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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 2Π(,\*) | (6,3,3,0) | (0,2,2,0) | 3.937a | **3.196** | **3.525** | **3.585** | **3.515** | **3.521** | **3.543** |
| 2Σ+(s,) | (6,3,3,0) | (1,1,1,0) | 3.845a | **3.523** | **3.718** | **3.838** | **3.808** | **3.823** | **3.808** |
| 2Φ(,\*) | (6,3,3,0) | (0,2,2,0) | 4.862a | **3.987** | **4.318** | **4.383** | **4.325** | **4.298** | **4.331** |
| 2Π(,\*) | (6,3,3,0) | (0,3,3,0) | 5.285a | **4.731** | **5.052** | **5.112** | **5.082** | **5.136** | **5.054** |
| 4Π(,\*) | (6,3,3,0) | (0,2,2,0) | 3.014a | **2.547** | **2.743** | **2.765** | **2.716** | **2.723** | **2.756** |
| 4Σ–(,s\*) | (6,3,3,0) | (0,1,1,1) | 5.053a | **4.920**b | **5.168** | **5.199** | **5.152** | **5.139**b | **5.189** |
| 4Σ+(s,\*) | (6,3,3,0) | (1,1,1,0) | 5.365a | **4.693** | **5.137** | **5.263** | **5.197** | **5.278** | **5.251** |
| 4Δ(s,\*) | (6,3,3,0) | (1,1,1,1) | 6.306a | **5.680** | **6.057** | **6.202** | **6.156** | **6.146** | **6.162** |

a Using reference (15e,12o) full valence active space. b Using a level shift of 0.4 a.u.