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CONTRIBUTION A L'ETUDE DU DEPLACEMENT ISOTOPIQUE ET DE LA STRUCTURE HYPERFINE DANS LE SPECTRE D'ARC DU XENON.

SOUTENUE LE 13 Juin 1975 DEVANT LA COMMISSION D'EXAMEN

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CONTRIBUTION A L'ETUDE

DU DEPLACEMENT ISOTOPIQUE ET DE LA STRUCTURE HYPERFINE

DANS LE SPECTRE D'ARC DU XENON

TABLE DES MATIERES

ARTICLE III

Hyperfine structure in the arc spectrum of xenon II.

ARTICLE IV

Etude paramétrique de la structure hyperfine du xénon I.

ANNEXE I

Etude paramétrique de la structure hyperfine des niveaux de la configuration $5p^5 8d$ du xénon 129.

ANNEXE II

Compléments sur l'étude paramétrique des configurations $5p^5$(6s,7s,5d,6d et 7d) et de la configuration $5p^5 8d$.

INTRODUCTION

I. GENERALITES. RESULTATS EXPERIMENTAUX (Articles 1 et 3).

Le déplacement isotopique et la structure hyperfine sont les deux effets qui traduisent l'influence de certaines propriétés des noyaux des atomes. L'étude de ces phenomènes permet d'atteindre aussi bien des paramètres nucléaires simples comme les moments dipolaire magnétique et quadrupolaire électrique, ou plus complexes comme la dimension et la forme des noyaux, que des paramètres liés aux électrons comme les constantes de structure hyperfine électronique.

L'étude du déplacement isotopique offre un intérêt particulier dans le xénon, à cause de la présence du nombre magique 82. Cette notion de nombre magique (2 ; 8 ; 20 ; 28 ; 50 ; 82 ; 126) a été introduite par la théorie des couches en physique nucléaire. Le noyau a une déformation minimale par rapport à la forme sphérique pour ces nombres de neutrons ou de protons, cette déformation étant nulle si les nombres de neutrons et de protons sont simultanément magiques . Il est donc intéressant d'étudier, au voisinage de ces nombres, le déplacement isotopique de volume, car il est lié aussi bien à la forme

qu'aux dimensions du noyau. Les effets de volume vont en croissant avec le nombre de masse ; l'étude des éléments ayant 82 neutrons est donc d'un grand intérêt. C'est pour cela que dans le Laboratoire Aimé Cotton ont été entreprises les études sur :

Baryum (Z=56)

N =	<u>82</u>	81	80	79	78	76	74
A =	138	137	136	135	134	132	130

par D. A JACKSON et DUONG HONG TUAN [1] ;

Cerium (Z=58)

N =	84	<u>82</u>	80	78
A =	142	140	138	136

par R.-J. CHAMPEAU [2] ;

Néodyme (Z=60)

N =	90	88	86	85	84	83	<u>82</u>
A =	150	148	146	145	144	143	142

par J.-M. HELBERT [3]

STRIGANOV et ses collaborateurs ont étudié les isotopes du samarium [4]

Samarium (Z=62)

N =	92	90	88	87	86	85	<u>82</u>
A =	154	152	150	149	148	147	144 .

Il restait à mesures les déplacements isotopiques du xénon

Xénon (Z=54)

N =	<u>82</u>	80	78	77	76	75	74	72	70
A =	136	134	132	131	130	129	128	126	124 .

Ce travail a été entrepris au Laboratoire Aimé Cotton, d'une part par R. VETTER [5] sur les raies laser infrarouges, d'autre part par D. A. JACKSON et moi-même sur les raies visibles.

Le déplacement isotopique des isotopes impairs n'étant accessible que si la structure hyperfine est connue, nous avons été amenés à mesurer les structures hyperfines de ces isotopes dans les raies visibles, celles dans le domaine infrarouge ayant été mesurées par S. LIBERMAN [6].

a) - Notations et conventions.

Sans vouloir reprendre la théorie du déplacement isotopique, il nous faut néanmoins préciser les notations et les conventions utilisées.

Les niveaux d'énergie seront toujours écrits dans la notation proposée par RACAH [7].

Dans le cas particulier du xénon, pour des raisons de quantité d'isotope enrichi disponible, l'isotope 136, le plus lourd, a été choisi comme repère de tous les déplacements isotopiques ; son déplacement a donc été fixé à zéro.

Le déplacement isotopique d'une transition a, de nombre d'ondes σ_a, entre les isotopes de nombre de masse $136-n$ et 136 peut s'écrire :

$$\Delta\nu_a\ (136-n\ ,\ 136) = \Delta\ M\ B_{a,n} + \Delta\ M\ S\ p_{a,n} + \Delta\ V_{a,n}$$

$\Delta\ M\ B$ est l'effet de masse normal ou de Bohr ; il peut être aisément calculé et sera souvent soustrait des valeurs expérimentales

$$\Delta\ M\ B_{a,n} = \frac{\sigma_a\ [(136-n) - 136]}{1836\ (136-n)\ 136} = \frac{-n\ \sigma_a}{1836 \times 136 \times (136-n)}\ .$$

Ces conventions conduisent à un effet de masse normal négatif dans toute transition.

Δ M S $p_{a,n}$ est appelé effet de masse spécifique.

$$\Delta \text{ M S } p_{a,n} = \frac{K_a\,[(136-n) - 136]}{(136-n)\ 136} = \frac{-n\ K_a}{136\ (136-n)} \quad .$$

Ces conventions entraînent que si l'effet de masse spécifique est positif, il est de sens opposé à l'effet de masse de Bohr.

K_a est un facteur purement électronique et ne dépend que de la transition étudiée,

Δ V est appelé effet de volume ou de champ,

$\Delta V_{a,n} = E_a\ C(136-n,\ 136)$

$C(136-n,\ 136)$ est un facteur nucléaire proportionnel à $\delta \langle r^2 \rangle$, variation du carré moyen de la distribution des charges entre les isotopes concernés,

E_a est la partie électronique du déplacement de volume et ne dépend que de la transition étudiée.

Précisons enfin que, par convention, nous considérons le déplacement isotopique pour une transition comme étant celui du niveau supérieur diminué de celui du niveau inférieur.

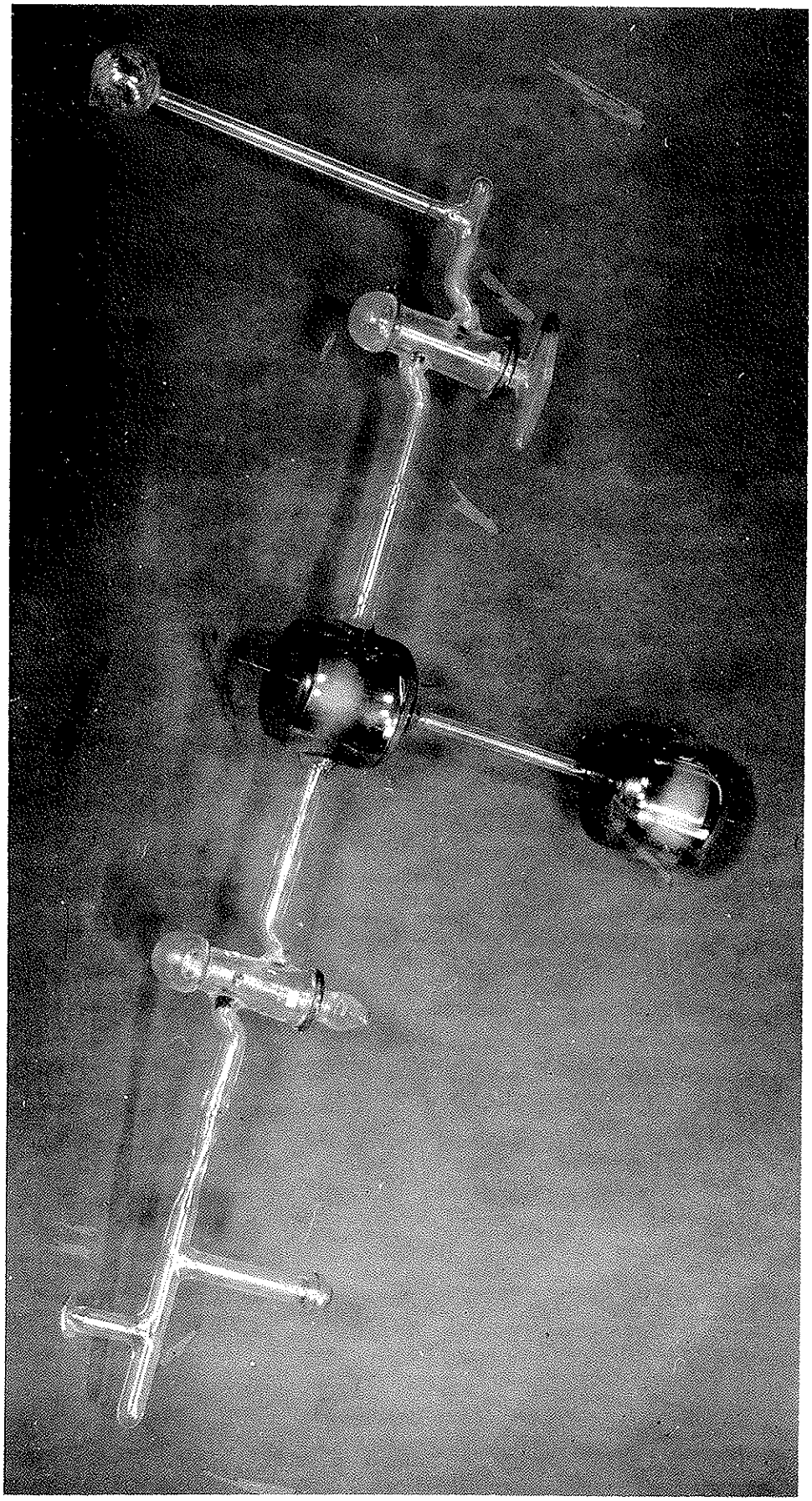

Fig. 1 - Tube à décharge

b) - Techniques et résultats expérimentaux.

Le xénon possède 9 isotopes stables dont les abondances naturelles sont les suivantes :

A	136	134	132	131	130	129	128	126	124
Abondance relative en %	8,93	10,52	26,93	21,24	4,05	26,24	1,91	0,088	0,095.

Les isotopes pairs donnent des composantes très voisines, car le déplacement isotopique est de l'ordre de 2 mK (1 mK = 10^{-3} cm^{-1}) pour une différence de 2 neutrons, ce qui est environ dix fois inférieur à la largeur Doppler. Les isotopes impairs donnent de multiples composantes à cause de la structure hyperfine. Le xénon naturel n'a donc pu être utilisé et il a fallu avoir recours aux isotopes très enrichis.

Le Centre de Spectrométrie de Masse du C. N. R. S. à ORSAY nous a gracieusement fourni les isotopes 134, 132, 131, 130, 129 et 128 enrichis à plus de 95 %, mais en très faible quantité (quelques mg), ainsi que les deux isotopes rares 126 et 124 en quantité encore plus faible (quelques microgrammes).

L'isotope 136 a été acheté en quantité suffisante pour pouvoir servir de repère à tous les autres isotopes. Nous avons utilisé un tube à décharge classique à électrodes froides, de type Geissler, constitué par deux boules reliées par un capillaire (Fig. 1). Au cours de la décharge, les parois du tube et les électrodes absorbent peu à peu le xénon ; le type de tube utilisé a été choisi pour minimiser cette consommation de xénon. Un tel tube a été fabriqué pour

chacun des neuf isotopes. Pour diminuer encore la consommation de xénon, nous avons introduit de l'hélium à la pression de 1 Torr, ce qui ne nécessite qu'une pression de l'ordre de 0,03 Torr de xénon pour obtenir le spectre d'arc dans de bonnes conditions.

Le déplacement dû à la pression de l'hélium est négligeable. Nous avons mesuré ce déplacement dans le cas des transitions $5p^5np \rightarrow 5p^56s$, qui sont les plus intéressantes pour l'étude de l'effet de volume. Avec une pression de 10 Torr (10 fois la pression utilisée), le déplacement est resté inférieur aux incertitudes de mesure ($\simeq$ 0,3 mK). En fait, pour l'étude du déplacement isotopique, la différence de pression d'hélium dans les deux tubes était de l'ordre de 0,1 Torr, d'où un déplacement certainement inférieur à 0,01 mK.

Le déplacement dû à la pression de xénon est de l'ordre de 1,5 à 3 mK par Torr, il est négligeable, eu égards aux pressions de xénon utilisées.

Nous nous sommes servis des mêmes tubes que précédemment pour mesurer la structure hyperfine des isotopes impairs, sauf pour huit raies faibles de l'isotope 129 pour lesquelles nous avons eu recours à un tube spécial (voir Article III, experimental procedure, Fig. 1).

Le fait que néanmoins nos tubes consomment du xénon nous a interdit la technique d'enregistrement photoélectrique raie par raie, car nous n'aurions jamais pu étudier toutes les raies dont nous disposions. Nous avons dû utiliser la technique photographique qui a l'avantage de donner sur une seule plaque de grandes régions du spectre pour une pose de quelques minutes.

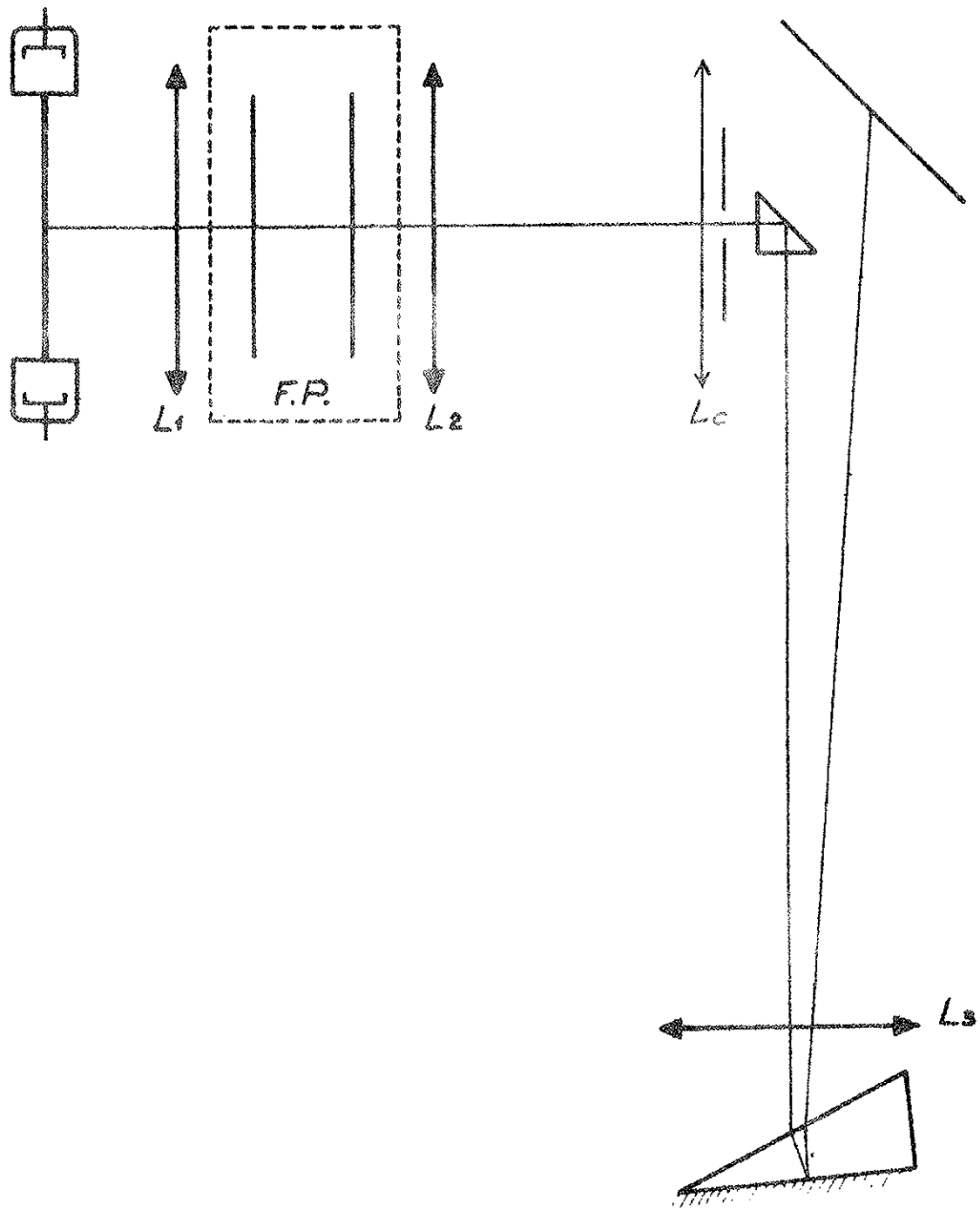

Fig:2 - Schéma de l'appareillage optique.

Nous nous sommes servi d'un spectrographe à prisme en montage Littrow, précédé d'un étalon Fabry-Perot plan (Fig. 2). Nous avons pu couvrir ainsi le domaine spectral allant de 4 500 Å à 9 045 Å, soit environ une octave.

Pour une raie donnée, la structure hyperfine ou le déplacement isotopique s'obtient facilement à partir des interférogrammes car la différence de nombres d'ondes est proportionnelle à la différence des carrés des diamètres des anneaux du Fabry-Perot.

Intéressons nous à l'écart entre 2 composantes données ; sa valeur est obtenue, pour un interférogramme, en effectuant la moyenne des mesures réalisées sur 5 ordres successifs. Pour connaître les incertitudes sur ces différences de nombres d'ondes entre composantes nous utilisons deux grandeurs :

- la déviation quadratique moyenne qui est la racine carrée de la somme des carrés des écarts à la moyenne, divisée par le nombre d'interférogrammes, car chacun fournit une mesure indépendante. Pour une raie donnée, elle est pratiquement constante quel que soit le nombre de mesures. Elle vaut environ 0,7 mK pour les raies bleues et 0,5 mK pour les raies infrarouges,

- l'incertitude statistique qui est égale à deux fois la déviation quadratique moyenne divisée par la racine carrée du nombre d'interférogrammes. La probabilité pour qu'une grandeur soit en dehors de l'intervalle défini par la valeur mesurée plus ou moins l'incertitude statistique n'est que de 5 % .

Pour réduire l'incertitude statistique nous avons été amenés à mesurer, pour chaque raie, entre 20 et 30 interférogrammes, pour chaque isotope dans le cas du déplacement isotopique, et entre 20 et 80 interférogrammes pour la structure hyperfine des isotopes impairs.

Les tableaux suivants permettent de se rendre compte de la quantité des résultats expérimentaux.

Déplacement isotopique
(l'isotope 136 étant pris comme référence)

Isotopes	134	132	130	128	126	124	131	129
Nombre de raies mesurées	37	37	37	37	3	12	10	23
Nombre de niveaux reliés entre eux *	42	42	42	42	-	12	5	19

Structure hyperfine

Isotopes	129 (I = 1/2)	131 (I = 3/2)
Nombre de raies mesurées	38	9
Nombre de constantes A déduites	29	8
Nombre de constantes B déduites	-	9
Nombre de constantes A à interpréter **	36	-
Nombre de constantes B à interpréter **	-	15

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* Les mesures de R. VETTER [5] sur les cinq isotopes pairs abondants nous ont permis d'atteindre les niveaux de la configuration $5p^5 5d$.

** Les mesures de S. LIBERMAN [6] ont été d'un grand secours pour compléter et corroborer nos résultats.

Le nombre des résultats expérimentaux a permis une interprétation paramétrique des phénomènes, aussi bien de déplacement isotopique que de structure hyperfine.

Une séparation des effets de masse et de volume a aussi été faite pour évaluer les variations relatives des carrés moyens de la distribution des charges et les comparer aux variations des énergies de liaison par nucléon.

II. ETUDES PARAMETRIQUES (Articles 2 et 4, Annexes 1 et 2).

a) - Principes des études paramétriques.

En spectroscopie atomique, le calcul des énergies par la méthode paramétrique est devenu classique. Il repose sur l'hypothèse du champ central [8]. Les énergies des niveaux sont les valeurs propres de l'Hamiltonien et les fonctions d'onde les vecteurs propres. La matrice de l'Hamiltonien H, qui est limité aux interactions électrostatiques Q, et de spin-orbite A, est construite sur les états d'ordre zéro appartenant à une ou plusieurs configurations. La méthode est paramétrique en ce sens que les intégrales radiales nécessaires pour la diagonalisation ne sont pas calculées à l'avance, mais ajustées de façon que les valeurs propres de H reproduisent au mieux les énergies expérimentales. L'écart quadratique moyen au sens de RACAH $(\overline{\Delta E})$ [9] permet de tester la qualité de l'étude :

$$\overline{\Delta E} = \left[\frac{\sum_i (E_i^{exp} - E_i^{cal})^2}{N - P} \right]^{\frac{1}{2}}$$

avec : E_i^{exp} énergie expérimentale du niveau i

E_i^{cal} énergie calculée du niveau i

N nombre de niveaux connus

P nombre de paramètres libres.

Les éléments de matrice sont de la forme :

$$H_{ij} = \sum_m \alpha_{ij}^m P_m$$

où les α_{ij}^m sont des coefficients purement angulaires et où les P_m sont les intégrales radiales d'interaction électrostatique R^k (intégrales de Slater) ou d'interaction spin-orbite $\zeta_{n\ell}$.

On introduit aussi souvent des corrections effectives d'interaction de configurations lointaines, en particulier la correction en $\alpha L(L+1)$ (correction de Trees [10]).

La méthode paramétrique est empirique en ce sens que, pour reproduire au mieux les énergies expérimentales, les paramètres tiennent compte de tous les phénomènes ayant une dépendance angulaire donnée ; ce sont donc tous, en fait, des paramètres effectifs.

La chaîne de programmes écrite au Laboratoire Aimé Cotton [11] permet d'effectuer tous les calculs. En fin d'étude nous obtenons :

- les énergies calculées E_i^{cal} ,
- la décomposition des fonctions d'ondes Ψ_i sur les vecteurs de la base choisie,

- la valeur numérique des paramètres P_m ,
- les coefficients des paramètres pour les différents niveaux étudiés.

Nous pouvons obtenir non seulement les coefficients des paramètres d'énergie mais aussi ceux de n'importe quel autre paramètre, en particulier ceux de la structure hyperfine et du déplacement isotopique. Le cas des coefficients des paramètres de déplacement isotopique est remarquablement simple, car ils sont, pour la plupart, identiques à ceux des paramètres d'énergie.

