# A short analysis of chemical bonds.

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**Abstract:** Nothing prohibits to give a definition of the multiplicity of bond: the multiplicity of bond is the energy of bond expressed in dimensionless units. It is easy to show, that relation multiplicity = f(L) and E = f(L), where multiplicity is multiplicity of bond, L – length of bond in Å, E – energy of bond in kj/mole will be described by function $y = a + b/x + c/x^2$ for any types of bond (C-N, C-O, C-S, N-N, N-O, O-O, C-P).

**Keywords:** chemical bond, bond energy, bond multiplicity, function.

## RESULTS AND DISCUSSION.

We'll find the dependence Multiplicity = f (L) and E = f (L) using function $y = a + b/x + c/x^2$ for C-O bonds, where the multiplicity — is multiplicity of bond, L – length of bond in Å, E – energy of bond in kj/mole.

For the length of bonds let us take the findings:

| | | | |
|---|---|---|---|
| $H_3C{-}OH$ | Lc-o = 1.434 Å | (6) | Multiplicity = 1 |
| $H_2C{=}O$ | Lc-o = 1.206 Å | (6) | Multiplicity = 2 |
| $C{\equiv}O$ | Lc-o = 1.12823 Å | (7) | Multiplicity = 3 |

$$Y = \frac{(y - y_1)}{(1/x - 1/x_1)}$$

$y = a + b/x + c/x^2$ $X = 1/x$

$b_1 = b + c/x_1$ $Y = b_1 + cX$

$$c = \frac{\left(\sum (1/x \cdot Y) - \left(\sum (1/x) \cdot \sum Y\right)/n\right)}{\left(\left(\sum 1/x^2\right) - \left(\sum (1/x)\right)^2/n\right)}$$

$$b_1 = \left(\sum Y\right)/n - c\left(\sum (1/x)\right)/n$$

n–the number of given value Y.

Let us find a from the equality: $\Sigma y = na + b\Sigma(1/x) + c\Sigma(1/x^2)$, when n = 3

Table 1. Calculation of ratios for relation Multiplicity = f(L) for C-O bond.

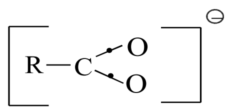
| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.43400 | 1 |
| | 0.82918740 | 0.68755174 | 7.58510526 | 6.28947368 | 1.20600 | 2 |
| | 0.88634410 | 0.78560586 | 10.58234503 | 9.37959905 | 1.12823 | 3 |
| ∑ | 1.71553149 | 1.47315760 | 18.16745029 | 15.66907273 | 3.76823 | 6 |

$1/x_1 = 0.69735007$  $x_1 = 1.43400$  $y_1 = 1$

$\Sigma(1/x^2) = 1.95945472$  $\Sigma(1/x) = 2.41288156$

c = 52.43899244  b = - 72.46498138  a = 26.03252883

$$\text{Multiplicity (C-O)} = 26.03252883 - \frac{72.46498138}{L} + \frac{52.43899244}{L^2}$$



Let us calculate from the equation:

$HCOO^{\ominus}\ Na^{\oplus}$  Lc-o = 1,27 Å  (8)  Multiplicity (L=1.27 Å) = 1.486

$NH_3^{\oplus}\ CH_2COO^{\ominus}$  Lc-o = 1,26 Å  (8)  Multiplicity (L=1.26 Å) = 1.551

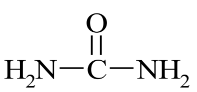
$CO_3^{2-}\ K_2^{2+}\ 3H_2O$  Lc-o = 1,29 Å  (9)  Multiplicity (Lc-o = 1.29 Å) = 1.370

$CO_3^{2-}\ Ca^{2+}$

O=CO  Lc-o = 1.162 Å  (4)  Multiplicity (Lc-o = 1.162 Å) = 2.507

So as we see, as expected theory of three-electrone bond, frequency of C-O bond in carboxylate anion is equal to 1.5. In carbonate anion frequency of C-O is equal to 1.37, while the carbon dioxide is equal to 2.5, which correlates well with the classical ideas.

