**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of BO2.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 2Πu(,) | (3,2,2,0,3,1,1,0) | (0,1,1,0,0,1,1,0) | 2.604 | **2.268** | **2.309** | **2.350** | **2.282** | **2.326** | **2.336** |
| 2Σu+(s,) | (3,2,2,0,3,1,1,0) | (0,0,0,0,1,1,1,0) | 3.444 | **2.991** | **3.013** | **3.071** | **3.025** | **3.066** | **3.068** |
| 2Σg+(s,) | (3,2,2,0,3,1,1,0) | (1,0,0,0,0,1,1,0) | 4.255 | **3.773** | **3.809** | **3.901** | **3.823** | **3.860** | **3.866** |

a Using reference (15e,12o) full valence active space.