **4.705** |
| 1A’(n,3s) | (5,2) | (3,0) | 5.872b | **6.066** | **6.316** | **6.377** | **6.378** | **6.310** | **6.339** |
| 3A’’(n,\*) | (4,2) | (1,1) | 1.313a | **0.753** | **0.996** | **1.130** | **1.084** | **1.091** | **1.120** |
| 3A’(,\*) | (2,2) | (2,0) | 5.517c | **5.373** | **5.522** | **5.539** | **5.544** | **5.496** | **5.537** |
| 1A’’[F](n,\*) | (4,2) | (1,1) | 1.833a | **1.315** | **1.554** | **1.663** | **1.623** | **1.620** | **1.656** |

a Reference (8e,6o) active space including valence nO, nN, NO, σNO and s\*NO, \*NO orbitals. b Reference (8e,7o) active space including valence nO, nN, NO, σNO and s\*NO, \*NO, Rydberg 3s orbitals. c Reference (4e,4o) active space including valence NO, σNO and s\*NO, \*NO orbitals.