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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA  (10 core)e | CASPT2  IPEA  (10 core)e | CASPT3  NOIPEA  (10 core)e | CASPT3  IPEA  (10 core)e | SC-NEVPT2  (10 core)e | PC-  NEVPT2  (10 core)e |
| 11Π | (3,2,2,0)a  (4,2,2,0)b  (6,3,3,1)c  (8,4,4,2)d | (1,1,1,0)  (1,1,1,0)  (1,1,1,0)  (1,1,1,0) | 0.297  0.421  0.432  0.432d | **0.502**  **0.530**  **0.543**  **0.551**d | **0.494**  **0.517**  **0.530**  **–** | **0.545**  **0.543**  **–**  **–** | **0.529**  **0.530**  **–**  **–** | **–**  **–**  **0.519**  **–** | **–**  **–**  **0.557**  **–** |
| 21Σ+ | (3,2,2,0)a  (4,2,2,0)b  (6,3,3,1)c | (2,0,0,0)  (2,0,0,0)  (2,0,0,0) | 3.810  3.636  3.597 | **3.845**  **3.774**  **3.681** | **3.932**  **3.854**  **3.763** | **3.806**  **3.739**  **–** | **3.841**  **3.772**  **–** | **3.933**  **3.883**  **3.792** | **3.869**  **3.817**  **3.718** |
| 11Δ | (3,2,2,0)a  (4,2,2,0)b  (6,3,3,1)c | (2,0,0,1)  (2,0,0,1)  (2,0,0,1) | 4.118  4.146  4.181 | **4.315**  **4.149**  **4.192** | **4.460**  **4.336**  **4.381** | **4.446**  **4.349**  **–** | **4.467**  **4.374**  **–** | **–**  **–**  **4.399** | **–**  **–**  **4.413** |
| 11Σ– | (3,2,2,0)a  (4,2,2,0)b  (6,3,3,1)c | (1,0,0,1)  (1,0,0,1)  (1,0,0,1) | 4.573  4.816  4.823 | **4.388**  **4.304**  **4.332** | **4.647**  **4.664**  **4.692** | **4.569**  **4.558**  **–** | **4.643**  **4.663**  **–** | **4.703**  **4.720**  **4.744** | **4.618**  **4.568**  **4.587** |
| 13Π | (3,2,2,0)a  (4,2,2,0)b  (6,3,3,1)c | (1,1,1,0)  (1,1,1,0)  (1,1,1,0) | 0.140  0.255  0.260 | **0.310**  **0.332**  **0.342** | **0.306**  **0.322**  **0.332** | **0.347**  **0.340**  **–** | **0.336**  **0.331**  **–** | **–**  **–**  **0.323** | **–**  **–**  **0.358** |
| 13Σ+ | (3,2,2,0)a  (4,2,2,0)b  (6,3,3,1)c | (2,0,0,0)  (2,0,0,0)  (2,0,0,0) | 1.332  1.356  1.349 | **1.606**  **1.512**  **1.514** | **1.637**  **1.569**  **1.570** | **1.606**  **1.542**  **–** | **1.610**  **1.549**  **–** | **1.621**  **1.562**  **1.554** | **1.637**  **1.562**  **1.554** |

a Using a reference (6e,7o) active space including 4s, 4p of Zn and 2p of O.

b Using a reference (8e,8o) active space including 4s, 4p of Zn and 2s, 2p of O.

c Using a reference (18e,13o) active space including 4s, 3d, 4p of Zn and 2s, 2p of O.

d Using a reference (18e,18o) active space including 4s, 3d, 4p, 4d of Zn and 2s, 2p of O. RASSCF and RASPT2 calculations with (18,5+8+5)[2,2].

e Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Zn (6,2,2,0).