Les études paramétriques de déplacement isotopique et de structure hyperfine sont donc doublement paramétriques. En effet, les coefficients des nouveaux paramètres sont obtenus à partir de l'étude paramétrique des énergies et il ne reste qu'à déterminer les valeurs des paramètres de la nouvelle étude, par la méthode de moindres carrés, de façon que les valeurs calculées (de déplacement isotopique ou de structure hyperfine) reproduisent au mieux les valeurs expérimentales.

b) - Etudes paramétriques réalisées.

L'interprétation paramétrique du déplacement isotopique qui a l'avantage de ne pas nécessiter de séparation en effets de masse et de volume, a été effectuée sur les niveaux des 4 configurations les plus profondes pour les isotopes 134, 132, 130 et 128, repérés par rapport au 136.

L'interprétation paramétrique de la structure hyperfine de l'isotope 129 a été effectuée pour 5 configurations impaires.

Ces interprétations passent obligatoirement par l'étude paramétrique des énergies des niveaux . Ce travail a été effectué par S. LIBERMAN [6] sur les configurations paires $5p^5$(6p et 7p) avec de bons résultats (écart quadratique moyen au sens de RACAH $\overline{\Delta E} = 24{,}6\ cm^{-1}$) , et sur les configurations impaires $5p^5$(6s et 5d) avec des résultats moins bons ($\overline{\Delta E} = 73\ cm^{-1}$) .

L'étude paramétrique des niveaux des configurations impaires a été reprise et élargie pour englober les configurations $5p^5$(6s,7s, 5d,6d et 7d) . Les résultats ont été fortement améliorés ($\overline{\Delta E} = 31{,}6\ cm^{-1}$) par la prise en compte des interactions entre les configurations $5p^5nd$ et celle entre $5p^56s$ et $5p^57s$. En ce qui concerne l'interaction entre les configurations $5p^56s$ et $5p^55d$, l'étude de la structure hyperfine a montré que les résultats obtenus ne sont qu'une première approximation ; la seule certitude que l'on puisse avoir est que le mélange de ces deux configurations ne se fait de façon appréciable que par l'intermédiaire des fonctions d'onde des niveaux 6s' 1/2 0 avec 5d 1/2 0 et 6s' 1/2 1 avec 5d 1/2 1 , mais les proportions indiquées par les calculs ne sont qu'un ordre de grandeur.

La configuration $5p^58d$ a été étudiée à part, car elle se mélange très peu aux autres (voir Annexe I).

STONE en 1959 [12] entreprend la première étude paramétrique de déplacement isotopique dans les configurations $np^5(n+1)s$ des gaz rares. Il faut toutefois attendre les cas du nickel [13] (BAUCHE, 1969) et du néon [14] (KELLER, 1972) pour avoir les premiers résultats vraiment satisfaisants. Si les études paramétriques de déplacement isotopique réussies sont si peu nombreuses jusqu'à présent, c'est qu'il faut réunir deux conditions indispensables pour mener à bien une telle étude :

- il faut disposer de valeurs expérimentales précises de déplacement isotopique des niveaux en nombre suffisant ;
- il faut connaître le couplage intermédiaire dans les configurations étudiées.

Le cas du néon est proche de celui du xénon à deux différences près :

- l'étude porte sur deux isotopes du néon pour cinq de xénon ;
- l'effet de volume est négligeable dans le néon, alors qu'il est important dans le xénon.

Le point remarquable, que l'on retrouve dans les deux études, porte sur les paramètres notés z_{2p} dans le néon et z_{5p} dans le xénon. Ces paramètres tiennent compte des effets des 5 électrons p de la seule sous-couche incomplète du coeur. Le paramètre z_{2p} prend des valeurs numériques très voisines dans les quatre configurations où il a pu être déterminé ; il en est de même pour le paramètre z_{5p}, ce qui indique que le coeur np^5 varie peu d'une configuration à l'autre.

Les contributions des effets de masse et de volume des différents paramètres ont pu être estimées et comparées à des valeurs obtenues a priori par des calculs Hartree-Fock ; l'accord est satisfaisant. En outre, le paramètre $g^1(5p,5d)$, qui tient compte des variations des effets isotopiques à l'intérieur de la configuration $5p^5 5d$, doit être théoriquement un paramètre de pur effet de masse ; ses valeurs numériques pour les isotopes successifs permettent de le vérifier facilement.

L'étude paramétrique des énergies des niveaux des configurations impaires $5p^5(6s \text{ et } 5d)$ effectuées par S. LIBERMAN a été choisie pour interpréter les résultats du déplacement isotopique, alors que celle portant sur les configurations $5p^5(6s,7s,5d,6d \text{ et } 7d)$ a été choisie pour interpréter les résultats de la structure hyperfine. En effet :

- le mélange des configurations $5p^5(6s \text{ et } 5d)$ est mal connu dans les deux cas ;
- les paramètres utiles de structure hyperfine sont les mêmes pour toutes les configurations $5p^5 nd$; il y a donc intérêt à utiliser la deuxième étude, même si nous connaissons peu de résultats sur les niveaux des configurations $5p^5(6d \text{ et } 7d)$.
- les paramètres de déplacement isotopique varient d'une configuration à l'autre et ne pourront être déterminés que si il y a suffisamment de résultats sur les niveaux de chaque configuration, ce qui n'est malheureusement pas le cas pour les d supérieurs.

Il faut donc s'attendre à une précision moins bonne dans la détermination des paramètres de déplacement isotopique des configurations $5p^5(6s \text{ et } 5d)$.

Les paramètres de structure hyperfine, comme les paramètres d'énergie $\zeta_{n\ell}$, sont liés aux quantités $\langle r^{-3} \rangle_{n\ell}$.

Les paramètres d'énergie du coeur (ζ_{5p}) dans les différentes configurations sont tous très voisins et très supérieurs aux paramètres d'énergie ζ_{nd} des électrons extérieurs successifs. Nous avons donc pu négliger les paramètres des électrons extérieurs et nous contenter de 4 paramètres, à savoir :

- un paramètre a_{6s} qui provient de la probabilité de présence de l'électron 6s au noyau ;
- trois paramètres pour l'électron 5p : a_{5p} , b_{5p} , c_{5p} (notation de Judd) indépendants de la configuration.

En l'absence d'effets relativistes et d'interactions de configurations lointaines, le paramètre a_{5p} est nul et les paramètres b_{5p} et c_{5p} sont égaux.

Il faut rapprocher cette étude de celles effectuées dans le même domaine des configurations $5p^N n\ell$ par LUC-KOENIG [15] et MORILLON [16] sur le tellure, l'iode et le xénon. Les calculs a priori de LUC-KOENIG ont montré l'importance des effets relativistes. Ils donnent la valeur du paramètre a_{5p} (a_{5p} = 14,81 mK) et celle du rapport b_{5p}/c_{5p} (0,74).

Les calculs S.U.H.F. (Spin-Unrestricted-Hartree-Fock) non relativistes montrent que, contrairement au tellure, dans le xénon les effets de polarisation du coeur sont très petits et ne contribuent que pour 1,6 mK au paramètre a_{5p} .

L'ensemble des 4 paramètres permet d'interpréter la structure hyperfine des niveaux des configurations $5p^5(6s,5d,6d.et\ 7d)$; l'interprétation peut être étendue à toutes les configurations $5p^5nd$ ainsi qu'à toutes les configurations paires $5p^5np$. En effet, nous avons repris l'étude de S. LIBERMAN sur les configurations paires, nous y avons introduit les nouvelles valeurs des constantes que nous avons mesurées et nous avons fixé le paramètre a_{5p} à la valeur calculée ; les paramètres b_{5p} et c_{5p} ont pris alors les mêmes valeurs que dans les configurations impaires, aux écarts types près.

III. SEPARATION DES EFFETS DE MASSE ET DE VOLUME (Articles 1 et 2).

Il n'y a que dans les éléments très légers que la séparation en effets de masse et de volume se fait aisément ; car ... l'effet de volume est négligeable pour les éléments dont le nombre atomique Z ne dépasse pas une limite qui peut être située vers 20, c'est-à-dire juste avant la première série des métaux de transition.

Pour les atomes dits "lourds", les déplacements sont en général très importants, de l'ordre de plusieurs dizaines de mK, et l'effet de volume est prépondérant. La limite inférieure peut être fixée au nombre de neutrons magique N=82 , les déplacements mesurés pour les isotopes avec $N > 82$ étant d'un ordre de grandeur supérieur aux déplacements mesurés pour les isotopes avec $N < 82$. Le cérium,

dont les isotopes stables s'étagent de N=78 à N=84 , est un exemple frappant de ce phénomène.

Le xénon fait malheureusement partie des atomes dits "moyens" . Les déplacements mesurés sont en général petits, quelques mK, et les effets de volume, de masse normal et de masse spécifique sont du même ordre de grandeur.

Voyons quels renseignements nous pouvons espérer tirer de la masse de nos résultats expérimentaux.

Commençons par enlever l'effet de masse de Bohr, nous obtenons les déplacements "réduits".

Pour deux transitions a et b , ces déplacements s'écrivent :

$$\Delta\nu_a\ (136\text{-}n, 136) = \frac{-n\ K_a}{136\ (136\text{-}n)} + E_a\ C\ (136\text{-}n, 136)$$

$$\Delta\nu_b\ (136\text{-}n, 136) = \frac{-n\ K_b}{136\ (136\text{-}n)} + E_b\ C\ (136\text{-}n, 136) \quad .$$

Formons les quantités $\Delta\nu_a \frac{136\text{-}n}{135n}$ et $\Delta\nu_b \frac{136\text{-}n}{135n}$, elles sont liées par la relation linéaire

$$\Delta\nu_a \frac{136\text{-}n}{135n} = \frac{E_a}{E_b}\ \Delta\nu_b \frac{136\text{-}n}{135n} - \frac{1}{136 \times 135}\left[K_a - \frac{E_a}{E_b} K_b\right] \quad .$$

La quantité $\Delta\nu_a \frac{136\text{-}n}{135n}$ est le déplacement "normalisé" de l'isotope 136-n à l'isotope 135 , et $\frac{-K_a}{136 \times 135} = M\ S\ p_a$ est l'effet de masse spécifique de la transition a entre les isotopes 136 et 135 .

Pour "normaliser" les déplacements des différents isotopes, il faut les diviser par les quantités suivantes :

isotope	134	132	130	128
diviseur	2,015	4,09	6,23	8,44

En portant en abscisses $\Delta\nu_b \frac{136-n}{135n}$ et en ordonnées $\Delta\nu_a \frac{136-n}{135n}$, nous obtenons une droite, dite droite de King [17], dont nous pouvons tirer deux renseignements :

- la pente $\frac{E_a}{E_b}$, rapport des effets de volume des deux transitions ;
- l'ordonnée à l'origine $M S p_a - \frac{E_a}{E_b} M S p_b$, différence entre l'effet de masse spécifique de la transition a et le produit de la pente par l'effet de masse spécifique de la transition b .

Malheureusement, il est impossible de séparer les effets de masse spécifique et de volume à partir des seules droites de King, même s'il était possible de les tracer pour toutes les transitions et tous les isotopes, car les équations ne sont pas indépendantes. Il faut une information supplémentaire pour obtenir cette séparation.

Cette information supplémentaire peut être obtenue par une mesure de déplacement isotopique dans le domaine des rayons X, pour lequel on peut séparer aisément les effets de masse et de volume.

D'autres méthodes font appel à des mesures de déplacement isotopique dans les atomes muoniques ou à des effets de masse spécifique connus dans des atomes de même nombre de masse et de numéro atomique

voisin. Il est dangereux de tracer des droites de King dans de telles conditions, car les paramètres nucléaires ne sont pas les mêmes.

Dans notre cas, l'information supplémentaire a été apportée par un calcul Hartree-Fock effectué par J. BAUCHE [18] en couplage L.S. . Ce calcul donne le déplacement de masse spécifique des deux termes Russell-Saunders ^1P et ^3P de la configuration $5p^5 6s$ par rapport au centre de gravité (C.G.) de la configuration $5p^5 6p$. Pour obtenir les effets de masse spécifique des niveaux de la configuration $5p^5 6s$, il faut connaître le couplage intermédiaire de cette configuration.

L'étude paramétrique que nous avons faite à ce sujet nous apprend que les configurations $5p^5 6s$ et $5p^5 5d$ sont mélangées par l'intermédiaire des fonctions d'onde des niveaux 6s' 1/2 0 , 6s' 1/2 1 avec 5d 1/2 0 , 5d 1/2 1 et que ce mélange n'a pu être parfaitement déterminé. Nous ne pourrons pas en déduire l'effet de masse spécifique des niveaux 6s' 1/2 0 et 6s' 1/2 1 .

Par contre les fonctions d'onde des niveaux 6s 3/2 1 et 6s 3/2 2 ont pu être parfaitement déterminées et nous connaissons leur décomposition sur les vecteurs de base du couplage Russell-Saunders ; nous pouvons donc raisonnablement calculer les effets de masse spécifique de ces deux niveaux pour le couple d'isotopes 136 - 135 .

Réf. $5p^5 6p$ (C.G.) = 0

6s 3/2 1 = −0,16 mK

6s 3/2 2 = −0,40 mK .

Hélas, les résultats des calculs Hartree-Fock sont rarement en bon accord avec les valeurs expérimentales et il faut les utiliser avec prudence. Les résultats antérieurs dans les spectres des séries 3d , 4f , 4d et 5d montrent que le signe et l'ordre de grandeur sont bons, mais que les valeurs calculées sont entre 1,5 et 2 fois trop grandes [19].

Voyons si les résultats expérimentaux nous permettent de préciser ces valeurs que, pour l'instant, nous sommes tentés de fixer à :

$$6s\ 3/2\ 1 \simeq -0,1\ mK$$

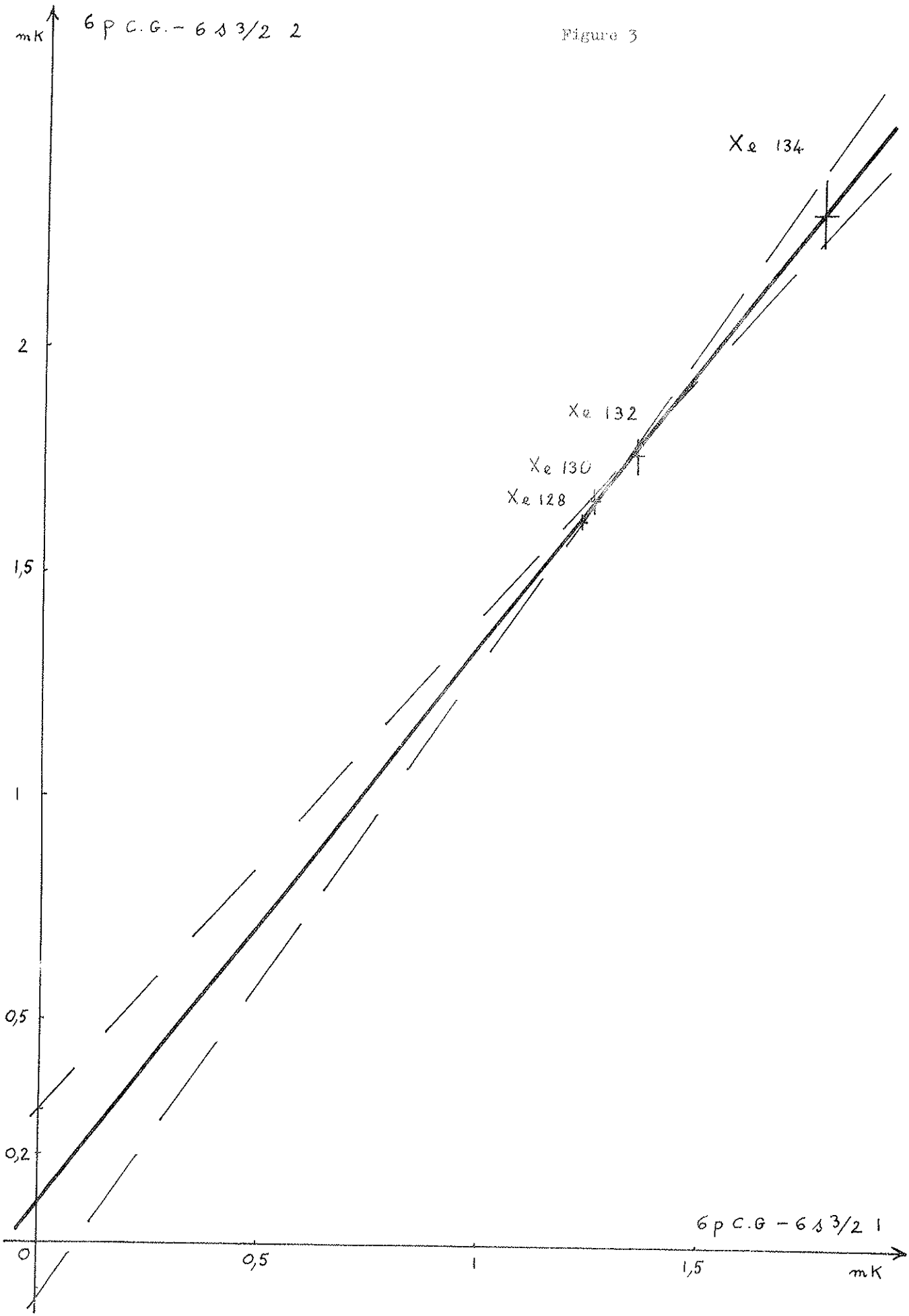
$$6s\ 3/2\ 2 \simeq -0,2\ mK \ .$$

Pour cela nous pouvons, par la méthode de moindres carrés, obtenir les déplacements résiduels (effet de masse normal enlevé) des niveaux des configurations $5p^5(6s,5d,6p \text{ et } 7p)$, pour les isotopes 134, 132, 130 et 128 . Le déplacement isotopique du niveau 6s 3/2 1 , qui intervient le plus grand nombre de fois, a été fixé à zéro pour tous les isotopes.

La précision sur les 10 niveaux de la configuration $5p^5 6p$ est de l'ordre de 0,2 mK , compte tenu que de nombreux niveaux sont déterminés par plusieurs transitions. On peut admettre une répartition gaussienne de l'incertitude de chaque niveau, si bien que le centre de gravité (C.G.) de ces 10 niveaux est connu avec une précision de l'ordre de $0,2\ mK / \sqrt{10}$.

Le niveau 6s 3/2 2 est relié indirectement au niveau 6s 3/2 1 de 7 façons différentes ; la précision dans les 7 transitions où

Figure 3


mK
6p C.G. – 6s 3/2 2
Xe 134
Xe 132
Xe 130
Xe 128
2
1,5
1
0,5
0,2
0
0,5
1
1,5
mK
6p C.G – 6s 3/2 1

intervient le niveau 6s 3/2 2 est de l'ordre de 0,25 mK ; on peut donc dire que le déplacement isotopique de ce niveau est connu avec une précision de l'ordre de 0,1 mK .

Traçons une droite de King (figure 3), de la façon décrite plus haut, en portant en abscisse la transition fictive

$$C.G.\ 5p^5 6p \rightarrow 6s\ 3/2\ 1$$

et en ordonnée la transition fictive

$$C.G.\ 5p^5 6p \rightarrow 6s\ 3/2\ 2 \quad .$$

Les valeurs des déplacements des isotopes 134, 132, 130 et 128 étant respectivement divisées par 2,015 - 4,09 - 6,23 et 8,44 , les abscisses des points sont connues avec les précisions 0,03 mK - 0,015 mK - 0,01 mK et <0,01 mK . Les ordonnées sont connues avec les précisions 0,08 mK - 0,04 mK - 0,03 mK et 0,02 mK .

Si l'on se contente de prendre la droite moyenne et les droites extrêmes qui coupent les 4 domaines d'incertitude, ce qui est la façon habituelle, mais non rigoureuse, de procéder, l'ordonnée à l'origine vaut $0,1 \pm 0,2$ mK . Cette valeur "expérimentale" est compatible avec celle que l'on peut déduire des calculs Hartree-Fock : 0,2 mK à partir des valeurs brutes et 0,07 mK à partir des valeurs réduites (voir plus haut les valeurs Hartree-Fock) ; mais elle n'apporte aucune précision supplémentaire.

Nous admettrons donc les valeurs suivantes pour l'effet de masse spécifique :

C.G. $5p^5 6p \rightarrow 6s\ 3/2\ 1 = 0,1$ mK

C.G. $5p^5 6p \rightarrow 6s\ 3/2\ 2 = 0,2$ mK .

L'incertitude, qui provient des calculs Hartree-Fock et de la correction apportée, peut être estimée à 0,1 mK .

Nous touchons ici une difficulté propre aux atomes dits "moyens" où les effets de déplacement isotopique sont très petits et où, malgré une grande précision absolue, la précision relative est souvent dérisoire.

IV. DEPLACEMENT ISOTOPIQUE ET ENERGIE DE LIAISON PAR NUCLEON.

Simon GERSTENKORN [20] a fait un rapprochement entre le déplacement isotopique de volume et la variation de l'énergie de liaison par nucléon.

