THE INVESTIGATION OF THE RELATIONSHIP ELECTRONIC ENERGY ~ [VIBRATIONAL FREQUENCY]^2 X [INTERNUCLEAR DISTANCE]^2, FOR CHEMICALLY ALIKE MOLECULES

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ABSTRACT

The first author has previously established the following relationship between the *minimum electronic energy* E_{min}, and the *lowest vibrational frequency* ω_{min} at this energy level, in regards to various *vibrational electronic states* of a given diatomic molecule: $E_{min} = 4\pi^2 \mathcal{M}_0 g_k \omega_{min}^2 r_{min}^2$. Here $\mathcal{M}_0$ is the *reduced mass* of the molecule, r_{min} the *internuclear distance* associated with ω_{min} , and g_k a *dimensionless coefficient* usually around *unity,* insuring the equality; for electronic states configured alike, we expect the coefficient g_k, to remain practically the same. This essentially discloses an interesting architecture of diatomic molecules.

INTRODUCTION

It was the author's original idea that the *special theory of relativity* imposes that, already at *rest,* the *"period of time"* T_0, the *"characteristic length"* $\mathcal{R}_0$, the *"clock mass"* M_0 to be associated with the internal dynamics of an atomistic or molecular wave-like object, and the total energy E_0, making the basis of the dynamics in question, ought to relate to each other in a given manner.[1, 2, 3, 4, 5, 6, 7, 8] More fundamentally, based on the *orchestration of electric charges,* these quantites are expected to be related to each other *two by two,* in just a unique way.[9, 10,11]

The cancellation of electric charges from the expressions in question, ultimately leads to a *compact relationship,* between the four quantites of interest.

In this article we are going to provide a *direct derivation* of this interesting *compact relationship.*

Thus let E(r) be the *electronic energy of the molecule,* at a given state, with respect to the *internuclear distance* r.

E(r) can be as usual, expressed, in terms of the *force constant* k_{min} , associated with ω_{min} as,[12]

$$E(r) = E_{min} + \frac{1}{2} k_{min} (r - r_{min})^2 . \qquad (1)$$

It should be emphasized that this relationship, does not display *characteristics* such as *"anharmonicity"* and *"dissociation";* but in this work we are dealing with only *the lowest vibrational level of the states* of concern. Thus, even when we look at an *exited electronic state,* Eq.(1) is quite valid, in regards to the *lowest vibrational level* of it.

E(r) vanishes at the *abscissa* r_{00} , which we can define with respect to r_{min}, as

$$r_{00} = p\, r_{min} \text{ [value which makes E(r), vanish] ;} \qquad (2)$$

p is an *unknown parameter* at this stage, though it appears to be roughly around 2.

Eqs.(1) and (2), provide us with the possibility of expressing E_{min}, as

$$E_{min} = \frac{1}{2}\, k_{min}\, (p-1)^2\, r_{min}^2 \,. \tag{3}$$

Next we define a quantity g_k as,

$$g_k = \frac{(p-1)^2}{2} \,. \tag{4}$$

Thus using the familiar expression,

$$\omega_{min} = \frac{1}{2\pi}\sqrt{\frac{k_{min}}{\mathcal{M}_0}} \,, \tag{5}$$

we can *finally* arrive at our target relationship:

$$E_{min} = 4\pi^2 \mathcal{M}_0 g_k \omega_{min}^2 r_{min}^2 \,. \tag{6}$$

Note that Eq.(4) depicts two values for p, and in fact, there are two roots r_{00}, fulfilling Eq.(2).

We expect Eq.(6) to be valid not only regarding the electronic states of a given molecule, but also regarding the ground states of *chemically alike molecules*, for which we expect g_k to remain practically constant.

Let then E_0 be the *magnitude of the ground state electronic energy*, ω_0 the *lowest vibration frequency* at E_0, and r_0 the *ground state internuclear distance* of the molecule of concern.

Eq.(6) then becomes

$$E_0 = 4\pi^2 \mathcal{M}_0 g_k \omega_0^2 r_0^2 \,. \tag{7}$$

Thus, we conjecture that the plot of E_0 versus $\omega_0^2 r_0^2$, should come out as a *straight line* for *chemically alike molecules,* the slope of which furnishes the coefficient g_k.

We can equally write

$$T_0 = 2\pi\sqrt{\frac{g_k \mathcal{M}_0}{E_0}}\; r_0 \tag{8}$$

where T_0 is the inverse of ϖ_0.

This equation suggests that, for *chemically alike molecules,* the period of vibration T_0, should behave proportionally to $\left\lfloor \sqrt{\mathcal{M}_0 / E_0}\; r_0 \right\rfloor$.

We have calculated the electronic ground state energy E_{0AB}, of the diatomic molecule AB, in consideration, from

$$E_{0AB} = I_{0A} + I_{0B} + D_{0AB} \, , \tag{9}$$

where D_{0AB} is the *dissociation energy* of the molecule AB, and I_{0A} and I_{0B} are respectively the *ionization energies of the atoms,* A and B.

The attached tables and figures succesfully display our prediction for all of the diatomic molecules, reassembled on the basis of their *chemical similarities.*

For each chemical family of concern, g_k is calculated and presented in Table 19.

Table 1

Molecules	T_0 (cm^{-1} x10^{3}c)	M_0 (amu)	R_0 (Å)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
H_2	0,24	0,5	0,74	31,64	2,58	0,26
Li_2	2,89	3,51	2,67	11,81	1,99	0,03
Na_2	6,34	11,49	3,08	11,01	2,01	0,02
K_2	10,88	19,49	3,92	9,19	1,91	0,07
NaK	8,06	14,48	3,50	10,03	1,92	0,06
NaRb	9,54	17,86	2,64	4,40	1,79	0,13
Rb_2	18,06	42,47	4,21	9,64	1,96	0,04
Cs_2	23,91	66,47	4,65	12,55	2,22	0,08
Average					2,04	0,09

Table 2

Molecules	T_0 (cm^{-1} x10^{3}c)	M_0 (amu)	R_0 (Å)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
N_2	0,43	7,00	1,09	190,53	2,06	0,02
P_2	1,29	15,49	1,89	125,87	1,94	0,04
PN	0,75	9,65	1,49	158,29	2,05	0,01
Average					2,02	0,02

Table 3

Molecules	T_0 (cm^{-1} x10^{3}c)	M_0 (amu)	R_0 ($\overset{\circ}{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert\mathrm{RelativeError}\rvert$ as Referred to the Average
O_2	0,64	8,00	1,21	102,56	1,90	0,13
S_2	1,39	15,99	1,89	72,46	1,60	0,06
Se_2	2,57	39,97	2,15	82,22	1,71	0,02
Te_2	4,00	63,83	2,59	58,35	1,48	0,12
SO	0,90	10,66	1,49	86,43	1,72	0,03
Average					1,67	0,07

Table 4

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\overset{\circ}{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert\mathrm{RelativeError}\rvert$ as Referred to the Average
F_2	11,21	9,50	1,44	37,59	15,50	0,28
Cl_2	17,96	17,49	1,99	28,4	11,50	0,05
Br_2	31,15	39,96	2,28	25,59	10,93	0,09
I_2	46,87	63,47	2,67	22,44	10,44	0,10
BrF	15,04	15,35	1,76	31,42	12,23	0,01
ClF	12,93	12,31	1,63	32,99	12,98	0,08
ICl	26,23	27,42	2,32	25,56	10,92	0,09
Average					12,07	0,11

Table 5

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\overset{\circ}{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert\mathrm{RelativeError}\rvert$ as Referred to the Average
LiH	7,36	0,88	1,59	21,48	22,90	0,07
NaH	8,83	0,97	1,89	20,93	21,70	0,02
KH	10,46	0,98	2,24	19,79	20,98	0,02
RbH	11,01	0,99	2,37	19,66	20,70	0,03
CsH	11,55	1,00	2,49	19,39	20,43	0,04
Average					21,34	0,03

Table 6

Molecules	T_0 (cm^{-1} x10^4c)	M_0 (amu)	R_0 $(\overset{\circ}{\mathrm{A}})$	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert\mathrm{RelativeError}\rvert$ as Referred to the Average
BeH	5,03	0,91	1,34	25,11	19,72	0,05
MgH	6,98	0,97	1,73	23,72	19,95	0,06
CaH	7,94	0,98	2,00	21,4	18,55	0,02
SrH	8,53	0,99	2,15	20,96	18,26	0,03
BaH	8,77	1,00	2,23	20,62	17,86	0,05
Average					18,87	0,04

