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ENERGY LEVELS OF THE SINGLE EXCITED STATES IN NaI AND Na-LIKE IONS *

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ABSTRACT

Energy levels of the single excited $1s^2 2s^2 2p^6 ns(^2S)$, $1s^2 2s^2 2p^6 mp(^2P)$, $1s^2 2s^2 2p^6 md(^2D)$ and $1s^2 2s^2 2p^6 nf(^2F)$; $n = 4 - 7$, $m = 3 - 6$ states for NaI and Na-like ions are calculated using the one configuration Hartree-Fock method. Good agreement is obtained between our results for the higher members of the NaI sequence and previous data from photo-absorption and beam foil experiments.

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1. INTRODUCTION

Single excitations in sodium and sodium-like ions form one of the simplest atomic systems in which an $n\ell$ electron is outside a closed $1s^2 2s^2 2p^6$ core. The spectra for these atoms and ions can be treated as one electron spectra (hydrogen-like) with no correlation with the core [1] and [2].

In present study we have performed single-configuration Hartree-Fock energy calculations for the $1s^2 2s^2 2p^6 ns(^2S)$, $1s^2 2s^2 2p^6 mp(^2P)$, $1s^2 2s^2 2p^6 md(^2D)$ and $1s^2 2s^2 2p^6 nf(^2F)$; $n = 4 - 7$, $m = 3 - 6$ one electron excited states in Na and Na-like ions using the computer code of Froese-Fischer [3].

The purpose of this study is to investigate the hydrogen-like trends of the energy levels of outer shell one electron excitation along the NaI isoelectronic sequence. Moreover, spectroscopic data for highly stripped ions are urgently needed for the development of Tokamak devices, both for plasma diagnostics and for estimating energy loss through impurity ions [4].

2. METHOD OF CALCULATION

The method of calculation was described elsewhere [5] and [6]. The Hartree-Fock programme of Froese-Fischer [3] was used in calculating the average energies of the various configurations and the method of Edlen [7] for extrapolating level intervals in terms of Slater parameters was applied to obtain the term energies of the levels.

3. RESULTS AND DISCUSSION

Our results of the energy levels calculated in Cm^{-1} of the various configurations relative to the ground state $1s^2 2s^2 2p^6 3s$ configuration are given in Tables 1 - 8 together with the experimental data of Moore [8] from photo-absorption measurements. A deviation of about 4.5% for NaI is observed between our results and the experimental data and which decreases with the increase of z along the isoelectron sequence until it reaches 9.4% for ArVIII. The relatively large deviation from the experimental

values obtained for NI and MgII is expected since we use in our calculations the single configuration one electron model. This method is suitable for the calculations of the energy levels of the higher members of the isoelectronic sequence, where the excitation energies of the excited electron are well separated from each other and lie high above the ground level.

Table 9 shows a good agreement between our calculations for the energy of the $1s^2 2s^2 2p^6 3p(^2P)$ level of SVI and ArVIII and the observed values of these levels from the spark spectra of SVI, Ref.[9] and the beam foil spectra of ArVIII, Ref.[10], respectively.

To study the systematic trends in the isoelectronic sequence from the point of view of the charge expansion theory of Layzer [11], we expand the energy in descending power of z (the atomic charge).

$$E = E_0 z^2 + E_1 z + E_2 + \ldots \quad ,$$

where E_0 is the zeroth order energy. Fig.1 shows the z-energy dependence of our calculated Hartree-Fock energies for the 4s, 4p and 4d levels of the NaI sequence. The linear relations obtained between E/z^2 and $1/z$ (see Fig.1), are indications of electrostatic interactions existing between the core electrons and the excited electron in the various members of the sequence. The deviation from linearity occurring at NaI and MgII might be due to the effects of configuration interactions in these light members of the sequence which are neglected in our calculations.

In order to check the hydrogenic behaviour of the term energies, we plotted in Figs. 2 and 3, our calculated energy values for NaI and PV against $1/n^2$ (where n is the principal quantum number). A linear behaviour is obtained for $n = 4$ up to 7 (i.e. for highly excited states), and a deviation from linearity from $n = 3$ to 4 (see Figs. 2 and 3). This deviation might be attributed to electron correlation effects with the same parity and angular momentum, which are appreciable in the case of low excited states having relatively small energy separations.

