| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | | |
| | | | | | | | | | | | | |
| 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 | | | | | |
| | | | | | | | | | | | | |
| | | | transition state (Tucker) | r C | aD | | | E of H(a0) | | | | |
| | | | 2.3 E-10 | 1.20654 | 5.29321E-11 | | | 13.605804 | | | | |
| a (m) | b (m) | c' (m) | 2c' (m) | eccentricity | R of Csp3 initial | R of C sp3 final | E coul sp3 | E Cl | Hybridization Factor | | | |
| 1.96252E-10 | 1.60448E-10 | 1.13010E-10 | 2.26020E-10 | 0.57584 | 0.91771 | 0.87495 | 14.82575 | -12.96764 | 0.91771432 | | | |
| 3.70862 | 3.03202 | 2.13558 | 4.27117 | | r (Cla) initial | r (Cla) final | | E Cl- | C HO to Cl hybridization factor | | | |
| | | | | | 2.68720 | 0.89582 | | -3.612724 | 0.81317 | | | |
| | | | | | r (Clb) initial | r (Clb) final | | E tolal Cl- | | | | |
| 2.00000 | | | | | 1.05158 | 0.89582 | | -16.58036 | | | | |
| 1.229761809 | | | | | | | | | | | | |
| | Ve (eV) | Vp (eV) | T (eV) | Vm (eV) | Et (eV) | E initial of Csp3 | E initial of Csp3 | E initial of Csp3 | delta E C (C-Cla) | delta E C (C-Clb) | | |
| Evib C-Cl (cm^-1) | -33.44629 | 12.74200 | 4.50926 | -2.25463 | -48.21577 | -14.63489 | -14.63489 | -14.63489 | -0.36229 | -0.36229 | | |
| 650 | Herzberg | | | delta Et(H2 MO) and E final of Csp3 | | | | | 152.34026 | r sp3 | E sp3 Final | |
| Evib C-Cl (eV) | | | | 16.07130 | -48.21573 | E final of Csp3 C-C | E final of Csp3 C=C | E final of Csp3 | | 0.87495 | 15.55033 | |
| 0.08059 | | | | | matchH2+Cl- | -15.35946 | -15.76868 | -15.56407 | | | 15.35946 | |
| | | | | | | | | | delta E Cla (Cla-C) | | | |
| eV/cm^-1 | w (s-1) | EK (eV) | | | Et (eV) sum of MO &AOs | E(eV) delta Csp3 C-C | E(eV) delta Csp3 C=C | E(eV) delta Csp3 | -0.36229 | | | |
| 0.000123985 | 3.69097E+15 | 2.42946 | | | -49.66491 | -0.72457 | -1.13379 | -0.92918 | | r sp3 | E sp3 Final | |
| kcal/mole/eV | | | | | | | Total E(eV) delta Csp3 C-C + C=C | 2X E(eV) delta Csp3 | | 0.89582 | 15.18804 | |
| 4.336340E-02 | | | | | | | -1.85837 | -1.85836 | | | | |
| kJ/mole/eV | | | | | | Avg E final of Csp3 | Avg E(eV) delta Csp3 | | delta E Clb (Clb-C) | | | |
| 0.010364101 | | | | | Emag | -15.56407 | -0.92918 | | -0.36229 | | | |
| | | | | C-Cl total bond E (eV) | 0.14803 | | | | | r sp3 | E sp3 Final | |
| | | | | 3.77116 | | | Et (eV) sum of AOs | | | 0.89582 | 15.18804 | |
| | | | | | | | -1.44915 | | | | | |
| | EDoppler (eV) | C-Cl Eocs (eV) | C-Cl ET (eV) | C-Cl total bond E (eV) | C-Cl total bond E (kcal/mole) | | | Et (eV) C HO to C-Cla bond | Et (eV) Cla AO to C-Cla bond | Et (eV) C HO to C-Clb bond | Et (eV) Clb AO to C-Clb bond | |
| | 0.07657 | 0.03628 | 49.73747 | 3.73930 | 86.23168 | | | -0.36229 | -0.36229 | -0.36229 | -0.36229 | |
| | | | | Delta (eV) | Delta (kcal/mole) | | | | | | | |
| | | | | -0.03186 | -0.73473 | | | | | | | |
| | | | | | | | | | | | | |
| | | | | | Cl-C bond intercept parameters | | | | | | | |
| | | | | | | | | | | | | |
| | | | angle of intersection with C | | | angle of intersection with Cla | | | angle of intersection with Clb | | | |
| | | | 3.183388284 | | | 3.068764188 | | | 3.068764188 | | | |
| | | | #NUM! | | | #NUM! | | | #NUM! | | | |
| | | theta prime | #NUM! | | theta prime | #NUM! | | theta prime | #NUM! | | | |
| | | theta C | #NUM! | | theta Cla | #NUM! | | theta Clb | #NUM! | | | |
| | | | #NUM! | | | #NUM! | | | #NUM! | | | |
| | | | #NUM! | | | #NUM! | | | #NUM! | | | |
| | | | #NUM! | | | #NUM! | | | #NUM! | | | |
| | | theta H2 MO | #NUM! | | theta H2 MO | #NUM! | | theta H2 MO | #NUM! | | | |
| | | dH2 MO | #NUM! | #NUM! | dH2 MO | #NUM! | #NUM! | dH2 MO | #NUM! | #NUM! | | |
| | | dC AO | #NUM! | #NUM! | dCla AO | #NUM! | #NUM! | dClb AO | #NUM! | #NUM! | | |
| | | | | | | | | | | | | |
| | r6 | E ele | exp | | | | | | | | | |
| | 1.20654 | 11.27671 | 11.2603 | | | | | | | | | |
| | Exp | | r sp3 | E sp3 | | | | | | | | |
| C3+ | 64.4939 | 10 | 0.919153831 | 14.80253 | | | | | | | | |
| C2+ | 47.8878 | | | 14.61166867 | | | | | | | | |
| C+ | 24.38332 | | | r3 | | | | | | | | |
| C | 11.2603 | | | 0.84317 | | | | | | | | |
| total | 148.02532 | | | | | | | | | | | |
| | | | Emag (a0) | Emag (r3) | | | | | | | | |
| | | | 0.114411043 | 0.19086 | | | | | | | | |
| | | | | | | | | | | | | |
| | | | Initial Parameters | | | | Final Parameters | | | | | |
| | Theory | | r sp3 | E sp3 | | Theory | | r sp3 | E sp3 | | | |
| C3+ | 64.3921 | 10 | 0.91771 | 14.825751 | C3+ | 64.3921 | 9.75 | 0.87495 | 15.55033 | | | |
| C2+ | 48.3125 | | | 14.63489 | C2+ | 48.3125 | | | 15.35946 | | | |
| C+ | 24.2762 | | | | C+ | 24.2762 | | | | | | |
| C | 11.27671 | | | | C2sp3 | 14.63489 | | | | | | |
| total | 148.25751 | | | | total | 151.61569 | | | | | | |
| | | | | | | | | | | | | |
| | | | | | | | Final Parameters | | | | | |
| | | | | | | Theory | | r sp3 | E sp3 | | | |
| | | | | | C3+ | 64.3921 | 9.5 | 0.85252 | 15.95955 | | | |
| | | | | | C2+ | 48.3125 | | | 15.76868 | | | |
| | | | | | C+ | 24.2762 | | | | | | |
| | | | | | C2sp3 | 14.63489 | | | | | | |
| | | | | | total | 151.61569 | | r sp3 | E sp3 | | | |
| | | | | | | | | 0.86359 | 15.75493 | | | |
| | | | | | | | | | 15.56407 | | | |