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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA  (14 core)b | CASPT2  IPEA  (14 core)b | SC-NEVPT2  (14 core)b | PC-  NEVPT2  (14 core)b |
| 1Σ+ | (7,2,2,2) | (2,0,0,0) | 2.668 | **3.009** | **3.149** | **3.047** | **3.030** |
| 1Π | (7,2,2,2) | (1,1,1,0) | 2.468 | **2.972** | **3.049** | **2.968** | **3.015** |
| 1Δ | (7,2,2,2) | (2,0,0,1) | 2.554 | **3.454** | **3.472** | **3.371** | **3.454** |
| 3Σ+ | (7,2,2,2) | (2,0,0,0) | 2.159 | **2.562** | **2.692** | **2.590** | **2.578** |
| 3Π | (7,2,2,2) | (1,1,1,0) | 2.162 | **2.779** | **2.845** | **2.739** | **2.818** |
| 3Δ | (7,2,2,2) | (2,0,0,1) | 2.309 | **3.214** | **3.229** | **3.124** | **3.203** |

a Using a (12e,13o) active space including 4s, 3d, 4d of Cu and 3pz, 4pz of Cl.

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

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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA  (14 core)c | CASPT2  IPEA  (14 core)c | SC-NEVPT2  (14 core)c | PC-NEVPT2  (14 core)c |
| 1Σ+ | (6,2,2,2)a  (7,2,2,2)b | (2,0,0,0)  (2,0,0,0) | 2.677 | **3.967** | **3.088** | **3.323** | **3.333** |
| 1Π | (6,2,2,2)a  (7,2,2,2)b | (1,1,1,0)  (1,1,1,0) | 2.555 | **2.902** | **2.965** | **2.929** | **2.971** |
| 1Δ | (6,2,2,2)a  (7,2,2,2)b | (2,0,0,1)  (2,0,0,1) | 2.754 | **3.525** | **3.533** | **3.435** | **3.539** |
| 3Σ+ | (6,2,2,2)a  (7,2,2,2)b | (2,0,0,0)  (2,0,0,0) | 2.177 | **2.513** | **2.626** | **2.539** | **2.529** |
| 3Π | (6,2,2,2)a  (7,2,2,2)b | (1,1,1,0)  (1,1,1,0) | 2.235 | **2.606** | **2.661** | **2.606** | **2.654** |
| 3Δ | (6,2,2,2)a  (7,2,2,2)b | (2,0,0,1)  (2,0,0,1) | 2.500 | **3.276** | **3.281** | **3.176** | **3.277** |

a Using a (12e,12o) active space including 4s, 3d, 4d of Cu and 3pz of Cl.

b Using a (12e,13o) active space including 4s, 3d, 4d of Cu and 3pz, 4pz of Cl.

c Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Cu and 1s, 2s, 2p of Cl (8,3,3,0).