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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA  (10 core)b | CASPT2  IPEA  (10 core)b | SC-NEVPT2  (10 core)b | PC-  NEVPT2  (10 core)b |
| 2Δ | (6,3,3,1)a | (2,0,0,1) | 1.038 | **0.855** | **0.840** | **0.884** | **0.874** |
| 2Π | (6,3,3,1)a | (1,1,1,0) | 2.073 | **2.013** | **2.027** | **2.039** | **2.014** |
| 2Δ | (6,3,3,1)a | (3,0,0,2) | 2.181 | **2.118** | **2.227** | **2.242** | **2.222** |

a Using a reference (9e,13o) active space including 4s, 3d, 4p of Ti and 2s, 2p of N.

b Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Ti and 1s of N (6,2,2,0).

c Core orbitals not correlated at PT2 level: 1s, 2s, 2p of Ti and 1s of N (4,1,1,0).