L'analyse par S. GERSTENKORN des déplacements isotopiques relatifs de volume $(D.I.R.)_V$, au voisinage des couches fermées, l'a amené à proposer la relation empirique suivante :

$$(D.I.R.)_V = \frac{\Delta V_{1,2}}{\Delta V_{1,3}} = \frac{E_1 - E_2}{E_1 - E_3} \quad ;$$

$(D.I.R.)_V$ est le déplacement isotopique relatif de volume pour les isotopes 1, 2 et 3 ;

E_1 , E_2 et E_3 sont les énergies de liaison par nucléon des isotopes

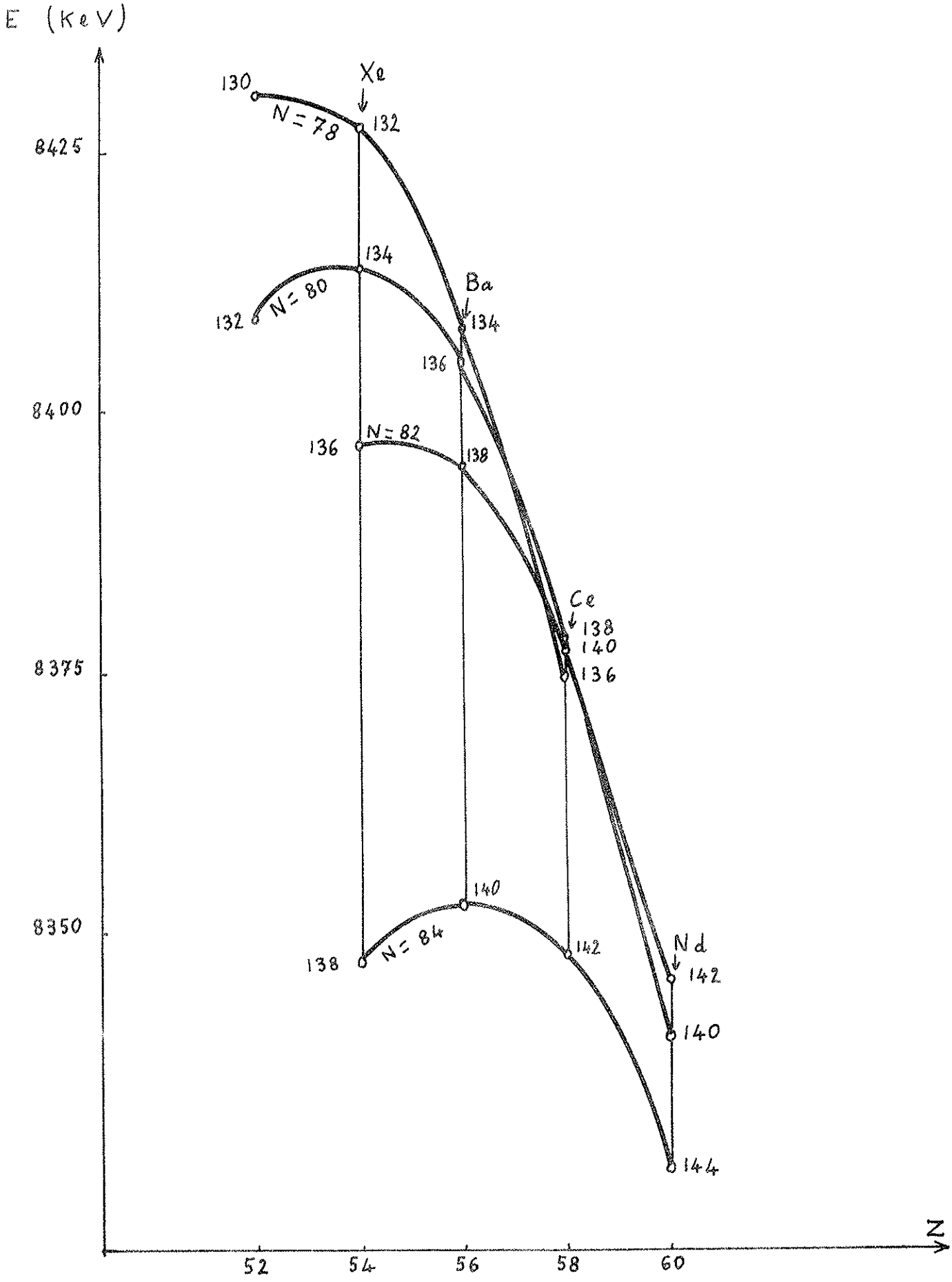

E (KeV)
8425
8400
8375
8350
Xe
Ba
Ce
Nd
130
132
134
136
138
140
142
144
N = 78
N = 80
N = 82
N = 84
52
54
56
58
60
N

Figure 4

1, 2 et 3 ; les valeurs en sont tabulées [21] et les rapports $\frac{E_1 - E_2}{E_1 - E_3}$ sont connus à quelques pour cent près.

Cette relation, valable au voisinage des couches fermées en neutrons ou en protons, se vérifie bien partout où elle a pu être appliquée. Elle a, entre autres, permis d'interpréter :

- l'inversion de la position des isotopes dans les cas du chrome, du strontium et du cérium ;

- la distorsion entre les composantes 134, 136 et 138 du baryum ;

- le "saut" après le nombre magique dans les cas du strontium, du cérium et du plomb.

La figure 4 représente la variation des énergies de liaison par nucléon E au voisinage de la couche fermée en neutrons N=82 .

Cependant, si cette relation rend compte des phénomènes cités ci-dessus, il serait hasardeux de vouloir en tirer des données quantitatives et de calculer à partir de la relation

$$\Delta V_{12} / \Delta V_{13} \simeq \Delta E_{12} / \Delta E_{13}$$

l'effet spécifique de masse dans le cas du xénon où les effets mesurés, et à plus forte raison leurs différences, sont particulièrement petits en valeur absolue.

Pour illustrer l'analogie entre énergie de liaison et $(D.I.R.)_V$, nous avons construit, pour chacun des éléments dont les nombres atomiques Z sont pairs et vont de 48 à 56, un graphique où sont portés en

fonction du nombre de masse A :

- l'énergie de liaison par nucléon E ;

- le déplacement isotopique relatif de volume ΔV entre isotopes pairs consécutifs ; cette quantité ΔV, pour les isotopes de nombres de masse A et A-2, est figurée par une flèche placée à l'abscisse A-1 et de hauteur proportionnelle à ΔV.

Nous pouvons distinguer plusieurs zones dans les courbes d'énergie E, en les considérant dans le sens des nombres de masse croissants :

- une zone I où la courbe est croissante ;

- une zone II située dans la partie décroissante entre le maximum et l'isotope N-4, "N" étant un nombre de neutrons magique ;

- une zone III entre l'isotope N-4 et l'isotope N ;

- une zone IV après l'isotope N.

Ces graphiques se trouvent aux figures 5 à 9 ; le cas du xénon est à la figure 8, et est privilégié car il est le seul où la suite des isotopes stables s'étend sur trois zones. Nous n'avons fait figurer que les isotopes pairs pour lesquels les déplacements isotopiques sont connus, ce qui explique qu'en général, sur les courbes d'énergies nous ne voyons pas l'ensemble des 4 zones énumérées plus haut.

Dans ces 5 graphiques nous constatons une analogie remarquable entre les énergies de liaison par nucléon et les déplacements isoto-

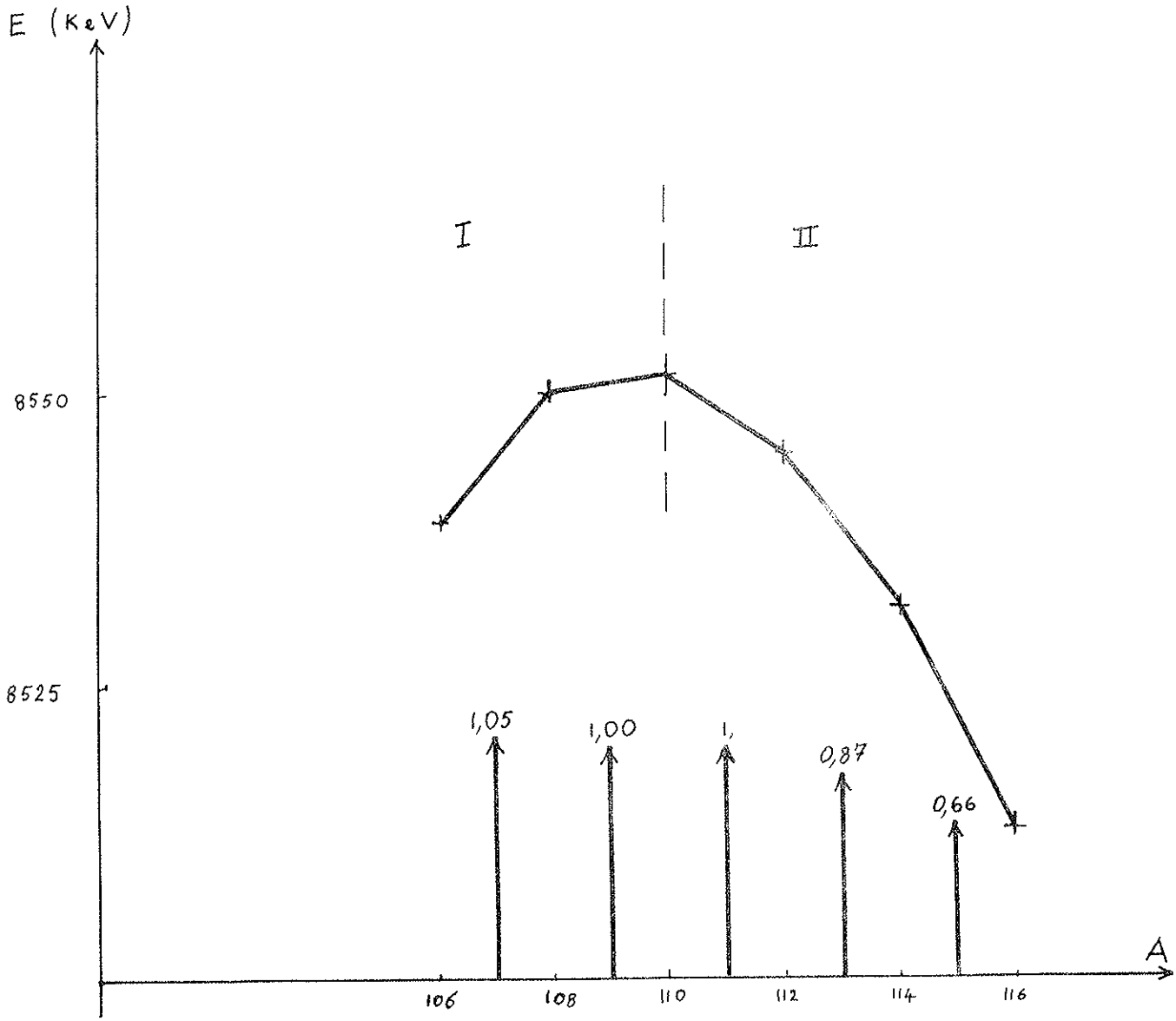


Figure 5

Energie de liaison par nucléon en KeV et déplacement isotopique relatif de volume du cadmium Z=48

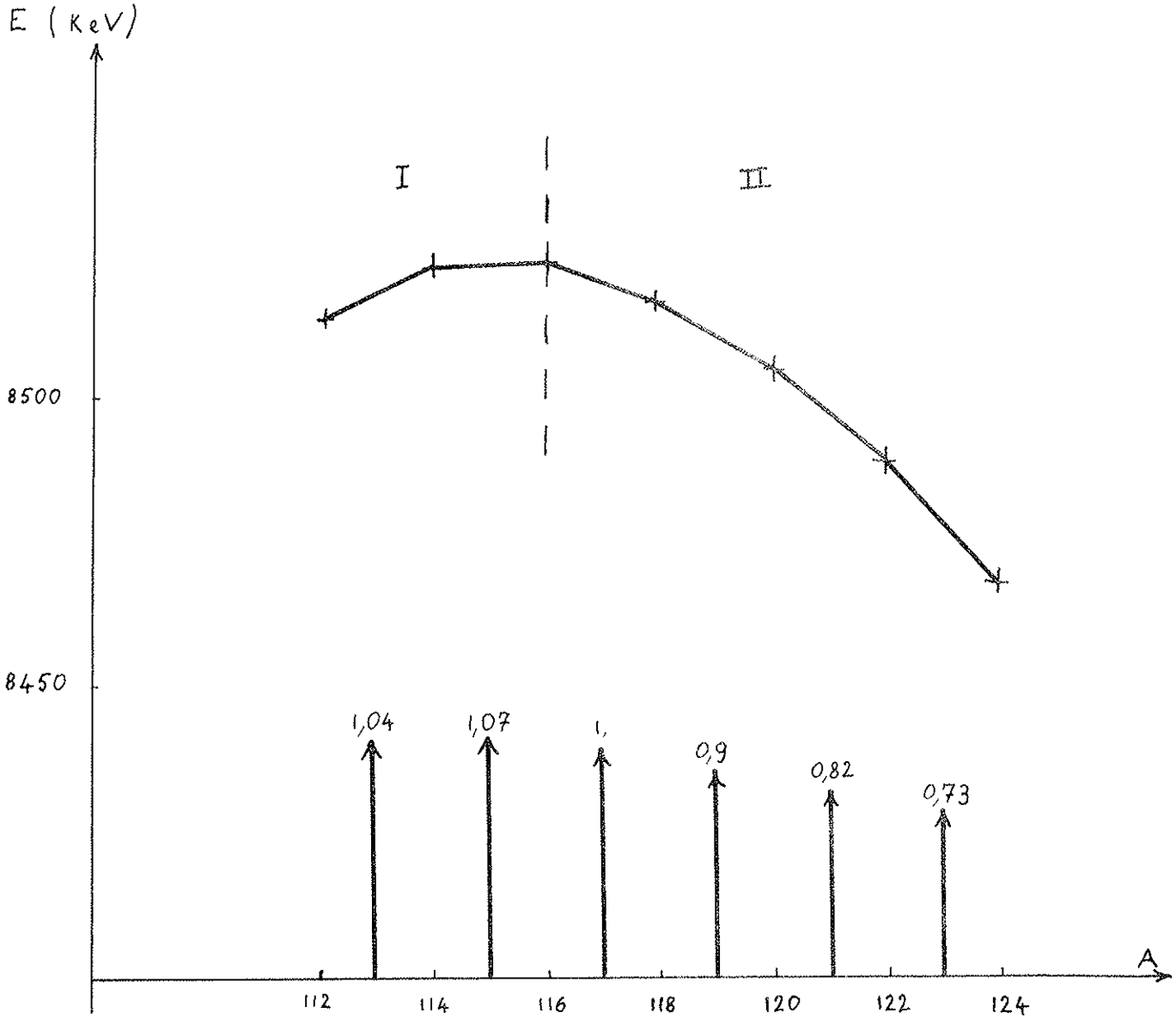


Figure 6

Energie de liaison par nucléon en KeV et
déplacement isotopique relatif de volume
de l'étain Z=50

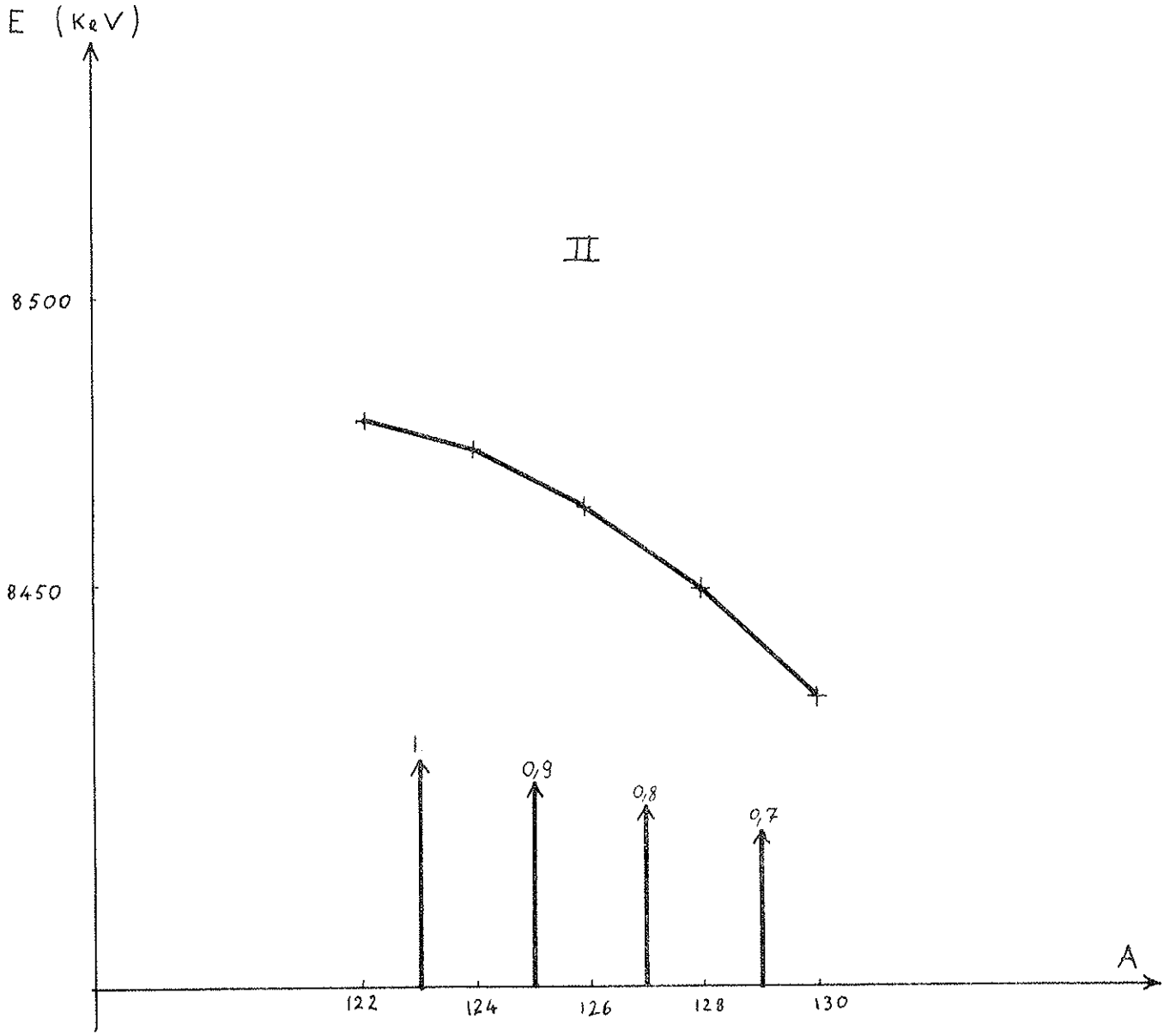


Figure 7

Energie de liaison par nucléon en KeV et déplacement isotopique relatif de volume du tellure Z=52

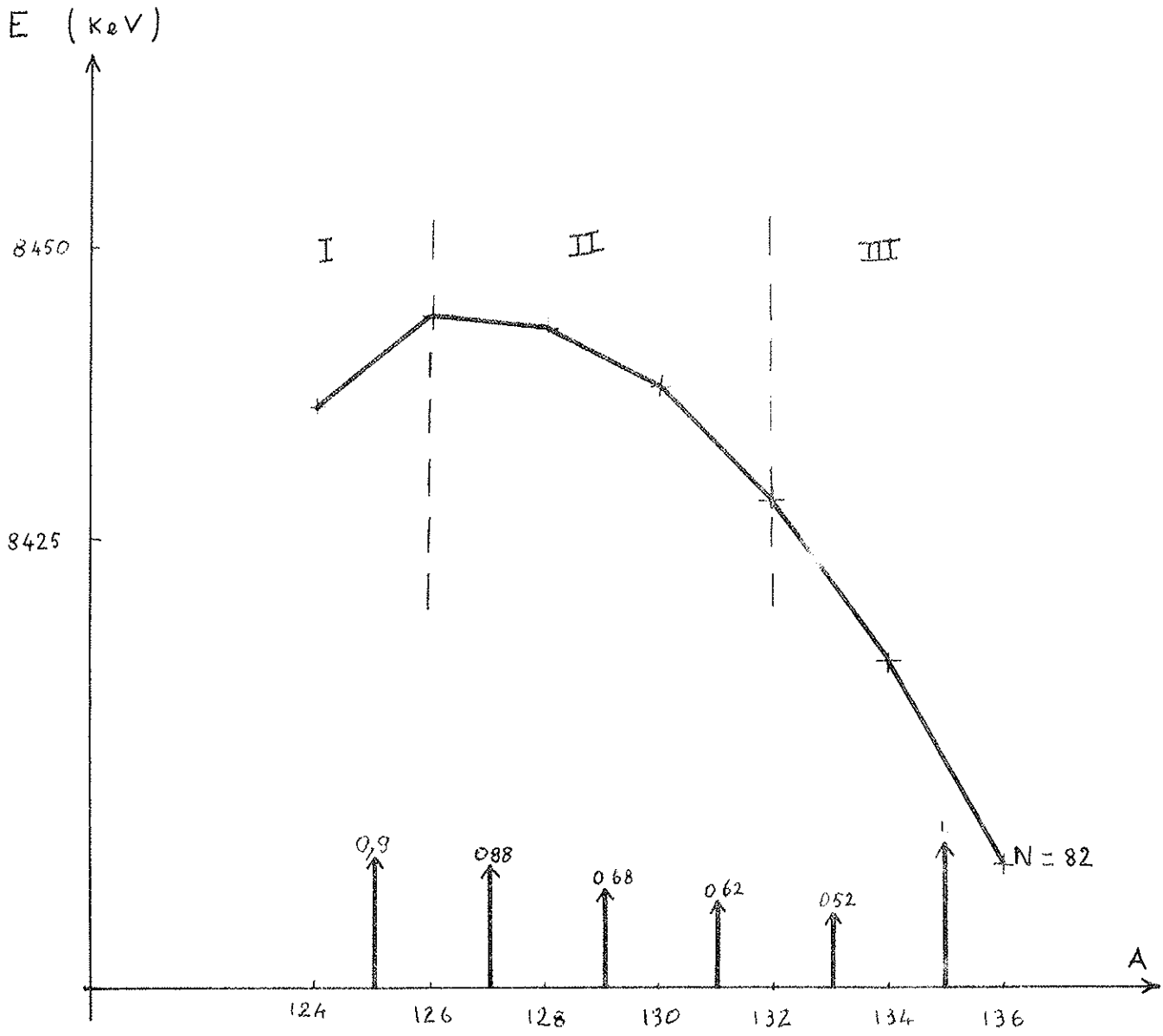


Figure 8

Energie de liaison par nucléon en KeV et déplacement isotopique relatif de volume du xénon Z=54

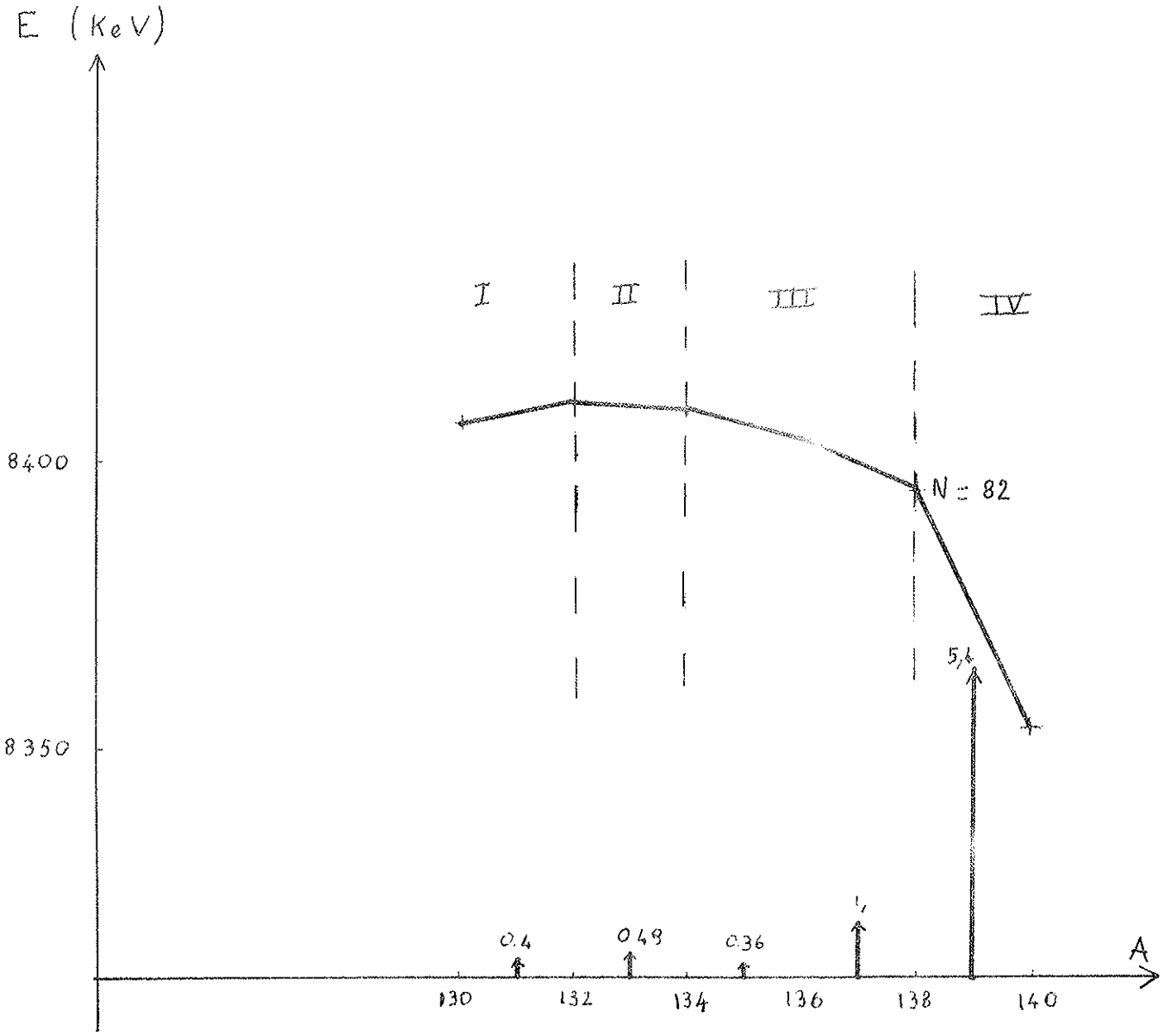


Figure 9

Energie de liaison par nucléon en KeV et déplacement isotopique relatif de volume du baryum Z=56

piques de volume, en tenant compte des correspondances suivantes, aux incertitudes expérimentales près :

- dans la zone I, nous sommes près du maximum de la courbe E , ce qui correspond au passage au fond de la vallée de stabilité : les ΔV sont égaux. Exemples : cadmium [22][23][24][25][26][27] et étain [28][29] ;

- dans la zone II E décroît de façon monotone, il en est de même pour ΔV . Exemples : cadmium, étain, tellure [30] et xénon. Nous pouvons penser que dans cette zone, les neutrons supplémentaires se placent à la périphérie sans qu'il y ait d'arrangement interne dans le noyau. Ceci conduirait bien pour ΔV à une loi en $EA^{1/3}$, expression représentant le terme de "surface" de l'énergie de liaison;

- la zone III reflète l'effet de fermeture de couche, les variations de E comme de ΔV étant nettement plus importantes pour le couple N,N-2 que pour le couple N-2,N-4 . Exemples : xénon et baryum [1];

- enfin la zone IV montre le "saut" après le nombre magique aussi bien dans la variation de E que dans la valeur de ΔV . Exemple : baryum [31].

