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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,b3u,b2u,b1g,b1u,b2g,b3g,au) | State-average  (Ag,B3u,B2u,B1g,B1u,B2g,B3g,Au) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Πg | (3,2,2,0,3,1,1,0) | (1,0,0,0,0,1,1,0) | 4.109a | **3.654** | **3.934** | **4.063** | **4.027** | **3.969** | **4.009** |
| 1Δg(n2,\*2) | (3,2,2,0,3,1,1,0) | (2,0,0,1,0,0,0,0) | 4.985a | **4.744**b | **5.027** | **5.209** | **5.255** | **5.123**b | **5.172** |
| 1Σ+g(n2,\*2) | (3,2,2,0,3,1,1,0) | (2,0,0,0,0,0,0,0) | 5.837a | **5.506**c | **5.776** | **5.993** | **5.986** | **5.826**c | **5.896** |

a All calculations using a full valence (12e,12o) active space. b Level shift of 0.4 au. c Level shift of 0.5 au.