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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1A2(,3s) | (2,3,0,2) | (1,0,0,2) | 5.256a | **6.041** | **6.156** | **6.268** | **6.280** | **6.024** | **6.061** |
| 1B2(,\*) | (0,4,0,2) | (1,0,2,0) | 7.778b | **6.025** | **6.594** | **6.431** | **6.197** | **6.711** | **6.798** |
| 1A1(,\*) | (0,3,0,2) | (3,0,0,0) | 6.727c,d | **6.102** | **6.658** | **6.828** | **6.774** | **6.623** | **6.690** |
| 1B1(,3py) | (0,3,1,2) | (1,1,0,0) | 6.072e | **6.630** | **6.792** | **6.720** | **6.712** | **6.595** | **6.654** |
| 1A2(,3pz) | (2,3,0,2) | (1,0,0,2) | 5.873a | **6.770** | **6.870** | **6.979** | **6.992** | **6.720** | **6.755** |
| 1B2(,3px) | (0,4,0,2) | (1,0,2,0) | 6.540b | **6.837** | **7.109** | **7.064** | **7.014** | **6.884** | **6.960** |
| 3B2(,\*) | (0,3,0,2) | (1,0,1,0) | 3.945c | **4.008** | **4.259** | **4.432** | **4.415** | **4.117** | **4.173** |
| 3A1(,\*) | (0,3,0,2) | (3,0,0,0) | 5.410c | **5.087** | **5.500** | **5.629** | **5.601** | **5.403** | **5.474** |
| 3A2(,3s) | (1,3,0,2) | (1,0,0,1) | 5.572f | **5.989** | **6.162** | **6.088** | **6.081** | **5.990** | **6.048** |
| 3B1(,3py) | (0,3,1,2) | (1,1,0,0) | 6.043e | **6.596** | **6.757** | **6.684** | **6.676** | **6.560** | **6.619** |

a Using reference (6e,7o) active space including valence , 3s and 3pz orbitals. b Using reference (6e,6o) active space including valence  and 3px orbitals. c Using reference (6e,5o) active space including valence  orbitals. d Strong double-excitation character. e Using reference (6e,6o) active space including valence  and 3py orbitals. f Using reference (6e,6o) active space including valence  and 3s orbitals.