Finally we conclude that the one configuration Hartree-Fock method is suitable for the calculations of the energy levels of the highly excited states (high n values) and moderately ionized atoms (large z) in the

sequence, work is in progress taking into account configuration interation effects in the energy level calculations.

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REFERENCES

[1] J. Migdalk and W.E. Baylis, J. Phys. B12 (1979) 2595.

[2] B.N. Chichkov and V.P. Shevelko, Physica Scripta 23 (1981) 1055.

[3] C. Froese Fischer, Comput. Phys. Commun. 1 (1969) 151.

[4] E. Oktay, Atomic and Molecular Processes in Controlled Thermonuclear Fusion, Eds. M.R.C. McDowell and A.M. Frendeci, NATO Adv. Study Inst. Series (1979) p.99.

[5] Th.M. El-Sherbini, Atomkernenergie (ATKE) 39 (1981) 53.

[6] Th.M. El-Sherbini and S.H. Allam, Ann. Physik 39, (1982) 107.

[7] B. Edlen, Handbuch der Physik, Ed. S. Flügge (Springer-Verlag, Berlin, 1964) Vol.27, p.80.

[8] C.E. Moore, Atomic Energy Levels, NBS Circular, No.467, Vol.1 (1949).

[9] I. Joelsson, P.O. Zetterberg and C.E. Magnusson, Physica Scripta 2 (1979) 145.

[10] F.H. Pinnington, R.N. Gosselin, J.A. O'Neill, J.A. Kernaham, K.E. Donnelly and R.L. Brooks, Physics Scripta 2 (1979) 151.

[11] D. Layzer, Ann. Phys. 8 (1959) 271; Monthly Not. Roy. Astron. Soc. 114 (1954) 692.

TABLE 1

Table 1 : Excitation energies of Na I levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$ together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s$ (^2S)	24574.0	25739.9	$1s^2 2s^2 2p^6 3d$ (^2D)	27755.4	29172.9
5s (^2S)	31837.7	33200.7	4d (^2D)	33098.1	34548.8
6s (^2S)	34948.2	36372.7	5d (^2D)	35572.3	37036.8
7s (^2S)	36563.0	38012.1	6d (^2D)	36916.3	38387.3
$1s^2 2s^2 2p^6 3p$ (^2P)	15955.5	16956.2	$1s^2 2s^2 2p^6 4f$ (^2F)	33112.4	34588.6
4p (^2P)	28927.8	30266.9	5f (^2F)	35580.6	37057.6
5p (^2P)	33620.9	35040.3	6f (^2F)	36921.4	38400.1
6p (^2P)	35847.7	37296.5	7f (^2F)	37699.4	39209.2

TABLE 2

Table 2 : Excitation energies of Mg II levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$ together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s\ (^2S)$	68025.2	69805.2	$1s^2 2s^2 2p^6 3d\ (^2D)$	69543.7	71490.4
$5s\ (^2S)$	90644.0	92786.2	$4d\ (^2D)$	91120.0	93312.1
$6s\ (^2S)$	100926.1	103198.1	$5d\ (^2D)$	101132.0	103421.1
$7s\ (^2S)$	106459.5	108784.7	$6d\ (^2D)$	106567.3	108900.9
$1s^2 2s^2 2p^6 3p\ (^2P)$	34643.9	35669.4	$1s^2 2s^2 2p^6 4f\ (^2F)$	91442.4	93800.0
$4p\ (^2P)$	78310.9	80620.8	$5f\ (^2F)$	101315.8	103690.2
$5p\ (^2P)$	95250.4	97454.9	$6f\ (^2F)$	106679.5	109062.6
$6p\ (^2P)$	103328.1	105623.1	$7f\ (^2F)$	109913.7	112301.8

