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

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2C  NOIPEA  (10 core)b | CASPT2C  IPEA  (10 core)b |
| 1Σ+(dz2,4s) | (7,3,3,2) | (2,0,0,0) | 2.076 | **2.477** | **2.539** |
| 1Π(dxz/dyz,4s) | (7,3,3,2) | (1,1,1,0) | 2.031 | **2.658** | **2.674** |
| 1Δ(dxy/dx2-y2,4s) | (7,3,3,2) | (2,0,0,1) | 2.349 | **3.045** | **3.045** |
| 1Π(dz2/dyz,4s) | (7,3,3,2) | (1,2,2,0) | 5.092 | **6.021** | **6.047** |
| 3Σ+(dz2,4s) | (7,3,3,2) | (2,0,0,0) | 1.497 | **1.933** | **1.987** |
| 3Π(dxz/dyz,4s) | (7,3,3,2) | (1,1,1,0) | 1.679 | **2.355** | **2.367** |
| 3Δ(dxy/dx2-y2,4s) | (7,3,3,2) | (2,0,0,1) | 2.103 | **2.791** | **2.793** |
| 3Π(dz2/dyz,4s) | (7,3,3,2) | (1,2,2,0) | 4.875 | **5.790** | **5.825** |

a All calculations using a (12e,15o) active space including 4s, 3d, 4p, 4d of Cu and 2pz of F.

b Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Cu and 1s of F (6,2,2,0).