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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA  (9 core)b | CASPT2  IPEA  (9 core)b | CASPT2C  NOIPEA  (5 core)c | CASPT2C  IPEA  (5 core)c |
| 1Σ+(dz2,4s) | (7,3,3,2) | (2,0,0,0) | 2.642 | **3.067** | **3.143** | **2.976** | **3.068** |
| 1Π(dxz/dyz,4s) | (7,3,3,2) | (1,1,1,0) | 2.784 | **3.652** | **3.623** | **3.569** | **3.553** |
| 1Δ(dxy/dx2-y2,4s) | (7,3,3,2) | (2,0,0,1) | 2.756 | **3.642** | **3.614** | **3.560** | **3.544** |
| 1Π(dz2/dyz,4s) | (7,3,3,2) | (1,2,2,0) | 4.656 | **5.260** | **5.449** | **5.192** | **5.397** |
| 1Σ+(dz2,4px/4py) | (7,3,3,2) | (3,0,0,0) | 5.516 | **5.932** | **6.038** | **5.878** | **5.995** |
| 3Σ+(dz2,4s) | (7,3,3,2) | (2,0,0,0) | 2.082 | **2.507** | **2.572** | **2.409** | **2.491** |
| 3Π(dxz/dyz,4s) | (7,3,3,2) | (1,1,1,0) | 2.523 | **3.428** | **3.393** | **3.342** | **3.321** |
| 3Δ(dxy/dx2-y2,4s) | (7,3,3,2) | (2,0,0,1) | 2.611 | **3.509** | **3.479** | **3.416** | **3.401** |
| 3Π(dz2/dyz,4s) | (7,3,3,2) | (1,2,2,0) | 3.973 | **4.651** | **4.746** | **4.594** | **4.702** |

a All calculations using a (12e,15o) active space including 4s, 3d, 4p, 4d of Cu and 1s of H.

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

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

**Table.** CASPT2/aug-cc-pVDZ vertical transition energies (eV) of CuH.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA  (9 core)b | CASPT2  IPEA  (9 core)b |
| 1Σ+(dz2,4s) | (7,3,3,2) | (2,0,0,0) | 2.652 | **3.031** | **3.102** |
| 1Π(dxz/dyz,4s) | (7,3,3,2) | (1,1,1,0) | 2.803 | **3.607** | **3.571** |
| 1Δ(dxy/dx2-y2,4s) | (7,3,3,2) | (2,0,0,1) | 2.798 | **3.593** | **3.558** |
| 1Π(dz2/dyz,4s) | (7,3,3,2) | (1,2,2,0) | 4.683 | **5.216** | **5.408** |
| 1Σ+(dz2,4px/4py) | (7,3,3,2) | (3,0,0,0) | 5.521 | **5.864** | **5.971** |
| 3Σ+(dz2,4s) | (7,3,3,2) | (2,0,0,0) | 2.101 | **2.471** | **2.536** |
| 3Π(dxz/dyz,4s) | (7,3,3,2) | (1,1,1,0) | 2.542 | **3.374** | **3.333** |
| 3Δ(dxy/dx2-y2,4s) | (7,3,3,2) | (2,0,0,1) | 2.655 | **3.457** | **3.422** |
| 3Π(dz2/dyz,4s) | (7,3,3,2) | (1,2,2,0) | 3.992 | **4.601** | **4.691** |

a All calculations using a (12e,15o) active space including 4s, 3d, 4p, 4d of Cu and 1s of H.

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

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