In urea C-O multiplicity of bonds equal to about 1.5, and C-N is approximately 1.7 (as shown below).


Lc-o = 1.27 Å  (10)

Multiplicity (Lc-o = 1.27 Å) = 1.486 ≈ 1.5  Multiplicity C−N = 1.686

Now let's find the dependence E = f (L) для C−O bonds.

For the bonds energy let's take the date:

C−O Lc-o = 1.434 Å Ec-o = 351.708 kj/mole (2)

C=O (for $H_2C=O$) Lc-o = 1.206 Å Ec-o = 686.668 kj/mole (2)

C≡O Lc-o = 1.12823 Å Ec-o = 1071.773 kj/mole (7)

Table 2. Calculation factors for dependency E = f(L) for C-O bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | <br>0.82918740<br>0.88634410 | <br>0.68755174<br>0.78560586 | <br>2540.70685895<br>3809.98813722 | <br>2106.72210526<br>3376.96049318 | 1.43400<br>1.20600<br>1.12823 | 351.708<br>686.668<br>1071.773 |
| Σ | 1.71553149 | 1.47315760 | 6350.69499617 | 5483.68259844 | 3.76823 | 2110.149 |

$1/x_1 = 0.69735007$ $x_1 = 1.43400$ $y_1 = 351.708$

$\Sigma(1/x^2) = 1.95945472$ $\Sigma(1/x) = 2.41288156$

c = 22207.04265404 b = - 31359.17576343 a = 11420.81052442

$$Ec\text{-}o = 11420.81052442 - \frac{31359.17576343}{L} + \frac{22207.04265404}{L^2}$$

Let us find from the equation:

E (L = 1.434 Å) = 351.708 kj/mole

E (L = 1.206 Å) = 686.668 kj/mole

E (L = 1.12823 Å) = 1072.542 kj/mole

O=CO Lc-o = 1.16213 Å (29)

E (L = 1.16213 Å) = 879.596 kj/mole = 210.088 kcal/mole

O=CO Lc-o = 1.162 Å E (average) = 192 kcal/mole D = 127 kcal/mole (11)

E (L = 1.162 Å) = 880.257 kj/mole = 210.246 kcal/mole

$\overset{\oplus}{N}H_3{-}CH_2COO^{\ominus}$ Lc-o = 1.26 Å E(L = 1.26 Å) = 520.383 kj/mole

HCO−OH Lc-o = 1.41 Å D ~ 90 kcal/mole (4)

E (L = 1.41 Å) = 350.243 kj/mole = 83.654 kcal/mole

$H_3C-OH$ $L_{c-o}$ = 1.434 Å D ~ 90 kcal/mole (4)

E (L = 1.434 Å) = 351.708 kj/mole = 84.004 kcal/mole

$CH_3CO-OH$ $L_{c-o}$ = 1.43 Å D ~ 90 kcal/mole (4)

E (L = 1.430 Å) = 351.038 kj/mole = 83.844 kcal/mole

So we can see the binding energy calculated from the equation for C-O bond nice correlated with experimental data.

We'll find the dependence Multiplicity = f (L) and E = f (L) for C−N bonds.

For the bonds energy let's take the date (2):

C−N E = 291.834 kj/mole

C=N E = 615.489 kj/mole

C≡N (for HC≡N) E = 866.709 kj/mole

For lengths of bonds let us take the date:

$CH_3-NH_2$ ($L_{C-N}$ = 1.4714 Å) (12)

HC≡N ($L_{C≡N}$ = 1.157 Å) (6)

C=N ($L_{C=N}$ = 1.28 Å) (14)

We'll find the dependence Multiplicity = f (L)

Table 3. Calculation coefficients for dependence Multiplicity = f (L) for C-N bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.4714 | 1 |
| | 0.78125000 | 0.61035156 | 9.84008359 | 7.68756531 | 1.2800 | 2 |
| | 0.86430424 | 0.74702181 | 10.82957888 | 9.36005089 | 1.1570 | 3 |
| ∑ | 1.64555424 | 1.35737337 | 20.66966247 | 17.04761620 | 3.9084 | 6 |

