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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 2D(s,2px,y) | (3,1,1,0) | (1,1,1,1) | 3.204a | **2.695** | **2.889** | **2.959** | **2.952** | **2.867** | **2.920** |
| 2Σ–(s,2px,y) | (3,1,1,0) | (0,1,1,1) | 3.219a | **3.093** | **3.246** | **3.314** | **3.309** | **3.261** | **3.305** |
| 2Σ+(s,2px,y) | (3,1,1,0) | (1,1,1,0) | 4.223a | **3.823** | **3.998** | **4.164** | **4.129** | **3.976** | **4.034** |
| 2Σ+(2px,y,3s) | (4,1,1,0) | (2,1,1,0) | 6.062b | **6.518** | **6.501** | **6.462** | **6.442** | **6.514** | **6.511** |
| 4Σ–(s,2px,y) | (3,1,1,0) | (0,1,1,1) | 0.261a | **0.511** | **0.588** | **0.662** | **0.683** | **0.673** | **0.679** |
| 4Π(s,3s) | (4,1,1,0) | (0,2,2,0) | 6.882b | **7.463** | **7.502** | **7.550** | **7.587** | **7.586** | **7.584** |

a Using reference (5e,5o) full valence active space. b Using reference (5e,6o) full valence active space plus one 3s orbital.