Cette correspondance avec les énergies de liaison par nucléon éclaire d'intéressante façon le problème du déplacement isotopique de volume. Nous pouvons ainsi prévoir les valeurs de ΔV pour les isotopes pairs radioactifs du xénon :

- pour l'isotope 122 : $\Delta V_{124-122} \simeq \Delta V_{126-124}$

car nous sommes dans la zone I ;

- pour l'isotope 138 il y a saut après le nombre magique N=82 (zone IV) :

$$\Delta V_{138-136} \simeq 4 \Delta V_{136-134} \quad .$$

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Isotope shifts in the arc spectrum of xenon

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Isotope shifts have been measured in the lines of the spectrum xenon I for all of the nine stable isotopes. For the five more abundant (heavier) isotopes of even mass number the measurements include 37 lines in the visible and the photographic infrared; but for the lightest isotopes ^{126}Xe and ^{124}Xe measurements could be made only in respectively 3 and 12 lines, on account of the very small amounts of enriched isotopes which were available. For the isotopes of odd mass-number precise measurements could be made only when the hyperfine structures were resolved. This was possible for 22 lines of ^{129}Xe, which has a nuclear spin of $\frac{1}{2}$ with correspondingly simple hyperfine structures but for only 10 lines of ^{131}Xe, which has a nuclear spin of $\frac{3}{2}$ with more complex hyperfine structures, with much narrower separations. The lines for which isotope shifts were measured were (with two exceptions) due to transitions either between the electron configurations $5p^5$, 6 or 7p and $5p^56s$ or the configurations $5p^5$, 6, 7, 8 or 9d and $5p^56p$. The shifts in 24 lines due to the first type of transitions are invariably in the opposite sense to the Bohr shift and from two to six times greater while those in 11 lines due to the second type of transitions are in the same sense as the Bohr shift, and two to three times greater.

The isotope shifts show departures from a linear relation between the neutron number and the isotope shift which resemble those found in lines of barium and caesium.

The large number of lines in which isotope shifts have been measured permits an extensive test of the hypothesis that the ratio of the field-shifts of the isotopes should be constant in all lines; the validity of this hypothesis is confirmed.

Introduction

There is an approximately linear relation between the differences in the mass numbers and the isotope shifts in the case of atoms which have nuclei with neutron numbers well removed from the magic numbers of neutrons 28, 50, 82 and 126. But if one of the isotopes of an element has a neutron number equal to a magic number, the isotope shifts (due to the field effect) are not proportional to the differences in neutron numbers for the isotopes with neutron numbers equal to and close to the magic number. The isotope shifts in the sequence of elements caesium, barium and cerium afford excellent examples of this anomaly. In the first two of these elements the shift between the lines of the isotopes with neutron numbers 82

and 80 is much greater than that between these of the isotopes with neutron numbers 80 and 78. In the resonance line, 8521 Å,* of caesium (Hühnermann & Wagner 1966, 1967, 1968) these two shifts are 3.6 and 1.2 mk; in the resonance line of barium (Jackson & Duong 1966) they are 5.6 and 2.3 mk. In the lines 5291 and 5615 Å or cerium (Champeau & Gerstenkorn 1968) the lines of the isotope with neutron number 82 lie between those of the isotopes with neutron numbers 80 and 78. Abnormally large odd–even staggering has also been observed in the first two of these elements; this is particularly pronounced in the case of barium. The shift between the lines of the isotopes with neutron numbers 82 and 81 is 7.7 mk, which is equivalent to 14.4 mk for a difference of two neutrons, which is between 3 and 4 times greater than the average of the shifts between two adjacent isotopes of even mass number.

The element xenon is of particular interest for furthering the investigation of these anomalies, since it has a sequence of seven stable isotopes of even neutron number starting with the same magic number, 82, and descending to 70; measurement of the shifts of these isotopes enables a complete comparison to be made with the shifts of the isotopes of even neutron number measured in the spectra of caesium and barium, and since the sequence extends farther from the magic neutron number it permits a better test of the linearity between isotope shift and neutron number when the neutron number is well removed from the magic number. The two odd isotopes with neutron numbers 77 and 75 are farther removed from the magic number 82 than those of barium with neutron numbers 81 and 79 or that of caesium with neutron number 79; it is thus possible to determine whether the abnormally large odd–even staggering observed in the spectra of these two elements is associated with the closeness of the neutron numbers to the magic number.

Preliminary measurements of isotope shifts in the visible and photographic infrared have been published previously (Jackson & Coulombe 1970). These were both less complete and less accurate than the measurements reported here. After the earlier publication photographic plates became available with sensitivity improved by a factor of approximately 3 for both the visible and infrared regions; and the enriched isotopes were available in greater quantities. On account of these two factors it was possible to use interferometers with higher resolving power and consequently improved accuracy of measurement, high luminosity being no longer the most important requirement. A greater number of recordings could be made, with a corresponding reduction of the statistical uncertainty. The measurements reported here are the result of a new series of measurements made under the new, improved conditions. The accuracy of the measurements was described in terms of the probable error in the earlier publication; this was assumed to be the mean deviation divided by the square root of the number of interferograms measured. The criterion used here is the statistical uncertainty, which is the square root of the mean of the squares of the deviations divided by one half of the square root of

* 1 Å = 10^{-10} m = 10^{-1} nm; 1 mk = 10^{-3} cm^{-1}; 1 Torr ≈ 133 Pa.

the number of interferograms measured. This is greater by a factor of approximately 2.5 than the probable error, but it is more useful for estimating the reliability measurements, since, in the absence of systematic errors, the chance of an error exceeding the statistical uncertainty is very small – of the order of 5 %

The light sources

For each isotope a different discharge tube was used since the method of measuring isotope shifts was the comparison of the wavelength of a line emitted by ^{136}Xe with that emitted by another of the isotopes. The method of mixing the required even isotope with ^{129}Xe could not be used, since the shifts were to be measured in as many as possible of the stronger lines in the blue and photographic infrared regions and in many of these lines there would be overlapping of the strong central components of ^{129}Xe by the single component of the even isotope. The discharge tubes were Geissler tubes of rather large dimensions, fitted with a side tube for storing the enriched sample of one of the isotopes of xenon. The end-pieces were approximately 60 mm long and 50 mm in diameter; they were fitted with cold electrodes in the form of hollow cylinders of sheet aluminium approximately 50 mm long and 40 mm in diameter. The capillary had an internal diameter of 5 mm and a length of approximately 100 mm. The tubes were operated with helium as a carrier gas at a pressure of 1 Torr, and with xenon at a much lower pressure. The partial pressure of the xenon was normally maintained at 0.02 Torr; this could be very conveniently controlled by observing the relative strengths of the lines 4923 Å of xenon and 5015 Å of helium, since under these conditions they are of equal intensity. For the very strong lines 8231 and 8819 Å it was necessary to use a lower pressure, not exceeding 0.005 Torr since these lines self-reverse at higher pressure. The tubes were operated with an alternating current of 20 mA; the potential between the electrodes was approximately 420 V at the normal pressure of xenon but about 20–30 V lower at the lower pressure. The requisite partial pressure of xenon was obtained by condensing the xenon in the reservoir by cooling with liquid nitrogen, opening the tap separating it from the discharge tube, allowing the reservoir to warm, until the lines of xenon could be seen in the spectrum, removing the excess of xenon by condensing in the reservoir, finally closing the tap when the lines of helium and xenon had the appropriate intensities.

When different tubes are used to compare the wavelengths of lines of different isotopes it is evident that the shifts owing to inevitable differences of pressure, of either the carrier gas, helium or of the xenon itself must be limited. To check this, approximate measurements were made both of the pressure shifts due to the carrier gas and due to xenon. With a difference of 10 Torr in the pressure of helium the shifts were less than 0.3 mk for lines of the type s–p. The pressure of the helium in the discharge tubes was set to 1 Torr, to an accuracy of ± 0.1 Torr; consequently the shifts would be less than about 0.01 mk. Measurements were also made to determine the effects of differences of the pressure of the xenon. The pressure shifts of lines of the s–p type of transition, for a pressure difference of 1 Torr were found to be

between 0.2 and 0.5 mk (towards longer wavelength) for the lines in the infrared, and about twice as great for the lines in the blue. The partial pressure of the xenon did not exceed 0.02 Torr and the difference in the pressure in the two tubes would be substantially less than this, so that possible errors owing to pressure shifts would be unlikely to be a significant source of error. The pressure shifts (due to xenon) of lines of the p–d type of transition were difficult to measure because they become weak when the pressure is increased; they appeared to be smaller than those of lines of the s–p type of transition, and in the opposite sense. The shifts due to the helium are rather large for lines of the types 6p–7, 8 or 9d, approximately +0.5 mk/Torr for 6p–7d and +3 mk/Torr for 6p–9d.

The spectrograph and interferometer

The spectrograph was a prismatic instrument of the Littrow type with a dispersion of 0.1 mm/Å in the blue decreasing to 0.02 mm/Å in the limit of the photographic infrared. The Fabry–Perot interferometer was external to the spectrograph and an achromatic objective of 50 cm focal length formed an image of the fringe system on the spectrograph slit. The capillary of the discharge tube was placed in the focus of another objective, also of 50 cm focal length, so that a sharply focused image of the capillary was formed on the spectrograph split. The discharge tube was held in a support with a fine adjustment which allowed the image of the capillary to be exactly alined with the spectrograph split in a few seconds, so that the operation of changing the tube with xenon 136 for a tube with another isotope could be effected in less than 1 min. A field lens placed close to the spectrograph slit formed an image of the interferometer plates on the objective of the spectrograph. This optical arrangement ensures that the light entering the spectrograph passes through exactly the same part of the etalon interferometer plates and with exactly the same intensity distribution when the discharge tubes are interchanged.

The procedure for making the photographic recordings was designed to avoid systematic errors. A series of four exposures was made on one photographic plate, starting with one isotope, followed by two exposures for the other isotope and finishing with the first isotope. This was immediately followed by another similar series of four exposures but starting with the other isotope. Each series enabled two independent measurements of the isotope shift to be made. In the case of the lightest isotopes, available in very small quantities, this procedure was changed; a series of three exposures was made, starting and finishing with the isotope 136 with the rare isotope in between.

For measuring the shifts of the isotopes with even mass numbers a spacer of 30 mm length was used. The reflecting surfaces were multilayer dielectric coatings. For the blue, orange and red lines 3-layer coatings with a maximum reflectance at 5000 Å were used. The instrumental width was approximately equal to the Doppler width for the blue lines; and about twice this for the orange and red lines; but as some of these are very weak, the corresponding gain in luminosity was necessary to avoid long exposures. For the infrared lines 5-layer coatings were used which

gave instrumental width rather narrower than the Doppler width at the wavelength of maximum reflectance (8000 Å) and about 30 % greater at the shortest and longest wavelengths.

The root mean square of the deviations of the values derived from the measurement of one pair of interferograms averaged 0.7 mk for the blue lines, 0.8 mk for the orange and red lines and 0.5 mk for the infrared lines. In most cases between 20 and 30 interferograms were measured; but for some of the weaker lines only 12 were measured, in these cases two independent series of measurements of the interferograms were made. It was found that the root mean squares of the deviations when the average of the two measurements was taken was reduced in the ratio 1:1.3.

For measuring the shifts of the isotopes of odd mass number the length of the spacer had to be chosen to suit the requirements of the hyperfine structure; in some lines this was as small as 12 mm while for others it was 50 mm. It was also necessary to use 5-layer coatings for the blue lines as well as for the infrared lines.

The enriched isotopes

The enriched isotopes were prepared and analysed by the Centre de Spectrométrie Nucléaire at de Spectrométrie du C.N.R.S. (Camplan, Meunier & Sarrouy 1970), except in the case of the isotope 136, which was obtained from Germany. This latter was required in much larger quantity than the other isotopes, since it was used as the comparison for all of the others; the quantity available was large compared with that used during the course of the research. The quantities of the other isotopes, with the exception of the two lightest, 126 and 124, were approximately 5 mg (of each isotope); this was amply sufficient to allow the requisite, large numbers of interferograms to be made. But the amounts available of the least abundant isotopes 126 and 124 were very small. Of the former there was less than 0.01 mg and it was possible to make interferograms only of the three strongest infrared lines, 8231, 8819 and 8280 Å; however, as many as 40 interferograms could be made of these lines so that the statistical uncertainty of the measurements was not greater than that of the other isotopes (0.2 mk). The amount available of the isotope 124 was substantially larger (approximately 0.1 mg) so that interferograms could be made of the four strongest infrared lines and also of the eight strongest of the blue lines. Between 12 and 20 interferograms could be made of the blue lines and the statistical uncertainties were between 0.4 and 0.6 mk, or about twice as great as for the other isotopes.

The analyses of the enriched isotopes are given in table 1.

The measurements of the isotope shifts

The results of the measurements of the isotope shifts of 37 lines in the visible and photographic infrared regions are given in table 2. In order to facilitate the observation of certain regularities the lines have been arranged in the order appropriate to their classification rather than in the order of increasing wavelength. The first and second columns indicate the wavelength of the line and its classification

according to Humphreys & Meggers (1933) with the notation proposed by Racah (1942). The third column gives the value of the unit Bohr shift, M_1, the Bohr shift between the isotope 136 and an imaginary isotope 135. In the remaining columns are given the total (measured) isotope shifts of the eight other isotopes relative to the isotope 136. The figure in parentheses after the isotope shift is the statistical uncertainty and that in square brackets is the difference between the measured value of the isotope shift and the value given by the difference of the shifts of the two levels concerned, these being the means of either two or three values found from different combinations by application of the Ritz combination principle. This method can be used for 18 lines if only the lines whose shifts were measured by the present authors are used; but if measurements of four of the lines in the far infrared made by Vetter (1970) and of one line measured by Shafer (1970) are also used, it can be applied to four more lines; these lines are identified by an asterisk.

TABLE 1. ANALYSES OF ENRICHED ISOTOPES OF XENON

	82	80	78	77	76	75	74	72	70
	136	134	132	131	130	129	128	126	124
136	93.1	6.9	—	—	—	—	—	—	—
134	0.94	91.22	2.32	2.16	0.50	2.69	0.18	—	—
132	0.579	0.707	94.8	1.822	0.275	1.692	0.08	—	—
131	0.245	0.297	0.734	98.05	0.112	0.541	—	—	—
130	0.092	0.142	0.541	0.342	98.21	0.649	0.025	—	—
129	0.194	0.232	0.675	0.352	0.099	98.4	—	—	—
128	0.44	0.61	1.92	1.55	0.31	3.06	92.1	—	—
126	⩽ 0.09	⩽ 0.1	⩽ 0.6	0.87	0.28	3.54	0.56	93.6	0.34
124	0.02	0.03	0.13	0.18	0.08	1.03	0.17	0.41	97.88

This comparison of the observed and calculated values of the isotope shifts gives a good check on the consistency of the measurements. It can be seen that none of these differences exceeds the statistical uncertainty, while many are substantially smaller; the average difference for the 22 lines is between one third and one half of the average value of the statistical uncertainties, and is thus approximately equal to the probable error. (The terms statistical uncertainty and probable error are defined on page 278.)

Comparison with other measurements

Koch & Rasmussen (1950) measured isotope shifts in three lines, but only for the isotopes 136, 134 and 132. Simultaneously with the present authors, Fischer, Hühnerman, Krömer & Schäfer (1973) have measured the isotope shifts of the stable isotopes in four lines, but of these lines one, 9799 Å, is not among the 37 lines measured by the present authors, since it is beyond the limit of sensitivity of the photographic plates used. Koch & Rasmussen gave no figures for the uncertainty of their measurements, but comparison with the uncertainties of measurements of the hyperfine structures of the lines of the isotopes 129 and 131, made with similar experimental equipment (Bohr, Koch & Rasmussen 1952), indicates that the uncertainty is not less than 0.5 mk, and since the shift between 132 and 136 is found