$1/x_1 = 0.67962485$ $x_1 = 1.4714$ $y_1 = 1$

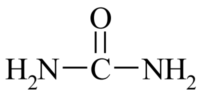
$\Sigma(1/x^2) = 1.81926331$ $\Sigma(1/x) = 2.32517908$

c = 11.91384503 b = - 7.56455294 a = 0.63817306

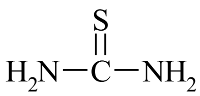
$$\text{Multiplicity (C-N)} = 0.63817306 - \frac{7.56455294}{L} + \frac{11.91384503}{L^2}$$

Let us find from the equation:

$C(N_3)_3^{\oplus}\ SbCl_6^{\ominus}$ $\quad L_{C-N} = 1{,}34\ \text{Å}$
$C(NH_2)_3^{\oplus}\ CO_3^{\ominus}$ $\quad L_{C-N} = 1{,}34\ \text{Å}$ (9) Multiplicity (L = 1.34 Å) = 1.628



$L_{C-N} = 1{,}33\ \text{Å}$ (10) Multiplicity ($L_{C-N}$ = 1.33 Å) = 1.686
$L_{C-O} = 1{,}27\ \text{Å}$



$L_{C-N} = 1{,}33\ \text{Å}$ (10) Multiplicity ($L_{C-N}$ = 1.33 Å) = 1.686
$L_{C-S} = 1{,}71\ \text{Å}$

We'll find the dependence E = f (L) for C-N bonds.

Table 4. Calculation coefficients for dependence E = f (L) for C-N bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.4714 | 291.834 |
| | 0.78125000 | 0.61035156 | 3184.79225580 | 2488.11894984 | 1.2800 | 615.489 |
| | 0.86430424 | 0.74702181 | 3112.82707944 | 2690.42962786 | 1.1570 | 866.709 |
| ∑ | 1.64555424 | 1.35737337 | 6297.61933524 | 5178.54857771 | 3.9084 | 1774.032 |

$1/x_1 = 0.67962485$ $\quad x_1 = 1.4714$ $\quad y_1 = 291.834$

$\Sigma(1/x^2) = 1.81926331$ $\quad \Sigma(1/x) = 2.32517908$

c = - 866.48412671 $\quad$ b = 4450.61712191 $\quad$ a = - 2332.69568587

$$E\ (\text{C-N}) = -2332.69568587 + \frac{4450.61712191}{L} - \frac{866.48412671}{L^2}$$

E (L = 1.33 Å) = 523.790 kj/mole

We'll find the dependence Multiplicity = f (L) and E = f (L) for C−S bonds. Firstly we'll find the dependence Multiplicity = f (L).

For lengths of bonds let us take the date:

| | | | |
|---|---|---|---|
| $H_3C-SH$ | Multiplicity = 1 | L = 1.818 Å | (15) |
| $H_2C=S$ | Multiplicity = 2 | L = 1.6108 Å | (16) |
| C≡S | Multiplicity = 3 | L = 1.53492 Å | (7) |

In the molecule CS multiplicity equal to 3, what confirming the spectral data of the compounds CS, HCP, CP (7), (17), namely the frequency of fluctuations and constant anharmonicity ($\omega_e x_e$), what for C≡P and C≡S bond are almost identical:

CS    $L_{C-S}$ = 1.53492 Å    D = 169.6 kcal/mole    $\omega_e$ = 1285.08 $cm^{-1}$
$\omega_e x_e$ = 6.46 $cm^{-1}$

CP    $L_{C-P}$ = 1.5583 Å    D = 122 kcal/mole    $\omega_e$ = 1239.67 $cm^{-1}$
$\omega_e x_e$ = 6.86 $cm^{-1}$

H−C≡P    $L_{C-P}$ = 1.5421 Å    $\nu_1$ = 3216.9 $cm^{-1}$
$L_{C-H}$ = 1.0667 Å    $\nu_2$ = 1278.4 $cm^{-1}$
$\nu_3$ = 674.7 $cm^{-1}$

