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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA  (9 core)m | CASPT2  IPEA  (9 core)m | CASPT2  NOIPEA  (5 core)o | CASPT2  IPEA  (5 core)o | SC-NEVPT2  (9 core)m | PC-  NEVPT2  (9 core)m |
| 12Π | (3,1,1,0)a  (5,2,2,1)b  (7,3,3,2)c | (1,1,1,0)  (1,1,1,0)  (1,1,1,0) | 2.657  2.682  2.713 | **2.799**  **2.830**  **2.838** | **2.818**  **2.851**  **2.862** | **2.800**  **2.833**  **–** | **2.819**  **2.853**  **–** | **–**  **–**  **–** | **–**  **–**  **–** |
| 22Σ+ | (3,1,1,0)a  (5,2,2,1)b  (7,3,3,2)c | (2,0,0,0)  (2,0,0,0)  (2,0,0,0) | 4.334  4.411  4.459 | **4.409**  **4.466**  **4.397** | **4.485**  **4.539**  **4.510** | **4.403**  **4.465**  **–** | **4.481**  **4.541**  **–** | **4.484**  **4.558**  **–** | **4.468**  **4.519**  **–** |
| 32Σ+ | (4,1,1,0)d  (6,2,2,1)e  (8,3,3,2)f | (3,0,0,0)  (3,0,0,0)  (3,0,0,0) | 4.733  4.765  4.839 | **5.056**  **5.091**  **5.089** | **5.040**  **5.093**  **5.097** | **5.038**  **5.082**  **–** | **5.022**  **5.083**  **–** | **5.028**  **5.067**  **–** | **5.021**  **5.041**  **–** |
| 42Σ+ | (5,1,1,0)g  (7,2,2,1)h  (9,3,3,2)i | (4,0,0,0)  (4,0,0,0)  (4,0,0,0) | 5.284  5.441  5.372 | **5.527**  **5.315**  **5.548**n | **5.558**  **5.524**  **5.598**n | **5.513**  **–**  **–** | **5.545**  **–**  **–** | **5.550**  **–**  **–** | **5.527**  **–**  **–** |
| 22Π | (3,2,2,0)j  (5,3,3,1)k  (7,4,4,2)l | (1,2,2,0)  (1,2,2,0)  (1,2,2,0) | 5.564  5.596  5.648 | **6.064**  **6.118**  **6.135**n | **6.045**  **6.100**  **6.106**n | **6.052**  **6.114**  **–** | **6.033**  **6.095**  **–** | **–**  **–**  **–** | **–**  **–**  **–** |

a Using a reference (3e,5o) active space including 4s, 4p of Zn and 1s of H.

b Using a reference (13e,10o) active space including 4s, 3d, 4p of Zn and 1s of H.

c Using a reference (13e,15o) active space including 4s, 3d, 4p, 4d of Zn and 1s of H.

d Using a reference (3e,6o) active space including 4s, 4p, 5s of Zn and 1s of H.

e Using a reference (13e,11o) active space including 4s, 3d, 4p, 5s of Zn and 1s of H.

f Using a reference (13e,16o) active space including 4s, 3d, 4p, 4d, 5s of Zn and 1s of H.

g Using a reference (3e,7o) active space including 4s, 4p, 5s, 5pz of Zn and 1s of H.

h Using a reference (13e,12o) active space including 4s, 3d, 4p, 5s, 5pz of Zn and 1s of H. (4p replaced by 4d)

i Using a reference (13e,17o) active space including 4s, 3d, 4p, 4d, 5s, 5pz of Zn and 1s of H.

j Using a reference (3e,7o) active space including 4s, 4p, 5px, 5py of Zn and 1s of H.

k Using a reference (13e,12o) active space including 4s, 3d, 4p, 5px, 5py of Zn and 1s of H.

l Using a reference (13e,17o) active space including 4s, 3d, 4p, 4d, 5px, 5py of Zn and 1s of H.

m Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Zn (5,2,2,0).

n Using density-fitting.

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