Table 7

Molecules	T_0 (cm^{-1} x10^4c)	M_0 (amu)	R_0 $(\overset{\circ}{\mathrm{A}})$	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert\mathrm{RelativeError}\rvert$ as Referred to the Average
BH	4,41	0,92	1,23	25,39	18,84	0,03
AlH	6,16	0,97	1,65	22,63	18,03	0,02
InH	7,02	0,99	1,84	21,85	17,93	0,02
TlH	7,43	1,00	1,87	21,87	18,58	0,01
Average					18,34	0,02

Table 8

Molecules	T_0 (cm^{-1} x10^4c)	M_0 (amu)	R_0 $(\overset{\circ}{\mathrm{A}})$	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert\mathrm{RelativeError}\rvert$ as Referred to the Average
CH	3,66	0,93	1,11	28,32	18,19	0,03
SnH	6,33	0,99	1,79	24,13	17,46	0,01
PbH	6,65	1,00	1,84	22,57	17,18	0,02
Average					17,61	0,02

Table 9

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\mathring{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
NH	3,03	0,94	1,04	31,92	16,98	0,018
BiH	6,11	1,00	1,81	23,57	16,39	0,018
Average					16,68	0,018

Table 10

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\mathring{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
HF	2,53	0,96	0,92	37,41	17,17	0,10
HCl	3,47	0,98	1,27	30,98	15,36	0,01
HBr	3,91	0,99	1,41	29,15	15,05	0,03
HI	4,48	1,00	1,60	27,10	14,58	0,06
Average					15,54	0,05

Table 11

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\mathring{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
ZnH	6,6	0,99	1,59	23,83	20,37	0,04
CdH	7,47	0,99	1,76	23,26	20,57	0,05
HgH	8,21	1,00	1,74	13,97	17,63	0,10
Average					19,52	0,07

Table 12

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\overset{\circ}{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{Relative Error} \rvert$ as Referred to the Average
CsF						
CsBr	52,63	49,92	3,14	19,61	10,50	0,16
CsI	71,63	64,94	3,41	17,72	10,98	0,12
NaCl	26,46	13,95	2,51	21,68	13,14	0,05
NaBr	31,98	17,86	2,64	20,80	13,07	0,04
NaI	35,15	19,45	2,90	18,75	11,90	0,05
KF	25,64	12,78	2,55	27,66	14,79	0,18
KCl	35,95	18,59	2,79	21,72	13,93	0,11
KBr	43,55	26,26	2,94	20,11	12,96	0,03
KI	47,48	29,89	3,23	18,12	11,45	0,09
RbCl	39,53	25,07	2,89	21,09	12,55	0,00
Average					12,57	0,08

Table 13

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\overset{\circ}{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{Relative Error} \rvert$ as Referred to the Average
BeO	6,83	5,77	1,33	79,26	19,03	0,02
MgO	12,90	9,59	1,75	75,10	20,63	0,10
BaO	15,00	14,33	1,94	68,64	16,92	0,10
SrO	15,50	13,53	1,92	69,95	18,36	0,02
Average					18,73	0,06

Table 14

Molecules	T_0 (cm^{-1} x10^{4}c)	M_0 (amu)	R_0 ($\overset{\circ}{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{Relative Error} \rvert$ as Referred to the Average
BeF	8,00	6,11	1,36	32,14	13,49	0,02
BeCl	12,00	7,17	1,70	26,58	13,59	0,03
MgF	14,10	10,60	1,75	29,26	13,39	0,02
CaF	17,20	12,88	2,02	26,68	12,25	0,07
Average					13,18	0,04

Table 15

Molecules	T_0 (cm^{-1} x10^4c)	M_0 (amu)	R_0 (Å)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
BO	5,37	6,52	1,20	91,27	16,74	0,03
AlO	10,37	10,04	1,62	77,28	17,76	0,03
Average					17,25	0,03

Table 16

Molecules	T_0 (cm^{-1} x10^4c)	M_0 (amu)	R_0 (Å)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
BF	7,26	6,72	1,26	30,01	12,18	0,07
BCl	12,06	8,38	1,72	25,25	12,17	0,07
BBr	14,77	9,66	1,88	24,20	12,43	0,09
AlCl	20,95	15,24	2,13	22,04	6,44	0,44
AlBr	26,64	20,11	2,29	20,19	11,67	0,02
InCl	31,71	26,82	2,31	23,28	12,79	0,12
InI	56,72	60,32	2,86	18,93	11,11	0,03
TlCl	35,09	29,87	2,55	22,81	12,03	0,05
TlBr	52,27	57,98	2,68	21,10	11,77	0,03
TlI	66,67	78,31	2,87	19,19	11,50	0,01
Average					11,41	0,09

Table 17

Molecules	T_0 (cm^{-1} x10^4c)	M_0 (amu)	R_0 (Å)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{RelativeError} \rvert$ as Referred to the Average
CO	4,67	6,86	1,13	94,28	15,32	0,00
CS	7,86	8,73	1,53	77,13	15,27	0,00
SiO	8,13	10,18	1,51	80,63	15,15	0,00
SiS	13,43	14,93	1,93	64,79	14,49	0,05
GeO	10,23	13,15	1,65	79,47	15,24	0,00
SnO	12,27	14,09	1,84	76,30	15,52	0,02
SnS	20,62	25,25	2,06	58,65	15,26	0,00
PbO	14,00	14,85	1,92	75,47	16,44	0,08
PbS	23,49	27,72	2,39	60,82	14,56	0,05
Average					15,25	0,02

Table 18

Molecules	T_0 (cm^{-1} x10^4c)	M_0 (amu)	R_0 ($\mathring{A}$)	E (ev)	$\frac{T_0}{R_0}\sqrt{\frac{E_0}{M_0}}$	$\lvert \text{Relative Error} \rvert$ as Referred to the Average
NO	5,33	7,47	1,15	98,21	16,81	0,02
PO	8,21	10,55	1,45	85,15	16,09	0,02
Average					16,45	0,02

Table 19 g_k's

Family of	**H_2**	**N_2**	**O_2**	**F_2**	**LiH**	**BeH**	**BH**	**CH**	**NH**
g_k	1.01	1.06	0.64	0.32	1.10	0.93	0.90	0.82	0.74

Family of	**HF**	**ZnH**	**CsF**	**BeO**	**BeF**	**BO**	**BF**	**CO**	**NO**
g_k	0.62	0.99	0.37	0.91	0.45	0.83	0.36	0.62	0.72

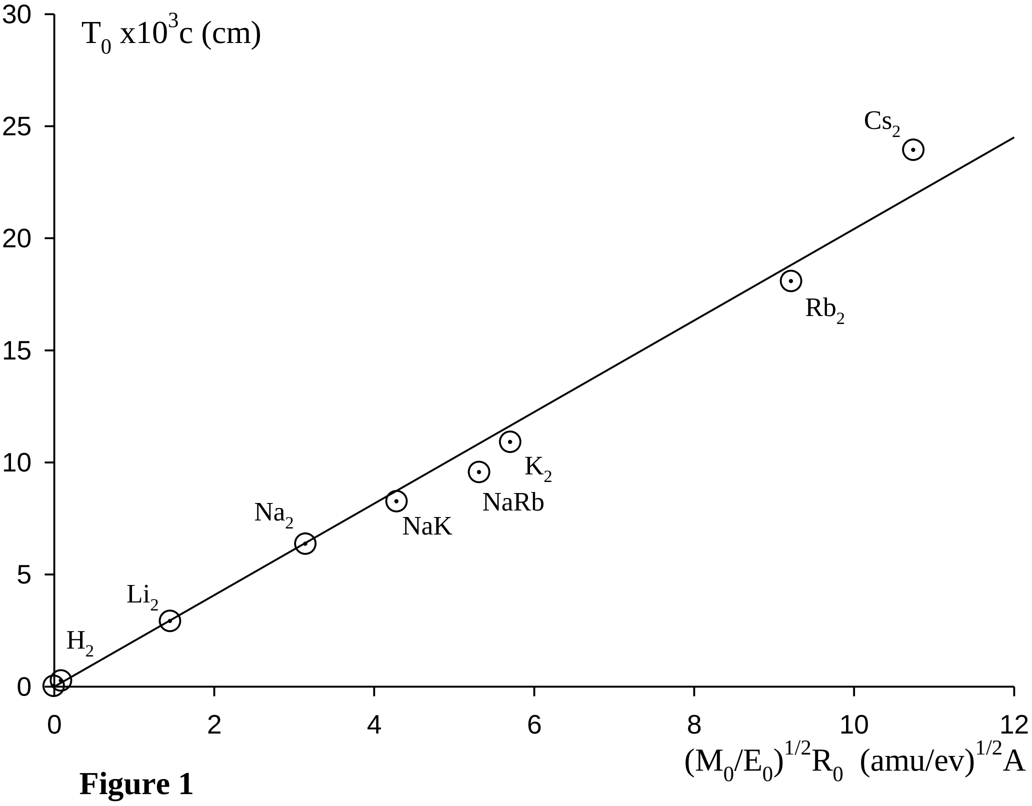

T_0 x10^3c (cm)
30
25
20
15
10
5
0
0
2
4
6
8
10
12
$(M_0/E_0)^{1/2}R_0$ $(\text{amu/ev})^{1/2}$A
Cs_2
Rb_2
K_2
NaRb
NaK
Na_2
Li_2
H_2