Table 5. Calculation coefficients for dependence Multiplicity = f (L) for C-S bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.81800 | 1 |
| | 0.62080954 | 0.38540448 | 14.13337066 | 8.77413127 | 1.61080 | 2 |
| | 0.65149975 | 0.42445193 | 19.71516575 | 12.84442560 | 1.53492 | 3 |
| ∑ | 1.27230929 | 0.80985641 | 33.84853640 | 21.61855688 | 4.96372 | 6 |

$1/x_1 = 0.55005501$    $x_1 = 1.81800$    $y_1 = 1$

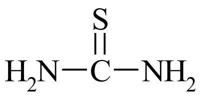
$\Sigma(1/x^2) = 1.11241692$    $\Sigma(1/x) = 1.82236429$

c = 181.87538814    b = - 198.81807222    a = 55.33256579

$$\text{Multiplicity (C-S)} = 55.33256579 - \frac{198.81807222}{L} + \frac{181.87538814}{L^2}$$

Let us find from the equation:

$CS_3^{2-}$ Lc-s = 1,71 Å (9) Multiplicity (Lc-s = 1.71 Å) = 1.263



$L_{C-S}$ = 1,71 Å (10)

$L_{C-N}$ = 1,33 Å

Multiplicity (C-S) = 1.263 Multiplicity (C-N) = 1.686

S=C=S Lc-s = 1.5529 Å (17)

Multiplicity (Lc-s = 1.5529 Å) = 2.722

In general, we see that oxygen sulfur analogs behave quite as expected:

a) thiourea and thiocarbonates anion have slightly lowered frequency of C-S bond (compared to the C-O) (1.263 to 1.507, and 1.263 to 1.370), due to more efficient delocalization of electrons on the sulfur atom is greater (compared to an oxygen atom )

b) carbon disulfide compared with carbon dioxide multiplicity of C-S bond slightly higher than the frequency of the C-O bond (2.7 against 2.5 in carbon dioxide) that can be explained by coupling undivided pair of electrons sulfur and oxygen with a double bond and therefore more coupling in the case of sulfur atom.

We'll find the dependence E = f (L) for C−S bonds.

For energies of bonds let us take the date:

C−S L = 1.818 Å E = 259.594 kj/mole (2)

C=S L = 1.6108 Å E = 728.538 kj/mole (2)

C≡S L = 1.53492 Å E = 709.606 kj/mole (7)

Table 6. Calculation coefficients for dependence E = f (L) for C-S bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.81800 | 259.594 |
| | 0.62080954 | 0.38540448 | 6627.75936908 | 4114.57621622 | 1.61080 | 728.538 |
| | 0.65149975 | 0.42445193 | 4436.03058434 | 2890.07282747 | 1.53492 | 709.606 |
| ∑ | 1.27230929 | 0.80985641 | 11063.78995342 | 7004.64904369 | 4.96372 | 1697.738 |

$1/x_1 = 0.55005501$ $x_1 = 1.81800$ $y_1 = 259.594$

$\Sigma(1/x^2) = 1.11241692$ $\Sigma(1/x) = 1.82236429$

c = - 71414.57485742 b = 90244.55278987 a = - 27772.64385690

$$E\ c\text{-}s = -27772.64385690 + \frac{90244.55278987}{L} - \frac{71414.57485742}{L^2}$$

Let us find from the equation:

SC=S Lc-s = 1.5529 Å E (L = 1.5529 Å) = 726.729 kj/mole = 173.576 kcal/mole

Ec-s (average) = 128 kcal/mole (11)

We'll find the dependence Multiplicity = f (L) and E = f (L) for N−N bonds.

