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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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,\*) | (1,3,1,3) | (1,1,0,0) | 4.289a | **3.360** | **3.739** | **3.839** | **3.801** | **3.921** | **3.935** |
| 1A2(n,\*) | (1,3,1,3) | (1,0,0,1) | 4.832a | **3.869** | **4.291** | **4.439** | **4.399** | **4.476** | **4.494** |
| 1A1(,\*) | (0,3,0,3) | (2,0,0,0) | 5.121b | **4.867** | **5.344** | **5.610** | **5.575** | **5.245** | **5.298** |
| 1A2(n,\*) | (1,3,1,3) | (1,0,0,2) | 6.259a | **5.190** | **5.727** | **5.946** | **5.882** | **5.894** | **5.929** |
| 1B2(n,3s) | (2,3,1,3) | (1,0,1,0) | 5.989c | **5.901** | **6.176** | **6.230** | **6.207** | **6.273** | **6.281** |
| 1B1(n,\*) | (1,3,1,3) | (1,2,0,0) | 7.156a | **5.941** | **6.502** | **6.709** | **6.638** | **6.671** | **6.716** |
| 1B2(,\*) | (0,5,0,4) | (1,0,1,0) | 7.543d | **6.818** | **7.263** | **7.268** | **7.189** | **7.166** | **7.246** |
| 3B1(n,\*) | (1,3,1,3) | (1,1,0,0) | 3.603a | **2.721** | **3.079** | **3.166** | **3.134** | **3.277** | **3.289** |
| 3A2(n,\*) | (1,3,1,3) | (1,0,0,1) | 4.493a | **3.592** | **4.010** | **4.174** | **4.144** | **4.175** | **4.200** |
| 3B2(,\*) | (0,3,0,3) | (1,0,1,0) | 3.934b | **4.126** | **4.437** | **4.664** | **4.650** | **4.238** | **4.304** |
| 3A1(,\*) | (0,3,0,3) | (2,0,0,0) | 4.928b | **4.475** | **4.874** | **4.972** | **4.941** | **4.828** | **4.885** |

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