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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 2Σ+(s,2px,y) | (3,1,1,0) | (1,1,1,0) | 4.546a | **4.180** | **4.174** | **4.183** | **4.154** | **4.168** | **4.176** |
| 2Σ–(2px,y,3s) | (4,1,1,0) | (0,1,1,1) | 7.388b | **7.721** | **7.916** | **8.001** | **8.012** | **7.947** | **7.961** |
| 2D(2px,y,3s) | (4,1,1,0) | (1,1,1,1) | 9.112b | **9.544** | **9.661** | **9.766** | **9.835** | **9.732** | **9.726** |
| 4Σ–(2px,y,3s) | (4,1,1,0) | (0,1,1,1) | 6.858b | **7.208** | **7.393** | **7.481** | **7.492** | **7.414** | **7.431** |

a Using reference (7e,5o) full valence active space. b Using reference (7e,6o) full valence active space plus one 3s orbital.