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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,b3u,b2u,b1g,b1u,b2g,b3g,au) | State-average  (Ag,B3u,B2u,B1g,B1u,B2g,B3g,Au) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Ag(p-p\*) | (0,0,0,0,3,2,3,2) | (3,0,0,0,0,0,0,0) | 6.895 | **5.942**b | **6.793** | **6.958** | **6.900** | **6.748**b | **6.809** |

a Using reference (10e,10o) active space including valence  orbitals. b Level shift = 0.4 au.