**Table.** MRPT/aug-cc-pVTZ vertical transition energies (eV) of NO2.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 | MS-PT2  IPEA | XMS-PT2  IPEA |
| 12B1(n,p\*) | (5,2,4,1) | (1,1,0,0) | 2.933a | **2.821** | **2.838** | **2.840** | **2.861** | **2.866** | **2.852** | **–** | **–** |
| 12B2(n,n) | (5,2,4,1) | (1,0,1,0) | 3.387a | **3.383** | **3.409** | **3.441** | **3.436** | **3.385** | **3.385** | **–** | **–** |
| 12A2(p,n) | (5,2,4,1) | (1,0,0,1) | 3.541a | **3.852** | **3.802** | **3.728** | **3.763** | **3.687** | **3.693** | **–** | **–** |
| 22A2(n,p\*) | (5,2,4,1) | (1,0,0,2) | 5.798a | **5.338** | **5.546** | **5.614** | **5.592** | **5.526** | **5.553** | **–** | **–** |
| 22B2(p,p\*)b | (5,2,4,1) | (1,0,2,0) | 6.286a | **5.734** | **5.942** | **6.024** | **5.993** | **5.941** | **5.966** | **–** | **–** |
| 32A2(n,p\*)b | (5,2,4,1) | (1,0,0,3) | 7.175a | **6.509** | **6.772** | **6.882** | **6.827** | **6.804** | **6.821** | **–** | **–** |
| 22A1(n,3s) | (6,2,4,1) | (2,0,0,0) | 6.639c | **7.354** | **7.407** | **7.595** | **7.722** | **7.578** | **7.509** | **–** | **–** |
| 32B2(p,p\*)d | (5,2,4,1) | (1,0,5,0) | 8.420a | **7.657**e | **7.957** | **8.116** | **8.002** | **7.996**e | **8.028** | **7.854** | **7.835** |
| 22B1(p,n) | (5,2,4,1) | (1,2,0,0) | 8.109a | **8.066** | **8.133** | **8.107** | **8.090** | **8.013** | **8.033** | **–** | **–** |
| 32A1(n,n) | (6,2,4,1) | (3,0,0,0) | 8.297c | **7.944** | **8.061** | **8.170** | **8.131** | **8.066** | **8.078** | **–** | **–** |
| 14A2(n,p\*) | (5,2,4,1) | (1,0,0,1) | 4.775a | **4.438** | **4.609** | **4.669** | **4.664** | **4.613** | **4.628** | **–** | **–** |
| 14B2(p,p\*) | (5,2,4,1) | (1,0,1,0) | 4.957a | **4.600** | **4.775** | **4.841** | **4.827** | **4.778** | **4.795** | **–** | **–** |

a Using reference (17e,12o) full valence active space. b Strong (>50%) double excitation character. c Using reference (17e,13o) full valence active space plus one 3s orbital. d Mixed withsignificant (s,n) character. e Using a level shift of 0.4 a.u.