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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| 1B1(n,\*) | (1,4,1,2) | (1,1,0,0) | 4.846a | **4.066** | **4.445** | **4.596** | **4.548** | **4.554** | **4.579** |
| 1A2(n,\*) | (1,4,1,2) | (1,0,0,1) | 5.515a | **4.362** | **4.802** | **4.899** | **4.843** | **5.001** | **5.016** |
| 1B2(,\*) | (0,6,0,3) | (1,0,1,0) | 5.275b | **4.982** | **5.417** | **5.605** | **5.573** | **5.362** | **5.410** |
| 1A2(n,\*) | (1,4,1,2) | (1,0,0,2) | 6.702a | **5.322** | **5.917** | **6.104** | **6.017** | **6.104** | **6.157** |
| 1B1(n,\*) | (1,4,1,2) | (1,2,0,0) | 7.204a | **5.653** | **6.307** | **6.490** | **6.404** | **6.532** | **6.580** |
| 1B2(n,3s) | (2,4,1,2) | (1,0,2,0) | 6.863c | **6.502** | **6.853** | **6.832** | **6.773** | **6.859** | **6.891** |
| 1A1(,\*) | (0,6,0,3) | (2,0,0,0) | 7.687b | **6.945** | **7.309** | **7.252** | **7.165** | **7.224** | **7.294** |
| 3B1(n,\*) | (1,4,1,2) | (1,1,0,0) | 4.449a | **3.673** | **4.050** | **4.207** | **4.168** | **4.183** | **4.205** |
| 3A1(,\*) | (0,6,0,3) | (2,0,0,0) | 4.225b | **4.248** | **4.570** | **4.726** | **4.712** | **4.444** | **4.506** |
| 3A2(n,\*) | (1,4,1,2) | (1,0,0,1) | 5.201a | **4.162** | **4.629** | **4.760** | **4.715** | **4.785** | **4.813** |
| 3B2(,\*) | (0,4,0,2) | (1,0,1,0) | 5.100d | **4.603** | **5.010** | **5.113** | **5.080** | **4.970** | **5.028** |

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