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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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(n(Be),p\*) | (4,4,4,0) | (1,2,2,0) | 4.228a | **4.161** | **4.171** | **4.181** | **4.174** | **4.163** | **4.166** |
| 2Σ+(n(Be),Ryd) | (7,2,2,0) | (4,0,0,0) | 6.202b | **6.172** | **6.187** | **6.215** | **6.218** | **6.211** | **6.209** |
| 2Σ+(n(Be),Ryd) | (7,2,2,0) | (4,0,0,0) | 6.053b | **6.211** | **6.198** | **6.190** | **6.221** | **6.232** | **6.225** |
| 2Π(n(Be),3px,y) | (4,4,4,0) | (1,2,2,0) | 7.004a | **7.081** | **7.082** | **7.079** | **7.091** | **7.098** | **7.097** |
| 2Σ+(n(Be),Ryd) | (7,2,2,0) | (4,0,0,0) | 7.584b | **7.691** | **7.684** | **7.691** | **7.715** | **7.717** | **7.711** |

a Using reference (9e,12o) full valence active space plus two 3px and two 3py orbitals. b Using reference (9e,11o) full valence active space plus one 3s, one 3pz and one 3dz2 orbitals.