Figure 1

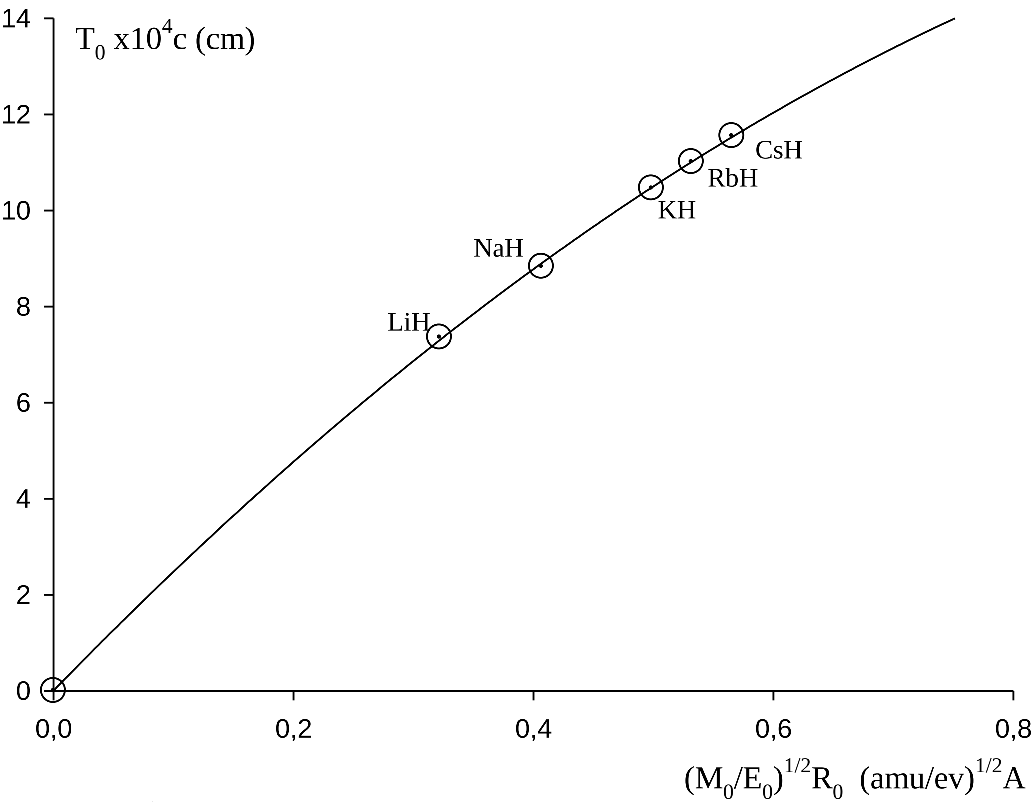

14
12
10
8
6
4
2
0
T_0 x10^4c (cm)
LiH
NaH
KH
RbH
CsH
0,0
0,2
0,4
0,6
0,8
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 2

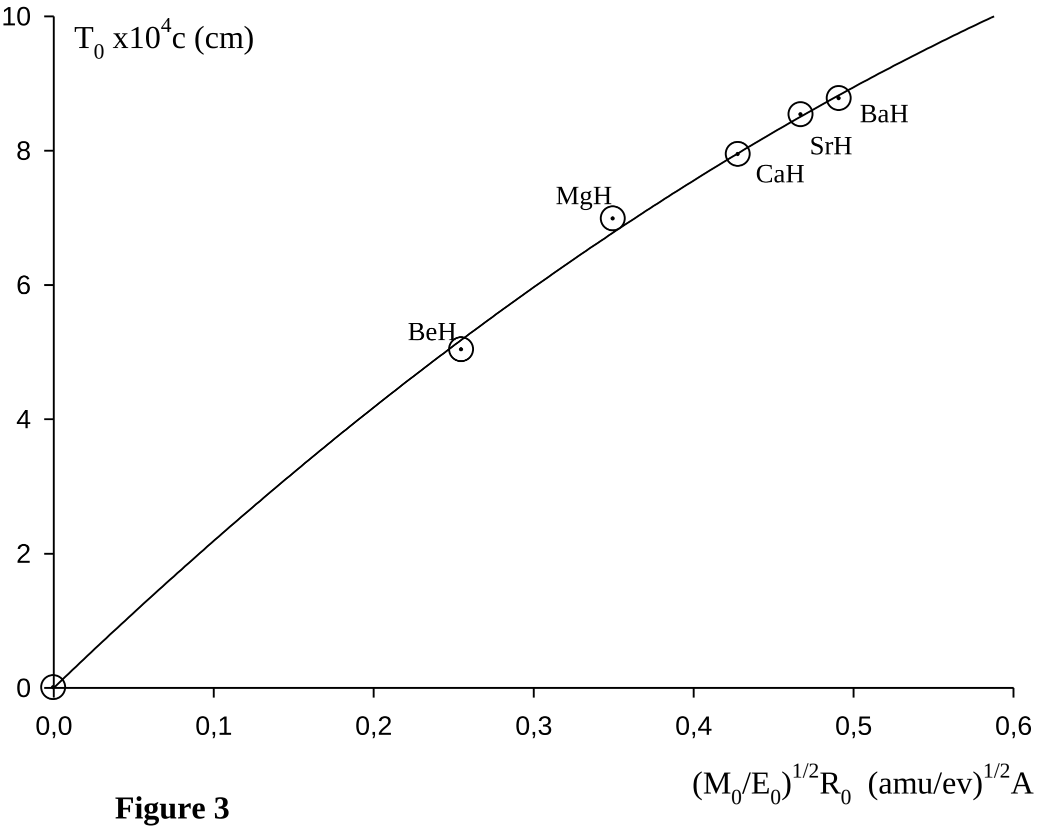

10
8
6
4
2
0
T_0 x10^4c (cm)
BaH
SrH
CaH
MgH
BeH
0,0
0,1
0,2
0,3
0,4
0,5
0,6
$(M_0/E_0)^{1/2}R_0$ $(amu/ev)^{1/2}$A

Figure 3

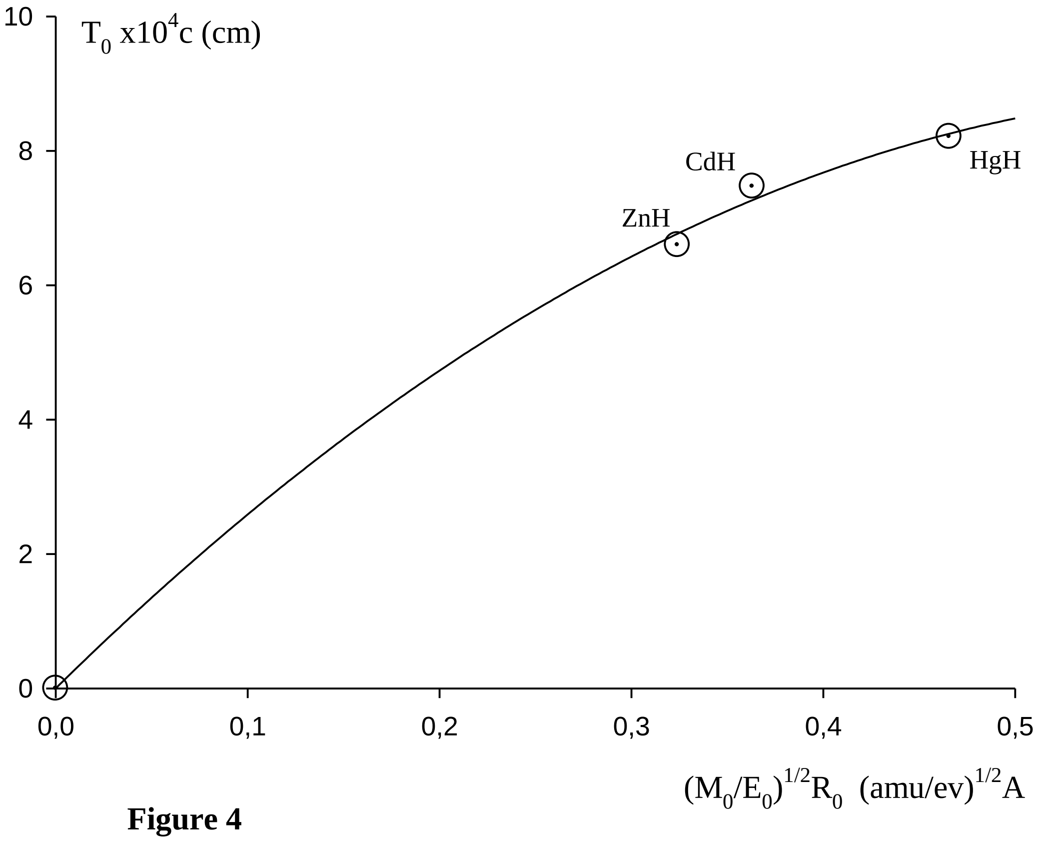

10
8
6
4
2
0
T_0 x10^4c (cm)
CdH
HgH
ZnH
0,0
0,1
0,2
0,3
0,4
0,5
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 4