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TABLE 3

Table 3 : Excitation energies of Al III levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$ together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s\ (^2S)$	124040.5	126162.6	$1s^2 2s^2 2p^6 3d\ (^2D)$	114106.5	115955.0
$5s\ (^2S)$	168016.5	170636.4	$4d\ (^2D)$	163293.2	165785.3
$6s\ (^2S)$	188684.9	191478.5	$5d\ (^2D)$	186143.5	188875.5
$7s\ (^2S)$	200042.4	202904.8	$6d\ (^2D)$	198532.7	201374.4
$1s^2 2s^2 2p^6 3p\ (^2P)$	52920.2	53694.1	$1s^2 2s^2 2p^6 4f\ (^2F)$	164728.0	167612.1
$4p\ (^2P)$	141384.7	143632.3	$5f\ (^2F)$	186945.6	189875.8
$5p\ (^2P)$	175783.4	178430.5	$6f\ (^2F)$	199016.6	201969.5
$6p\ (^2P)$	192815.3	195620.9	$7f\ (^2F)$	206201.4	209261.0

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TABLE 4

Table 4 : Excitation energies of Si IV levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$ together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s\ (^2S)$	191629.7	193981.5	$1s^2 2s^2 2p^6 3d\ (^2D)$	158883.4	160376.8
$5s\ (^2S)$	262465.9	265420.4	$4d\ (^2D)$	247383.8	250010.6
$6s\ (^2D)$	296499.4	299679.6	$5d\ (^2D)$	288474.5	291499.2
$7s\ (^2S)$	315462.2	318744.5	$6d\ (^2D)$	310717.5	313923.4
$1s^2 2s^2 2p^6 3p\ (^2P)$	70884.2	71289.6	$1s^2 2s^2 2p^6 4f\ (^2F)$	250898.3	254129.4
$4p\ (^2P)$	215894.5	218269.5	$5f\ (^2F)$	290402.1	293721.0
$5p\ (^2P)$	273569.4	276506.5	$6f\ (^2F)$	311868.4	315231.6
$6p\ (^2P)$	302482.3	305645.0	$7f\ (^2F)$	324699.9	328201.5

TABLE 5

Table 5 : Excitation energies of P V levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$ together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s\ (^2S)$	270450.9	272961.1	$1s^2 2s^2 2p^6 3d\ (^2D)$	203137.1	204197.1
$5s\ (^2S)$	373445.1	376639.2	$4d\ (^2D)$	342706.2	345398.4
$6s\ (^2S)$	423718.2	427157.0	$5d\ (^2D)$	407400.4	410631.1
$7s\ (^2S)$	452010.3	455573.0	$6d\ (^2D)$	442367.8	445814.0
$1s^2 2s^2 2p^6 3p\ (^2P)$	88670.6	88651.7	$1s^2 2s^2 2p^6 4f\ (^2F)$	349132.6	352595.8
$4p\ (^2P)$	301762.0	304161.8	$5f\ (^2F)$	410868.2	414458.7
$5p\ (^2P)$	387997.5	391101.7	$6f\ (^2F)$	444420.7	448061.7
$6p\ (^2P)$	424117.7	435100.4	$7f\ (^2F)$	464772.2	468580.0

TABLE 6

Table 6 : Excitation energies of S VI levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$ together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s\ (^2S)$	360354.0	362983.0	$1s^2 2s^2 2p^6 3d\ (^2D)$	246775.1	247452.0
$5s\ (^2S)$	500701.5	504112.0	$4d\ (^2D)$	449060.3	451785.0
$6s\ (^2S)$	570034.4	573823.0	$5d\ (^2D)$	542636.7	546021.0
$7s\ (^2S)$	609350.9		$6d\ (^2D)$	593155.4	596877.0
$1s^2 2s^2 2p^6 3p\ (^2P)$	106380.1	107137.0	$1s^2 2s^2 2p^6 4f\ (^2F)$	459030.2	462658.0
$4p\ (^2P)$	398807.5	401164.0	$5f\ (^2F)$	547945.8	551848.0
$5p\ (^2P)$	518784.7	522030.0	$6f\ (^2F)$	596277.0	600170.0
$6p\ (^2P)$	579942.9	583679.0	$7f\ (^2F)$	630120.8	

