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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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-p\*,p\*) | (2,2,2,2,1,1,1,1) | (2,0,0,0,0,0,0,0) | 4.217 | **3.971** | **4.039** | **4.086** | **4.056** | **4.031** | **4.041** |

a Using reference (12e,12o) active space including valence , σCC, σ\*CC orbitals.