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

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA  (9 core)b | CASPT2  IPEA  (9 core)b | CASPT2  NOIPEA  (5 core)c | CASPT2  IPEA  (5 core)c | SC-NEVPT2  (9 core)b | PC-  NEVPT2  (9 core)b | SC-NEVPT2  (5 core)c | PC-  NEVPT2  (5 core)c |
| 1Δ | (5,2,2,1) | (2,0,0,1) | 0.490 | **0.514** | **0.515** | **0.562** | **0.582** | **0.532** | **0.535** | **0.590** | **0.596** |
| 1Π | (5,2,2,1) | (1,1,1,0) | 0.814 | **0.742** | **0.764** | **0.740** | **0.794** | **0.774** | **0.769** | **0.772** | **0.769** |
| 1Σ+ | (5,2,2,1) | (2,0,0,0) | 2.310 | **1.920** | **2.040** | **1.683** | **1.868** | **2.003** | **1.983** | **1.766** | **1.744** |
| 1Π | (5,2,2,1) | (1,2,2,0) | 2.115 | **2.077** | **2.129** | **2.040** | **2.149** | **2.153** | **2.149** | **2.202** | **2.199** |
| 3Δ | (5,2,2,1) | (2,0,0,1) | 0.270 | **0.278** | **0.280** | **0.271** | **0.294** | **0.293** | **0.295** | **0.301** | **0.306** |
| 3Π | (5,2,2,1) | (1,1,1,0) | 0.537 | **0.496** | **0.510** | **0.483** | **0.528** | **0.523** | **0.523** | **0.510** | **0.511** |
| 3Σ+ | (5,2,2,1) | (2,0,0,0) | 0.833 | **0.785** | **0.813** | **0.804** | **0.865** | **0.825** | **0.827** | **0.887** | **0.890** |
| 3Π | (5,2,2,1) | (1,2,2,0) | 1.812 | **1.809** | **1.853** | **1.878** | **1.950** | **1.842** | **1.839** | **1.966** | **1.964** |

a All calculations using a (4e,10o) active space including 4s, 3d, 4p of Sc and 1s of H.

b Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Sc (5,2,2,0).

c Core orbitals not correlated at PT2 level: 1s, 2s, 2p of Sc (3,1,1,0).