TABLE 7

Table 7 : Excitation energies of Cl VII levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$ together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s\ (^2S)$	461268.0	464003.0	$1s^2 2s^2 2p^6 3d\ (^2D)$	289910.0	290166.0
$5s\ (^2S)$	644107.6	647677.0	$4d\ (^2D)$	566402.3	569142.0
$6s\ (^2S)$	735289.8		$5d\ (^2D)$	694060.7	697598.0
$7s\ (^2S)$	822507.8		$6d\ (^2D)$	762921.0	
$1s^2 2s^2 2p^6 3p\ (^2P)$	124088.1	124891.0	$1s^2 2s^2 2p^6 4f\ (^2F)$	580378.3	584086.0
$4p\ (^2P)$	506950.0	509197.0	$5f\ (^2F)$	701423.4	705898.0
$5p\ (^2P)$	665789.9		$6f\ (^2F)$	767226.9	771549.0
$6p\ (^2P)$	747238.5		$7f\ (^2F)$	799450.4	

Table 8 : Excitation energies of Ar VIII levels (in cm^{-1}) relative to the ground level $1s^2 2s^2 2p^6 3s$, together with the experimental data of Moore (8) for comparison.

Level	This work	Ref. (8)	Level	This work	Ref. (8)
$1s^2 2s^2 2p^6 4s$ (^2S)	573160.6	575910.0	$1s^2 2s^2 2p^6 3d$ (^2D)	332701.5	332727.0
5s (^2S)	803599.7	812422.0	4d (^2D)	694740.5	697471.0
6s (^2S)	919402.2		5d (^2D)	861619.6	865084.0
7s (^2S)	985790.9		6d (^2D)	951585.4	955560.0
$1s^2 2s^2 2p^6 3p$ (^2P)	141854.8	142776.0	$1s^2 2s^2 2p^6 4f$ (^2F)	713062.3	716818.0
4p (^2P)	626156.2	628240.0	5f (^2F)	871187.5	875248.0
5p (^2P)	828942.1	832245.0	6f (^2F)	957157.0	
6p (^2P)	933432.8		7f (^2F)	998314.8	

Table 9 : A comparison between our calculations for $1s^2 2s^2 2p^6 3p$ (^2P) level of S VI and Ar VIII and the experimental data of Joelsson et al (9) and Pinnington et al (10).

Level	S VI		Ar VIII	
	This work	Ref. (9)	This work	Ref. (10)
$1s^2 2s^2 2p^6 3p$ (^2P)	106380.1	105873.6	141854.8	142856.9

FIGURE CAPTIONS

Fig. Hartree-Fock excitation energies for $1s^2 2s^2 2p^6 4s(^2S)$, $1s^2 2s^2 2p^6 4p(^2P)$ and $1s^2 2s^2 2p^6 4d(^2D)$ levels of NaI sequence as a function of nuclear charge.

Fig.2 Hartree-Fock term energies of NaI as a function of the principal quantum number.

Fig.3 Hartree-Fock term energies of PV as a function of the principal quantum number.

