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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,b3u,b2u,b1g,b1u,b2g,b3g,au) | State-average  (Ag,B3u,B2u,B1g,B1u,B2g,B3g,Au) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Dg(p,p-s\*,s\*) | (2,1,1,0,2,1,1,0) | (2,0,0,1,0,0,0,0) | 2.487 | **2.277** | **2.271** | **2.144** | **2.119** | **2.096** | **2.126** |
| 1S+g(p,p-s\*,s\*) | (2,1,1,0,2,1,1,0) | (2,0,0,0,0,0,0,0) | 2.842 | **2.518** | **2.558** | **2.478** | **2.423** | **2.397** | **2.439** |
| 3S–g(p,p-s\*,s\*) | (2,1,1,0,2,1,1,0) | (1,0,0,1,0,0,0,0) | 1.742 | **1.461** | **1.476** | **1.328** | **1.266** | **1.279** | **1.318** |

a Using reference (8e,8o) active space including full valence space.