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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,au,bu,bg) | State-average  (Ag,Au,Bu,Bg) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1Ag(p-p\*) | (0,3,0,3) | (2,0,0,0) | 5.618 | **5.171** | **5.571** | **5.667** | **5.636** | **5.472** | **5.556** |

a Using reference (6e,6o) active space including valence  orbitals.