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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA  (14 core)c | CASPT2  IPEA  (14 core)c | SC-NEVPT2  (14 core)c | PC-  NEVPT2  (14 core)c |
| 2Δ | (5,2,2,1)a  (6,3,3,2)b | (2,0,0,1)  (2,0,0,1) | 1.059  0.821 | **0.977**  **1.009** | **0.935**  **0.936** | **0.911** | **0.934** |
| 2Π | (5,2,2,1)a  (6,3,3,2)b | (1,1,1,0)  (1,1,1,0) | 2.032  1.512 | **1.627**  **1.498** | **1.739**  **1.476** | **1.736**  **1.485** | **1.608**  **1.434** |
| 2Σ+ | (5,2,2,1)a  (6,3,3,2)b | (2,0,0,0)  (2,0,0,0) | 1.680  1.768 | **1.518**  **1.587** | **1.566**  **1.634** | **1.523**  **1.633** | **1.566**  **1.574** |
| 2Π | (5,2,2,1)a  (6,3,3,2)b | (1,2,2,0)  (1,2,2,0) | 2.583  2.229 | **2.299**  **2.280** | **2.368**  **2.215** | **2.362** | **2.338** |

a Using a reference (9e,10o) active space including 4s, 3d of Sc and 3s, 3p of S.

b Using a reference (9e,14o) active space including 4s, 3d of Sc and 3s, 3p, four 3d of S.

c Core orbitals not correlated at PT2 level: 1s, 2s, 2p, 3s, 3p of Sc and 1s, 2s, 2p of S (8,3,3,0).