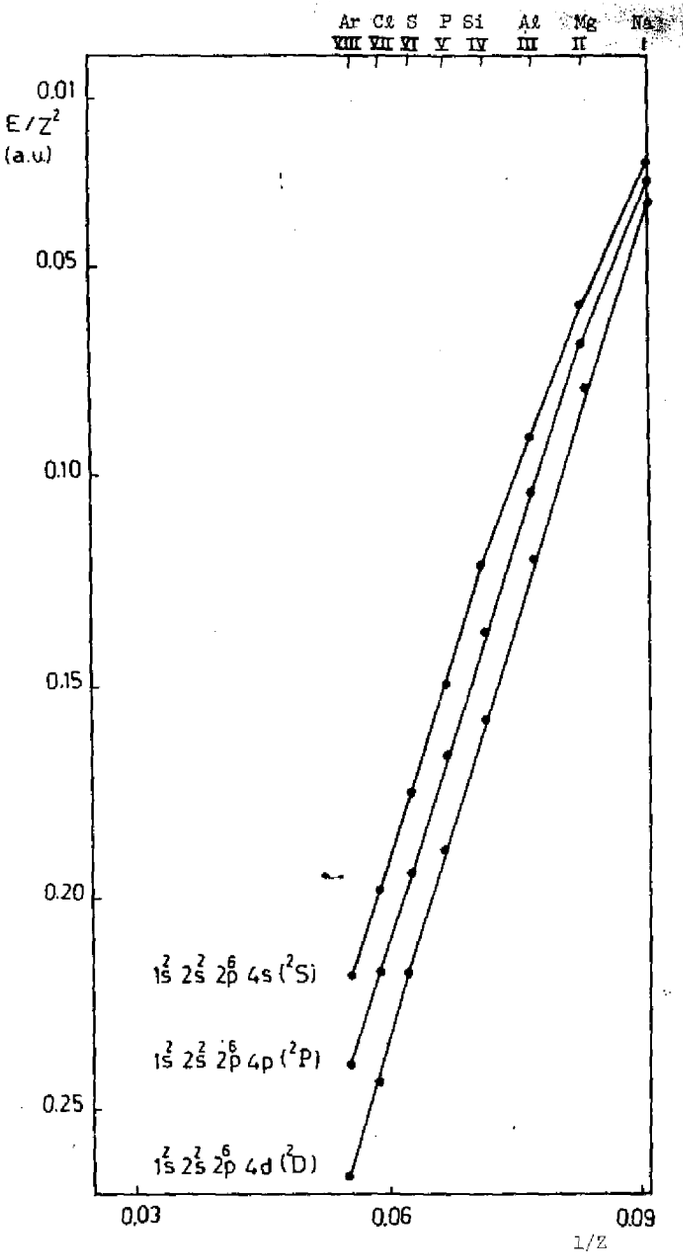

Fig.1

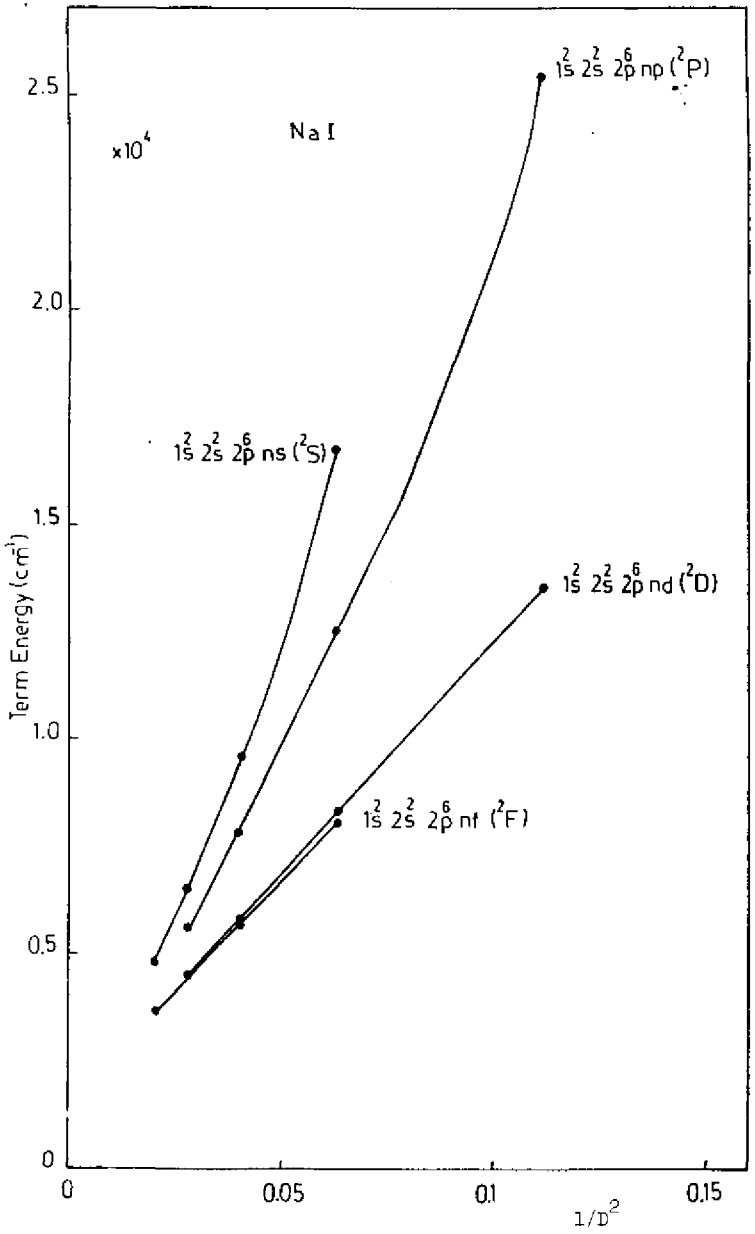
Na I
×10⁴
Term Energy (cm⁻¹)
1/D²
0
0.5
1.0
1.5
2.0
2.5
0.05
0.1
0.15
1s² 2s² 2p⁶ np (²P)
1s² 2s² 2p⁶ ns (²S)
1s² 2s² 2p⁶ nd (²D)
1s² 2s² 2p⁶ nf (²F)

