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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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) | (1,2,0,0) | 5.425a | **4.809** | **5.153** | **5.192** | **5.146** | **5.133** | **5.180** |
| 1B2(,\*) | (0,7,0,3) | (1,0,2,0) | 5.034b | **4.764** | **5.177** | **5.342** | **5.311** | **5.093** | **5.153** |
| 1A2(n,\*) | (2,4,0,2) | (1,0,0,2) | 6.298c | **5.029** | **5.457** | **5.351** | **5.289** | **5.593** | **5.632** |
| 1A1(,\*) | (0,4,0,2) | (2,0,0,0) | 7.899d | **6.269** | **6.921** | **6.801** | **6.690** | **6.927** | **7.036** |
| 1A1(n,3s) | (2,4,0,2) | (2,0,0,0) | 6.403c | **6.673** | **6.899** | **7.002** | **6.993** | **6.960** | **6.969** |
| 1A2(,3s) | (2,4,0,2) | (1,0,0,2) | 6.598c | **6.865** | **7.079** | **6.889** | **6.864** | **6.805** | **6.880** |
| 1B2(,\*) | (0,7,0,3) | (1,0,2,0) | 7.447b | **7.667** | **7.920** | **7.879** | **7.832** | **7.725** | **7.795** |
| 1B1(,3py) | (1,4,1,2) | (1,2,0,0) | 7.123a | **7.507** | **7.701** | **7.474** | **7.453** | **7.397** | **7.475** |
| 1A1(,\*) | (0,4,0,2) | (4,0,0,0) | 9.492d | **6.626** | **7.665** | **7.311** | **6.970** | **7.700** | **7.873** |
| 3A1(,\*) | (0,4,0,2) | (2,0,0,0) | 3.981d | **4.063** | **4.398** | **4.617** | **4.601** | **4.217** | **4.290** |
| 3B1(n,\*) | (1,4,0,2) | (1,1,0,0) | 4.648e | **4.206** | **4.478** | **4.598** | **4.577** | **4.552** | **4.572** |
| 3B2(,\*) | (0,7,0,3) | (1,0,2,0) | 4.826b | **4.533** | **4.856** | **4.910** | **4.876** | **4.744** | **4.813** |
| 3A1(,\*) | (0,4,0,2) | (3,0,0,0) | 5.107d | **4.634** | **5.091** | **5.223** | **5.190** | **5.020** | **5.088** |
| 3A2(n,\*) | (1,4,0,2) | (1,0,0,1) | 5.941e | **4.963** | **5.326** | **5.369** | **5.330** | **5.507** | **5.532** |
| 3B2(,\*) | (0,7,0,3) | (1,0,2,0) | 6.933b | **5.994** | **6.403** | **6.370** | **6.287** | **6.346** | **6.431** |

a Using reference (8e,8o) active space including valence , nN and 3py orbitals. b Using reference (6e,10o) active space including valence  and four 3px orbitals. c Using reference (8e,8o) active space including valence , nN and 3s orbitals. d Using reference (6e,6o) active space including valence  orbitals. e Using reference (8e,7o) active space including valence  and nN orbitals.