B1LYP/6-311G(df,p) f = 0.40,  12/9/08

This is input for linear regression.  In the first column are the
calculated diagonal efg's.  In the second are the corresponding
experimental nqcc's, followed by molecule and structure type.

```
 19.897546    -3438.17688     IF  re
 -9.948773     1719.08844
 -9.948773     1719.08844
 10.595592    -1828.059       HI  re
 -5.297796      914.0295
 -5.297796      914.0295
 11.034578    -1934.13022     CH3I  re
 -5.517289      967.06511
 -5.517289      967.06511
 13.744342    -2420.85        ICN  re
 -6.872171     1210.425
 -6.872171     1210.425
 12.778527    -2254.284       HCCI re
 -6.3892635    1127.142
 -6.3892635    1127.142
  6.849466    -1180.90        CH2I2 r*
 -0.860656      144.24
 -5.988810     1036.66
 16.908176    -2951.982       HOI ro
 -8.325914     1454.864
 -8.582262     1497.118
  9.385353    -1626.36        CH3-CHI-CH3  rs
 -5.067648      883.805
 -4.317705      742.555
  8.451029    -1478.06        CH3CH2I  rs
 -3.235915      564.56
 -5.215114      913.50
  5.568384     -940.00        OIO  ro
  0.480727     -109.84
 -6.049111     1049.84
  8.224867    -1421.9         CH2ICl ro
 -2.228064      392.6
 -5.996803     1029.3
 11.073747    -1912.39        INNN  ro
 -3.074568      537.11
 -7.999179     1375.28
 14.317382    -2451.02        I2  re
 -7.158691     1225.51
 -7.158691     1225.51
  6.316466    -1107.92        g-CH3-O-CH2I  rs
 -1.706692      303.255
 -4.609774      804.665
  9.398429    -1654.62        CH2=CHI  rs
 -4.448865      769.32
 -4.949564      885.30
  6.043130    -1041.2049      (CH3)3SiI ro
```

```
 -3.021565      520.60245
 -3.021565      520.60245

    ***************************************************

Following are the linear regression statistics.

Number of observations                  = 48
Mean of independent variable            = 5.551115e-17
Mean of dependent variable              = 9.473903e-15
Standard dev. of ind. variable          = 8.197694
Standard dev. of dep. variable          = 1424.965
Correlation coefficient                 = -0.999944
Regression coefficient (SLOPE)          = -173.8154
Standard error of coefficient           = 0.271311
t - value for coefficient               = -640.65
Regression constant (INTERCEPT)         = 1.91226e-14
Standard error of constant              = 2.200835
t - value for constant                  = 8.688793e-15

Analysis of variance
Source           d.f     Sum of squares  Mean Square     F
Regression         1    9.542401e+07    9.542401e+07    410432.4
Residual           46   10694.83        232.4963
Total              47   9.543471e+07

    ************************************************************

Finally, calculated diagonal nqcc's, molecule by molecule, are given below:

               b = -173.8154     Q = -0.73975110

      qii          Xii           expt       |diff|    %Diff

    19.897546  -3458.499900  -3438.1770   20.322899   0.591  IF
    -9.948773   1729.249950   1719.0885   10.161449   0.591
    -9.948773   1729.249950   1719.0885   10.161449   0.591

    10.595592  -1841.677053  -1828.0590   13.618093   0.745  HI
    -5.297796    920.838526    914.0295    6.809046   0.745
    -5.297796    920.838526    914.0295    6.809046   0.745

    11.034578  -1917.979580  -1934.1302   16.150669   0.835  CH3I
    -5.517289    958.989790    967.0651    8.075335   0.835
    -5.517289    958.989790    967.0651    8.075335   0.835

    13.744342  -2388.978291  -2420.8501   31.871807   1.317  ICN
    -6.872171   1194.489146   1210.4250   15.935903   1.317
    -6.872171   1194.489146   1210.4250   15.935903   1.317

    12.778527  -2221.104771  -2254.2839   33.179164   1.472  HCCI
    -6.389264   1110.552386   1127.1420   16.589582   1.472
```

| | | | | | |
|---|---|---|---|---|---|
| -6.389264 | 1110.552386 | 1127.1420 | 16.589582 | 1.472 | |
| 6.849466 | -1190.542667 | -1180.9000 | 9.642642 | 0.817 | CH2I2 |
| -0.860656 | 149.595266 | 144.2400 | 5.355261 | 3.713 | |
| -5.988810 | 1040.947401 | 1036.6600 | 4.287367 | 0.414 | |
| 16.908176 | -2938.901361 | -2951.9819 | 13.080573 | 0.443 | HOI |
| -8.325914 | 1447.172065 | 1454.8640 | 7.691948 | 0.529 | |
| -8.582262 | 1491.729295 | 1497.1180 | 5.388747 | 0.360 | |
| 9.385353 | -1631.318878 | -1626.3600 | 4.958893 | 0.305 | CH3-CHI-CH3 |
| -5.067648 | 880.835260 | 883.8050 | 2.969733 | 0.336 | |
| -4.317705 | 750.483618 | 742.5550 | 7.928625 | 1.068 | |
| 8.451029 | -1468.918979 | -1478.0601 | 9.141080 | 0.618 | CH3CH2I |
| -3.235915 | 562.451857 | 564.5600 | 2.108140 | 0.373 | |
| -5.215114 | 906.467122 | 913.5000 | 7.032878 | 0.770 | |
| 5.568384 | -967.870888 | -940.0000 | 27.870888 | 2.965 | OIO |
| 0.480727 | -83.557755 | -109.8400 | 26.282241 | 23.928 | |
| -6.049111 | 1051.428643 | 1049.8400 | 1.588677 | 0.151 | |
| 8.224867 | -1429.608541 | -1421.9000 | 7.708516 | 0.542 | CH2ICl |
| -2.228064 | 387.271834 | 392.6000 | 5.328173 | 1.357 | |
| -5.996803 | 1042.336707 | 1029.3000 | 13.036658 | 1.267 | |
| 11.073747 | -1924.787755 | -1912.3900 | 12.397740 | 0.648 | INN |
| -3.074568 | 534.407264 | 537.1100 | 2.702721 | 0.503 | |
| -7.999179 | 1390.380491 | 1375.2800 | 15.100462 | 1.098 | |
| 14.317382 | -2488.581467 | -2451.0200 | 37.561448 | 1.532 | I2 |
| -7.158691 | 1244.290734 | 1225.5100 | 18.780724 | 1.532 | |
| -7.158691 | 1244.290734 | 1225.5100 | 18.780724 | 1.532 | |
| 6.316466 | -1097.899059 | -1107.9200 | 10.020985 | 0.904 | g-CH3-O-CH2I |
| -1.706692 | 296.649351 | 303.2550 | 6.605654 | 2.178 | |
| -4.609774 | 801.249708 | 804.6650 | 3.415270 | 0.424 | |
| 9.398429 | -1633.591688 | -1654.6200 | 21.028307 | 1.271 | CH2=CHi |
| -4.448865 | 773.281246 | 769.3200 | 3.961239 | 0.515 | |
| -4.949564 | 860.310442 | 885.3000 | 24.989545 | 2.823 | |
| 6.043130 | -1050.389053 | -1041.2050 | 9.184097 | 0.882 | (CH3)3SiI |
| -3.021565 | 525.194527 | 520.6025 | 4.592049 | 0.882 | |
| -3.021565 | 525.194527 | 520.6025 | 4.592049 | 0.882 | |

Average Absolute Difference is 12.195819

Root Mean Square Difference is 14.926780

Average Absolute Expt NQCC is 1239.654054