For energies of bonds let us take the date:

N−N E = 160.781 kj/mole (2)

N=N E = 418.000 kj/mole (40)

N≡N E = 945.333 kj/mole (18)

For lengths of bonds let us take the date:

$H_2N{-}NH_2$ L = 1.4530 Å (26)

HN=NH L = 1.2300 Å (27)

N≡N L = 1.0976 Å (28)

Firstly we'll find the dependence Multiplicity = f (L)

Table 7. Calculation coefficients for dependence Multiplicity = f (L) for N−N bond.

| | $1/x$ | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.4530 | 1 |
| | 0.81300813 | 0.66098222 | 8.01430493 | 6.51569507 | 1.2300 | 2 |
| | 0.91107872 | 0.83006443 | 8.97474845 | 8.17670231 | 1.0976 | 3 |
| ∑ | 1.72408685 | 1.49104665 | 16.98905339 | 14.69239737 | 3.7806 | 6 |

$1/x_1 = 0.68823125$ $x_1 = 1.4530$ $y_1 = 1$

$\Sigma(1/x^2) = 1.96470890$ $\Sigma(1/x) = 2.41231809$

c = 9.79339013 b = - 6.68791795 a = 0.96407492

$$\text{Multiplicity (N-N)} = 0.96407492 - \frac{6.68791795}{L} + \frac{9.79339013}{L^2}$$

We'll find the dependence E = f (L) for N-N bonds.

Table 8. Calculation coefficients for dependence E = f (L) for N-N bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.4530 | 160.781 |
| | 0.81300813 | 0.66098222 | 2061.43150049 | 1675.96056951 | 1.2300 | 418.000 |
| | 0.91107872 | 0.83006443 | 3520.57842393 | 3207.52407428 | 1.0976 | 945.333 |
| Σ | 1.72408685 | 1.49104665 | 5582.00992443 | 4883.48464379 | 3.7806 | 1524.114 |

$1/x_1 = 0.68823125$  $x_1 = 1.4530$  $y_1 = 160.781$

$\Sigma(1/x^2) = 1.96470890$  $\Sigma(1/x) = 2.41231809$

c = 14878.53765631  b = - 20274.81508318  a = 7067.14065437

$$E\text{ (N-N)} = 7067.14065437 - \frac{20274.81508318}{L} + \frac{14878.53765631}{L^2}$$

Let us find from the equation:

$N_2^{\oplus}$  L = 1,116 Å,  Multiplicity = 2.835,  E = 846.001 kj/mole

experimentally found  E = 843.26 kj/mole  (19)

As we see in the latter case are almost the same value of energy of equation identified and obtained experimentally.

We'll find the dependence Multiplicity = f (L) for N−O bonds.

For lengths of bonds let us take the date:

$NH_2{-}OH$  $L_{N-O}$ = 1,453 Å  (20)  Multiplicity = 1

$CH_3{-}NO_2$  $L_{N-O}$ = 1,224 Å  (12)  Multiplicity = 1.5

NO  $L_{N-O}$ = 1,1507 Å  (19)  Multiplicity = 2.5

Table 9. Calculation coefficients for dependence Multiplicity = f (L) for N-O bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.4530 | 1.0 |
| | 0.81699346 | 0.66747832 | 3.88312664 | 3.17248908 | 1.2240 | 1.5 |
| | 0.86903624 | 0.75522398 | 8.29623106 | 7.20972544 | 1.1507 | 2.5 |
| Σ | 1.68602970 | 1.42270230 | 12.17935770 | 10.38221452 | 3.8277 | 5.0 |

$1/x_1 = 0.68823125$ $x_1 = 1.4530$ $y_1 = 1.0$

$\Sigma(1/x^2) = 1.89636455$ $\Sigma(1/x) = 2.37426095$

$c = 84.79763896$ $b = -123.75637485$ $a = 46.00756377$

$$\text{Multiplicity (N-O)} = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$N_2O$ N−N = 1.1282 Å (30)

N−O = 1.1843 Å

Multiplicity (N−O) (L = 1.1843 Å) = 1.969 ≈ 1.97

Multiplicity (N−N) (L = 1.1282 Å) = 2.730

$NO_3^-$ L (N−O) = 1.243 Å (31)

Multiplicity (L = 1.243 Å) = 1.328 ≈ 1.33

We'll find the dependence E = f (L) for N−O bond.

