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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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\*) | (0,4,0,4) | (2,0,0,0) | 4.879 | **4.326** | **4.741** | **4.814** | **4.783** | **4.680** | **4.751** |

a Using reference (8e,8o) active space including valence  orbitals.