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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (a’,a”) | State-average  (A’,A”) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1A’’(,3s) | (2,5) | (1,3) | 5.043a | **5.662** | **5.876** | **5.925** | **5.931** | **5.683** | **5.735** |
| 1A’(,3p) | (0,9) | (3,0) | 6.180b | **6.452** | **6.686** | **6.766** | **6.730** | **6.555** | **6.609** |
| 1A’’(,3p) | (4,6) | (1,7) | 5.433c | **6.465** | **6.574** | **6.797** | **6.831** | **6.439** | **6.467** |
| 1A’’(n,\*) | (2,5) | (1,3) | 7.131a | **6.566** | **6.941** | **7.007** | **6.960** | **6.849** | **6.915** |
| 1A’’(,3p) | (4,6) | (1,7) | 5.735c | **6.672** | **6.870** | **7.171** | **7.208** | **6.767** | **6.795** |
| 1A’’(,3s) | (4,6) | (1,7) | 5.680c | **6.696** | **6.893** | **7.253** | **7.298** | **6.794** | **6.816** |
| 1A’(,\*) | (0,9) | (3,0) | 6.735b | **6.461** | **6.880** | **7.060** | **7.003** | **6.833** | **6.890** |
| 1A’(n,3s) | (2,5) | (2,0) | 6.361a | **6.909** | **7.096** | **7.197** | **7.202** | **7.068** | **7.086** |
| 3A’(,\*) | (0,9) | (3,0) | 4.552b | **4.526** | **4.784** | **4.879** | **4.855** | **4.676** | **4.730** |
| 3A’’(,3s) | (2,5) | (1,3) | 5.034a | **5.633** | **5.856** | **5.903** | **5.906** | **5.663** | **5.716** |
| 3A’(,\*) | (0,9) | (3,0) | 5.685b | **5.482** | **5.848** | **5.955** | **5.909** | **5.721** | **5.799** |
| 3A’’(n,\*) | (2,5) | (1,3) | 6.578a | **6.097** | **6.443** | **6.513** | **6.480** | **6.369** | **6.428** |

a Using reference (8e,7o) active space including valence , nN and 3s orbitals. b Using reference (6e,9o) active space including valence  and four 3pz orbitals. c Using reference (8e,10o) active space including valence , nN, 3s and three 3p orbitals.