TABLE 2. ISOTOPE SHIFTS/mk IN THE ARC SPECTRUM OF XENON RELATIVE TO ^{136}Xe

lines (Å)	classification	M_i	134	132	131	130	129	128	126	124
4624	$6s\frac{3}{2}$–$7p\frac{3}{2}$	0.64	2.9_6 (0.25) [−0.06]	4.0_6 (0.25) [−0.11]	—	5.3 (0.2) [−0.04]	6.8_5 (0.2)	7.2 (0.25) [−0.06]	—	10.5 (0.6)
4671	$6s\frac{3}{2}$–$7p\frac{3}{3}$	0.63	2.9_5 (0.2)	4.2_6 (0.3)	—	5.1 (0.25)	6.9_5 (0.25)	7.2$_5$ (0.3)	—	10.7 (0.5)
4697	$6s\frac{3}{2}$–$7p\frac{2}{2}$	0.63	3.1_0 (0.2) [0.13]	4.0_9 (0.25) [0.09]	—	5.2 (0.3) [−0.11]	6.7_5 (0.15) [0.07]	7.5 (0.3) [0.13]	—	10.8 (0.4)
4807	$6s\frac{3}{2}$–$7p\frac{1}{0}$	0.62	2.3_9 (0.2)	2.9 (0.4)	4.8_5 (0.15)	3.7 (0.3)	5.2 (0.4)	4.7 (0.4)	—	7.1 (0.6)
4830	$6s\frac{3}{2}$–$7p\frac{1}{1}$	0.61	2.3 (0.25) [0.12]	3.0 (0.3) [0.10]	—	3.9 (0.25) [−0.03]	—	4.0 (0.4) [−0.39]	—	—
4843	$6s\frac{3}{2}$–$7p\frac{2}{2}$	0.61	2.0 (0.3) [0.09]	2.7 (0.4) [0.17]	—	3.0 (0.3) [0.05]	—	4.2 (0.2) [0.07]	—	—
4923	$6s\frac{1}{2}$–$7p\frac{2}{2}$	0.60	1.8 (0.2) [−0.13]	2.2 (0.3) [−0.13]	—	3.0 (0.25) [0.08]	4.0_9 (0.15) [−0.07]	4.1 (0.3) [−0.13]	—	5.5 (0.5)
4501	$6s\frac{3}{2}$–$6p\frac{1}{1}$	0.66	4.3_9 (0.25) [0.22]	6.0_5 (0.25) [0.05]	—	8.4 (0.3) [0.08]	10.7 (0.45)	11.0 (0.3) [0.13]	—	17.1 (0.7)
4524	$6s\frac{3}{2}$–$6p\frac{3}{2}$	0.66	4.4_5 (0.25) [−0.04]	6.2 (0.3) [0.02]	—	8.9 (0.4) [0.27]	10.7 (0.8) [−0.44]	11.2 (0.3) [−0.11]	—	—
4583	$6s\frac{1}{2}$–$6p\frac{1}{0}$	0.65	3.2$_5$ (0.3) [0.22]	4.0_6 (0.3) [−0.09]	6.8_6 (0.2)	5.5 (0.25) [−0.06]	8.2 (0.45) [0.20]	7.6 (0.4) [0.40]	—	11.6 (0.6)
4734	$6s\frac{1}{2}$–$6p\frac{2}{2}$	0.63	3.4_0 (0.2) [−0.05]	4.4 (0.3) [−0.13]	—	6.2 (0.25) [−0.06]	8.6 (0.3) [0.01]	8.2 (0.25) [0.02]	—	12.7 (0.5)
4916	$6s\frac{1}{2}$–$6p\frac{1}{1}$	0.60	2.8_9 (0.25) [−0.11]	3.5 (0.25) [−0.08]	—	5.1 (0.25) [−0.06]	—	6.7 (0.25) [0.01]	—	—
7642	$6s\frac{3}{2}$–$6p'\frac{1}{1}$	0.39	2.8_2 (0.2) [−0.10]	5.0 (0.3) [−0.11]	6.8_5 (0.4)	6.7_5 (0.15) [−0.12]	9.2 (0.3)	9.1_5 (0.2) [−0.05]	—	—
8206	$6s\frac{3}{2}$–$6p'\frac{2}{1}$	0.36	3.0_9 (0.2) [0.11]	4.3_8 (0.15) [0.04]	6.4 (0.25)	6.1_5 (0.15) [0.05]	7.8_5 (0.15)	8.1_5 (0.2) [−0.01]	—	—
7887	$6s\frac{1}{2}$–$6p'\frac{1}{0}$	0.38	2.2_6 (0.2) [−0.15]	3.5$_6$ (0.25) [0.06]	5.1 (0.25)	4.7_9 (0.15) [0.01]	6.6_5 (0.2) [−0.10]	6.0 (0.2) [−0.16]	—	—
8346	$6s\frac{1}{2}$–$6p'\frac{2}{2}$	0.36	2.8_5 (0.2) [0.08]	3.8_5 (0.2) [0.07]	—	5.3_6 (0.15) [−0.04]	6.8_6 (0.15) [−0.07]	7.2 (0.2) [0.06]	—	—
8231	$6s\frac{3}{2}$–$6p\frac{2}{2}$	0.36	3.2 (0.3) [−0.13]	4.9 (0.3) [−0.07]	7.6 (0.5)	6.7_5 (0.3) [−0.01]	9.0 (0.5)	8.8_5 (0.3) [−0.07]	11.2$_2$ (0.3)	14.0 (0.3)
8409*	$6s\frac{3}{2}$–$6p\frac{1}{1}$	0.35	3.2$_5$ (0.2) [−0.13]	4.8_6 (0.15) [−0.06]	7.7 (0.2)	6.8_5 (0.1) [0.02]	8.8_6 (0.2)	9.0$_5$ (0.25) [0.06]	—	—
8819	$6s\frac{3}{2}$–$6p\frac{2}{3}$	0.31	3.3$_5$ (0.2)	5.1_6 (0.2)	—	7.0$_5$ (0.2)	9.0 (0.3)	9.1$_5$ (0.15)	11.8 (0.15)	14.7 (0.15)
9045*	$6s\frac{1}{2}$–$6p\frac{2}{2}$	0.33	3.3 (0.2) [−0.05]	4.9_9 (0.15) [0.03]	—	6.8_6 (0.2) [−0.03]	8.9_5 (0.3)	8.9$_5$ (0.25) [−0.06]	—	—
8280*	$6s\frac{3}{2}$–$6p\frac{1}{0}$	0.36	2.6_9 (0.15) [0.13]	3.4$_5$ (0.15) [0.03]	5.4 (0.2)	4.6_5 (0.2)	6.0_5 (0.2)	6.1_6 (0.2)	7.5$_5$ (0.2)	9.3$_5$ (0.15)
8052	$6s\frac{3}{2}$–$6p\frac{1}{1}$	0.33	2.3$_5$ (0.2) [0.02]	3.4$_5$ (0.15) [0.06]	—	4.5_9 (0.15) [0.10]	—	5.8_5 (0.2) [0.01]	—	9.2$_0$ (0.25)
7967	$6s\frac{1}{2}$–$6p'\frac{1}{1}$	0.37	2.4$_5$ (0.25) [0.05]	3.6_9 (0.25) [0.02]	5.2$_6$ (0.25)	5.0_6 (0.15) [0.07]	6.4$_5$ (0.25)	6.8_9 (0.15) [0.04]	—	—
8649	$6s\frac{1}{2}$–$7p\frac{1}{1}$	0.34	1.8_9 (0.25) [0.06]	2.1$_6$ (0.25) [−0.09]	—	3.1$_6$ (0.2) [0.00]	—	4.4$_5$ (0.25) [0.19]	—	—
8739	$6p\frac{1}{1}$–$6d\frac{3}{2}$	0.34	−1.0$_5$ (0.2)	−2.15 (0.25)	−3.1 (0.2)	−3.2$_6$ (0.2)	−3.8$_5$ (0.25)	−4.1$_6$ (0.25)	—	—
8862	$6p\frac{1}{1}$–$6d\frac{1}{1}$	0.33	−1.0 (0.3)	−2.2 (0.3)	—	−3.4$_5$ (0.2)	—	−4.5 (0.25)	—	—
6187	$6p\frac{1}{1}$–$7d\frac{3}{2}$	0.46	−1.7 (0.5)	−3.0 (0.5)	—	−4.1 (0.4)	−4.5 (0.5)	−4.9 (0.4)	—	—
6882	$6p\frac{3}{2}$–$7d\frac{5}{2}$	0.43	−1.3 (0.4)	−1.7 (0.5)	—	−2.6 (0.25)	—	−3.8 (0.35)	—	—
7129	$6p\frac{3}{2}$–$7d\frac{3}{2}$	0.42	−1.1$_5$ (0.25)	−1.8$_6$ (0.25)	—	−3.0 (0.25)	—	−4.2 (0.2)	—	—
5895	$6p\frac{1}{1}$–$8d\frac{3}{2}$	0.50	−2.0 (0.4)	−2.6 (0.4)	—	−3.5 (0.5)	—	−4.5 (0.3)	—	—
6182	$6p\frac{3}{2}$–$8d\frac{5}{2}$	0.48	−1.5 (0.6)	−1.9 (0.8)	—	−3.2 (0.4)	—	−4.4 (0.4)	—	—
6318	$6p\frac{3}{2}$–$8d\frac{3}{2}$	0.47	−1.7 (0.4)	−2.4 (0.4)	—	−3.7 (0.4)	—	−4.6 (0.4)	—	—
6099	$6p\frac{1}{1}$–$8d\frac{5}{2}$	0.49	−2.2 (0.6)	−2.8 (1.0)	—	−3.5 (1.0)	—	−4.5 (0.4)	—	—
5934	$6p\frac{3}{2}$–$9d\frac{5}{2}$	0.50	−1.5 (0.4)	−1.9 (0.5)	—	−3.3 (0.4)	—	−4.1 (0.5)	—	—
6533	$6p\frac{3}{2}$–$9d\frac{3}{2}$	0.45	−2.0 (0.4)	−2.6 (0.9)	—	−3.7 (0.5)	—	−4.5 (0.4)	—	—
7585	$5d\frac{1}{1}$–$6f\frac{5}{2}$	0.39	0.5$_5$ (0.25)	1.1 (0.25)	—	1.8_6 (0.2)	1.8 (0.3)	2.2 (0.25)	—	—
8171*	$6p\frac{3}{2}$–$5d'\frac{3}{2}$	0.36	−0.6 (0.3) [−0.10]	−1.4$_5$ (0.3) [0.04]	—	−2.2$_6$ (0.2) [0.10]	−3.1 (0.25)	−3.6 (0.3) [−0.05]	—	—

from the sum of those between 136 and 134 and 134 and 132 (the shifts measured by these authors) the uncertainty could be increased. Fischer *et al.* (1973) measured the shifts with respect to the isotope 129; for comparison with the present authors' results these have been converted to shifts with reference to the isotope 136. This would tend to increase the uncertainty (except in the shift 129–136) by an amount less than 0.2 mk. The isotope shifts, in mk, relative to 136, are given in table 3. In the case of the measurements by Fischer *et al.* of the shifts in the line 8231 Å, it was necessary to assume the present authors' value for the shift 129–136 since this was not measured by the former; and for the isotopes 131 and 132, the difference of the present authors' values for 131–136 and 132–136 was taken. The uncertainties are given in parentheses after the isotope shifts. In the case of the measurements of Fischer *et al.* they are the uncertainties given by these authors without any increase for the conversion of the reference from the isotope 129 to the isotope 136.

The agreement between the values found by Fischer *et al.* and those found by the present authors is good. The average value of the differences is 0.21 mk and the average value of the differences from the mean values of the two series of measurements is 0.11 mk. In only one instance, the shift of the isotope 134 in the line 8206 Å, is the difference from the mean greater than the statistical uncertainties (by 0.1 mk); but if the statistical uncertainty of the measurement by Fischer *et al.* is increased by 0.2 mk (the value for the shift 129–136, which has been neglected) the difference is reduced to within the limits of the statistical uncertainties. The agreement with the values found by Koch & Rasmussen is fairly satisfactory; the differences are within the limits of the uncertainties.

King diagrams of the isotope shifts

The King diagram (King 1963, 1964; Stacey 1964) provides a method of testing the validity of the hypothesis of the constancy of the ratios of the field-shifts of different lines in a spectrum by eliminating the influence of the mass effects; alternatively, if this hypothesis is accepted, it provides a means of testing the accuracy of the measurements of the isotope shifts. It also gives the ratio of the field shifts of any pair of lines and the difference in the total mass-shifts if the field-shifts are approximately equal.

It would evidently be possible to make King diagrams of all the possible pairs of all the available lines, but in the present case this would scarcely be practical since the isotope shifts in 37 lines have been measured and consequently the number of possible pairs would be greater than 600. It was therefore decided to select one line and to construct the King diagrams with this line as a reference line, providing the values for the abscissae, and each one of the other 36 lines providing the values for the ordinates.

The line 8280 Å has been selected as the reference line for the following reasons. It is sufficiently strong to permit the isotope shift of ^{126}Xe, which was available in a very small quantity, to be measured; it does not self-reverse and is therefore

TABLE 3. COMPARISON OF MEASUREMENTS BY KOCH & RASMUSSEN (K.R.) AND BY FISCHER ET AL. (F.) WITH THOSE OF THE PRESENT AUTHORS (J.C.)

		isotope							
line (Å)	authors	134	132	131	130	129	128	126	124
8231	K.R.	3.5 (0.5)	5.6 (0.5÷)	—	—	—	—	—	—
	J.C.	3.2 (0.3)	4.9 (0.3)	—	—	—	—	—	—
8280	K.R.	2.9 (0.5)	4.0 (0.5÷)	—	—	—	—	—	—
	J.C.	2.6 (0.15)	3.4_5 (0.15)	—	—	—	—	—	—
8819	K.R.	3.6 (0.5)	6.1 (1.0)	—	—	—	—	—	—
	J.C.	3.3 (0.2)	5.1 (0.2)	—	—	—	—	—	—
7887	F.	1.8 (0.3)	3.1 (0.6)	5.1 (0.6)	4.7 (0.3)	6.2 (0.2)	5.8 (0.2)	7.6 (0.1)	9.5 (0.1)
	J.C.	2.2 (0.25)	3.5 (0.25)	5.1 (0.25)	4.7 (0.3)	6.0_5 (0.2)	6.0 (0.15)	—	—
8206	F.	2.4 (0.2)	4.2 (0.2)	6.2 (0.2)	5.8 (0.2)	7.7 (0.2)	7.9 (0.2)	10.0 (0.1)	12.5 (0.1)
	J.C.	3.0 (0.2)	4.3 (0.15)	6.4 (0.25)	6.1_5 (0.15)	7.8_5 (0.15)	8.1_5 (0.2)	—	—
8231	F.	—	(131–132)	2.8 (0.1)	—	(9.0)	—	11.1 (0.1)	13.8 (0.1)
	J.C.	3.2 (0.3)		2.7 (0.3)	—	9.0 (0.5)	8.0_5 (0.3)	11.2_5 (0.3)	14.0 (0.3)

not liable to shifts due to asymmetrical self-absorption which are a source of difficulty in the case of the much stronger line 8231 Å; the hyperfine structure of ^{131}Xe is satisfactorily resolved, while that of the line 8231 Å is not, and the other lines in which the resolution is satisfactory are too weak to allow the isotope shifts of ^{126}Xe (or ^{124}Xe) to be measured.

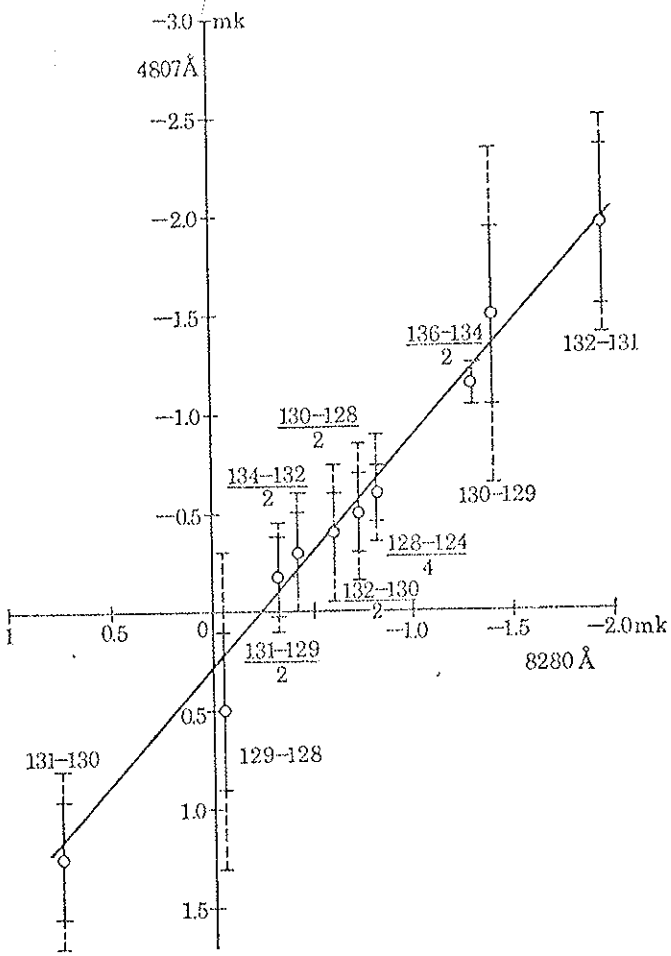

FIGURE 1. King diagram of the isotope shifts of the lines 8280 and 4807 Å of Xe I.

The method used for constructing the King diagrams can be seen from figure 1, which is the diagram for the pair of lines 8280 Å, the reference line and 4807 Å, the comparison line. The abscissae are given by the differences of the isotope shifts of adjacent pairs of isotopes in the reference line and the ordinates are given by the differences of the isotope shifts of the same pair of isotopes, in the line 4807 Å, the comparison line. If the difference of the mass numbers of the pairs is 2 units (an adjacent pair of even or of odd isotopes) these differences are divided by 2; and if

the difference of the mass numbers is 4 units (the isotopes 128 and 124) the differences in the isotope shifts are divided by 4. To enable a comparison to be made of the divergences of the points from the straight line and the statistical uncertainties, vertical lines have been drawn through the points; the unbroken part of the line is equal to the statistical uncertainty of the measurement of one of the pair of isotopes and the broken part is equal to that of the other. When the mass numbers of the pair differ by two units the length of the line is one half, and when they differ by four units, one quarter of the statistical uncertainties. It is apparent that the divergences of the points are less than the statistical uncertainties (reduced to one half or one quarter when appropriate) even when that of only one of the two measurements is taken.

TABLE 4. AVERAGE VALUES OF DIVERGENCES, Δ, OF POINTS IN THE KING DIAGRAMS OF 36 PAIRS OF LINES OF Xe I AND OF THE STATISTICAL UNCERTAINTIES, u (IN mk) OF THE ISOTOPE SHIFTS

isotope pair	136* −134	134* −132	132* −130	130* −128	128† −124	131* −129	132 −131	131 −130	130 −129	129 −128
$\Sigma\Delta/n$	−0.07	0.06	−0.05	−0.02	0.08	0.25	0.08	0.04	0.10	0.04
$\Sigma\|\Delta\|/n$	0.15	0.19	0.19	0.16	0.34	0.32	0.33	0.16	0.25	0.25
$\Sigma u/n$	0.30	0.64	0.67	0.62	0.76	0.57	0.54	0.39	0.56	0.60
$\Sigma\|\Delta\|/\Sigma u$	0.50	0.34	0.28	0.26	0.45	0.56	0.61	0.41	0.45	0.42
n	36	36	36	36	10	9	9	9	22	22

* Δ multiplied by 2. † Δ multiplied by 4.

Similar King diagrams have been made for all the other lines whose isotope shifts were measured, also with the line 8280 Å as the reference line. A summary of the information obtained from the diagram is given in table 4 (average values for the differences of the mass-shifts of certain groups of lines were also derived from these diagrams; these are given on page 288). The first row indicates the pair of isotopes concerned. The second row ($\Sigma\Delta/n$) is the sum of the divergences (multiplied by the factor 1, 2 or 4 according to the differences of mass 1, 2 or 4) for all the lines the sign being taken into consideration, divided by the number of lines. Evidently if the measurements of the isotope shifts of the reference line had been perfect, this quantity would be equal to zero to within the statistical uncertainty of the divergences (irrespective of sign) of all the lines; this is of the order of 0.1 mk. This is the case for all the pairs except 129–131, so that, except for this pair, the divergences have not been much increased by attributing the whole to the comparison line and none to the reference line. The small value of the quantity $\Sigma\Delta/n$ indicates a high degree of accuracy of the measurements of the shifts of the reference line; the errors in the measurements of the shifts of the even isotopes are probably less than 0.1 mk and probably less than 0.2 mk in those of the odd isotopes. The third row is $\Sigma|\Delta|/n$, the average value of the divergences when they are added without the sign being taken into consideration; this is a measure of the average error of the difference of two measurements of the shifts, which is evidently greater than

average of the two measurements, though probably less than the sum. The next row gives the average values of the sum of the statistical uncertainties of the shifts of the pair of isotopes, and the fifth row gives the ratio of the average values of the divergences and the statistical uncertainties. The mean for all the isotopes and all the lines of this ratio is 0.39 which is approximately equal to the ratio of probable errors to statistical uncertainties. The last row gives the number of lines measured for each pair of isotopes (the figures for the pairs 128–126 and 126–124 have been omitted since they occur in only two King diagrams; the divergences are between 0.1 and 0.3 mk and are smaller than the statistical uncertainties).

The divergences of the points from the straight line are in every diagram within the limits of the statistical uncertainties. This gives a satisfactory confirmation of the hypothesis of constant ratios of field-shifts, in all lines, for both even and odd isotopes; this hypothesis has been questioned by Hansen, Steudel & Walther (1967).

The ratios of the field-shifts in lines due to transitions of the types s–p, relative to that of the line 8280 Å, can be found from the King diagrams with precisions of 0.2–0.3. They can be separated conveniently into three categories – high, intermediate and low – and their values are:

high		intermediate				low			
4501	1.5	4624	1.0	7642	1.0	4843	0.9	7887	0.8
4524	1.5	4671	1.2	8206	1.1	4916	0.8	7967	0.9
4583	1.4	4697	1.1	8231	1.2	4923	0.7	8649	0.8
4734	1.4	4807	1.1	8346	1.0			8952	0.8
		4830	1.0	8409	1.2				
				8819	1.2				
				9045	1.2				

The lines in the orange and red, due to transitions of the types 6p–7, 8 or 9d, have negative slopes in the King diagrams, with an average value of approximately −0.5. The ratios of the field shifts of the infrared lines other than those due to transitions of the types s–p are discussed below (page 289).

Evaluation of the mass-effect of the isotope shifts of xenon

There are four methods with which approximate estimates of the magnitude of the total mass-shifts can be made, if calculated values of the specific mass-shifts are not available. Firstly, the King diagrams can give the differences of the mass-shifts of the two lines although they cannot give the absolute values; but if two groups of lines, widely separated in their wavelengths, due to similar combinations of electron configurations, have differences of mass-shifts which are small and are approximately equal to the Bohr shifts, this is an indication that the total mass-shifts are unlikely to differ greatly from the Bohr shifts. Secondly, in the case of spectra which have some lines in which the relation between the total isotope shifts and the differences of mass numbers differs substantially from linear, if there are other lines in which this relation is nearly linear, it follows that, for these lines, the field-shifts are small compared with the total mass-shifts, and the straight line of

a King diagram constructed with a line of the first type as the reference line, is nearly horizontal. Thirdly the empirical relation between the differences in nuclear binding energies and the relative isotope shifts (due to the field effect) discovered by Gerstenkorn (1969) by means of which the field- and mass-effects can be separated is applicable to the stable isotopes of xenon. The fourth method of evaluating the mass-shifts depends on the construction of a King diagram in which the reference line is a line of another element, with similar ratios of the field-shifts, due to a similar combination of electron configurations and with a known value of the mass-effect; the King diagram gives an approximate value of the difference of the mass-effect of the two lines. This method is, however, most uncertain; it cannot be regarded as quantitative.

In the arc spectrum of xenon there are two widely separated groups of lines due to similar combinations of electron configuration whose isotope shifts have been measured by the present authors. The first is a group of 12 lines with wavelengths between 4500 and 4930 Å due to transitions from the levels 7p or 6p′ to the levels 6s and the other is a group of 12 lines in the region 7880–9050 Å due to transitions from the levels 6 or 7p to the levels 6s or 6s′. The differences of the mass-shifts of lines of these two groups can be found from the King diagrams; it is the value of the ordinate at the point at which the straight line cuts the y-axis. The mean value of the differences per unit difference of mass of the blue and the infrared lines is 0.24 ± 0.15 mk, and with only one exception the greatest divergence is 0.2 mk (the exception is the line 4501 Å for which the difference is -0.1 mk, within the estimated uncertainty of 0.5 mk). The mean values of the Bohr shifts for the blue and for the infrared lines are respectively 0.62 and 0.35 mk and the differences is thus 0.27 mk. This good agreement of the mean value of the differences of the Bohr shifts and the mean value of the observed differences of the mass-shifts for two widely separated groups of lines indicates that the total mass-shifts are unlikely to differ from the Bohr shifts by amounts substantially greater than the difference of the Bohr shifts.

There are 4 lines among the 37 lines whose isotope shifts were measured by the present authors which have shifts very nearly proportional to the differences of mass. The straight lines of their King diagrams are nearly horizontal, but in each case there is a small slope which shows that the field effect is not quite zero, but is smaller than that of the reference line approximately in the ratio of the tangent of the angle of the slope. The mass-shift per unit mass, M_1, is found by dividing the shift between the isotopes 136 and 128 by the factor 8.44 and applying the appropriate correction (to eliminate the small field effect) found from the slope of the straight line of the King diagram and the approximately known value of the field effect of the reference line. The mass-shift, M_1, can also be found approximately from the value of the ordinate at the point at which the straight line cuts the y-axis.

