A short analysis of chemical bonds.

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Translation from Ukrainian to English made by Bezverkhniy Vitaliy Volodymyrovich.

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

$y = a + b/x + c/x^2$ $\quad X = 1/x \quad$ $Y = \dfrac{(y - y_1)}{(1/x - 1/x_1)}$

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

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

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

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.

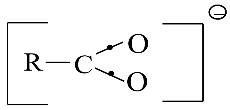
	1/x	1/x²	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	x (L, Å)	y (multiplicity)
					1.43400	1
	0.82918740	0.68755174	7.58510526	6.28947368	1.20600	2
	0.88634410	0.78560586	10.58234503	9.37959905	1.12823	3
∑	1.71553149	1.47315760	18.16745029	15.66907273	3.76823	6

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

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

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

$H_2N-C(=O)-NH_2$ 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)
					1.43400	351.708
	0.82918740	0.68755174	2540.70685895	2106.72210526	1.20600	686.668
	0.88634410	0.78560586	3809.98813722	3376.96049318	1.12823	1071.773
∑	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 Ǻ) = 351.708 kj/mole

E (L = 1.206 Ǻ) = 686.668 kj/mole

E (L = 1.12823 Ǻ) = 1072.542 kj/mole

O=CO Lc-o = 1.16213 Ǻ (29)

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

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

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

$\overset{\oplus}{NH_3}$—$CH_2\overset{\ominus}{COO}$ Lc-o = 1.26 Ǻ E(L = 1.26 Ǻ) = 520.383 kj/mole

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

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

H_3C−OH Lc-o = 1.434 Ǻ D ~ 90 kcal/mole (4)

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

CH_3CO−OH Lc-o = 1.43 Ǻ D ~ 90 kcal/mole (4)

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

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:

$CH_3{-}NH_2$ ($L_{C\text{-}N}$ = 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

$C(N_3)_3^{\oplus}\ SbCl_6^{\ominus}$ $L_{C-N} = 1{,}34$ Å

$C(NH_2)_3^{\oplus}\ CO_3^{\ominus}$ $L_{C-N} = 1{,}34$ Å

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

Let us find from the equation:

(9) Multiplicity (L = 1.34 Å) = 1.628

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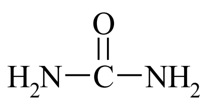
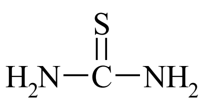


$L_{C-N} = 1{,}33$ Å (10)

$L_{C-O} = 1{,}27$ Å

Multiplicity ($L_{C\text{-}N}$ = 1.33 Å) = 1.686



$L_{C-N} = 1{,}33$ Å (10)

$L_{C-S} = 1{,}71$ 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.

	$1/x$	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	x (L, Å)	y (E, kj/mole)
					1.4714	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

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

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

c = - 866.48412671 b = 4450.61712191 a = - 2332.69568587

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

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 $L_{c\text{-}s}$ = 1.53492 Å D = 169.6 kcal/mole $\omega_e = 1285.08\ cm^{-1}$

$\omega_e x_e = 6.46\ cm^{-1}$

CP $L_{c\text{-}p}$ = 1.5583 Å D = 122 kcal/mole $\omega_e = 1239.67\ cm^{-1}$

$\omega_e x_e = 6.86\ cm^{-1}$

H−C≡P $L_{c\text{-}p}$ = 1.5421 Å $\nu_1 = 3216.9\ cm^{-1}$

$L_{c\text{-}H}$ = 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-} L_{C-S} = 1,71 Å (9) Multiplicity (L_{C-S} = 1.71 Å) = 1.263

S
||
$H_2N-C-NH_2$ 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 L_{C-S} = 1.5529 Å (17)

Multiplicity (L_{C-S} = 1.5529 Å) = 2.722

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	$1/x^2$	$\frac{(y-y_1)}{(1/x-1/x_1)}$	$\frac{((1/x)(y-y_1))}{(1/x-1/x_1)}$	x (L, Å)	y (E, kj/mole)
					1.81800	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 $L_{c\text{-}s}$ = 1.5529 Å E(L = 1.5529 Å) = 726.729 kj/mole = 173.576 kcal/mole

