**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of BH2.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 12B1(s,) | (3,1,2,0) | (1,1,0,0) | 1.228a | **1.171** | **1.185** | **1.185** | **1.186** | **1.183** | **1.188** |
| 22A1(s,3s) | (4,1,2,0) | (2,0,0,0) | 5.284b | **5.674** | **5.651** | **5.626** | **5.628** | **5.702** | **5.692** |
| 12B2(s,s) | (3,1,2,0) | (1,0,1,0) | 6.181a | **6.357** | **6.374** | **6.403** | **6.392** | **6.410** | **6.414** |
| 12A2(s,) | (3,1,2,0) | (1,0,0,1) | 6.157a | **6.267** | **6.369** | **6.406** | **6.403** | **6.390** | **6.423** |
| 22B2(s,3py) | (3,1,3,0) | (1,0,2,0) | 6.018c | **6.536** | **6.485** | **6.462** | **6.475** | **6.550** | **6.529** |
| 32A1(s,3pz) | (5,1,2,0) | (3,0,0,0) | 6.140d | **6.653** | **6.613** | **6.607** | **6.618** | **6.693** | **6.674** |
| 22B1(s,3px) | (3,2,2,0) | (1,2,0,0) | 6.448e | **6.827** | **6.811** | **6.777** | **6.772** | **6.849** | **6.845** |
| 22A2(s,) | (3,1,2,0) | (1,0,0,2) | 7.202a | **6.828** | **7.018** | **7.018** | **6.986** | **6.961** | **7.029** |
| 14A2(s,) | (3,1,2,0) | (1,0,0,1) | 5.230a | **5.230** | **5.347** | **5.356** | **5.348** | **5.340** | **5.381** |

a Using reference (5e,6o) full valence active space. b Using reference (5e,7o) full valence active space plus one 3s orbital. c Using reference (5e,7o) full valence active space plus one 3py orbital. d Using reference (5e,8o) full valence active space plus one 3s and one 3pz orbital.e Using reference (5e,7o) full valence active space plus one 3px orbital.