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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| State | Active space  (ag,b3u,b2u,b1g,b1u,b2g,b3g,au) | State-average  (Ag,B3u,B2u,B1g,B1u,B2g,B3g,Au) | CASSCF | CASPT2  NOIPEA | CASPT2  IPEA | SC-NEVPT2 | PC-NEVPT2 | CASPT3  NOIPEA | CASPT3  IPEA |
| 1B3u(n,\*) | (1,2,1,1,1,2,1,1) | (1,1,0,0,0,0,0,0) | 2.995a | **1.911** | **2.313** | **2.402** | **2.347** | **2.533** | **2.543** |
| 1Au(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,0,0,1) | 4.375a | **3.004** | **3.494** | **3.629** | **3.576** | **3.777** | **3.775** |
| 1Ag(double) | (1,2,1,1,1,2,1,1) | (2,0,0,0,0,0,0,0) | 5.419a | **4.318** | **4.566** | **4.688** | **4.608** | **4.951** | **4.917** |
| 1B1g(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,1,0,0,0,0) | 5.406a | **4.332** | **4.828** | **5.019** | **4.953** | **4.998** | **5.019** |
| 1B2u(,\*) | (0,2,0,1,0,2,0,1) | (1,0,1,0,0,0,0,0) | 5.035b | **4.840** | **5.305** | **5.596** | **5.558** | **5.231** | **5.259** |
| 1B2g(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,1,0,0) | 5.433a | **4.904** | **5.378** | **5.677** | **5.634** | **5.379** | **5.415** |
| 1Au(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,0,0,2) | 6.366a | **4.916** | **5.507** | **5.701** | **5.619** | **5.801** | **5.803** |
| 1B3g(double) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,0,1,0) | 6.590a | **5.218** | **5.853** | **6.200** | **6.149** | **6.215** | **6.201** |
| 1B2g(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,2,0,0) | 6.792a | **5.178** | **5.959** | **6.211** | **6.135** | **6.279** | **6.268** |
| 1B1g(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,2,0,0,0,0) | 7.183a | **5.893**c | **6.587**c | **6.833** | **6.757** | **6.715**c | **6.794**c |
| 3B3u(n,\*) | (1,2,1,1,1,2,1,1) | (1,1,0,0,0,0,0,0) | 2.380a | **1.307** | **1.696** | **1.778** | **1.726** | **1.931** | **1.941** |
| 3Au(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,0,0,1) | 4.055a | **2.778** | **3.259** | **3.410** | **3.364** | **3.522** | **3.525** |
| 3B1g(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,1,0,0,0,0) | 4.662a | **3.623** | **4.102** | **4.293** | **4.243** | **4.300** | **4.316** |
| 3B1u(,\*) | (0,4,0,1,0,2,0,2) | (1,0,0,0,2,0,0,0) | 3.901d | **4.289** | **4.550** | **4.701** | **4.702** | **4.344** | **4.393** |
| 3B2u(,\*) | (0,2,0,1,0,2,0,1) | (1,0,1,0,0,0,0,0) | 4.676b | **4.199** | **4.555** | **4.608** | **4.577** | **4.552** | **4.595** |
| 3B2g(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,1,0,0) | 5.165a | **4.533** | **5.021** | **5.304** | **5.266** | **5.071** | **5.101** |
| 3Au(n,\*) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,0,0,2) | 6.117a | **4.435** | **5.068** | **5.217** | **5.132** | **5.410** | **5.415** |
| 3B3g(double) | (1,2,1,1,1,2,1,1) | (1,0,0,0,0,0,1,0) | 6.562a | **4.861** | **5.388** | **5.570** | **5.506** | **5.848** | **5.829** |
| 3B1u(,\*) | (0,4,0,1,0,2,0,2) | (1,0,0,0,2,0,0,0) | 5.322d | **5.078** | **5.464** | **5.589** | **5.558** | **5.391** | **5.436** |

a Using reference (14e,10o) active space including valence  and nN orbitals. b Using reference (6e,6o) active space including valence  orbitals. c Level shift = 0.4 au. d Using reference (6e,9o) active space including valence  and three 3px orbitals.