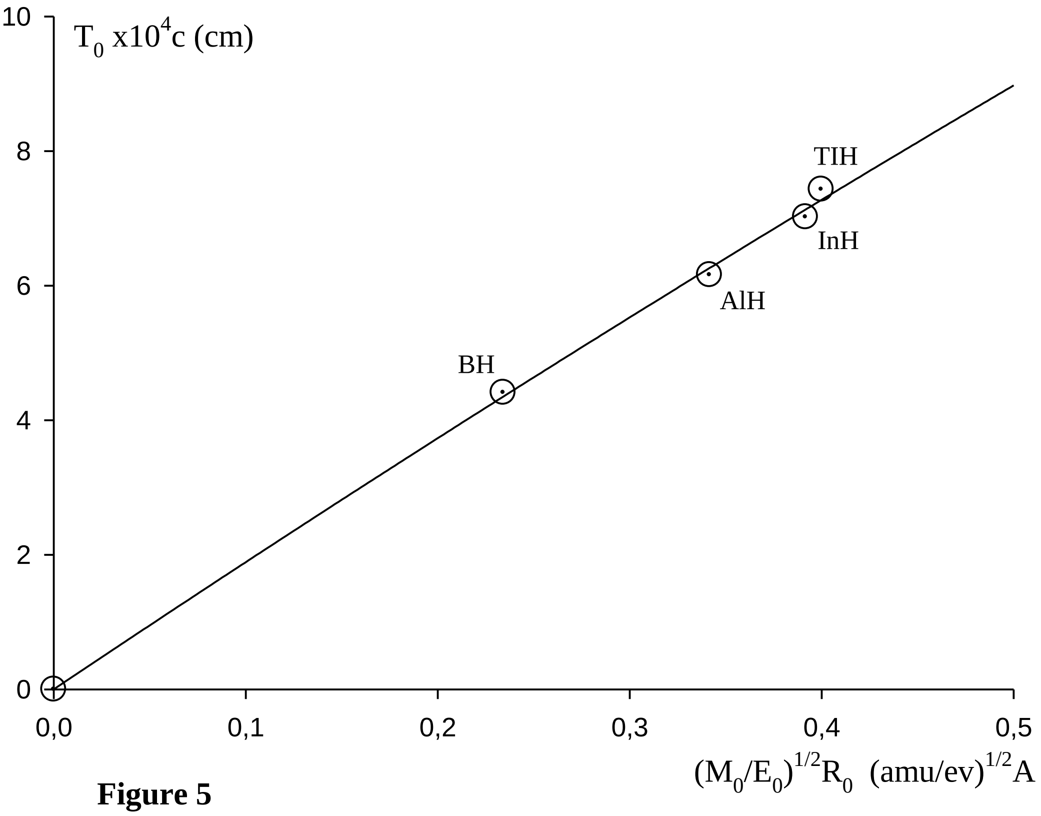

10
8
6
4
2
0
T_0 x10^4c (cm)
TlH
InH
AlH
BH
0,0
0,1
0,2
0,3
0,4
0,5
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 5

