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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1Ag(p,p-p\*,p\*) | (0,0,1,1,3,3,1,1) | (2,0,0,0,0,0,0,0) | 4.945a | **4.301** | **4.472** | **4.565** | **4.566** | **4.696** | **4.672** |
| 1B2g(n-p\*) | (0,0,1,1,3,3,1,1) | (1,0,0,0,0,1,0,0) | 6.539a | **5.005**b | **5.761** | **6.004** | **5.932** | **5.950**b | **6.028** |
| 1B1u(n-p\*)c | (0,0,1,1,3,3,1,1) | (1,0,0,0,1,0,0,0) | 6.543a | **5.002**b | **5.774** | **6.020** | **5.944** | **5.954**b | **6.036** |
| 1Ag(p-p\*) | (0,0,0,0,3,3,1,1) | (2,0,0,0,0,0,0,0) | 6.526d | **5.849** | **6.287** | **6.431** | **6.390** | **6.303** | **6.343** |
| 1Au(n-p\*) | (0,0,1,1,3,3,1,1) | (1,0,0,0,0,0,0,2) | 6.684a | **5.547**b | **6.210** | **6.548** | **6.502** | **6.352**b | **6.422** |
| 1B3g(n-p\*)e | (0,0,1,1,3,3,1,1) | (1,0,0,0,0,0,2,0) | 6.697a | **5.479**b | **6.234** | **6.574** | **6.530** | **6.492**b | **6.451** |

a Using reference (12e,10o) active space including valence  and the two nO orbitals. b Level shift = 0.4 au. c Denoted 1B3u in article using a different symmetry convention. d Using reference (8e,8o) active space including valence  orbitals. e Denoted 1B1g in article using a different symmetry convention.