

CN parameters copy

| | | | | | | | | | |
|------------------|---------------|---------------|---------------|---------------|-----------------------|-------------------|-------------------|----------|----------|
| pi | nu 0 | e | h bar | m sub e | a0 | c | mp | | |
| 3.1415927E+00 | 1.2566371E-06 | 1.6021892E-19 | 1.0545888E-34 | 9.1095345E-31 | 5.2917706E-11 | 2.9979246E+08 | 1.6726486E-27 | | |
| | epsilon 0 | uB | | | aH | | md | | |
| | 8.85E-12 | 9.27E-24 | | | 5.29465E-11 | | 3.3435860E-27 | | |
| | | | r C-N | | | | | | |
| | r3 | | 1.17181E-10 | crc | aD | | | | |
| | 0.5902 | | | | 5.29321E-11 | | | | |
| a (m) | b (m) | c' (m) | 2c' (m) | eccentricity | C r 2p (r5) | C r6 (initial) | | | |
| 1.29853E-10 | 1.15871E-10 | 5.86153E-11 | 1.17231E-10 | 0.45140 | 0.88084 | 1.20654 | | | |
| 2.45386 | 2.18964 | 1.10767 | 2.21534 | | | | | | |
| | | | | a-c' | N r 2p (r6) | N r7 (initial) | | | |
| | | | | 1.346192343 | 0.76366 | 0.93084 | | | |
| 1 | | | | | | | | | |
| 0.5 | | | | | | | | | |
| | Ve (eV) | Vp (eV) | T (eV) | Vm (eV) | Et (eV) H2-type MO | E of H(a0) | E of H(a0) | E(C) | E(C+) |
| | -23.90105 | 12.28328 | 4.87009 | -2.43504 | -9.18273 | 13.60580 | 13.60580 | 11.2603 | 24.38332 |
| eV/cm^-1 | | | | | | delta 1/r (a0^-1) | delta 1/r (a0^-1) | E(N) | E(N+) |
| 0.000123985 | | | | | | 0.30647 | 0.23518 | 14.53414 | 29.6013 |
| | | | | | Et (eV) sum of MO & A | delta E C AO | delta E N AO | | |
| Evib (0) (cm^-1) | w (s-1) | EK (eV) | | | -33.52149 | -8.33948 | -15.99929 | | |
| 2068.59 | 1.07550E+16 | 7.07912 | | | | | | | |
| Evib (0) (eV) | | | | | | | | | |
| 0.25647 | | | | | -25.79444 | | | | |
| | EDoppler (eV) | CN Eocs (eV) | CN ET (eV) | CN ED (eV) | ED (kcal/mole) | Rel. Error | | | |
| | 0.17645 | 0.04821 | 33.56970 | 7.77526 | 179.30477 | -0.00028 | | | |
| | | | | | | | | | |
| kcal/mole/ev | | | | | | | | | |
| 4.336340E-02 | | | | | | | | | |
| Do N-O | | | | | | | | | |
| 750.0 | 298K (CRC) | | | | | | | | |
| 179.2543021 | | | | | | | | | |
| 7.7731 | | | | | | | | | |
| | | | | | | | | | |
| C | | | | | | | | | |
| Z | r3 | denom | 1st term | 2nd term | num | 3 rd term | r5 | | |
| 6 | 0.84317 | 2.51355326 | 0.397843171 | 0.158279189 | 4.277451462 | 1.701754855 | 0.88084 | | |
| | | | | | | | | | |
| N | | | | | | | | | |
| Z | r3 | denom | 1st term | 2nd term | num | 3 rd term | r6 | | |
| 7 | 0.69385 | 2.534919283 | 0.309080314 | 0.095530641 | 3.519942238 | 1.388581586 | 0.76366 | | |