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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A1(p,p-p\*,p\*) | (0,3,0,2) | (2,0,0,0) | 5.013 | **4.580** | **4.798** | **4.785** | **4.760** | **4.753** | **4.792** |
| 1A1(p-p\*) | (0,3,0,2) | (3,0,0,0) | 7.814 | **5.979** | **6.650** | **6.484** | **6.368** | **6.622** | **6.760** |

a Using reference (4e,5o) active space including valence  orbitals.