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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 2Π(s\*,p) | (3,1,1,0) | (1,1,1,0) | 2.585a | **2.502** | **2.527** | **2.512** | **2.509** | **2.508** | **2.521** |
| 2Σ+(s\*,3s) | (4,1,1,0) | (3,0,0,0) | 5.397b | **5.513** | **5.515** | **5.495** | **5.483** | **5.524** | **5.527** |
| 2Σ+(s,s\*) | (4,1,1,0) | (3,0,0,0) | 5.520b | **5.709** | **5.768** | **5.744** | **5.730** | **5.778** | **5.806** |
| 2Σ+(s\*,3pz) | (5,1,1,0) | (4,0,0,0) | 6.004c | **6.134** | **6.144** | **6.125** | **6.110** | **6.158** | **6.164** |
| 2Π(s\*,3px,y) | (3,3,3,0) | (1,5,5,0) | 6.216d | **6.352** | **6.349** | **6.335** | **6.332** | **6.364** | **6.364** |
| 2Σ+(s\*,3dz2) | (6,1,1,0) | (5,0,0,0) | 7.166e | **7.138** | **7.172** | **7.138** | **7.110** | **7.160** | **7.176** |
| 2Π(s\*,3p’x,y) | (3,3,3,0) | (1,5,5,0) | 7.211d | **7.229** | **7.312** | **7.298** | **7.284** | **7.283** | **7.322** |
| 2Σ+(s\*,3p’z) | (7,1,1,0) | (6,0,0,0) | 7.229f | **7.425** | **7.409** | **7.412** | **7.414** | **7.446** | **7.437** |
| 2D(s\*,3dxy,x2–y2) | (4,1,1,1) | (2,0,0,1) | 7.730g | **7.814** | **7.809** | **7.810** | **7.811** | **7.822** | **7.820** |
| 2Π(s,p) | (3,3,3,0) | (1,5,5,0) | 7.817d | **7.691** | **7.827** | **7.802** | **7.776** | **7.778** | **7.834** |
| 4Π(s,p) | (3,1,1,0) | (1,1,1,0) | 5.490a | **5.795** | **5.826** | **5.808** | **5.812** | **5.840** | **5.858** |

a Using reference (3e,5o) full valence active space. b Using reference (3e,6o) full valence active space plus one 3s orbital. c Using reference (3e,7o) full valence active space plus one 3s and one 3pz orbitals. d Using reference (3e,9o) full valence active space plus two 3px and two 3py orbitals. e Using reference (3e,8o) full valence active space plus one 3s, one 3pz and one 3dz2 orbitals. f Using reference (3e,9o) full valence active space plus one 3s, two 3pz and one 3dz2 orbitals. g Using reference (3e,7o) full valence active space plus one 3dxy and one 3dx2–y2 orbitals.