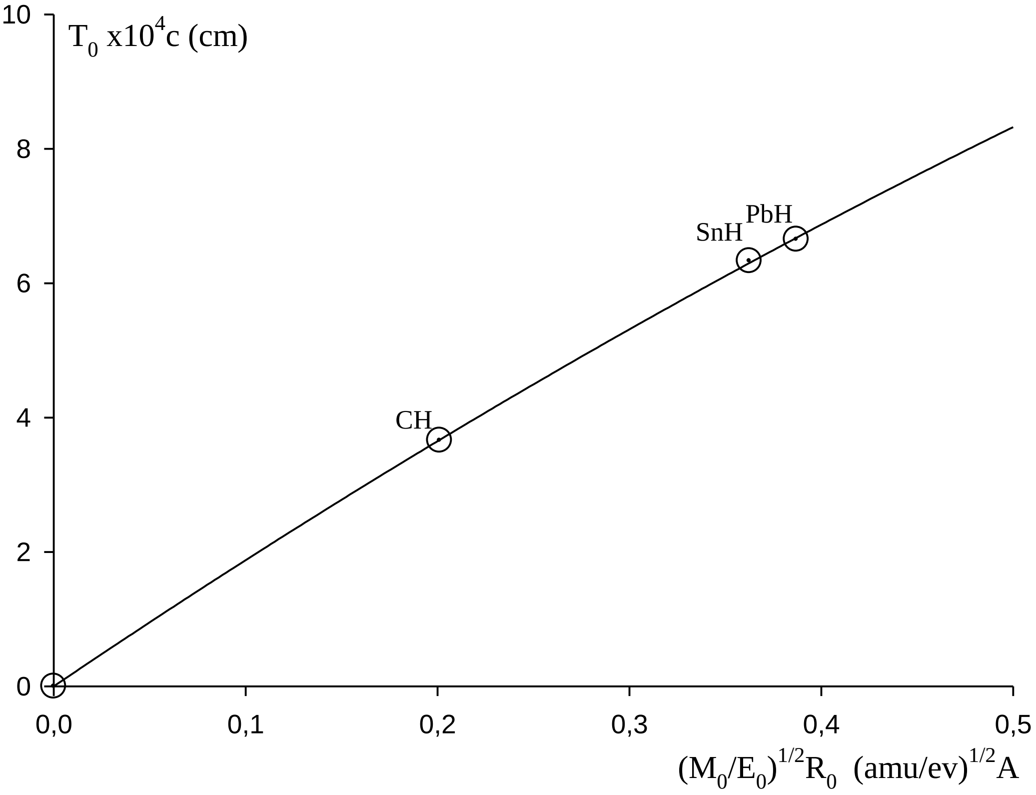

10
T_0 x10^4c (cm)
8
6
4
2
0
PbH
SnH
CH
0,0
0,1
0,2
0,3
0,4
0,5
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 6

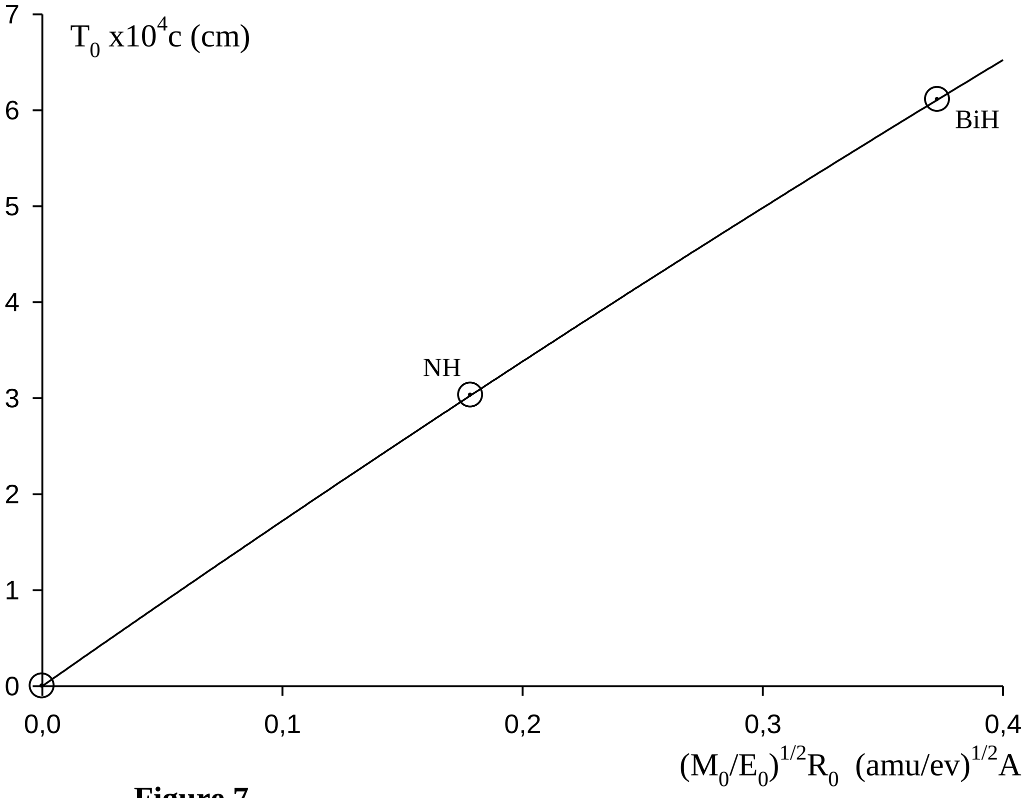


Figure 7

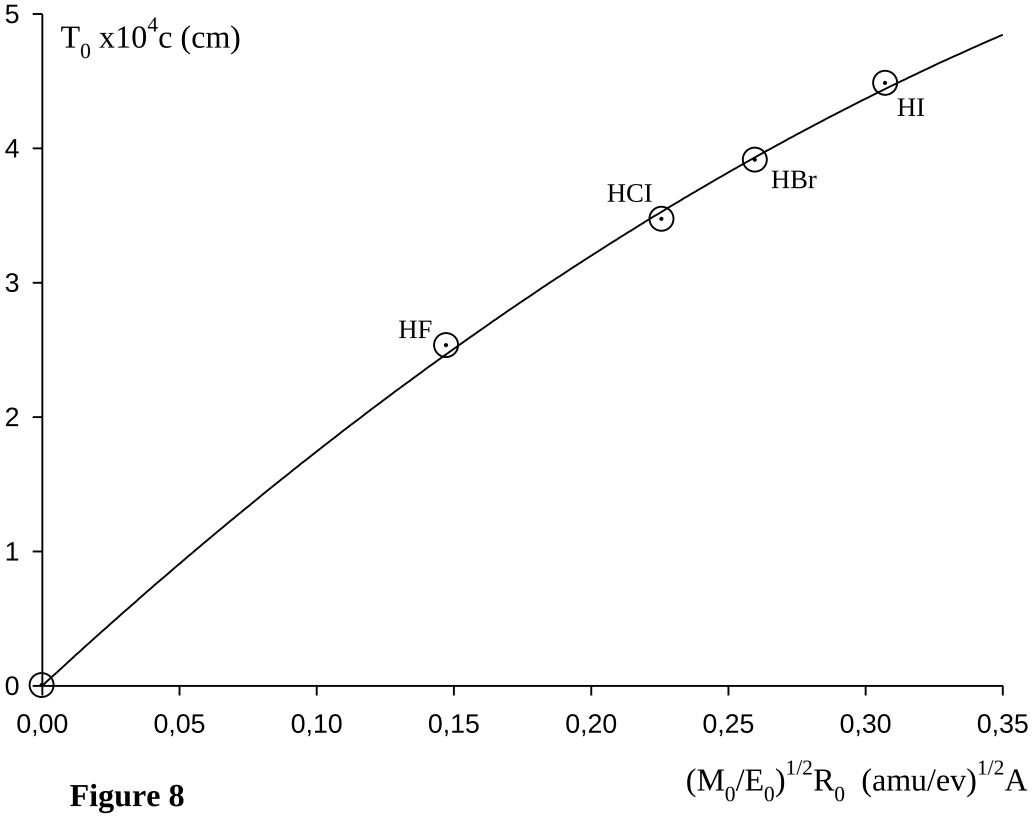

5
4
3
2
1
0
T_0 x10^4c (cm)
HI
HBr
HCI
HF
0,00
0,05
0,10
0,15
0,20
0,25
0,30
0,35
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 8

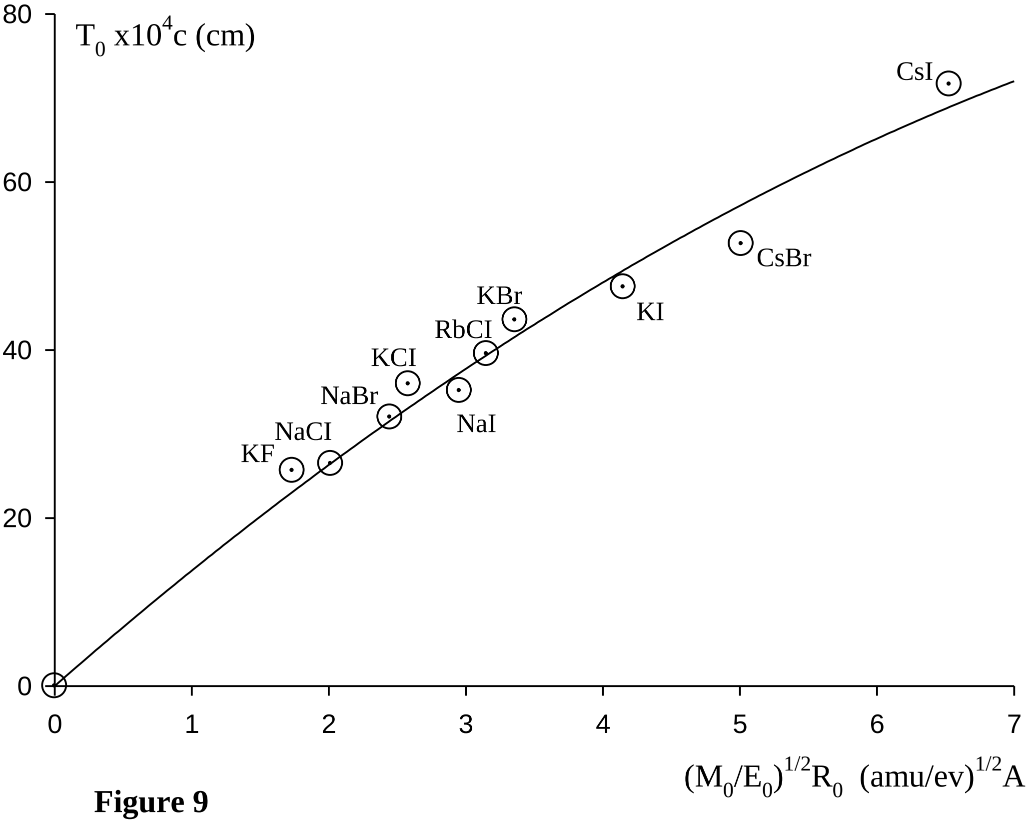
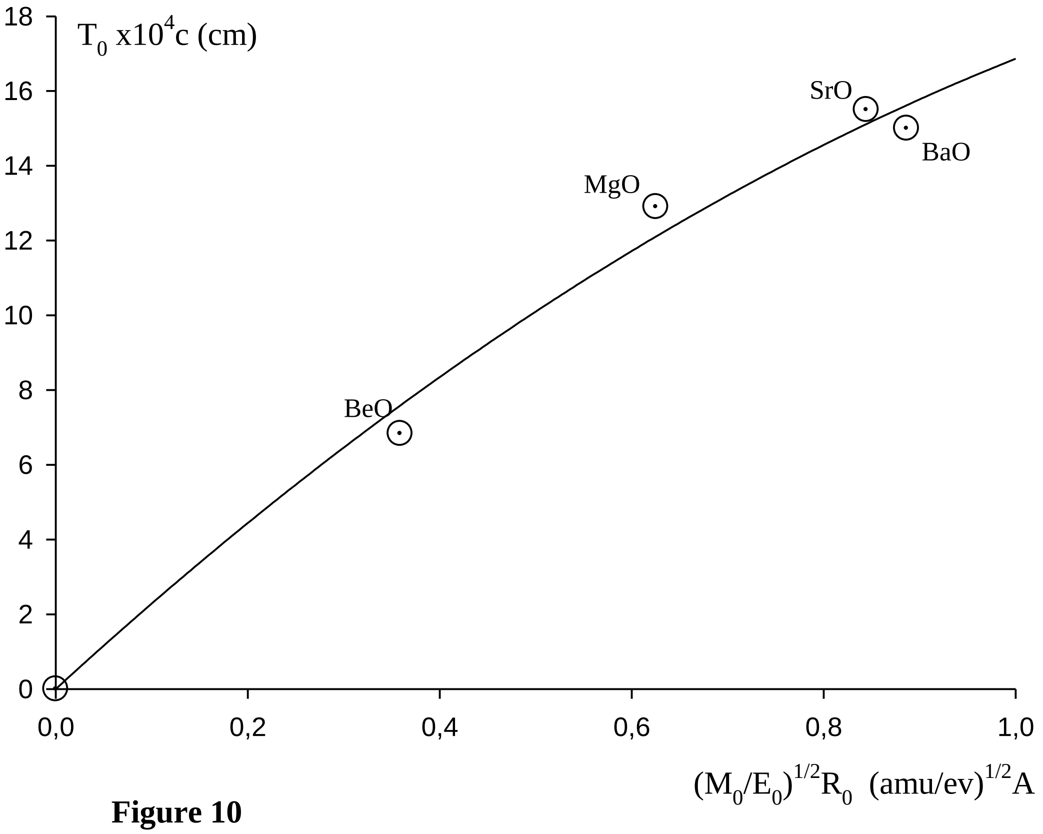