For energies of bonds let us take the date:

N−O E = 221.900 kj/mole (22)

N=O E = 607.086 kj/mole (22)

NO L = 1.15070 Å E = 626.847 kj/mole (19)

N−O L = 1.453 Å ($NH_2$−OH) (20)

Lengths L when N=O Multiplicity = 2 calculated by the formula:

$$\text{Multiplicity (N-O)} = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$$2 = 46.00756377 - \frac{123.75637485}{L} + \frac{84.79763896}{L^2}$$

$44.00756377\,L^2 - 123.75637485\,L + 84.79763896 = 0$

L = 1.18208253 Å

The value of L = 1.63007893 Å is not considered as the basis of bond lengths, it is clear that this multiplicity <1.

So, N=O Multiplicity = 2 L = 1.18208253 Å

N−O L = 1.453 Å E = 221.900 kj/mole

N=O L = 1.18208253 Å E = 607.086 kj/mole

NO L = 1.1507 Å E = 626.847 kj/mole

Table 10. Calculation coefficients for dependence E = f (L) for N−O bond.

| | 1/x | 1/x² | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.45300000 | 221.900 |
| | 0.84596462 | 0.71565614 | 2442.00695125 | 2065.85148606 | 1.18208253 | 607.086 |
| | 0.86903624 | 0.75522398 | 2239.68925320 | 1946.37112471 | 1.15070000 | 626.847 |
| ∑ | 1.71500086 | 1.47088013 | 4681.69620445 | 4012.22261077 | 3.78578253 | 1455.833 |

$1/x_1 = 0.68823125$ $x_1 = 1.4530$ $y_1 = 221.900$

$\Sigma(1/x^2) = 1.94454237$ $\Sigma(1/x) = 2.40323211$

c = - 8769.11638979 b = 15895.54907490 a = - 6564.31416262

$$E\ (N\text{-}O) = -6564.31416262 + \frac{15895.54907490}{L} - \frac{8769.11638979}{L^2}$$

Let us find from the equation:

$CH_3{-}NO_2$ $L_{N-O} = 1{,}224$ Å E (L = 1.224 Å) = 569.050 kj/mole

We'll find the dependence Multiplicity = f (L) for C−P bond.

$H_2P{-}CH_3$ $L_{C-P}$ = 1.858 Å (23) Multiplicity = 1

$(CH_3)_3P{=}CH_2$ $L_{C=P}$ = 1.640 Å (24) Multiplicity = 2

H−C≡P $L_{C\equiv P}$ = 1.5421 Å (17), (25) Multiplicity = 3

$L_{C\equiv P}$ = 1.54 Å (25)

$L_{C\equiv P}$ = 1.5421 Å (17)

Table 11. Calculation coefficients for dependence Multiplicity = f (L) for C−P bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.8580 | 1 |
| | 0.60975610 | 0.37180250 | 13.97761468 | 8.52293578 | 1.6400 | 2 |
| | 0.64846638 | 0.42050864 | 18.14005571 | 11.76321621 | 1.5421 | 3 |
| ∑ | 1.25822247 | 0.79231114 | 32.11767039 | 20.28615199 | 5.0401 | 6 |

$1/x_1 = 0.53821313$ $x_1 = 1.8580$ $y_1 = 1$

$\Sigma(1/x^2) = 1.08198452$ $\Sigma(1/x) = 1.79643561$

c = 107.52805439 b = - 109.46128312 a = 28.76548555

$$\text{Multiplicity (C-P)} = 28.76548555 - \frac{109.46128312}{L} + \frac{107.52805439}{L^2}$$

Let we see O-O bonds.