These four lines, their classifications and the unit mass-shifts are:

8171 Å	8733 Å	8862 Å	7585 Å
$6p^{\frac{3}{2}}2–5d'^{\frac{3}{2}}2$	$6p^{\frac{1}{2}}1–6d^{\frac{3}{2}}2$	$6p^{\frac{1}{2}}1–6d^{\frac{1}{2}}1$	$5d^{\frac{5}{2}}4–5f^{\frac{5}{2}}5$
0.4 ± 0.2 mk	0.5 ± 0.2 mk	0.5 ± 0.2 mk	-0.3 ± 0.2 mk

The values of the unit mass-shifts were determined by both of the two methods described above: the differences are less than 0.05 mk. The corrections applied for the residual field-shifts, necessary with the first method, are small, ranging between 0 and 0.07 mk. The shifts of the first three of these lines are approximately equal to the Bohr shifts (0.37, 0.34 and 0.34 mk); the differences are less than the uncertainties and the (unit) specific mass-shift must be less than 0.2 mk. The shifts of the line 7585 Å are, however, in the opposite sense to the Bohr shift and the unit specific mass-shift must be approximately -0.6 mk.

The isotope shifts of 13 lines in the far infrared have been measured by Vetter (1970). Nine of these lines are due to transitions of the type 6p–5d, two of the type 6p′–5d′ and one of the type 7p–5d′. All of these 12 lines have shifts in the same sense as the Bohr shift and nearly proportional to the mass-shifts, with the exception of the line 2.518 μm in which the shifts are very small. The unit mass-shifts determined by the two methods described above range between 0.6 and 1.0 mk; the field shifts are small – between $-\frac{1}{20}$ and $\frac{1}{5}$ of the estimated field-shifts of the line 8280 Å. Since the Bohr shift for unit mass in this region is between 0.1 and 0.05 mk there are evidently specific mass-shifts, in the same sense as the Bohr shift, of between 0.5 and 0.9 mk for unit mass-difference.

The line 3.6518 μm, $7s\frac{3}{2}2–7p\frac{1}{2}1$, has isotope shifts of a type quite different from those of the 12 lines discussed in the preceding paragraph; they resemble those of lines due to transitions of the type 6s–7p. The field shifts are smaller than those of the line 8280 Å in the ratio 0.43:1.

The empirical relation between the differences of nuclear binding energies and the field effect of the isotope shifts found by Gerstenkorn (1969, 1971, 1973) applies to sequences of three isotopes with even neutron numbers, the heaviest having a magic number of neutrons; the three heaviest stable isotopes of xenon satisfy this condition. This relation is

$$\frac{E_N - E_{(N-4)}}{E_N - E_{(N-2)}} = \frac{F_{(N,N-4)}}{F_{(N,N-2)}} = R,$$

where N is a magic number of neutrons; E_N, $E_{(N-2)}$ and $E_{(N-4)}$ are the binding energies of nuclei with N, $N-2$ and $N-4$ neutrons; $F_{(N,N-2)}$ and $F_{(N,N-4)}$ are the field effects of the isotope shifts between isotopes with N and $N-2$ and isotopes with N and $N-4$ neutrons. If the ratios of the field effects can be found by means of this relation the value of the total mass-effects can be calculated for these isotopes, and hence for all the other isotopes. This relation has been tested for six elements for which the nuclear binding energies and the field effects of the isotope shifts are known; it has been found to be correct within the limits of the experimental uncertainties for all except one of these elements. The exception is barium, for which the ratio of the differences of the binding energies is 1.56 ± 0.1 (Wapstra & Gove 1971); while the ratio of the field effects of the isotope shifts is 1.35 ± 0.1 for the line 5536 Å of Ba I (Jackson & Duong 1964) and 1.36 ± 0.1 for the line 4934 Å of Ba II (Fischer, Hartmann & Hühnermann 1969). The ratio of the differences of the nuclear binding energies of xenon is 1.79 ± 0.03 (Wapstra & Gove 1971); if it is assumed that a

similar difference between the ratio of the differences of the nuclear binding energies and the field-shifts can be expected in the case of xenon, since the structures of the nuclei are similar, then the ratio of the field-shifts, R, should be 1.56.

The total mass-shifts between the isotopes 136 and 134 have been calculated for the value 1.56 of the ratio R from the equations:

$$(1.56-a)\,F = (2.015a-4.092)\,M_1$$
$$F = (T-M),$$

where a is the ratio of the total isotope shifts of the pairs 136, 132 and 136, 135 and F, M and T are the field, the mass and the total shifts between the isotopes 135 and 134. The mass-shift for unit difference of mass (136–135) is equal to $M/2.015$. The values of M_1 thus calculated are in agreement with the Bohr shifts for the 12 blue lines and for 12 infrared lines due to the transitions of the types 6s or 6s′–6p′, 6p or 7p; but the uncertainties are rather high (0.3–0.6 mk).

Calculations made recently by M. J. Bauche (private communication to the present authors) have shown that the specific mass-shifts for these lines are smaller than the Bohr shifts; for the line 8280 Å the calculated value of the total mass-shift is within 0.1 mk of the value given by the present authors' measurements of the isotope shifts 136–134 and 136–132 combined with the value of 1.56 for the Gerstenkorn ratio. It is 0.2 mk greater than the Bohr shift, but the mean value of the mass-shifts of the other infrared lines (of the type s–p) found from the King diagrams is 0.2 mk smaller than that of the line 8280 Å, and thus equal to the Bohr shift.

From (i) the observed agreement between the differences of the mass-shifts of two widely spaced groups of lines with the differences of the Bohr shifts, (ii) the values of the total mass-shifts calculated from the (corrected) Gerstenkorn ratio and (iii) the values of the specific mass-shifts calculated by M. J. Bauche it can be concluded that the unit mass-shifts of the lines of xenon owing to transitions of the type 6s or 6s′–6p′, 6p or 7p are unlikely to differ from the Bohrs shifts by more than a few millikaysers.

The field effect of the isotope shifts

The most suitable lines for investigating the field effect of the isotope shifts are those due to the transitions from the p and p′ levels to the s and s′ levels since in these lines the field-shifts predominate and the mass-shifts have been shown in the preceding section to be small, and approximately equal to the Bohr shift. For these lines it will be assumed that the unit mass-shift, M_1, is equal to the Bohr shift calculated for isotopes 136 and an imaginary isotope 135 ($M_1 = 2966/\lambda$): to obtain the mass-shifts for the other isotopes the value of M_1 must be multiplied by the following factors:

134	132	131	130	129	128	126	124
−2.02	−4.09	−5.15	−6.23	−7.33	−8.44	−10.72	−13.06

it may be noted that the change of mass-shift with change of mass number differs substantially from a linear relation; for the lightest isotope it exceeds this by nearly

10 %. The field-shifts are found by subtracting the mass-shift from the observed (total) shift, and it is evident that even a small error in the value of M_1 can produce a significant error in the value of the mass-shifts for the lighter isotopes. If it is assumed that the value of M_1 may differ by only 0.2 mk from that of the Bohr shift the corresponding error in the field-shift for ^{134}Xe is 0.4 mk, increasing to nearly 3 mk for ^{124}Xe: thus for all except the heaviest isotope it is large compared with the statistical uncertainties of the measurements.

TABLE 5. FIELD SHIFTS/mk OF THE LINES: 4501 AND 4524 Å (MEAN) AND 8648 Å OF Xe I; 8649 AND 8943 Å (MEAN) OF Cs I; 5536 Å OF Ba I; 4934 Å OF Ba II.

mass number (Xe) ...	(135)	134	(133)	132	131	130	129	128	126	124
neutron number ...	81	80	79	78	77	76	75	74	72	70
Xe I (4501 and 4524 Å)	—	5.7	—	8.8	(12.8)	12.7	15.5	16.6	(20.7)	24.9
Xe I (8469 Å)	—	2.5	—	3.5	(5.3)	5.2	(6.9)	7.4	—	—
Cs I (8521 and 8943 Å)	—	3.6	6.0	4.8	6.4	5.1_5	—	7.5	10.5	—
Ba I (5536 Å)	7.7	5.6	10.6	7.9	—	10.6	—	13.3	—	—
Ba II (4934 Å)	10.0	7.2	14.0	10.2	—	14.2	—	17.2	—	—

In view of this it is considered unnecessary to give a table of the field-shifts of all of these lines, but table 5 gives the field-shifts for two lines 4501 and 4525 Å, which have the greatest, and the line 8649 Å which has the smallest field-shifts. The field-shifts for the resonance lines of Cs I, 8521 and 8943 Å (Hühnermann & Wagner 1966, 1967, 1968; Otten & Ullrich 1969; Marrus, Wang & Yellin 1969), the resonance line of Ba I, 5536 Å (Jackson & Duong 1966) and one of the resonance lines of Ba II, 4934 Å (Fischer *et al*, 1969) are also given. In the case of barium I the mass-shift, M_1, is assumed to be 0.73 mk, which is 0.2 mk greater than the Bohr shift; for the line of Ba II it is assumed to be equal to the Bohr shift: for the resonance lines of caesium it is assumed to be zero, since Bauche (see, for example, Marrus *et al.* 1969) has calculated that the specific mass-shift is approximately equal to the Bohr shift but in the opposite sense. The errors in these values of M_1 are probably less than 0.5 mk. The mass numbers refer to the isotopes of xenon; for the isotopes of caesium they are increased by 1 unit and for those of barium by 2 units. For all of these lines the transitions are similar, a 6p electron changing to a 6s electron consequently similar values of the field-shifts indicate nuclear field-effects of the same order of magnitude. It is evident that the field-shifts for both Ba I and Ba II closely resemble those of the lines of xenon with the greatest shifts while those of Cs I are more similar to those of Xe I with the smallest shifts (no indication is given of the precision of these figures because the unknown uncertainties due to lack of exact values for the mass-shifts are larger than the uncertainties of measurement).

There are eight lines between the wavelengths 5895 and 7120 Å due to transitions of the type 6p–7, 8 or 9d, which all have shifts in the same sense as the Bohr shift. The statistical uncertainties of the measurements are rather high (with the exception of those of the line 7120 Å), but it is apparent from the figures in table 2 that there is for all of these lines a similar departure from the linear relation between isotope

shift and difference of mass number, indicating a significant field effect. The differences of the mass-shifts from that of the line 8280 Å cannot be determined for these lines from the King diagrams because the field-shifts are in the opposite sense. However, if it is assumed that the ratio, R, is equal to 1.56, the value of the unit mass-effect, M_1, can be calculated; the values for the eight lines cover the range 0.0 ± 0.3 m (for the line 7120 Å) to -0.6 ± 0.6 mk (for the line 5934 Å), with an average value of -0.2 mk).

The differences of the isotope shifts of the eight lines are within the range of the statistical uncertainties of the measurements, consequently it is of interest to find the mean values for each isotope, since the statistical uncertainties are thus substantially reduced. The values of the total shifts and the field shifts on the assumption that R is equal to 1.56 (giving the average value of M_1 as -0.2 mk) are, relative to the isotope 136:

	isotope			
	134	132	130	128
total shift/mk	-1.6_5	-2.4	-3.5	-4.4
field shift/mk	-2.0_5	-3.2	-4.7	-6.1

The uncertainties of the average total shifts are less than 0.3 mk but those of the field-shifts are greater due to the uncertainties of the values of the mass-shifts, which increase from 0.5 mk for the isotope 134 to four times this for the isotope 128.

The ratios of the field-shifts of the isotopes (relative field-shifts)

To find the field-shifts from the observed shifts it is necessary to find the value of the unit mass-shift, M_1, and a small error in M_1 gives rise to errors in the values of the field shifts up to 12 times greater. However, an accurate knowledge of the ratios of the field-shifts of the various isotopes is of great interest and it will be shown that the errors in the relative field-shifts due to errors in the value of M_1 are proportionally much smaller than the errors in the values of the field-shifts. The relative field-shifts have been calculated for all the lines due to transitions of the type 6s or 6s′–6 or 7p or 6p′, since the lines have relatively large field-shifts. For each line the ratios have been normalized so that the field-shift for the isotope 128 is equal 8.00. This isotope was chosen as the basis of the normalization because it is that with the neutron-number farthest removed from the magic number, for which the shifts could be measured in all the lines. The effect of changes in the value of M_1 has been calculated for the line 8231 Å which has approximately the average values of the isotope shifts of lines due to transitions of the type s–p. The field-shifts have been calculated first on the assumption that M_1 is equal to 0.35 mk and then for a value differing from this by 0.35 mk. The results of these calculations are shown in table 6, in which the first row indicates the isotope concerned, the second row the total isotope shift relative to the isotope 136, the third gives the ratio of the field-shifts if M_1 is assumed to be equal to 0.35 mk (the Bohr shift) and the last row shows the

amounts by which these ratios are changed if M_1 is changed by 0.35 mk. The change is positive if M_1 is reduced and negative if it is increased. It is evident that except in the case of the isotope 131 the changes do not exceed the statistical uncertainties of the ratios, and in the case of the isotope 131 the change is approximately four times smaller than the proportional change in the field-shift. In the case of the lighter isotopes, the changes are negligible compared with the uncertainties of the measurements, while the changes of the absolute values are ten times greater than the uncertainties of the measurements.

TABLE 6. EFFECT OF CHANGING THE VALUE OF THE UNIT MASS-SHIFT BY 0.35 mk ON THE RATIOS OF THE FIELD-SHIFT

isotope	134	132	131	130	129	128	126	124
total shift/mk	3.2	4.9	7.6	6.7_5	9.0	8.8_5	11.2_5	14.0
ratio of field-shifts (M_1 = 0.35 mk)	2.6_5	4.3	6.3_5	6.0_5	7.8_5	8.0_6	10.1_5	12.6
change of ratio (M_1 = 0 or 0.7 mk)	0.2_5	0.1_5	0.5	0.0_5	0.3	0	0	0.0_5

The relative field-shifts have been calculated for all the lines due to transitions of the types 6s or 6s′–6 or 7p or 6p′; but for brevity, in table 7, the mean values are given of all lines due to combinations of the same two electron configurations. The first column gives the final and initial electron configurations, the figure in parentheses showing the number of lines; the next eight columns give the relative field-shifts, the figure in parentheses is the mean value of the statistical uncertainties of the lines of the group and the second figure in parentheses is the number of lines in which the shifts were measured if less than the number given in the first column.

The first two rows show the mass number and the neutron number of the isotope; the next five rows give the relative field shifts of the five groups with transitions of the type s–p, and the next row gives the relative field shifts for the group of eight lines with transitions of the type 6p–7, 8 or 9d (the figure for the isotope 134 is in parentheses, as it has no significance since it follows from the assumption of the value 1.56 for the ratio R for determining the value of the unit mass-shift). The ninth row gives the mean values of the relative field-shifts for each isotope, the values for each of the groups being weighted in proportion to the number of lines measured and in inverse proportion to the statistical uncertainty; the tenth row gives the statistical uncertainty of the mean values of the relative field-shifts derived from the divergences of the values given by each of the groups from the mean value.

It is evident from the figures given in table 7 that the values of the relative field-shifts for the six different groups of lines differ by less than the statistical uncertainties for every isotope in all the groups.

The effect on the relative field-shifts of the addition of increasing numbers of

TABLE 7. RELATIVE FIELD-SHIFTS (128 − 136 = 8.00)

	M 134 N 80	132 78	131 77	130 76	129 75	128 74	126 72	124 70
configurations								
6s–6p (6)	2.72 (0.2)	4.30 (0.2)	6.36 (0.3) (3)	6.06 (0.2)	7.69 (0.4)	8.00	10.1 (0.3) (3)	12.59 (0.3) (4)
6s–7p (7)	2.71 (0.3)	4.19 (0.3)	6.25 (0.4) (1)	6.26 (0.4)	7.56 (0.3) (5)	8.00	—	12.15 (0.5) (5)
6s′–6p′ (4)	2.71 (0.3)	4.23 (0.3)	5.96 (0.5) (3)	6.00 (0.3)	7.58 (0.6)	8.00	—	—
6s–6p′ (5)	2.76 (0.3)	4.15 (0.3)	6.22 (0.5) (1)	6.03 (0.3)	7.70 (0.3) (3)	8.00	—	12.35 (0.3) (3)
6s′–7p (2)	2.65 (0.2)	4.00 (0.3)	5.76 (0.5) (1)	5.90 (0.3)	7.4 (0.6) (1)	8.00	—	—
6p–7, 8, 9d (8)	(2.7)	4.2 (0.5)	—	6.1 (0.5)	—	8.00	—	—
mean	2.72	4.20	6.15	6.09	7.62	8.00	10.1_0	12.4_2
statistical uncertainty	0.05	0.08	0.2	0.11	0.07	—	0.3	0.2

neutrons can be seen best by a comparison of the differences of the relative field-shifts of successive pairs of even isotopes; these differences are:

isotope pair	124–126	126–128	128–130	130–132	132–134	134–136
difference of relative field-shifts	2.3_2 (0.3)	2.1_0 (0.3)	1.9_1 (0.1)	1.8_9 (0.1)	1.4_8 (0.1)	2.7_2 (0.05)

The addition of four successive pairs of neutrons, starting with the lightest isotope, produces approximately equal changes in the isotope shifts, although the effects to the first two pairs of neutrons appear to be rather greater than those of the third and fourth pairs. These small changes in the differences are less than the uncertainties. They might be regarded as without significance; but the values of the isotope shifts found by Fischer *et al.* (1973) give differences of the relative field-shifts of the first three pairs of isotopes which differ from those found by the present

TABLE 8. RELATIVE FIELD-SHIFTS IN Xe I, Cs I AND Ba I

mass number (Xe) ...	(135)	134	(133)	132	131	130	129	128	126	74
neutron number ...	81	80	79	78	77	76	75	74	72	70
Xe I	—	2.7_2	—	4.2	6.1	6.0_9	7.6_3	8.00	10.1	12.42
Cs I	—	3.8	6.4	5.1	6.8	5.5	—	8.00	11	—
Ba I	4.6	3.4	6.4	4.7	—	6.4	—	8.00	—	—

authors by only 0.1, the values being 2.4, 2.2 and 1.9_5. However, the changes in the differences of the relative field-shifts of the first four pairs of isotopes are comparatively small. This confirms the conclusions made from the values of the field shifts of the resonance lines of barium (Jackson & Duong 1966) that the addition of pairs of neutrons to nuclei of even neutron number produces approximately the same change of the field-shift until the neutron number is four less than the magic number; but in the case of xenon the observations have smaller uncertainties and are more extensive, and consequently of greater significance. They cover a large range, including four pairs, starting with the isotope with the neutron number 12 less than the magic number, whereas in the case of barium there are only two pairs, starting with the isotope with the neutron number 8 less than the magic number.

A comparison of the degree of odd–even staggering in xenon with that in caesium and barium can be made by means of table 8 in which are given the relative field-shifts in the lines of Xe I and in the resonance lines of Cs I and Ba I. It is apparent that the staggering in Ba I is much greater than that in Xe I; in the former, the field-shifts of the odd isotopes are approximately equal to those of the even isotopes with three fewer neutrons, whereas in the latter the field-shift of the isotope 131 is only a little greater than that of the isotope 130 and that of the isotope 129 is substantially less than that of the isotope 128. Since the neutron numbers of the odd isotopes of barium differ by one and by three units from the magic number, while those of the odd isotopes of xenon differ from it by 5 and by 7 units, it appears that the much greater odd–even staggering in barium is related to the proximity of the neutron numbers of the odd isotopes to the magic number. It should not, however,

be overlooked that the staggering of these two isotopes is approximately equal although the neutron number of the lighter is 3 units less than the magic number, while that of the heavier is only 1 unit less than the magic number.

The isotope shifts of two isotopes with odd neutron numbers have been measured in the case of caesium; these are the isotopes 134 and 132, with three and five neutrons less than the magic number. Assessment of the degree of odd–even staggering is difficult because the isotope 131 ($N = 76$) appears to have a shift about 1 mk too small in comparison with the other isotopes of even neutron number and the shifts of the isotopes 129 and 127 appear to be too high; but these last two have uncertainties of nearly 2 mk. It appears qualitatively that the staggering of the isotope with three neutrons less than the magic number is rather less than that of the similar isotope of barium, that the staggering of the isotope with five neutrons less than the magic number is less than this but more than that of the corresponding isotope of xenon. With the exception of 133, all of these isotopes of caesium are artificial, radioactive isotopes; the heaviest has a life of 30 a, the next 3×10^6 a, but those lighter than 133 have lives decreasing from 7 d to 6 h.

It can be concluded that the odd–even staggering increases as the neutron number of the odd isotope approaches the magic number and that it increases as the atomic number increases from 54 to 56.

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Interpretation of the isotope shifts in the arc spectrum of xenon

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From the experimental results of Jackson & Coulombe (1974) and Vetter (1970) in the arc spectrum of xenon, the isotope shifts of 30 levels in the low configurations $5p^56s$, $5p^56p$, $5p^55d$ and $5p^57p$ are obtained, for the mass numbers 136, 134, 132, 130 and 128. A parametric study of these shifts for each isotope is made, with 3 parameters for the even levels and 6 for the odd levels. Following the conclusions of Jackson & Coulombe (1974), the respective contributions of mass- and field-effects to the shifts of the levels and to the parameters are evaluated from King diagrams. The *ab initio* values obtained for the parameters through the Hartree–Fock non-relativistic and relativistic methods show a satisfactory agreement with the experimental values.

1. Introduction

The principles of parametric study of isotope shifts in atomic spectra were first given by Stone (1959) and their application to the configurations $np^5(n+1)s$ of the rare gases.

In the case of the rare gases Bauche & Keller (1971) and Keller (1973) have been able to interpret, by means of the introduction of new types of parameters, the measurements by Odintsov (1965) and Keller & Lesprit (1973) of shifts in the arc spectrum of neon. The experimental values of the shifts in the arc spectrum of xenon found by Vetter (1970) and Jackson & Coulombe (1974) offer the possibility of making a second extensive parametric study of the isotope shifts in a rare gas. There are two significant differences in this case and that of neon: first the shifts between seven even and two odd isotopes have been measured instead of only two even isotopes; secondly the shifts are due to both the mass- and the field-effects while in neon the field-effect is almost certainly small compared with the mass-effect.

Experimental values of the shifts of the levels, found from the measured shifts of the lines, are given. The method by which the mass-effects of the lines are separated from the field-effect has been described in an earlier publication (Jackson & Coulombe 1974).

2. The isotope shifts of the levels

The isotope shifts of the levels relative to a reference level involved in the lines whose shifts have been measured have been found by applying the Ritz combination principle. The level $6p\frac{1}{2}1$ has been selected as the reference level because it is probable that its field isotope shift is relatively small (the notation of the levels is

that of Racah 1942). The isotope shifts of a large number of lines have been measured and a number of levels can be found from two or more different combinations.