T_0 x10^4c (cm)
80
60
40
20
0
0
1
2
3
4
5
6
7
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A
CsI
CsBr
KI
KBr
RbCI
KCI
NaBr
NaI
NaCI
KF

Figure 9



T_0 x10^4c (cm)
18
16
14
12
10
8
6
4
2
0
0,0
0,2
0,4
0,6
0,8
1,0
$(M_0/E_0)^{1/2}R_0$ $(amu/ev)^{1/2}$A
SrO
BaO
MgO
BeO

Figure 10

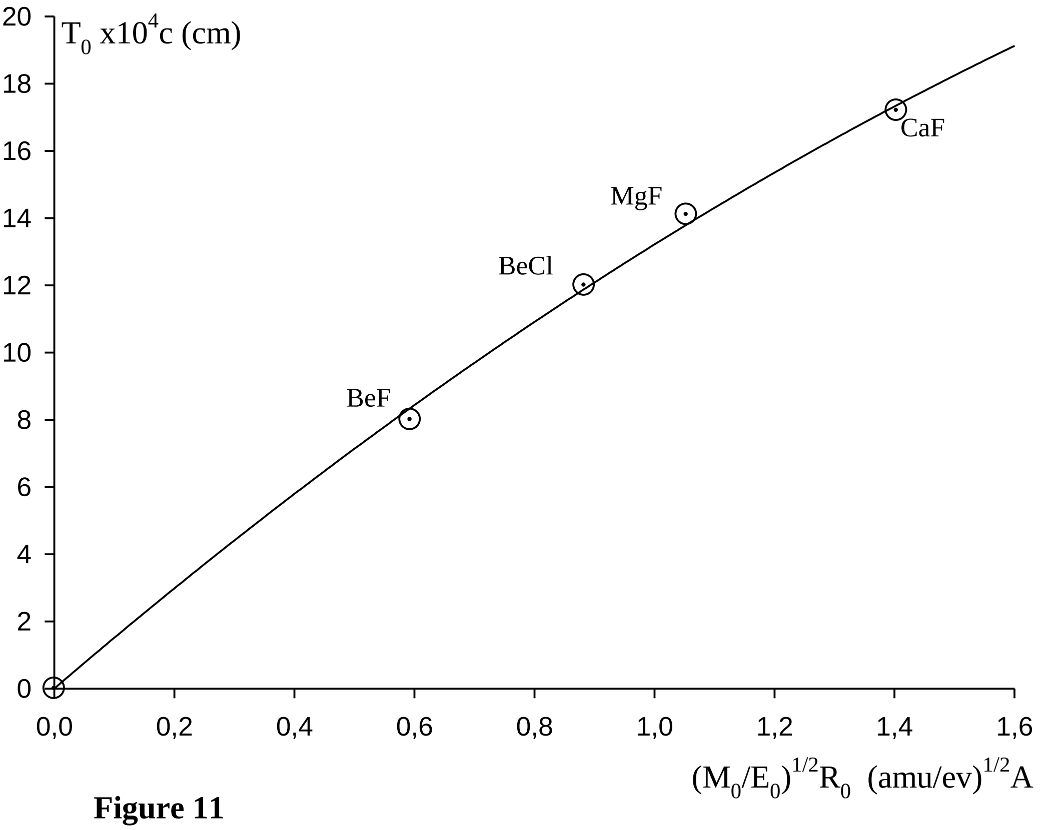

T_0 x10^4c (cm)
20
18
16
14
12
10
8
6
4
2
0
0,0
0,2
0,4
0,6
0,8
1,0
1,2
1,4
1,6
BeF
BeCl
MgF
CaF
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 11

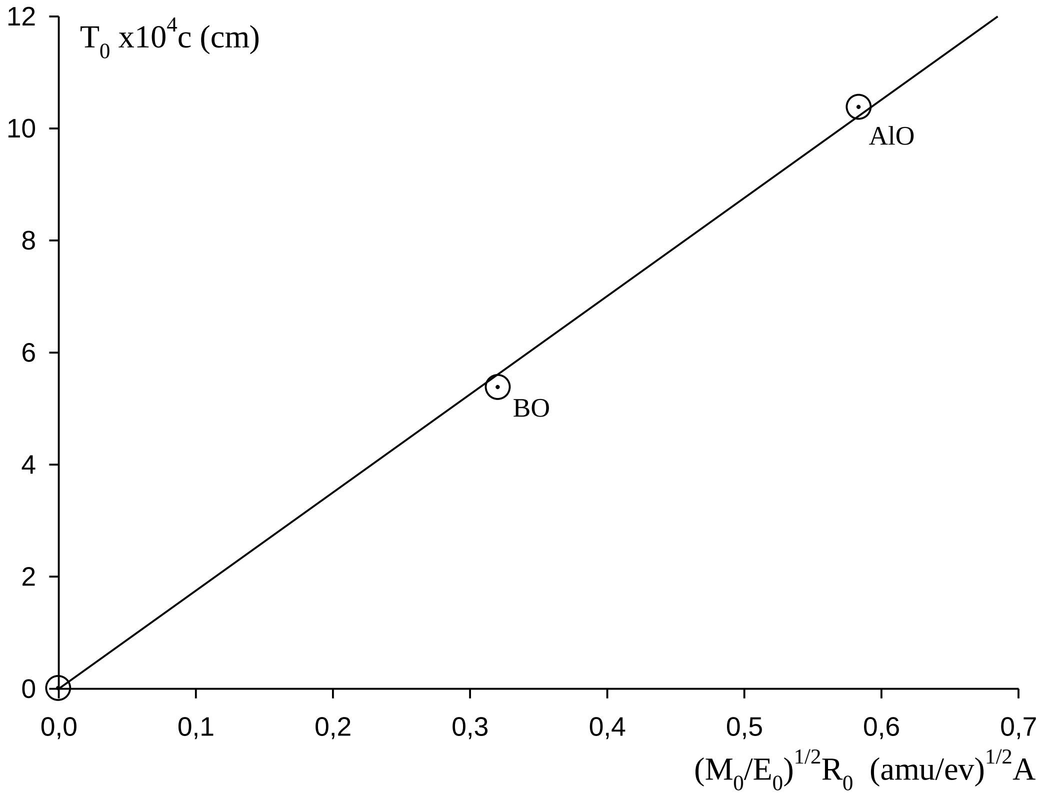

12
10
8
6
4
2
0
$T_0 \times 10^4 c$ (cm)
AlO
BO
0,0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 12