For lengths of bonds let us take the date:

$O_3$ $L_{o\text{-}o} = 1.2717$ Å (32)

$O_2$ $L_{o\text{-}o} = 1.20735$ Å (33)

$H_2O_2$ $L_{o\text{-}o} = 1.452$ Å (34)

For energies of bonds let us take the date (35)

$O_2 = 2O$ $119.11 \cdot 4.184 = 498.356$ kj/mole

$O_3 = O_2 + O$ $25.6 \cdot 4.184 = 107.110$ kj/mole - this dissociation energy

O−O $E = 33.2 \cdot 4.187 = 139.008$ kj/mole (2)

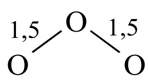
But energy O-O bond at 1.5 multiplicity we find the following manner:

$O_3 = O_2 + O$ 107.110 kj/mole

$O_2 = O + O$ 498.356 kj/mole

$O_3 = O + O + O$ 498.356 kj/mole + 107.110 kj/mole

If these three oxygen atoms forming a molecule of ozone

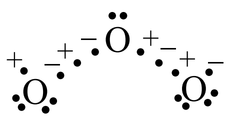



then this energy is released from the two formed three-electrone bonds, so

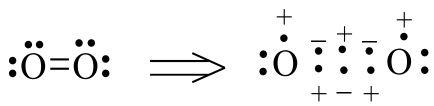
$$302.733 = \frac{(498.356 + 107.110)}{2}$$

$E_{o\text{-}o}$ when multiplicity 1.5 = 302.733 kj/mole

HO−OH Multiplicity (O-O) = 1



Multiplicity (O-O) = 1.5



Multiplicity (O-O) = 2

Multiplicity O-O bond in the molecule of oxygen equal to 2, despite two three-electrone bond as is the interaction of unpaired electrons on the oxygen atoms with three-elecrone bond that follows a compliance rules of octet.

$H_2O_2$ Lo-o = 1.452 Å Multiplicity = 1 E = 139.008 kj/mole

$O_3$ Lo-o = 1.2717 Å Multiplicity = 1.5 E = 302.733 kj/mole

$O_2$ Lo-o = 1.20735 Å Multiplicity = 2 E = 498.356 kj/mole

Table 12. Calculation coefficients for dependence Multiplicity = f (L) for O−O bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (Multiplicity) |
|---|---|---|---|---|---|---|
| | | | | | 1.45200 | 1.0 |
| | 0.78634898 | 0.61834472 | 5.12065557 | 4.02662230 | 1.27170 | 1.5 |
| | 0.82826024 | 0.68601502 | 7.16563335 | 5.93500920 | 1.20735 | 2.0 |
| ∑ | 1.61460922 | 1.30435975 | 12.28628893 | 9.96163149 | 3.93105 | 4.5 |

$1/x_1 = 0.68870523$ $x_1 = 1.452$ $y_1 = 1.0$

$\Sigma(1/x^2) = 1.77867464$ $\Sigma(1/x) = 2.30331446$

c = 48.79304255 b = - 66.85172754 a = 23.89786759

$$\text{Multiplicity (O-O)} = 23.89786759 - \frac{66.85172754}{L} + \frac{48.79304255}{L^2}$$

Table 13. Calculation coefficients for dependence E = f (L) for O−O bond.

| | 1/x | $1/x^2$ | $\frac{(y-y_1)}{(1/x-1/x_1)}$ | $\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$ | x (L, Å) | y (E, kj/mole) |
|---|---|---|---|---|---|---|
| | | | | | 1.45200 | 139.008 |
| | 0.78634898 | 0.61834472 | 1676.75866772 | 1318.51747088 | 1.27170 | 302.733 |
| | 0.82826024 | 0.68601502 | 2574.95601441 | 2132.73368486 | 1.20735 | 498.356 |
| ∑ | 1.61460922 | 1.30435975 | 4251.71468213 | 3451.25115574 | 3.93105 | 940.097 |

$1/x_1 = 0.68870523$ $x_1 = 1.452$ $y_1 = 139.008$

$\Sigma(1/x^2) = 1.77867464$ $\Sigma(1/x) = 2.30331446$

c = 21430.93279023 b = - 29935.02909385 a = 10590.40848780

$$E\ (O\text{-}O) = 10590.40848780 - \frac{29935.02909385}{L} + \frac{21430.93279023}{L^2}$$

