**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of H2BO.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 12B1(p,n) | (5,2,3,0) | (0,1,1,0) | 2.140 | **2.204** | **2.179** | **2.158** | **2.172** | **2.155** | **2.149** |
| 12A1(s,n) | (5,2,3,0) | (1,0,1,0) | 3.479 | **3.508** | **3.511** | **3.538** | **3.549** | **3.513** | **3.512** |
| 22B2(s,n) | (5,2,3,0) | (0,0,2,0) | 4.855 | **4.687** | **4.736** | **4.788** | **4.723** | **4.716** | **4.735** |
| 22B1(n,p\*) | (5,2,3,0) | (0,2,1,0) | 6.722 | **6.061** | **6.203** | **6.232** | **6.101** | **6.200** | **6.225** |
| 22A1(s\*,n) | (5,2,3,0) | (2,0,1,0) | 7.651 | **7.306** | **7.417** | **7.531** | **7.428** | **7.390** | **7.426** |
| 32B2(p,p\*)b | (5,2,3,0) | (0,0,3,0) | 7.596 | **7.441** | **7.631** | **7.724** | **7.675** | **7.622** | **7.665** |
| 14B2(p,p\*) | (5,2,3,0) | (0,0,2,0) | 6.813 | **6.652** | **6.820** | **7.078** | **6.883** | **6.826** | **6.856** |
| 14B1(s,p\*) | (5,2,3,0) | (0,1,1,0) | 8.495 | **7.969** | **8.177** | **8.176** | **8.081** | **8.104** | **8.176** |

a Using reference (11e,10o) full valence active space. b Involving strong double (np,np\*) character.