**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of CH3.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 | MS-PT2  IPEA | XMS-PT2  IPEA |
| 12A1’(,3s) | (5,2,1,0) | (1,0,1,0) | 5.227a | **5.917** | **5.867** | **5.799** | **5.802** | **5.893** | **5.879** | **–** | **–** |
| 12E’(s,) | (4,2,1,0) | (1,1,1,0) | 7.611b | **7.087** | **7.090** | **7.083** | **7.036** | **7.079** | **7.083** | **–** | **–** |
| 22E’(,3px/y) | (6,3,1,0) | (3,2,1,0) | 6.320c | **7.160** | **7.094** | **7.032** | **7.040** | **7.153** | **7.129** | **–** | **–** |
| 12A2”(,3pz) | (4,2,2,0) | (0,0,2,0) | 6.974d | **7.670** | **7.621** | **7.548** | **7.555** | **7.656** | **7.641** | **–** | **–** |
| 32E’(,3px/y) | (7,4,1,0) | (4,3,1,0) | 7.922e | **7.944** | **8.018** | **8.013** | **7.956** | **8.036** | **8.053** | **8.355** | **8.453** |

a Using reference (7e,8o) full valence active space plus one 3s orbital. b Using reference (7e,7o) full valence active space. c Using reference (7e,10o) full valence active space plus one 3s, one 3px and one 3py orbitals. d Using reference (7e,8o) full valence active space plus one 3pz orbital. e Using reference (7e,12o) full valence active space plus one 3s, one 3px, one 3py , one 3dx2-y2 and one 3dxy orbitals.