The evaluation of the shifts of the levels has been confined to the even isotopes 134, 132, 130 and 128, since the measurements of the shifts of the odd isotopes 131 and 129 and the rare even isotopes 126 and 124 were not made for all of the lines for which the shifts of the more abundant even isotopes were measured. The results are given in table 1. The values given are the residual shifts of the levels, which have been obtained from the measured shifts of the lines less the Bohr shifts. To obtain the total shifts of the levels, the quantity M_1† multiplied by the factor -2.015, -4.09, -6.22 and -8.44 respectively for the isotopes 134, 132, 130 and 128 must be added. The values of M_1 are given in table 1. For the s and p levels the specific mass-shifts are unlikely to exceed a few millikaysers‡ per unit mass. For all except one of the 5d levels the specific mass-shift, M_1', is substantially larger; this is considered in detail below. The value of M_1' is given in the last column. To obtain the field shift the quantity M_1' multiplied by the appropriate factor must be subtracted from the residual shift. The shift of a level is designated positive when the level of the lighter isotope is higher.

The residual shift $S(M,i)$ of a level i for the isotope of mass M has been found for each of the four isotopes by means of the method of least squares for a system consisting of 38 equations of the type

$$S(M,i)-S(M,j)=\sigma(M,ij)$$

(where $\sigma(M,ij)$ is the residual shift of the line $i \rightarrow j$) and the equation

$$S(M,6p_{\frac{1}{2}}1)=0.$$

Of these equations, 12 were found from the measurements made by Vetter (1970), one from the measurements made by Shafer (1971) and 25 from the measurements made by Jackson & Coulombe (1974). The uncertainties of the experimental values given in table 1 are $\sqrt{2}$ times the uncertainties of the measurements of the shifts of the lines made by Jackson & Coulombe (1974).

A parametric study of isotope shifts is feasible and significant only in configurations where the shifts of many levels are known experimentally; this investigation is therefore limited to the even configurations $5p^56p$ and $5p^57p$ and to the odd configurations $5p^55d$ and $5p^56s$, in which the shifts of respectively 10, 5, 11 and 4 levels have been measured, out of 10, 10, 12 and 4 existing levels. Due to the configuration mixing, all levels of a given parity are treated together.

3. Parameters

The main field-shift contribution arises from the s electrons, and is constant inside any configuration (Stone 1959). Therefore, in the cases where two configurations are treated together, e.g. $5p^56p$ and $5p^57p$, two parameters can be introduced: the

† $M_1 = [\sigma(136)-\sigma(134)]/2.015$.
‡ 1 mk $= 10^{-3}$ cm^{-1}.

first, the parameter a with coefficient unity for levels of both configurations, and the other the parameter d whose coefficient for a given level is equal to the fraction of unity for which this level belongs to the second configuration. The parameter d accounts at the same time for all the mass-shift contributions which are equal for all levels of a configuration. The specific mass-shift operator has exactly the same angular dependence as that part of the electrostatic Coulomb operator which generates the Slater integrals $G^k(nl, n'l')$ with $k = 1$. Following Stone (1959) and Bauche (1969), we are thus led to introduce parameters denoted $g^1(5p, 6s)$, $g^1(5p, 5d)$ and $r^1(5d5p, 5p6s)$ in the odd configurations $5p^5 5d$ and $5p^5 6s$.

When the field-shift is the dominant contribution, its second order effects may be of appreciable importance. They lead to the introduction of one effective isotope-shift

TABLE 1. RESIDUAL ISOTOPE SHIFTS OF LEVELS OF Xe I

(^{136}Xe = 0), (experimental uncertainties: 0.3 mk for ^{131}Xe, 0.2 mk for ^{132}Xe and ^{130}Xe, 0.5 mk for ^{128}Xe)

						mass-shift	
					calculated value	Bohr	specific
	^{131}Xe	^{132}Xe	^{130}Xe	^{128}Xe	^{132}Xe	M_1	M_1'
$6s\frac{3}{2}2$	-4.1_5	-6.4_0	-9.2_5	-12.2_5	-6.5_0	0.30	-0.2
$6s\frac{3}{2}1$	-3.0_5	-4.7_0	-6.6_5	-8.8_5	-4.8_0	0.27	-0.1
$6s'\frac{1}{2}0$	-2.5_5	-4.4_0	-6.0_5	-8.2_5	-4.0_0	0.03	-0.5
$6s'\frac{1}{2}1$	-1.8_0	-2.9_0	-4.0_5	-5.5_5	-3.0_5	0.00	-0.2
$5d\frac{1}{2}0$	-1.5_0	-2.9_0	-4.2_0	-5.6_5	-3.2_5	-0.08	-0.5
$5d\frac{1}{2}1$	-1.4_0	-2.7_5	-4.1_5	-5.6_0	-2.7_5	-0.08	-0.6
$5d\frac{3}{2}4$	-1.5_0	-2.8_5	-4.6_0	-6.3_5	-2.4_5	-0.09	-0.8
$5d\frac{3}{2}3$	-1.2_0	-2.5_0	-3.9_0	-5.3_0	-2.4_0	-0.11	-0.6_5
$5d\frac{3}{2}2$	-1.3_0	-2.7_5	-4.3_5	-5.9_5	-2.4_0	-0.09	-0.8
$5d\frac{3}{2}1$	0.3_5	0.5_5	0.8_5	1.1_5	0.5_5	-0.20	0.0_5
$5d\frac{5}{2}2$	-1.0_0	-2.2_5	-3.5_5	-4.8_5	-2.4_0	-0.14	-0.6_5
$5d\frac{5}{2}3$	-1.1_0	-1.9_5	-3.2_0	-4.4_0	-2.4_5	-0.16	-0.5
$5d'\frac{3}{2}2$	0.1_5	0.0_5	-0.2_5	-0.4_5	-0.0_5	-0.42	-0.5_5
$5d'\frac{3}{2}1$	—	—	—	—	2.8_5	-0.49	0.0_5
$5d'\frac{5}{2}2$	0.3_5	-0.1_5	-0.2_0	-0.3_5	0.0_0	-0.42	-0.5
$5d'\frac{5}{2}3$	0.5_5	0.1_0	-0.0_5	-0.2_0	0.0_0	-0.43	-0.5_5
$6p\frac{1}{2}1$	0	0	0	0	0	0	0
$6p\frac{5}{2}2$	-0.1_5	-0.2_0	-0.3_5	-0.4_5	0.0_0	-0.03	0.0
$6p\frac{5}{2}3$	-0.1_5	0.0_5	-0.1_0	-0.2_5	0.0_0	-0.04	0.0
$6p\frac{3}{2}1$	-0.0_5	-0.1_0	-0.2_0	-0.2_5	0.0_0	-0.05	0.0
$6p\frac{3}{2}2$	-0.1_0	0.0_5	-0.2_0	0.7_5	0.0_0	-0.06	0.0
$6p\frac{1}{2}0$	0.1_5	-0.2_0	0.2_5	0.2_5	0.0_0	-0.09	-0.1
$6p'\frac{3}{2}1$	1.1_0	1.3_5	2.3_0	2.9_5	1.7_0	-0.33	0.0_5
$6p'\frac{3}{2}2$	1.6_5	2.4_0	3.5_0	4.6_0	2.2_5	-0.36	0.0_5
$6p'\frac{1}{2}1$	1.2_5	2.3_0	3.2_0	4.2_0	2.0_5	-0.36	0.0_5
$6p'\frac{1}{2}0$	1.3_0	2.1_0	2.9_5	3.8_0	2.1_0	-0.38	0.0_5
$7p\frac{1}{2}1$	—	—	—	—	0.6_5	-0.32	-0.0_5
$7p\frac{5}{2}2$	0.1_0	0.1_0	0.0_0	0.4_5	0.2_5	-0.33	-0.0_5
$7p\frac{5}{2}3$	0.0_5	0.4_0	-0.1_5	0.4_0	0.1_5	-0.34	-0.0_5
$7p\frac{3}{2}1$	0.6_0	0.7_0	-1.2_0	1.6_5	0.8_5	-0.34	-0.0_5
$7p\frac{3}{2}2$	0.1_0	0.3_0	0.1_0	0.4_5	0.3_5	-0.34	-0.0_5
$7p\frac{1}{2}0$	0.4_5	0.7_0	0.9_0	1.0_5	0.5_5	-0.35	-0.0_5

parameter for each Slater integral containing at least one unpaired s-electron (Bauche 1969). In our case, this gives two parameters with respectively the same angular coefficients as $G_1(5p, 6s)$ and $R^1(5d5p, 5p6s)$, for the odd levels; these parameters were already introduced above to account for mass shift. In all the configurations $2p^5nl$ of Ne I (Keller 1973), a parameter denoted z_{2p} was introduced, having the same angular coefficients as the spin-orbit constant ζ_{2p}. In xenon, we introduced one z_{5p} parameter for each configuration, which accounts essentially for all the field-shift contributions in the core, for example, those due to the $5p_{\frac{1}{2}}$ electrons.

In table 2 each type of parameter is classified according to the isotope shift effects and orders of perturbation which it accounts for. The parameter z_{5p} contributes to the mass effect in the first order of perturbation only through the relativistic corrections (Stone 1961, 1963).

TABLE 2. TYPES OF ISOTOPE-SHIFT PARAMETERS IN THE ARC SPECTRUM OF XENON

	field shift		mass shift,
	first order	second order	first order
a	×	×	×
d	×	×	×
$g^1(5p, 6s)$		×	×
$g^1(5p, 5d)$			×
$r^1(5p6s, 5d5p)$		×	×
z_{5p}	×	×	×

4. RESULTS

The parametric determination of the wave functions of the levels of xenon I has already been effected by Liberman (1969), for intermediate coupling and configuration mixing. It has been seen above that each of the isotope-shift parameters has the same angular coefficients as one of the energy parameters; constructing the formal expansion of the isotope shift of each relevant level in terms of the chosen parameters is a simple task.

An attempt has been made to solve for each isotope, by the least-squares method, two systems of fifteen linear equations: one for the even levels, with four unknowns, and one for the odd levels, with seven unknowns. The results for the parameters are presented in table 3. In this table, the Slater-like parameters are replaced by multiples, exactly as for the corresponding energy integrals (Condon & Shortley 1935): the definitions are:

$$g_1(5p, 6s) = \tfrac{1}{3}g^1(5p, 6s), \quad g_1(5p, 5d) = \tfrac{1}{15}g^1(5p, 5d).$$

The two parameters $z_{5p}(5p^57p)$ and $r^1(5d5p, 5p6s)$ could not be determined, the former for lack of experimental evidence and the latter because the theoretical uncertainty was too large.

For brevity the calculated values of the shifts of the levels obtained from the parameter values presented in table 3 are given only for ^{132}Xe, in column 6 of table 1. In this column the calculated values are also given of the only known levels of the configurations $5p^5 7p$ and $5p^5 5d$ for which experimental values are not available; these are $7p\,^3_2 1$ and $5d'\,^3_2 1$ (the latter has the largest negative calculated shift in table 1; the calculated values for the isotopes 134, 130 and 128 are respectively 1.8_0, 4.3_0 and 5.7_0.

TABLE 3. VALUES OF THE ISOTOPE-SHIFT PARAMETERS (mk) (WITH STANDARD DEVIATIONS) AND OF THE R.M.S. DEVIATIONS FOR THE LEVELS

	^{134}Xe	^{132}Xe	^{130}Xe	^{128}Xe
a (even levels)	0.52 ± 0.04	0.83 ± 0.06	1.18 ± 0.07	1.49 ± 0.08
$d(5p^5 7p)$	0.13 ± 0.08	0.17 ± 0.12	0.06 ± 0.13	0.45 ± 0.15
$z_{5p}(5p^5 6p)$	1.13 ± 0.06	1.67 ± 0.09	2.59 ± 0.10	3.32 ± 0.12
$\overline{\Delta T}$ (even levels)	0.12	0.19	0.19	0.23
a (odd levels)	0.52 ± 0.07	1.32 ± 0.11	2.16 ± 0.16	2.98 ± 0.22
$d(5p^5 6s)$	-2.78 ± 0.17	-3.85 ± 0.27	-5.10 ± 0.40	-6.70 ± 0.55
$z_{6p}(5p^5 5d)$	1.05 ± 0.10	1.65 ± 0.16	2.53 ± 0.23	3.38 ± 0.32
$z_{5p}(5p^5 6s)$	0.83 ± 0.16	1.16 ± 0.26	1.92 ± 0.38	2.43 ± 0.54
$g_1(5p, 5d)$	0.15 ± 0.02	0.30 ± 0.03	0.47 ± 0.05	0.63 ± 0.07
$g_1(5p, 6s)$	0.96 ± 0.21	1.65 ± 0.34	2.36 ± 0.49	3.10 ± 0.68
$\overline{\Delta T}$ (odd levels)	0.20	0.32	0.47	0.65

The specific mass-shifts of the upper levels 5d and 5d' have been found from King diagrams (King 1964) in which the reference line is the line 8280 Å† ($6p\,^1_2 0 \rightarrow 6s\,^3_2 1$) for which the specific mass-effect is assumed to be small. They are relatively large for all of these levels except $5d\,^3_2 1$. The experimental and the calculated residual shifts can be corrected for the effects of these large specific mass-shifts; without these corrections there are large variations in the values of the residual shifts of these levels, over a range of 3 mk for ^{132}Xe.

For all four isotopes and for both parities, the values of $\overline{\Delta T}$ are also given in table 3. $\overline{\Delta T}$ is the root mean square of the differences between the experimental and the calculated shifts, as defined by Racah (1950).

The deviations in table 3 increase roughly in proportion to the value of the parameter, with increasing mass difference; for a given mass difference they increase for z_{5p} in the order $5p^5 6p$, $5p^5 5d$, $5p^5 6s$. This indicates that not the experimental uncertainties but shortcomings in the theoretical interpretation are primarily responsible for the lack of accuracy in the parametric results; secondly, these inadequacies are more serious in the odd than in the even system of levels.

In the interpretation, either the completeness of the list of isotope-shift parameters or the quality of the wavefunction expansions can be questioned. With regard to the parameters, several separate and equally unsuccessful additions were made, among which were: (i) the parameters z_{5d}, z_{6p} and z_{7p}, with definitions

† 1 Å = 10^{-10} m = 0.1 nm.

analogous to that of z_{5p}; (ii) instead of a and the g^1 parameters, one parameter for each term, as was done in Ne I (Bauche & Keller 1971); (iii) one parameter to account for the relativistic-correction operator Δ_1 defined by Stone (1963). In addition, on the principle of a method introduced by King & Van Vleck (1939) in the sp configurations, it was taken into account that, in an approximation better than the central field, the 6s (or 5p) radial function is closer to (or further from) the nucleus in the 6s′ than in the 6s levels; this phenomenon would yield different values of $g^1(5p, 6s)$ in the 6s and 6s′ levels, but allowance for it did not improve the interpretation.

As concerns the quality of the wavefunction expansions, the r.m.s. deviation between theoretical and experimental energies is 73 cm^{-1} for the odd configurations, compared to only 25 cm^{-1} for the even (Liberman 1969). Unfortunately, it appears difficult to improve the wavefunctions of the odd levels: the rapid convergence of the upper odd configurations to the ground levels of the ion makes the classical scheme of parametric studies inadequate for an accurate interpretation.

It is concluded that the limiting factor in the accuracy of the parametric results is the quality of the wavefunctions. As a consequence, the stochastic parts of the errors in the parameter values, in table 3, are mainly not of experimental origin; the changes in the parameters from ^{134}Xe to ^{128}Xe are probably better determined than the standard deviations indicate, because the same imperfect parameter coefficients were used for all isotopes.

5. Separation of mass and field effects

In table 3, the parameter $g_1(5p, 5d)$ alone is nearly exactly proportional to the Bohr shift. Therefore it is almost purely a mass-shift parameter, in agreement with table 2.

With regard to the field effect, Jackson & Coulombe (1974) concluded that the unit mass-shift in the line $\lambda = 8280$ Å ($6p\frac{1}{2}0 \rightarrow 6s\frac{1}{2}1$) is unlikely to differ from the Bohr shift by more than a few millikaysers; following this conclusion we can separate the mass and field parts of the isotope shift and obtain the values of the relevant electronic quantities (specific-mass-shift contributions and screening factors) by drawing a King diagram. In this diagram, the residual shifts in the line $\lambda = 8280$ Å are plotted on the horizontal axis and the parameter values on the vertical axis. Here it is not necessary to treat the even and odd levels separately. In a new calculation, the shifts of all thirty experimental levels were interpreted in one least-squares fit with the same z_{5p} and g_1 parameters as above, one parameter a with coefficient unity for all levels and one parameter d for each of the configurations $5p^57p$, $5p^55d$ and $5p^56s$. In this way were obtained the values of the d parameters listed in table 4. With regard to the results given in tables 3 and 4 it has been assumed that the coefficients of the g_1 and z_{5p} parameters are those relative to the centre of gravity of the relevant configuration, i.e. that their weighted average value in all the J-levels of that configuration is zero.

From table 4 it can be seen that $d(5p^5 5d)$ is an almost pure mass-shift parameter, and that $d(5p^5 7p)$ is very small and probably positive. The numbers in table 3 show that the values of the parameters $z_{5p}(5p^5 6p)$ and $z_{5p}(5p^5 5d)$ are not significantly different: the latter will not be further considered.

If it is assumed that the mass-shift contributions in the transition $\lambda = 8280$ Å are approximately equal to the Bohr shift (Jackson & Coulombe 1974) the mass-shift contribution, P_m, to any plotted parameter and the ratio ρ for each parameter P can be found from the King diagram; ρ is the ratio of the field-shift part of the parameters P and $d(5p^5 6s)$. The quantity ρ is the extension to any parameter of the definition of the screening factors for the configurations. These results are given in the second and fourth columns of table 5. For each quantity, the uncertainty is assumed to be equal to half the difference between the values obtained from the lines of maximum and minimum slope which can be drawn through the four rectangles defining the uncertainties.

TABLE 4. VALUES OF THE ISOTOPE-SHIFT PARAMETERS (mk) FOR THE CENTRES OF GRAVITY OF THE CONFIGURATIONS

	^{134}Xe	^{132}Xe	^{130}Xe	^{128}Xe
a	0.52 ± 0.05	0.83 ± 0.09	1.18 ± 0.12	1.49 ± 0.16
$d(5p^5 7p)$	0.13 ± 0.10	0.17 ± 0.17	0.06 ± 0.22	0.45 ± 0.30
$d(5p^5 5d)$	-1.04 ± 0.07	-2.15 ± 0.12	-3.34 ± 0.16	-4.47 ± 0.22
$d(5p^5 6s)$	-3.82 ± 0.11	-6.00 ± 0.17	-8.44 ± 0.23	-11.17 ± 0.31

TABLE 5. ELECTRONIC ISOTOPE-SHIFT QUANTITIES: COMPARISON BETWEEN EXPERIMENT AND THEORY

	mass-shift contribution P_m/mk (for $\Delta M = 2$)		$\rho = P_i/[d(5p^5 6s)]_i$	
parameter P	experimental	Hartree–Fock	experimental	Hartree–Fock
$d(5p^5 5d)$	-1.1 ± 0.3	-0.6	0.03 ± 0.1	-0.09
$d(5p^5 6s)$	-0.6 ± 0.7	-0.5	(1)	(1)
$z_{5p}(5p^5 6p)$	0.14 ± 0.27	—	-0.31 ± 0.13	—
$z_{5p}(5p^5 6s)$	0.07 ± 0.7	—	-0.23 ± 0.3	—
$g_1(5p, 5d)$	0.15 ± 0.09	0.13	0 ± 0.04	0.01
$g_1(5p, 6s)$	0.36 ± 0.9	0.4	-0.18 ± 0.4	-0.11

6. *Ab initio* evaluations

For mass-shifts, the Hartree–Fock method gives reasonable estimates for a number of elements of intermediate atomic mass (Bauche 1974). The Hartree–Fock computer code of Froese-Fischer (1970) has been applied to the centres of gravity of the three lowest configurations studied and to some of their Russell–Saunders terms. The results for the specific mass-shifts are given in the second column of table 6. From these are derived the *ab initio* values of the mass-shift contributions to the d and g_1 parameters, which are given in column 3 of table 5.

The Hartree–Fock results also yield some information concerning the field shifts, through the evaluation of $|\Psi(0)|^2$, as applied successfully by Wilson (1968). The quantities $4\pi|\Psi(0)|^2$ are listed in column 3 of table 6, in atomic units, with the centre of gravity of $5p^5 6p$ again taken as a reference. The computed ρ factors are listed in column 5 of table 5. The fact that a second order isotope-shift parameter such as $g_1(5p, 6s)$ can be evaluated from the Hartree–Fock results for $|\Psi(0)|^2$ follows from Brillouin's theorem (Bauche & Klapisch 1972; Labarthe 1972).

The agreement between experimental and Hartree–Fock quantities in table 5 is good; the differences are substantially smaller than the estimated uncertainties of the former.

TABLE 6. HARTREE–FOCK VALUES OF THE SPECIFIC SHIFTS AND OF THE ELECTRONIC DENSITIES AT THE NUCLEUS

	specific shift/mk (for $\Delta M = 2$)	(electronic density at $r = 0$)/a.u.
$5p^5 6p$ c.g.†	0	0
$5p^5 6p\ ^3S$	0.0	0
$5p^5 5d$ c.g.	−0.6	−2
$5p^5 5d\ ^3P$	−2.1	−6
$5p^5 5d\ ^1P$	0.6	0
$5p^5 6s$ c.g.	−0.5	22
$5p^5 6s\ ^3P$	−0.8	24
$5p^5 6s\ ^1P$	0.0	19

† Reference state.

It is satisfactory that the three z_{5p} parameters, although determined independently, have almost the same value. They deal with the difference between the isotope shifts of the core states, $5p^5$ $J = \frac{1}{2}$ and $\frac{3}{2}$, which certainly does not change much from one configuration $5p^5 nl$ to the other. They cannot be evaluated by means of the non-relativistic Hartree–Fock method, which ignores all magnetic interactions in the atom.

The field-shift part of any z_{5p} parameter is essentially due to the $5p_{\frac{1}{2}}$ field-shift contribution and to the screening effect of the $5p^5$ subshell on the s electrons of the core. The $5p_{\frac{1}{2}}$ contribution is larger in the $5p^5$ $J = \frac{3}{2}$ state, which contains two $5p_{\frac{1}{2}}$ electrons. For the screening effect, Desclaux (1971, 1974) has communicated to us the results of relativistic Hartree–Fock calculations on the two ground levels of Xe II, $5p^5$ $J = \frac{1}{2}$ and $\frac{3}{2}$. In these results, the quantity $4\pi|\Psi(0)|^2$ for a $5p_{\frac{1}{2}}$ electron amounts to respectively 24.2 and 23.6 atomic units in the $J = \frac{1}{2}$ and $J = \frac{3}{2}$ states, and its total value for all s and p electrons is respectively 3 398 253 and 3 398 273 atomic units. The resulting sign of z_{5p} is confirmed by the experimental results given in table 5.

It appears that the overall coherence of our interpretation tends to confirm the conclusion of Jackson & Coulombe (1974) concerning the low value of the specific mass-shift in the $\lambda = 8280$ Å line.