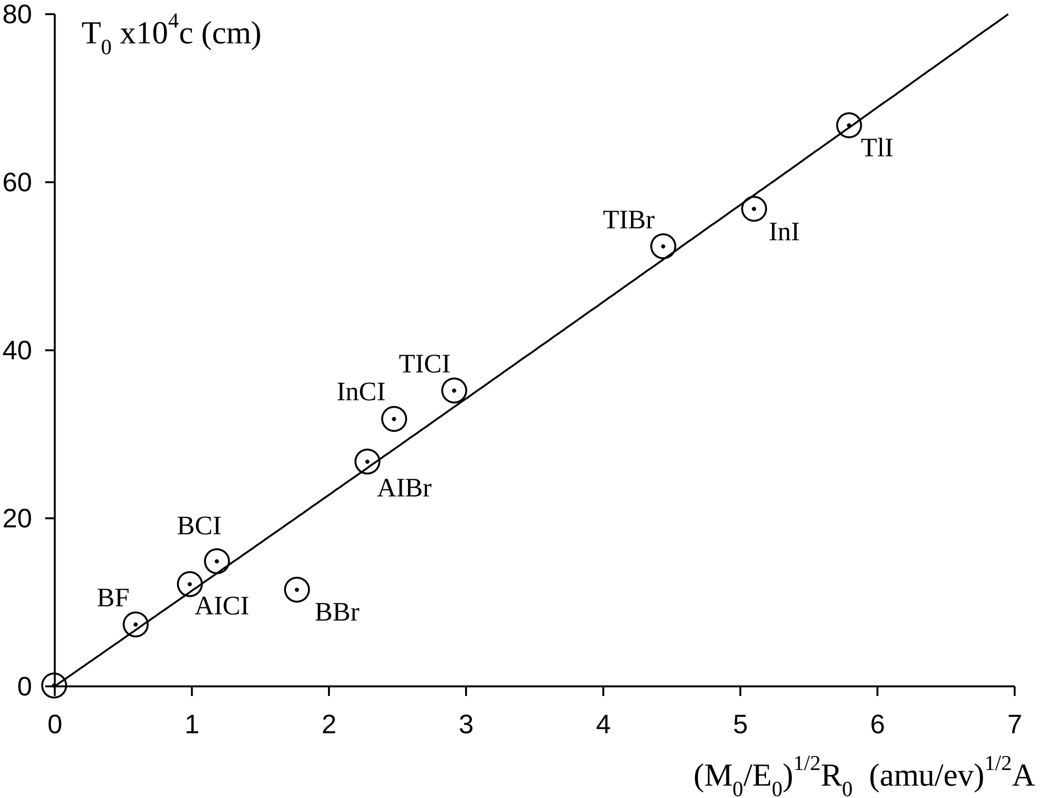
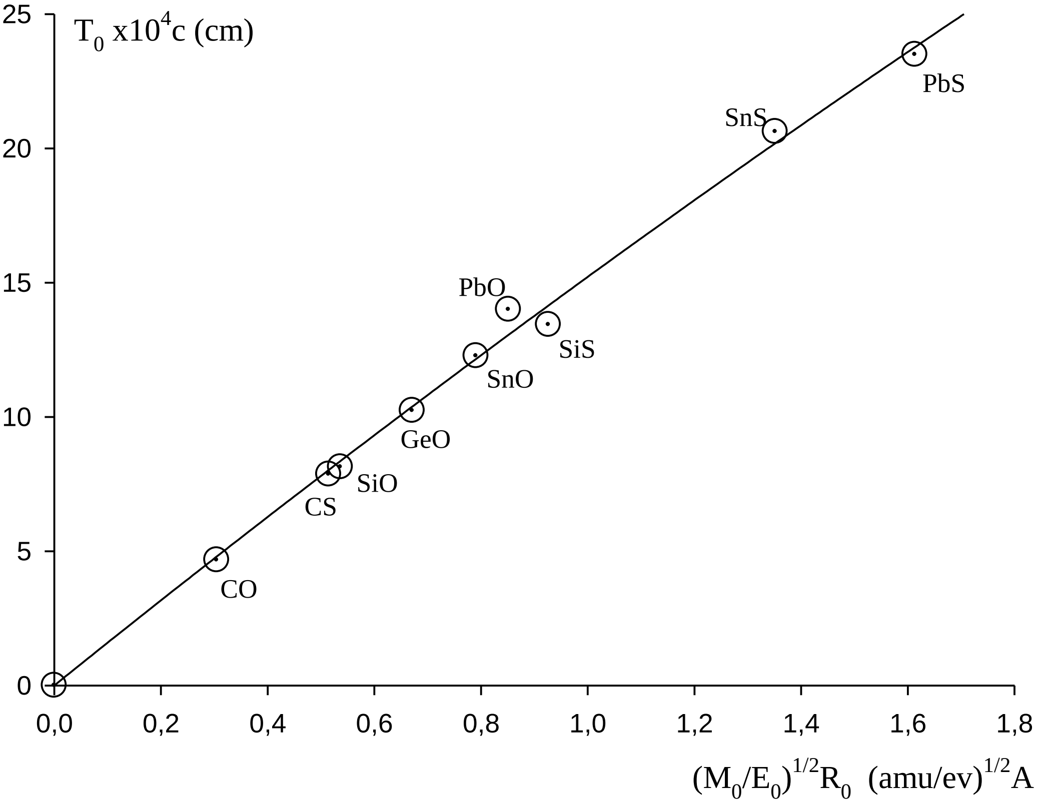

80
60
40
20
0
T_0 x10^{4}c (cm)
TlI
TIBr
InI
TICI
InCI
AIBr
BCI
BF
AICI
BBr
0
1
2
3
4
5
6
7
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 13



25
20
15
10
5
0
T_0 x10^4c (cm)
PbS
SnS
PbO
SiS
SnO
GeO
SiO
CS
CO
0,0
0,2
0,4
0,6
0,8
1,0
1,2
1,4
1,6
1,8
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 14

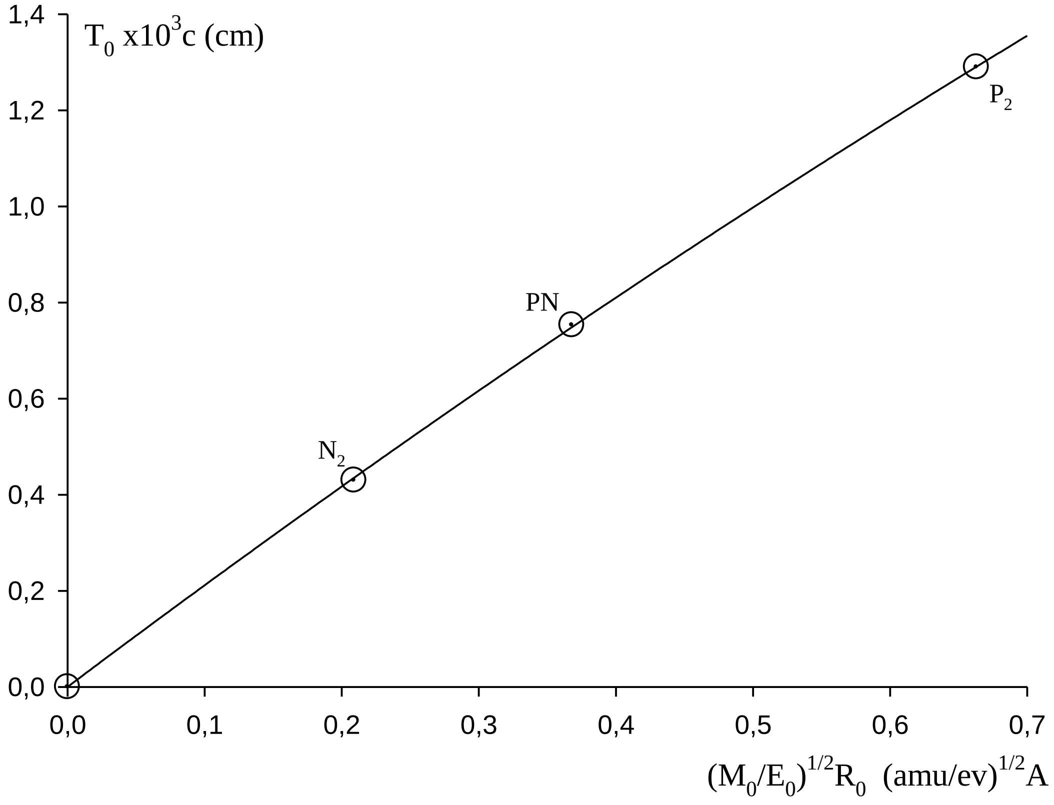
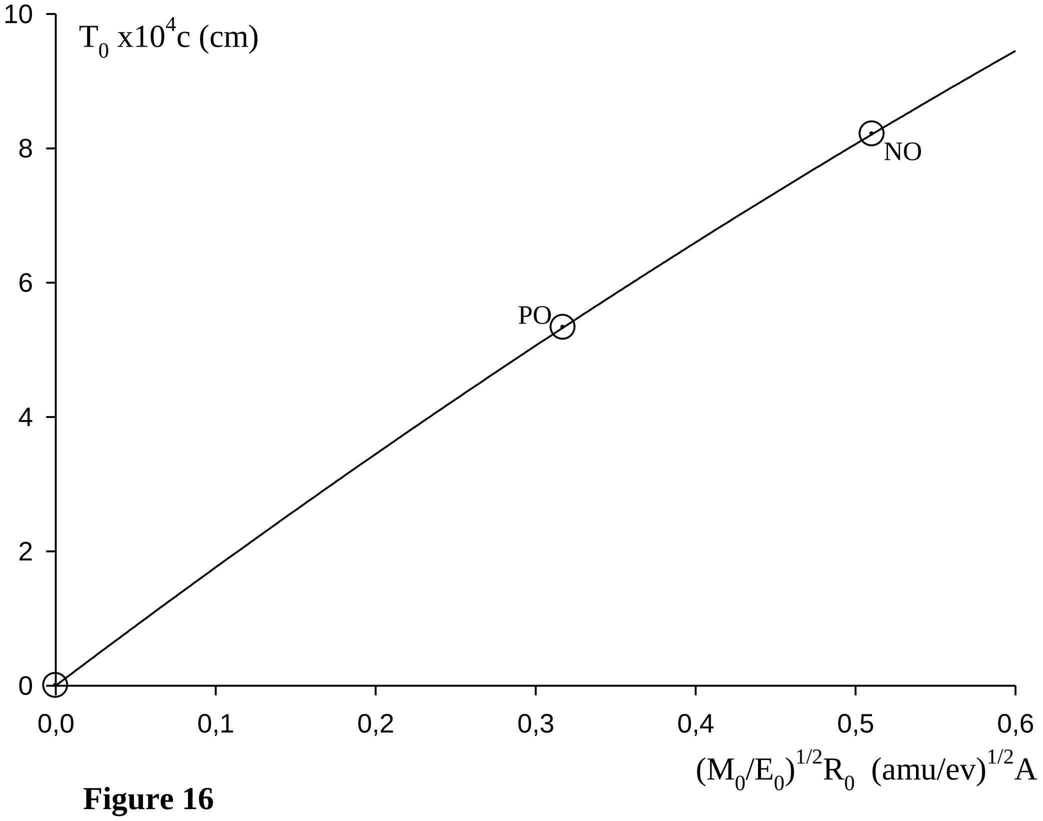

