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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA  (14 core)b | CASPT2  IPEA  (14 core)b | SC-NEVPT2  (14 core)b | PC-  NEVPT2  (14 core)b |
| 11Π | (5,3,3,0)a | (1,1,1,0) | 0.628 | **0.720** | **0.774** | **0.714** | **0.724** |
| 21Σ+ | (5,3,3,0)a | (2,0,0,0) | 3.852 | **3.856** | **3.978** | **3.973** | **3.915** |
| 11Δ | (5,3,3,0)a | (2,0,0,1) | 4.053 | **4.046** | **4.231** | **4.209** | **4.216** |
| 11Σ– | (5,3,3,0)a | (1,0,0,1) | 4.303 | **4.079** | **4.335** | **4.302** | **4.258** |
| 13Π | (5,3,3,0)a | (1,1,1,0) | 0.442 | **0.521** | **0.573** | **0.515** | **0.524** |
| 13Σ+ | (5,3,3,0)a | (2,0,0,0) | 2.040 | **2.249** | **2.314** | **2.314** | **2.306** |

a Using a reference (8e,11o) active space including 4s, 4p of Zn and 3s, 3p, 3dz2, 3dxz, 3dyz of S.

b Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Zn and 1s, 2s, 2p of S (8,3,3,0).