$E_{c\text{-}s}$ (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
∑	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)

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
∑	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 · 4.184 = 498.356 kj/mole

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

O−O E = 33.2 · 4.187 = 139.008 kj/mole (2)

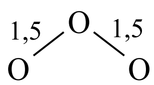
But energy O-O bond at 1.5 multiplicity we find the following manner:

$O_3 = O_2 + O$ 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

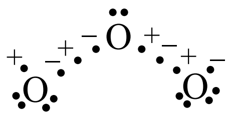
If these three oxygen atoms forming a molecule of ozone



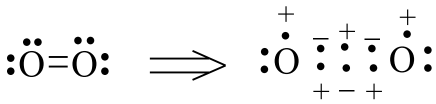
then this energy is released from the two formed three-electrone bonds, so

Eo-o when multiplicity 1.5 = 302.733 kj/mole $302.733 = \frac{(498.356 + 107.110)}{2}$

HO−OH Multiplicity (O-O) = 1



Multiplicity (O-O) = 1.5



Multiplicity (O-O) = 2

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/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)
	 0.78634898 0.82826024	 0.61834472 0.68601502	 5.12065557 7.16563335	 4.02662230 5.93500920	1.45200 1.27170 1.20735	1.0 1.5 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/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)
	 0.78634898 0.82826024	 0.61834472 0.68601502	 1676.75866772 2574.95601441	 1318.51747088 2132.73368486	1.45200 1.27170 1.20735	139.008 302.733 498.356
∑	1.61460922	1.30435975	4251.71468213	3451.25115574	3.93105	940.097

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

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

$c = 21430.93279023$ $b = -29935.02909385$ $a = 10590.40848780$

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

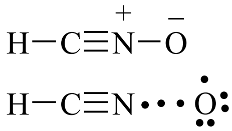
HCNO $L_{C\text{-}H} = 1.0266$ Å (36)

$L_{C\text{-}N} = 1.1679$ 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



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

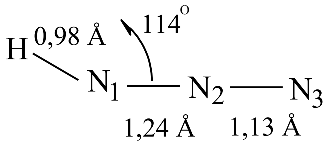
HNCS $L_{H\text{-}N} = 0.988$ Å (36) H−N=C=S

$L_{N\text{-}C} = 1.216$ Å

$L_{C\text{-}S} = 1.560$ Å

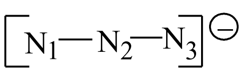
Multiplicity ($L_{C\text{-}N} = 1.216$ Å) = 2.475

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



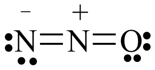
Multiplicity ($L_{N1\text{-}N2}$ =1.24 Å) = 1.940 (MO ~ 1.65) (37)

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



Multiplicity ($L_{N\text{-}N}$ =1.18 Å) = 2.330 $L_{N\text{-}N}$ ~ 1.18 Å (37)

N_2O $\Longrightarrow$



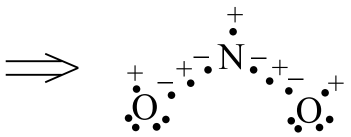
N−N = 1.1282 Å (30)

N−O = 1.1843 Å

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

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

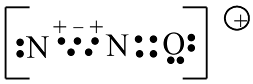
NO_2



$L_{N\text{-}O}$ = 1.197 Å (38)

Multiplicity (N−O) = 1.802

$N_2O^{\oplus}$



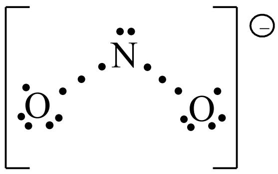
N−N = 1.154 Å (30)

N−O = 1.185 Å

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

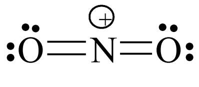
Multiplicity ($L_{N\text{-}O}$ = 1.185 Å) = 1.959

$NO_2^{\ominus}$



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

REFERENCES.

