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

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a1,b1,b2,a2) | State-average  (A1,B1,B2,A2) | CASSCF | CASPT2  NOIPEA  (10 core)c | CASPT2  IPEA  (10 core)c | CASPT2  NOIPEA  (6 core)d | CASPT2  IPEA  (6 core)d | SC-NEVPT2  (10 core)c | PC-  NEVPT2  (10 core)c | SC-NEVPT2  (6 core)d | PC-  NEVPT2  (6 core)d |
| 2Δ | (6,3,3,1)a | (2,0,0,1) | 1.855 | **1.812** | **1.794** | **1.678** | **1.684** | **1.773** | **1.797** |  |  |
| 2Π | (6,3,3,1)a | (1,1,1,0) | 2.074 | **2.029** | **2.037** | **2.049** | **2.059** | **2.049** | **2.040** |  |  |
| 2Σ+ | (7,3,3,1)b | (2,0,0,0) | 2.688 | **2.550** | **2.569** | **2.536** | **2.559** | **2.614** | **2.591** | **2.609** | **2.583** |
| 2Π | (6,3,3,1)a | (1,2,2,0) | 3.349 | **3.655** | **3.632** | **3.601** | **3.583** | **3.527** | **3.502** |  |  |

a Using a reference (9e,13o) active space including 4s, 3d, 4p of Sc and 2s, 2p of O.

b Using a reference (9e,14o) active space including 4s, 3d, 4p, 4dz2 of Sc and 2s, 2p of O.

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

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