**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of N2+.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,b3u,b2u,b1g,b1u,b2g,b3g,au) | State-average  (Ag,B3u,B2u,B1g,B1u,B2g,B3g,Au) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 2Πu(,s) | (2,1,1,0,2,1,1,0) | (1,1,1,0,0,0,0,0) | 1.367 | **1.482** | **1.437** | **1.356** | **1.350** | **1.343** | **1.346** |
| 2Σu+(s\*,s) | (2,1,1,0,2,1,1,0) | (1,0,0,0,1,0,0,0) | 3.250 | **3.243** | **3.291** | **3.378** | **3.333** | **3.307** | **3.312** |
| 2Πg(s,p\*) | (2,1,1,0,2,1,1,0) | (1,0,0,0,0,1,1,0) | 9.027 | **8.680** | **8.776** | **8.900** | **8.870** | **8.830** | **8.828** |
| 4Σu+(p,p\*) | (2,1,1,0,2,1,1,0) | (1,0,0,0,1,0,0,0) | 6.874 | **6.423** | **6.633** | **6.735** | **6.678** | **6.644** | **6.672** |
| 4Δu(p,p\*) | (2,1,1,0,2,1,1,0) | (1,0,0,0,1,0,0,1) | 8.502 | **7.807** | **8.023** | **8.122** | **8.069** | **7.999** | **8.036** |
| 4Σu–(p,p\*) | (2,1,1,0,2,1,1,0) | (1,0,0,0,0,0,0,1) | 9.309 | **8.694** | **8.923** | **9.082** | **9.018** | **8.918** | **8.952** |
| 4Πg(pp,sp\*) | (2,1,1,0,2,1,1,0) | (1,0,0,0,0,1,1,0) | 9.125 | **8.998** | **9.065** | **9.046** | **9.010** | **8.952** | **8.985** |

a Using reference (9e,8o) full valence active space.