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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1D(2s,2s-2p,2p) | (3,2,2,1,2,1,1,0) | (3,0,0,0,0,0,0,0) | 7.115a | **7.129** | **7.137** | **7.133** | **7.133** | **7.139** | **7.142** |

a Using reference (2e,12o) active space including full valence space plus 3p and 3d orbitals.