HCNO $L_{C\text{-}H} = 1.0266$ Å (36)

$L_{C\text{-}N} = 1.1679$ Å

$L_{N\text{-}O} = 1.1994$ Å

Multiplicity ($L_{C\text{-}N} = 1.1679$ Å) = 2.897

Multiplicity ($L_{N\text{-}O} = 1.1994$ Å) = 1.772

$H-C\equiv \overset{+}{N}-\overset{-}{O}$

H−C≡N•••O:

HNCO $L_{H\text{-}N} = 0.987$ Å (36) H−N=C=O

$L_{N\text{-}C} = 1.207$ Å

$L_{C\text{-}O} = 1.171$ Å

Multiplicity ($L_{N\text{-}C} = 1.207$ Å) = 2.549

Multiplicity ($L_{C\text{-}O} = 1.171$ Å) = 2.392

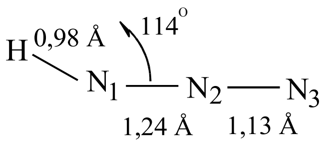
HNCS $L_{H\text{-}N} = 0.988$ Å (36) H−N=C=S

$L_{N\text{-}C} = 1.216$ Å

$L_{C\text{-}S} = 1.560$ Å

Multiplicity ($L_{C\text{-}N} = 1.216$ Å) = 2.475

Multiplicity ($L_{C\text{-}S} = 1.560$ Å) = 2.620



Multiplicity ($L_{N1-N2}$ =1.24 Å) = 1.940 (MO ~ 1.65) (37)

Multiplicity ($L_{N2-N3}$ =1.13 Å) = 2.715 (MO ~ 2.64)

$[N_1-N_2-N_3]^{\ominus}$ Multiplicity ($L_{N-N}$ =1.18 Å) = 2.330 $L_{N-N}$ ~ 1.18 Å (37)

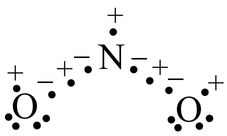
$N_2O$ $\Longrightarrow$ 

N−N = 1.1282 Å (30)

N−O = 1.1843 Å

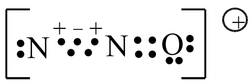
Multiplicity ($L_{N-N}$ = 1.1282 Å) = 2.730

Multiplicity ($L_{N-O}$ = 1.1843 Å) = 1.969

$NO_2$ $\Longrightarrow$ 

$L_{N-O}$ = 1.197 Å (38)

Multiplicity (N−O) = 1.802

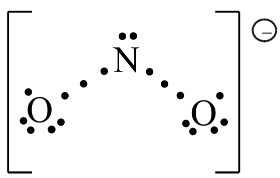
$N_2O^{\oplus}$ 

N−N = 1.154 Å (30)

N−O = 1.185 Å

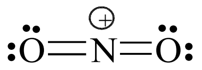
Multiplicity ($L_{N-N}$ = 1.154 Å) = 2.523

Multiplicity ($L_{N-O}$ = 1.185 Å) = 1.959

$NO_2^{\ominus}$ 

N−O = 1.236 Å (39)

Multiplicity (N−O) = 1.388 ≈ 1.39



$L_{N\text{-}O}$ = 1.200 Å (30)

Multiplicity (N−O) = 1.765

## CONCLUSION.

As exemplified in many chemical bonds (C-N, C-O, C-S, N-N, N-O, O-O) using the equation $y = a + b/x + c/x^2$ to describe the multiplicity dependence = f(L) i E = f(L) (where multiplicity - is multiplicity of bond , L - length of bond in Å, E - energy of bond in kj /mole), gives good results and determine the multiplicity of power relations in many organic and inorganic compounds. In fact, to determine the multiplicity or energy of bond we can known length of the bonds must solve simple quadratic equation. Conversely, knowing the multiplicity or energy or bond can determine its length (again solving basic equation). This method is simple, but gives good results when analyzing the chemical bonds that are nice to coincide with the experimental data or other theoretical calculations.

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37. See (14), p. 564.

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