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

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 | MS-PT2  IPEA | XMS-PT2  IPEA |
| 2Σ+(s,) | (6,3,3,0) | (1,1,1,0) | 1.645a | **1.508** | **1.585** | **1.642** | **1.613** | **1.619** | **1.627** | **–** | **–** |
| 2Π(,) | (6,3,3,0) | (0,2,2,0) | 5.667a | **5.391** | **5.469** | **5.547** | **5.515** | **5.497** | **5.496** | **–** | **–** |
| 2Π(,\*) | (6,3,3,0) | (0,3,3,0) | 6.808a | **5.825**c | **6.249** | **6.410** | **6.284** | **6.291**c | **6.297** | **–** | **–** |
| 2Φ(,\*) | (6,3,3,0) | (0,2,2,0) | 7.375a | **6.327** | **6.825** | **6.969** | **6.885** | **6.913** | **6.857** | **–** | **–** |
| 4Π(,\*) | (6,3,3,0) | (0,2,2,0) | 6.151a | **5.484** | **5.748** | **5.870** | **5.769** | **5.756** | **5.780** | **–** | **–** |
| 4Σ+(s,\*) | (6,3,3,0) | (1,1,1,0) | 6.001a | **5.263**c | **5.670** | **5.849** | **5.754** | **5.766**c | **5.795** | **–** | **–** |
| 4Δ(s,\*) | (6,3,3,0) | (1,1,1,1) | 6.751a | **5.916** | **6.414** | **6.591** | **6.526** | **6.580** | **6.528** | **–** | **–** |
| 4Σ–(s,\*) | (6,3,3,0)  (7,3,3,0) | (0,1,1,1)  (0,1,1,2) | 7.405a  7.580b | **6.489**c  **6.372**c | **6.964**  **7.007** | **7.170**  **7.223** | **7.041**  **7.047** | **7.014**c  **7.085**c | **7.057**  **7.103** | **–**  **6.982** | **–**  **6.962** |
| 4Σ–(,3s) | (7,3,3,0)  (7,3,3,0) | (0,1,1,1)  (0,1,1,2) | 7.098b  7.183b | **7.013**  **7.006**c | **7.253**  **7.253** | **7.425**  **7.434** | **7.407**  **7.402** | **7.389**  **7.343**c | **7.376**  **7.359** | **–**  **7.145** | **–**  **7.167** |

a Using reference (15e,12o) full valence active space. b Using reference (15e,13o) full valence active space plus one 3s orbital. c Using a level shift of 0.4 a.u.