**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of C2H.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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(p,s) | (5,2,2,0) | (1,1,1,0) | 0.958a | **0.864** | **0.818** | **0.714** | **0.696** | **0.730** | **0.733** |
| 2Σ+(p,p\*) | (5,2,2,0) | (2,0,0,0) | 7.562a,b | **6.776**c | **7.133** | **7.254** | **7.160** | **7.052**c | **7.136** |
| 2Σ–(p,p\*) | (5,2,2,0) | (1,0,0,1) | 8.581a | **7.305** | **7.728** | **7.763** | **7.606** | **7.513** | **7.646** |
| 2Δ(p,p\*) | (5,2,2,0) | (2,0,0,1) | 8.560a | **7.569** | **7.909** | **7.963** | **7.861** | **7.764** | **7.862** |
| 4Σ+(p,p\*) | (5,2,2,0) | (2,0,0,0) | 5.234a | **4.874** | **5.208** | **5.281** | **5.235** | **5.164** | **5.212** |
| 4Δ(p,p\*) | (5,2,2,0) | (2,0,0,1) | 6.561a | **5.933** | **6.216** | **6.251** | **6.186** | **6.104** | **6.183** |
| 4Σ–(p,p\*) | (5,2,2,0) | (1,0,0,1) | 7.452a | **6.688** | **7.048** | **7.140** | **7.012** | **6.887** | **6.997** |

a Using reference (9e,9o) full valence active space. b Significant (50%) double excitation character. c Using a level shift of 0.4 a.u.