1. Ingold K. Theoretical essentials of the organic chemistry. Mir, Moscow, 1973, p. 143 (Russian translation from Structure and mechanism in organic chemistry. Second edition, INGOLD C.K. Cornell University press Ithaca and London, 1969).

2. See (1), p. 116.

3. Vedeneev VI, LV Gurvich, VN Kondratiev, VA Medvedev, EL Frankiewicz Energy break chemical bonds. The ionization potentials and electron affinities. Directory. Publisher of the USSR Academy of Sciences, Moscow, 1962, p. 69-70.

4. Cottrell T.L. The Strengths of Chemical Bonds. Butterworths Scientific Publications, London, 1958.

5. Grey G. Electrons and Chemical Bonding. Mir, Moscow, 1967, p. 141 (Russian translation from Electrons and chemical Bonding, Harry B. Gray, New York, Amsterdam, 1965).

6. See (1), p. 140.

7. KS Krasnov, Filippenko NV, Popov VA etc. The molecular constants of inorganic compounds:. Directory. Chemistry, Leningrad, 1979, p. 36.

8. See (1), p. 144.

9. Wells A. Structural inorganic chemistry. “Mir”, Moscow, 1988, vol. 3, p. 17 (Russian translation from c Structural inorganic chemictry, fifth Edition, Wells A. F. Clarendon Press, Oxford, 1986).

10. See (9), p. 17-18.

11. See (5), p. 117.

12. See (7), p. 416.

13. See (7), p. 367.

14. Wells A. Structural inorganic chemistry. “Mir”, Moscow, 1987, vol. 2, p. 566 (Russian translation from Structural inorganic chemictry, fifth Edition, Wells A. F. Clarendon Press, Oxford, 1986).

15. See (7), p. 365.

16. See (7), p. 198.

17. See (7), p. 106.

18. LV Gurvich, Karachevtsev GV, Kondratiev VN, Lebedev A., Medvedev VA, Potapov VK Hodeev S. Energy break chemical bonds. The ionization potentials and electron affinities. Nauka, Moscow, 1974, p. 97.

19. See (7), p. 42.

20. See (7), p. 312.

21. See (7), p. 216.

22. Matthieu G., R. Panico course of theoretical foundations of organic chemistry. Mir, Moscow, 1975, p. 20 (Russian translation from MÉCANISMES RÉACTIONNELS EN CHIMIE ORGANIQUE MATHIEU J., PANICO R., Hermann, 1972).

23. See (14), p. 612.

24. Kolodyazhni OI Chemistry phosphorus ylides. Naukova Dumka, Kiev, 1994, p. 255.

25. See (14), p. 611.

26. Wells A. Structural Inorganic Chemistry. Mir, Moscow, 1987, vol. 2, p. 558 (Russian translation from Wells A. F. Structural inorganic chemictry, Fifth Edition, Clarendon Press, Oxford).

27. Wells A. Structural Inorganic Chemistry. Mir, Moscow, 1987, vol. 2, p. 562 (Russian translation from Wells A. F. Structural inorganic chemictry, Fifth Edition, Clarendon Press, Oxford).

28. Gordon A., Ford R. Sputnik chemist. Physico-chemical properties, methods, bibliography. Mir, Moscow, 1976, p. 127 (Russian translation from THE CHEMIST'S COMPANION. A HANDBOOK OF PRACTICAL DATA, TECHNIQUES, AND REFERENCES. ARNOLD J. GORDON Pfizer, Inc., RICHARD A. FORD Montgomery College, A WILEY-INTERSCIENCE PUBLICATION, JOHN WILEY AND SONS, New York – London – Sydney – Toronto, 1972).

29. See (7), p. 110.

30. See (7), p. 124.

31. See (7), p. 218.

32. See (7), p. 130.

33. See (7), p. 46-47.

34. See (7), p. 236.

35. See (18), p. 106.

36. See (7), p. 200.

37. See (14), p. 564.

38. See (7), p. 122.

39. See (14), p. 577.

40. See (14), p. 543.