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

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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,\*) | (1,2,0,1,1,2,0,1) | (1,1,0,0,0,0,0,0) | 4.761a | **3.655** | **4.090** | **4.224** | **4.174** | **4.295** | **4.312** |
| 1Au(n,\*) | (1,2,0,1,1,2,0,1) | (1,0,0,0,0,0,0,1) | 5.903a | **4.257** | **4.762** | **4.816** | **4.766** | **5.096** | **5.102** |
| 1B2u(,\*) | (0,2,0,1,0,2,0,1) | (1,0,1,0,0,0,0,0) | 4.973b | **4.649** | **5.126** | **5.365** | **5.323** | **5.034** | **5.089** |
| 1B2g(n,\*) | (1,2,0,1,1,2,0,1) | (1,0,0,0,0,1,0,0) | 5.796a | **5.272** | **5.679** | **5.925** | **5.880** | **5.699** | **5.734** |
| 1Ag(n,3s) | (2,2,0,1,1,2,0,1) | (2,0,0,0,0,0,0,0) | 6.693c | **6.271** | **6.655** | **6.733** | **6.699** | **6.803** | **6.810** |
| 1B1g(n,\*) | (1,2,0,1,1,2,0,1) | (1,0,0,1,0,0,0,0) | 7.159a | **6.068** | **6.614** | **6.799** | **6.752** | **6.757** | **6.779** |
| 1B1u(,\*) | (0,4,0,1,0,2,0,2) | (1,0,0,0,3,0,0,0) | 8.043d | **6.716** | **7.138** | **6.893** | **6.807** | **7.118** | **7.202** |
| 1B1g(,3s) | (1,2,0,1,0,2,0,1) | (1,0,0,1,0,0,0,0) | 6.727e | **7.267** | **7.414** | **7.334** | **7.329** | **7.177** | **7.236** |
| 1B2u(n,3py) | (1,2,1,1,1,2,0,1) | (1,0,2,0,0,0,0,0) | 7.495f | **6.933** | **7.339** | **7.287** | **7.249** | **7.396** | **7.427** |
| 1B1u(n,3pz) | (1,2,0,1,2,2,0,1) | (1,0,0,0,3,0,0,0) | 7.831g | **7.085** | **7.555** | **7.489** | **7.419** | **7.591** | **7.644** |
| 1B1u(,\*) | (0,4,0,1,0,2,0,2) | (1,0,0,0,3,0,0,0) | 9.646d | **7.962** | **8.589** | **8.424** | **8.247** | **8.575** | **8.679** |
| 3B3u(n,\*) | (1,2,0,1,1,2,0,1) | (1,1,0,0,0,0,0,0) | 4.156a | **3.083** | **3.485** | **3.606** | **3.561** | **3.707** | **3.723** |
| 3B1u(,\*) | (0,4,0,1,0,2,0,2) | (1,0,0,0,2,0,0,0) | 3.982d | **4.149** | **4.439** | **4.578** | **4.573** | **4.284** | **4.339** |
| 3B2u(,\*) | (0,2,0,1,0,2,0,1) | (1,0,1,0,0,0,0,0) | 4.623b | **4.092** | **4.437** | **4.456** | **4.421** | **4.406** | **4.465** |
| 3Au(n,\*) | (1,2,0,1,1,2,0,1) | (1,0,0,0,0,0,0,1) | 5.845a | **4.213** | **4.732** | **4.798** | **4.751** | **5.069** | **5.073** |
| 3B2g(n,\*) | (1,2,0,1,1,2,0,1) | (1,0,0,0,0,1,0,0) | 5.245a | **4.658** | **5.043** | **5.255** | **5.214** | **5.109** | **5.138** |
| 3B1u(,\*) | (0,4,0,1,0,2,0,2) | (1,0,0,0,2,0,0,0) | 5.149d | **4.921** | **5.286** | **5.373** | **5.349** | **5.194** | **5.248** |

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  and three 3px orbitals. e Using reference (6e,7o) active space including valence  and 3s orbitals. f Using reference (10e,9o) active space including valence , nN and 3py orbitals. g Using reference (10e,9o) active space including valence , nN and 3pz orbitals.