**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of CH2N.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 12B2(p,n) | (5,3,2,0) | (0,1,1,0) | 4.289a | **4.196** | **4.181** | **4.138** | **4.120** | **4.111** | **4.119** |
| 12A1(s,n) | (5,3,2,0) | (1,1,0,0) | 4.464a | **4.354** | **4.358** | **4.416** | **4.409** | **4.383** | **4.380** |
| 22B2(n,p\*) | (5,3,2,0) | (0,1,2,0) | 5.134a | **4.562** | **4.730** | **4.779** | **4.682** | **4.640** | **4.689** |
| 22B1(p,p\*) | (5,3,2,0) | (0,2,0,0) | 6.600a,b | **6.228** | **6.383** | **6.441** | **6.425** | **6.333** | **6.373** |
| 22A1(n,3s) | (6,3,2,0) | (2,1,0,0) | 6.268c | **6.784** | **6.776** | **6.764** | **6.784** | **6.800** | **6.788** |
| 12A2(s,p\*) | (5,3,2,0) | (0,1,0,1) | 7.938a | **7.417** | **7.610** | **7.736** | **7.691** | **7.609** | **7.647** |
| 32B1(n,3px) | (5,4,2,0) | (0,3,0,0) | 7.204d | **7.787** | **7.766** | **7.744** | **7.771** | **7.747** | **7.743** |
| 32A1(n,3pz) | (7,3,2,0) | (3,1,0,0) | 7.190e | **7.806** | **7.787** | **7.795** | **7.820** | **7.840** | **7.819** |
| 14B1(p,p\*) | (5,3,2,0) | (0,2,0,0) | 5.309a | **5.154** | **5.282** | **5.317** | **5.312** | **5.240** | **5.273** |
| 14A2(s,p\*) | (5,3,2,0) | (0,1,0,1) | 6.861a | **6.362** | **6.539** | **6.657** | **6.615** | **6.566** | **6.593** |

a Using reference (11e,10o) full valence active space. b Strong (63%) double excitation character. c Using reference (11e,11o) full valence active space plus one 3s orbital. d Using reference (11e,11o) full valence active space plus one 3px orbital. e Using reference (11e,12o) full valence active space plus one 3s and one 3pz orbitals.