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

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCFa | CASPT2  NOIPEA  (10 core)b | CASPT2  IPEA  (10 core)b | CASPT2  NOIPEA  (6 core)c | CASPT2  IPEA  (6 core)c | SC-NEVPT2  (10 core)b | PC-  NEVPT2  (10 core)b | SC-NEVPT2  (6 core)c | PC-  NEVPT2  (6 core)c |
| 1Δ | (5,2,2,1) | (2,0,0,1) | 0.506 | **0.550** | **0.554** | **0.598** | **0.631** | **0.568** | **0.584** | **0.569** | **0.594** |
| 1Π | (5,2,2,1) | (1,1,1,0) | 1.265 | **1.318** | **1.344** | **1.330** | **1.404** | **1.394** | **1.409** | **1.307** | **1.322** |
| 1Σ+ | (5,2,2,1) | (2,0,0,0) | 2.490 | **2.278** | **2.366** | **2.004** | **2.169** | **2.390** | **2.382** | **2.071** | **2.055** |
| 1Π | (5,2,2,1) | (1,2,2,0) | 2.337 | **2.421** | **2.478** | **2.468** | **2.591** | **2.560** | **2.569** | **2.638** | **2.650** |
| 3Δ | (5,2,2,1) | (2,0,0,1) | 0.262 | **0.288** | **0.292** | **0.279** | **0.313** | **0.312** | **0.318** | **0.257** | **0.267** |
| 3Π | (5,2,2,1) | (1,1,1,0) | 0.840 | **0.885** | **0.896** | **0.860** | **0.908** | **0.928** | **0.933** | **0.816** | **0.819** |
| 3Σ+ | (5,2,2,1) | (2,0,0,0) | 1.391 | **1.366** | **1.389** | **1.302** | **1.362** | **1.396** | **1.408** | **1.311** | **1.323** |
| 3Π | (5,2,2,1) | (1,2,2,0) | 2.263 | **2.393** | **2.422** | **2.427** | **2.516** | **2.496** | **2.503** | **2.504** | **2.513** |

a Using a reference (4e,10o) active space including 4s, 3d, 4p of Sc and 2pz of F.

b Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Sc and 1s of F (6,2,2,0).

c Core orbitals not correlated at PT2 level: 1s, 2s, 2p of Sc and 1s of F (4,1,1,0).