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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,b3u,b2u,b1g,b1u,b2g,b3g,au) | State-average  (Ag,B3u,B2u,B1g,B1u,B2g,B3g,Au) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1B2u(,\*) | (0,0,0,0,2,1,2,1) | (1,1,0,0,0,0,0,0) | 4.977a | **4.660** | **5.136** | **5.355** | **5.323** | **5.014** | **5.091** |
| 1B1u(,\*) | (0,0,0,0,4,1,2,2) | (1,1,2,0,0,0,0,0) | 7.268b | **6.231** | **6.647** | **6.484** | **6.429** | **6.580** | **6.675** |
| 1E1g(,3s) | (1,0,0,0,2,1,2,1) | (1,0,0,0,0,1,1,0) | 5.902c | **6.570** | **6.697** | **6.758** | **6.754** | **6.505** | **6.555** |
| 1A2u(,3px,y) | (0,1,1,0,2,1,2,1) | (1,0,0,0,2,0,0,1) | 6.143d | **7.069** | **7.210** | **7.397** | **7.398** | **7.021** | **7.074** |
| 1E2u(,3px,y) | (0,1,1,0,2,1,2,1) | (1,0,0,0,2,0,0,1) | 6.210d | **7.118** | **7.261** | **7.450** | **7.451** | **7.077** | **7.127** |
| 1E2g(2,\*2) | (0,0,0,0,2,1,2,1) | (2,0,0,1,0,0,0,0) | 8.103a | **7.816**e | **8.314** | **8.550** | **8.512** | **8.162**e | **8.263** |
| 1A1g(2,\*2) | (0,0,0,0,2,1,2,1) | (3,0,0,1,0,0,0,0) | 11.444a | **9.326**e | **10.236** | **10.381** | **9.995** | **10.315**e | **10.468** |
| 3B1u(,\*) | (0,0,0,0,4,1,2,2) | (1,0,1,0,0,0,0,0) | 3.846b | **3.916** | **4.220** | **4.330** | **4.324** | **4.077** | **4.139** |
| 3E1u(,\*) | (0,0,0,0,4,1,2,2) | (1,1,1,0,0,0,0,0) | 4.850b | **4.513** | **4.889** | **4.944** | **4.922** | **4.800** | **4.866** |
| 3B2u(,\*) | (0,0,0,0,4,1,2,2) | (1,1,0,0,0,0,0,0) | 6.747b | **5.404** | **5.849** | **5.587** | **5.511** | **5.809** | **5.902** |

a Using reference (6e,6o) active space including valence  orbitals. b Using reference (6e,9o) active space including valence  and three 3pz orbitals. c Using reference (6e,7o) active space including valence  and 3s orbitals. d Using reference (6e,8o) active space including valence , 3px and 3py orbitals. e Level shift = 0.4 au.