1,4
1,2
1,0
0,8
0,6
0,4
0,2
0,0
T_0 x10^3c (cm)
P_2
PN
N_2
0,0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 15



10
8
6
4
2
0
T_0 x10^4c (cm)
NO
PO
0,0
0,1
0,2
0,3
0,4
0,5
0,6
$(M_0/E_0)^{1/2}R_0$ $(amu/ev)^{1/2}$A

Figure 16

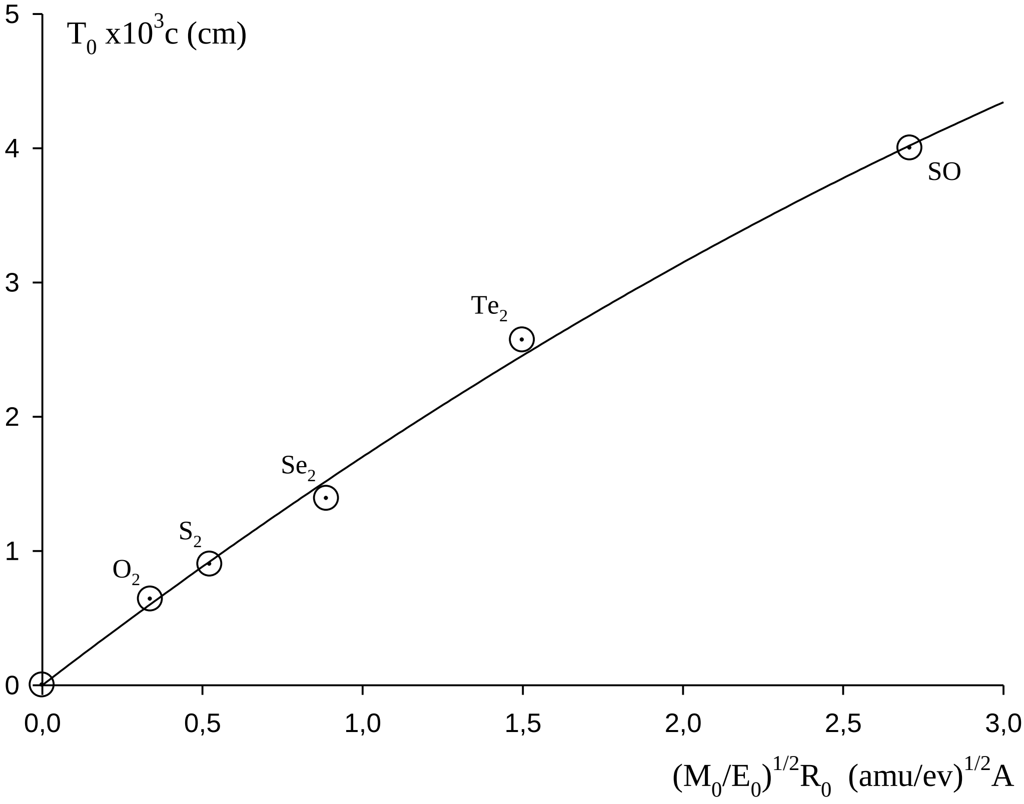

5
4
3
2
1
0
T0 x10^3c (cm)
SO
Te2
Se2
S2
O2
0,0
0,5
1,0
1,5
2,0
2,5
3,0
(M0/E0)^1/2R0 (amu/ev)^1/2A

Figure 17

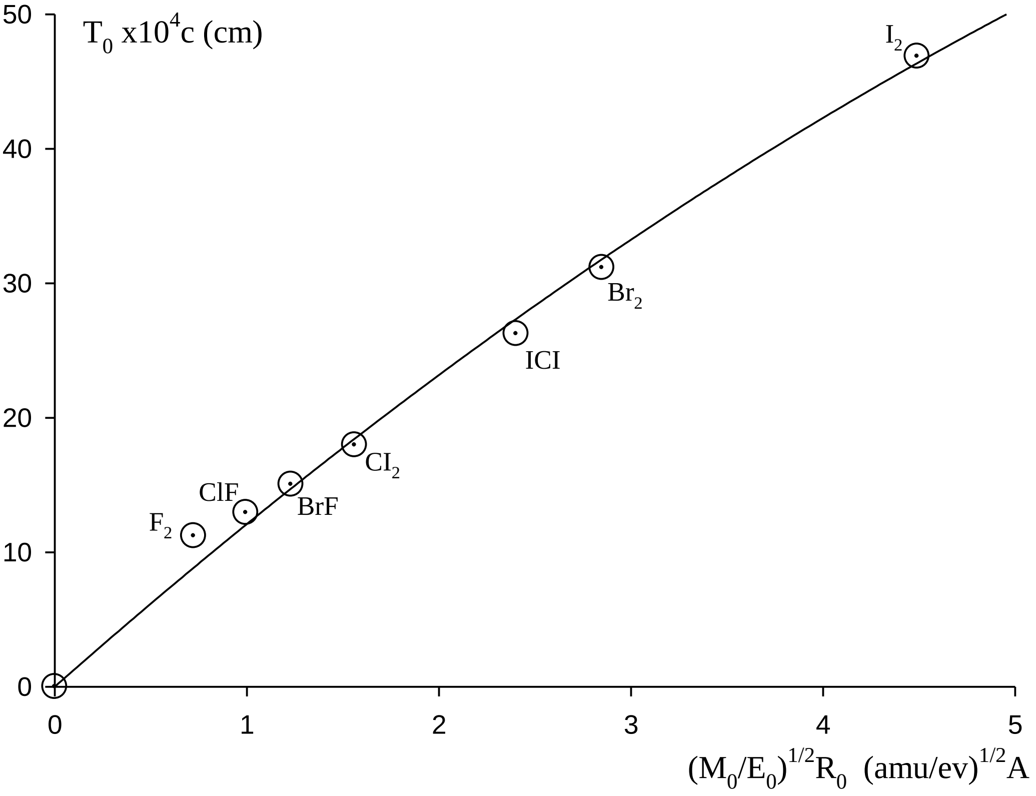

50
40
30
20
10
0
T_0 x10^4c (cm)
I_2
Br_2
ICI
CI_2
ClF
BrF
F_2
0
1
2
3
4
5
$(M_0/E_0)^{1/2}R_0$ (amu/ev)$^{1/2}$A

Figure 18

CONCLUSION

The foregoing results show that our prediction, i.e Eq.(6), together with the *constancy of the coefficient* g_k, *for members of a given chemical family,* indeed holds fairly succesfully. The constant $(T_0/R_0)\left(\sqrt{M_0/E_0}\right)\{(cm^{-1}x10^3c/A)\sqrt{amu/ev}\}$, i.e. $\sqrt{g_k}$, varies between, approximately 1 and 2, throughout different families.

One can show that g_k happens to be roughly, *inversely proportional to the dissociation energy of the molecule.* [13] As one can observe from Table 19, it indeed decreases as the bond becomes stronger. Thus, the smaller g_k is, the higher is the number of the covalent bonds, making the overall bond of the diatomic molecule, or the higher is the number of free electrons an atom possesses, the looser will be the bond it will make with, say, an halogen, thus the higher will g_k be, etc.

It is easy to check that, Eq.(6) amazingly holds, even for the Bohr hydrogen atom, for which however, g_k becomes unity.

Note that we have found nothing similar to the line we pursued herein.

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