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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1Σ–u(,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,0,0,0,1) | 6.128 | **5.011** | **5.423** | **5.387** | **5.325** | **5.356** | **5.455** |
| 1Δu(,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,1,0,0,1) | 6.386 | **5.305** | **5.680** | **5.668** | **5.610** | **5.625** | **5.718** |
| 3Σ+u(,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,1,0,0,0) | 4.541 | **3.671** | **4.107** | **4.131** | **4.081** | **4.088** | **4.168** |
| 3Δu(,\*) | (0,2,2,0,0,2,2,0) | (1,0,0,0,1,0,0,1) | 5.277 | **4.448** | **4.818** | **4.821** | **4.782** | **4.782** | **4.862** |

a All calculations using a full valence (8e,8o)  active space.