Fig.2

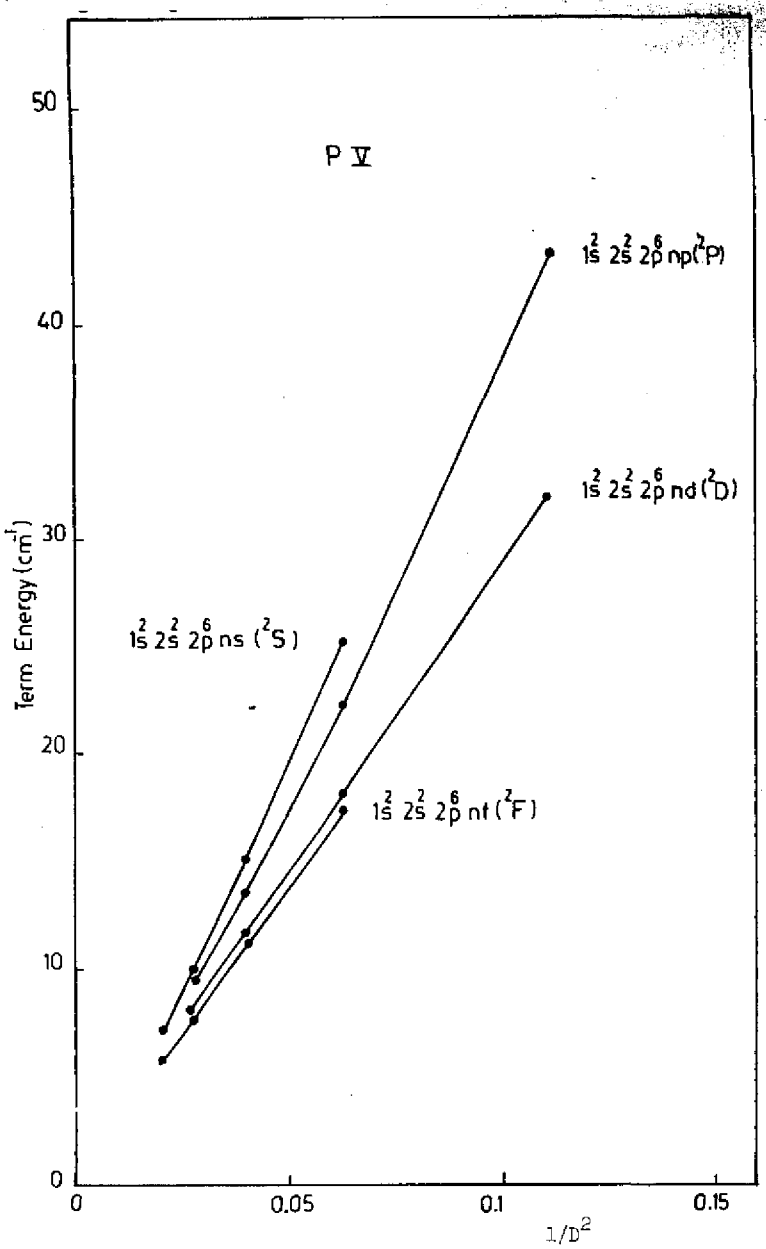
P V
Term Energy (cm⁻¹)
1/D²
0
10
20
30
40
50
0.05
0.1
0.15
1s² 2s² 2p⁶ np(²P)
1s² 2s² 2p⁶ nd(²D)
1s² 2s² 2p⁶ ns (²S)
1s² 2s² 2p⁶ nf (²F)

Fig.3