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

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 12B1(,\*) | (0,2,0,1) | (0,1,0,1) | 3.666a | **3.277** | **3.450** | **3.550** | **3.540** | **3.380** | **3.422** | **–** | **–** |
| 12A1(,3s) | (1,2,0,1) | (1,0,0,1) | 4.603b | **5.189** | **5.112** | **4.991** | **4.996** | **5.001** | **5.001** | **–** | **–** |
| 22A1(,3pz) | (2,2,0,1) | (2,0,0,1) | 4.792c | **5.711** | **5.582** | **5.623** | **5.634** | **5.521** | **5.499** | **–** | **–** |
| 12B2(,3py) | (0,2,1,1) | (0,0,1,1) | 5.188d | **5.875** | **5.786** | **5.656** | **5.661** | **5.665** | **5.665** | **–** | **–** |
| 22B1(,\*) | (0,4,0,1) | (0,4,0,1) | 5.618e | **6.122** | **6.104** | **6.011** | **5.989** | **5.991** | **6.004** | **5.784** | **5.775** |
| 32A1(,3pz) | (4,0,0,1) | (4,2,0,1) | 5.825f | **6.637** | **6.530** | **6.492** | **6.482** | **6.450** | **6.435** | **6.498** | **6.500** |
| 42A1(s,) | (4,0,0,1) | (4,2,0,1) | 8.087f | **6.056** | **6.240** | **5.828** | **5.781** | **6.486** | **6.525** | **6.127** | **6.126** |
| 22B2(,4dyz) | (0,2,3,1) | (0,0,3,1) | 5.935g | **6.759** | **6.652** | **6.577** | **6.568** | **6.562** | **6.550** | **6.608** | **6.610** |
| 32B2(s,) | (0,2,3,1) | (0,0,3,1) | 7.994g | **6.374** | **6.513** | **6.303** | **6.275** | **6.795** | **6.807** | **6.460** | **6.458** |
| 32B1(,\*) | (0,4,0,1) | (0,4,0,1) | 6.674e | **6.969** | **7.002** | **6.883** | **6.845** | **6.922** | **6.944** | **6.589** | **6.575** |
| 42B1(,\*) | (0,4,0,1) | (0,4,0,1) | 8.718e | **6.593** | **7.141** | **6.671** | **6.490** | **7.301** | **7.395** | **7.791** | **7.834** |
| 14A2(,\*) | (0,2,0,1) | (0,0,0,2) | 5.503a | **5.896** | **6.003** | **6.187** | **6.185** | **5.837** | **5.881** | **–** | **–** |

a Using reference (3e,3o) active space including valence  orbitals. b Using reference (3e,4o) active space including valence  and 3s orbitals. c Using reference (3e,5o) active space including valence  and 3s, 3pz orbitals. d Using reference (3e,4o) active space including valence  and 3py orbitals. e Using reference (3e,5o) active space including valence  and two 3px orbitals. f Using reference (5e,7o) active space including valence , one valence s, 3s and two 3pz orbitals. g Using reference (5e,6o) active space including valence , one valence s, 3py and 4dyz orbitals.