The authors gratefully acknowledge the use of the Hartree–Fock numerical computer code of C. Froese-Fischer. They also thank J.-P. Desclaux for having kindly applied his relativistic Hartree–Fock code to the problem of xenon, and J. Sinzelle for essential help in the computational work; and take this opportunity of thanking Professor Pierre Jacquinot for the interest he has taken in this research.

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Isotope shifts in the arc spectrum of xenon. II

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New measurements of the isotope shifts of a group of lines in the orange and red, due to transitions of the type 6p–7, 8 and 9d, have now been made, since the uncertainties of earlier measurements (Jackson & Coulombe 1974) were relatively large, between 0.4 and 1.0 mk.† The uncertainties of the new measurements have been reduced to between 0.2 and 0.5 mk and the number of lines investigated has been increased from 8 to 13. The isotope shifts of 2 lines due to the forbidden transitions 6s′–5f and one line due to the transition 5d–7f have also been measured.

Introduction

Earlier measurements of the shifts of 8 lines due to transitions 6p–7, 8 and 9d indicated a significant field effect, of the order of one half of the average value of the field-effects of lines due to transitions of the type 6s or 6s′–6 or 7p or 6p′, and in the opposite sense (Jackson & Coulombe 1974). The detection of the field-effect depends on the difference of the ratio of the observed shifts 136–132 : 136–134 from 2.03 or of the ratio 136–130 : 136–134 from 3.09 The observed shifts of the isotope 134. differed by amounts between -0.2 and -0.5 mk from the values required by these ratios, but the experimental uncertainties were between 0.4 and 0.6 mk (the uncertainties of the values of the shifts of the isotope 130 are relatively unimportant since the uncertainty in the value of the shift required for the isotope 134 is only one third of that of the isotope 130). Thus for any one line the difference between the observed shift and that corresponding to a pure mass-shift was within the limits of the experimental uncertainty; but for all of the eight lines this difference was in the same sense and the differences in the values of the shifts for the various lines were within the experimental uncertainties. It appeared appropriate to take the average values of the shifts for all eight lines, and thus reduce the experimental uncertainties. The value of the field shift found from these average values was approximately -0.5 that of the field shift of the line 8280 Å and the value of the unit mass-shift M_1^T (mass + specific) was -0.2 mk, with an uncertainty of 0.3 mk.

In view of this rather unexpectedly large field effect it seemed necessary to measure the isotope shifts with an improved precision so that the experimental uncertainties for individual lines would be smaller than the observed differences of the isotope shifts from those required for pure mass-shifts; and also to find whether

† 1 mk = 10^{-3} cm^{-1}; 1 Å = 10^{-10} m = 0.1 nm; 1 Torr ≈ 133 Pa.

the small differences between the shifts of the different lines were significant. The new measurements were made only with the isotopes 134, 130 and 128 (relative to 136), and for the three weakest lines, only with the isotopes 134 and 130. In this particular instance this is not a serious shortcoming, since the relevant quantities, the field-shifts and the specific mass-shifts can be found from a King (1963) diagram made with the line 8280 Å as the reference line whose isotope shifts are known with uncertainties of only 0.15 or 0.2 mk. The points defining the line are given by dividing the shifts (136–134), (136–130) and (136–128) respectively by the factors 2.015, 6.23 and 8.44. The tangent of the slope of the line gives the ratio of the field-shifts of the comparison line and the reference line and the amount by which the (total) mass-shift differs from that of the reference line is given by the value of the point at which the King straight line cuts the y-axis plus the mass-shift of the reference line multiplied by the tangent of the slope. The values used for the shifts of the line 8280 Å were not the direct measurements but were the values given by the mean value of the differences of the values of the upper and lower levels found by the application of the Ritz combination principle (Jackson & Coulombe 1974). These are, in milikaysers (136 = 0)

134	132	130	128
2.4_5	3.4_0	4.6_5	6.1_0

They differ from the directly measured shifts by -0.15 and -0.05 mk respectively for the isotopes 134 and 132, and for the two other isotopes they are equal to the direct measurements. The errors of these values are unlikely to exceed 0.15 mk. The specific mass shift of the line 8280 Å is assumed to be zero (Jackson & Coulombe 1974).

The experimental procedure

The method by which the isotope shifts were measured was the same as that described in the earlier paper (Jackson & Coulombe 1974). However, for the stronger lines 6184, 6318, 6470, 6473, 6488, 6499 and 6504 Å the Fabry–Perot interferometer was used with a plate separation of 5 cm, instead of 2 cm or 3 cm used in the earlier work; and special precautions were taken to ensure that the pressure of the carrier gas, helium, was equal in the tube with ^{136}Xe and that with either ^{134}Xe, ^{130}Xe or ^{128}Xe. The pressure of the helium was 1 Torr and, in the earlier work, was adjusted in separate fillings of the two tubes with a precision of $\pm$ 0.05 Torr. For lines due to transitions between the electron configurations 6s and 6 or 7p this precision is adequate since the corresponding difference in the pressure shifts is less than 0.05 mk. The shifts of lines due to transitions between the electron configurations 6p–7, 8 or 9d are much greater, increasing from approximately 1 mk/Torr for transitions 6s–7p to approximately 4 mk/Torr for transitions 6s–9p; in the latter case a difference of pressure of the helium of 0.05 Torr corresponds to a difference of the shift of 0.2 mk, which is not negligible in the case of the new measurements. To eliminate this source of error the two tubes were connected to the filling system (each with the xenon

confined in the reservoir) and filled simultaneously with helium; they were left connected for several minutes to ensure complete equilibrium. When the tubes were removed from the filling system the partial pressure of the xenon was adjusted by controlling the relative strengths of the lines of xenon and helium (Jackson & Coulombe 1973).

The measurements of the isotope shifts

The results of the new measurements of the isotope shifts are given in table 1. These are the observed shifts (relative to the isotope 136) and are thus the sums of the field-shifts and the Bohr and specific mass-shifts. The figures in curved brackets after the isotope shifts are the statistical uncertainties of the measurements (the root mean square of the deviations divided by one half of the square root of the number of measurements). Comparison with the earlier measurements shows some significant differences but in every case the difference is less than the uncertainty given for the earlier measurements.

The figures in square brackets after the measured shifts of the isotope 132 are the shifts found from King diagrams made in the manner described above. Their precision is better than that of the direct measurements since the uncertainty is approximately the mean of the uncertainties of the new measurements of the shifts of the isotope 134 and 136. It can be seen that the differences between the direct measurements and the interpolated values are several times smaller than stated uncertainties in most of the lines and not greater in any line.

The ratios of the field-shifts of the lines, given in table 1 are the ratios of the field shifts of the lines to that of the line 8280 Å; the unit specific mass-shifts are derived from the difference of the total mass-shift found from the King diagram and the Bohr shift. To obtain the mass-shift for the isotopes 134, 132, 130 or 128 (relative to 136), the unit mass-shift is multiplied respectively by the factors -2.02, -4.09, -6.23 or -8.44. The figures in curved brackets after the ratios of the field-shifts and the specific mass-shifts are the estimated uncertainties.

The King diagrams were used also to check the consistency of the measurements. The divergence of the point given by the isotope 128 from the straight line drawn through the points given by the isotopes 134 and 130 was measured; multiplied by the factor 8.44 this gives the error of the measurement of the shift of the isotope 128 assuming those of the isotopes 134 and 130 to be correct. The values found were between 0.2 and -0.2 mk, thus in every line less than the statistical uncertainty.

The classification of the lines is due to Humphreys & Meggers (1933) and the notation is that proposed by Racah (1942).

TABLE 1. ISOTOPE SHIFTS (mk) IN THE ARC SPECTRUM OF XENON, RELATIVE TO ^{136}Xe; RATIOS OF FIELD-SHIFTS (8280 Å ≡ 1); UNIT MASS-SHIFTS: M_1, Bohr, M_1' SPECIFIC

		total isotope shifts					mass-shift	
line/Å	classification	134	132	130	128	ratio of the field shifts	bohr M_1	specific M_1'
6470	$6p\frac{1}{2}1-7d\frac{3}{2}2$	-1.6_0 (0.2)	—	-3.5_0 (0.2)	−4.6 (0.3)	-0.5_0 (0.15)	0.46	-0.2_5 (0.15)
6473	$6p\frac{1}{2}1-7d\frac{3}{2}1$	−1.2 (0.3)	—	−3.6 (0.3)	−4.9 (0.4)	-0.0_5 (0.2)	0.46	0.0_5 (0.2)
6488	$6p\frac{1}{2}1-7d\frac{5}{2}2$	-1.6_0 (0.2)	−3.0 (0.5) [−2.6]	-3.8_0 (0.2)	−4.8 (0.4)	-0.4_0 (0.15	0.46	−0.3 (0.15)
6882	$6p\frac{3}{2}2-7d\frac{7}{2}3$	−1.3 (0.3)	−1.7 (0.5) [−1.9]	−2.6 (0.3)	−3.8 (0.4)	-0.5_0 (0.2)	0.42	-0.6_0 (0.2)
7120	$6p\frac{3}{2}3-7d\frac{7}{2}4$	−1.2 (0.3)	−1.8 (0.3) [−2.0]	−3.0 (0.3)	−4.0 (0.2)	-0.2_5 (0.2)	0.42	-0.2_0 (0.2)
5857	$6p\frac{1}{2}1-8d\frac{3}{2}2$	−1.6 (0.3)	−2.5 (0.5) [−2.5]	−3.7 (0.5)	−4.4 (0.7)	-0.5_5 (0.2)	0.51	−0.5 (0.2)
5895	$6p\frac{1}{2}1-8d\frac{1}{2}1$	−1.5 (0.3)	−2.6 (0.4) [−2.4]	−3.5 (0.5)	−4.5 (0.3)	-0.5_0 (0.2)	0.50	−0.4 (0.2)
5931	$6p\frac{1}{2}1-8d\frac{1}{2}0$	−1.7 (0.4)	—	−3.6 (0.5)	—	-0.7_0 (0.3)	0.50	-0.7_5 (0.3)
6182	$6p\frac{3}{2}2-8d\frac{7}{2}3$	−1.4 (0.2)	−1.9 (0.8) [−2.2]	-3.0_5 (0.2)	−4.4 (0.4)	-0.5_5 (0.2)	0.48	−0.6 (0.2)
6318	$6p\frac{3}{2}3-8d\frac{7}{2}4$	-1.6_0 (0.2)	−2.4 (0.5) [−2.5]	-3.5_0 (0.25)	−4.8 (0.3)	-0.5_5 (0.15)	0.47	−0.5 (0.15)
6499	$6p\frac{3}{2}1-8d\frac{5}{2}2$	−1.9 (0.25)	−2.8 (1.0) [−2.6]	-3.5_0 (0.2)	−4.5 (0.4)	-0.8_0 (0.2)	0.46	-0.8_5 (0.15)
5825	$6p\frac{3}{2}2-9d\frac{7}{2}3$	−1.7 (0.4)	—	−3.5 (0.5)	—	−0.6 (0.6)	0.51	−0.6 (0.4)
5934	$6p\frac{3}{2}3-9d\frac{7}{2}4$	−1.6 (0.3)	−1.9 (0.5) [−2.4]	−3.5 (0.5)	−4.1 (0.5)	-0.5_5 (0.25)	0.51	−0.5 (0.3)
6533	$6p\frac{5}{2}2-9s\frac{3}{2}1$	−1.6 (0.3)	−2.6 (0.9) [−2.3]	−3.5 (0.5)	−4.5 (0.4)	−0.5 (0.2)	0.46	−0.4 (0.8)
6504	$5d\frac{7}{2}4-7f\frac{9}{2}5$	−0.1 (0.3)	0.5 (0.5) [0.5]	1.0 (0.4)	1.6 (0.4)	−0.4 (0.2)	0.44	−1.0 (0.3)
5824	$6s'\frac{1}{2}0-5f\frac{3}{2}1$	1.5 (0.3)	—	2.8 (0.3)	—	0.7_0 (0.2)	0.51	−0.2 (0.2)
6180	$6s'\frac{1}{2}1-5f\frac{3}{2}2$	1.0 (0.5)	—	1.5 (0.5)	—	—	0.48	—

The ratios of the field-shifts and the specific mass-shifts of lines due to the transitions 6p–7, 8 and 9d

It can be seen from the values of the isotope shifts and the uncertainties of the measurements given in table 1 that field-shifts can be detected in the individual lines, as a result of the increased precision. The amounts by which the shifts of the isotope 134 exceed one third of those of the isotope 130 are greater than the widest limits of the uncertainties (taking the lower limit for the isotope 134 and the upper limit for the isotope 130) in twelve of the thirteen lines. The ratios of the field shifts are negative in all of the lines and are thus in the opposite sense to that of the line 8280 Å (and those of all the other lines due to transitions between the configurations $6s5p^5$ and 6 and $7p5p^5$); they are in the same sense as the Bohr shift. The mean value of the ratios of the isotope shifts for the eight lines previously measured (Jackson & Coulombe 1974) is -0.5 in agreement with the earlier value of 'approximately -0.5'.

The specific mass-shifts are all negative (in the opposite sense to the Bohr shift). The mean value of M_1' for the eight lines measured previously is -0.6 mk; the earlier value was -0.2 ± 0.5 mk. It is apparent from table 1 that both the ratios of the field-shifts and the specific mass-shifts are (numerically) greater in the lines due to the transitions 6p–8 and 9d than those due to the transitions 6p–7d. There are however within these groups differences of the isotope shifts 136–134 from the mean value for the group which are greater in some lines than the experimental uncertainties. These differences cannot be explained by differences in the field shifts of the p levels. These are known, and are small (Jackson & Coulombe 1974); for the levels $6p_{\frac{3}{2}}^{\frac{5}{2}}2$ and $6p_{\frac{3}{2}}^{\frac{5}{2}}3$ they differ from that for the level $6p_{\frac{1}{2}}^{\frac{1}{2}}1$ by 0.1_5 mk and for the isotope 130 the mean difference is 0.2_5 mk. A new series of King diagrams was made for the lines with lower levels $6p_{\frac{3}{2}}^{\frac{5}{2}}2$ or 3 with the values of the shifts changed by these amounts to find the values of the ratios of the field-shifts and specific mass-shifts if the effect of the differences of the shifts of the p levels from those of the $6p_{\frac{1}{2}}^{\frac{1}{2}}1$ level is eliminated. The changes are small compared with the experimental uncertainties, and are approximately equal for all the lines; the mean value is $+0.05$ for the ratio of the field-shifts and $+0.03$ mk for the unit specific mass-shift, M_1'.

In the case of the first four lines in table 1 these differences may be due to the different amount of mixing of the upper levels with 5 and 6d levels; but for the rest of the lines the effects of mixing of the upper levels are negligible. It appears that the possibility of small differences in the values of the field-shifts and specific mass-shifts of levels having the same electron configurations cannot be excluded; but these differences are smaller than the differences between the ratios of the field-shifts and specific mass-shifts of lines with the upper levels 8d or 9d and lines with the upper levels 7d.

The isotope shifts of two lines due to the transitions 6p–6d (Jackson & Coulombe 1974) and eight lines due to the transitions 6p–5d (Vetter 1970) have been measured, consequently a comparison can be made of the ratios of the field-shifts and specific mass-shifts of lines due to the five types of transitions, 6p–5, 6, 7, 8 and 9d. The

ratios of the field-shifts and the specific mass-shifts of these lines have been found from King diagrams by the same method as that used for lines due to the transitions 6p–7, 8 and 9d.

The mean values of the ratios of the field-shifts and specific mass-shifts of the lines due to these five types of transitions are:

transition	6p–5d	6p–6d	6p–7d	6p–8d	6p–9d
ratio of the field-shift	0.04 (0.1)	−0.2 (0.2)	−0.3 (0.3)	−0.6 (0.2)	−0.6 (0.3)
unit specific mass-shift/mk	0.7 (0.2)	0.0 (0.2)	−0.2 (0.3)	−0.6 (0.3)	−0.6 (0.3)

The figure in brackets after the mean value is the greatest divergence from the mean value; but for the transitions 6p–6d and 6p–9d the experimental uncertainties are given, since they are greater than the divergences. The specific mass-shift of the line 26518 Å, $6p_{\frac{1}{2}}0–5d_{\frac{3}{2}}1$ has been excluded from the average since its value, $M_1 = -0.01$ mk, is so different from those of the other lines due to the transitions 6p–5d that it can be regarded as anomalous.

The large changes of the ratios of the field-shifts and the specific mass-shifts between the transitions 6p–5d and 6p–8 and 9d are probably due mainly to the d levels since these quantities change relatively little between the various 6p levels. The negative values of the ratios of the field-shifts are compatible with the attribution of the greater part of the field-shifts to the upper (d) levels; with a normal field-shift, due only to the volume effect, if the shift of the upper level is greater than that of the lower level, the shift of the line is in the same sense as the Bohr shift, corresponding, in this case, to a negative ratio of the field-shifts of the lines.

The field-shifts of the levels

The relatively small differences in the shifts of the 6p levels (covering a range of ±0.15 mk for the isotope 134) and in the shifts of the 6p levels and 7p levels (0.35 mk for the isotope 134) suggest that the field-shifts of these levels are small compared with those of the 6s levels. If the value of zero is assumed for the field-

Table 2. Approximate values of the field-shifts $^{134}Xe–^{136}Xe$ (mk) of levels and configurations of Xe I

$6s_{\frac{3}{2}}1$	$6s_{\frac{3}{2}}2$	$7s_{\frac{3}{2}}2$	$9s_{\frac{3}{2}}1$	$6s'_{\frac{1}{2}}0$	$6s'_{\frac{1}{2}}1$				
−3.0	−3.9	−0.7	−1.5	−2.5	−1.8				
	6p	7p	6p′	5d	6d	7d	8d	9d	5d′
	0.0	0.3	1.3	0.0	−0.5	−0.9	−1.8	−1.8	1.3

shifts of the 6p levels, the field-shifts of the other levels can be found from the ratios of the field shifts of the lines given in table 1, and from the values of isotope shifts previously published (Vetter 1970; Jackson & Coulombe 1974). These are approximate values, since for the d levels mean values of the different members of the five configurations are taken although the range of the ratios of the field-shifts of the

lines concerned is in some cases as great as $\pm 0.1_5$ (corresponding to ± 0.2 mk for the isotope 134); also the value zero assumed for the field-shifts of the p levels may be incorrect, but, here the correction required would be equal for all the levels. The approximate values of the field-shifts of these configurations are given in table 2, and, for comparison the field-shifts of six s and s′ levels are also given. (A negative sign signifies that the level of the isotope 134 is the lower.)

The progressive increase of the (negative) shift as the configuration changes from 5d to 8 or 9d (and from 7s to 9s) could be explained by a diminishing of the screening of the core.

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ÉTUDE PARAMÉTRIQUE DE LA STRUCTURE HYPERFINE DU XÉNON I

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Résumé. — Après une étude paramétrique de la structure fine de l'ensemble des 5 configurations $5p^5(6s, 7s, 5d, 6d$ et $7d)$ de Xe I, une étude paramétrique de la structure hyperfine de l'isotope 129 est présentée. Quatre paramètres suffisent pour interpréter l'ensemble des résultats expérimentaux et retrouver les constantes de structure hyperfine du cœur $5p^5$.

Abstract. — A phenomenological study of the multiplet structures of the mixed odd-low configurations $5p^5(6s, 7s, 5d, 6d$ and $7d)$ in Xe I is followed by a phenomenological study of the hyperfine structure of the levels of the isotope 129. Four parameters are sufficient for interpreting the experimental results and for finding the hyperfine structure constants of the core $(5p^5)$.

1. **Introduction.** — L'extension des mesures de structure hyperfine de Jackson et Coulombe [1] dans le spectre d'arc de l'isotope 129 du xénon a permis de déterminer de nouvelles constantes de structure hyperfine pour les niveaux suivants :

1 niveau de la configuration $5p^5$ 5d
2 niveaux de la configuration $5p^5$ 6d
5 niveaux de la configuration $5p^5$ 7d

Une formule établie par S. Liberman [2] dans l'hypothèse d'un couplage j-l pur, ne donne des résultats en accord avec les mesures que pour les niveaux qui ne sont pas tributaires du couplage, comme le niveau 7d 7/2 4 qui est le seul de $J = 4$ dans la configuration $5p^5$ 7d (la notation des niveaux est celle proposée par Racah [3]); ceci est dû au fait que le couplage réel est trop éloigné du couplage j-l.

Une étude paramétrique de la structure hyperfine du xénon a déjà été effectuée par S. Liberman [4] en 1969, sur les configurations paires $5p^5$ 6p et 7p d'une part et les configurations impaires $5p^5$ 6s et 5d d'autre part. Les résultats pour les configurations paires sont excellents; ils sont un peu moins bons pour les configurations impaires. (Voir dans le tableau IV les résultats antérieurs.)

Pour interpréter l'ensemble des 19 constantes de structure hyperfine maintenant connues dans les configurations impaires, nous avons entrepris l'étude paramétrique de la structure hyperfine des 4 configurations $5p^5(6s, 5d, 6d$ et $7d)$, en espérant retrouver les constantes de structure hyperfine du cœur $5p^5$ établies avec précision dans le cas des configurations paires [4].

2. **Etude paramétrique des énergies des niveaux.** — Avant de procéder à l'étude paramétrique des structures hyperfines, nous avons dû entreprendre l'étude paramétrique des énergies des niveaux de ces 4 configurations impaires, auxquelles nous avons ajouté la configuration $5p^5$ 7s pour essayer d'en déterminer l'influence.

Les énergies de ces niveaux sont comprises entre 67 000 cm^{-1} et 103 400 cm^{-1} au-dessus du niveau fondamental. Les configurations sont presque toujours imbriquées les unes dans les autres, ce qui laisse supposer de fortes interactions. Pour traiter l'ensemble des 5 configurations, il faut introduire 52 paramètres, alors que nous ne connaissons que 38 niveaux. Il a fallu procéder à quelques approximations pour parvenir à déterminer selon les méthodes de Racah [5], [6] 37 paramètres effectifs dont seulement 28 sont libres.

Pour construire les matrices de l'ensemble des 5 configurations, nous nous sommes servis des matrices des coefficients des configurations $5p^5(6s$ et $5d)$ utilisées par S. Liberman.

Le tableau I donne la liste des 37 paramètres qui ont été déterminés.

Le tableau II donne, pour les 44 niveaux théoriques, les énergies et facteurs de Landé calculés, en regard des énergies et facteurs de Landé expérimentaux quand ils sont connus.

Les paramètres sont classés en différents groupes.

1) Paramètres internes à la configuration $5p^5$ 6s.

$S*$ donne la différence des hauteurs moyennes de $5p^5$ 6s et $5p^5$ 5d,

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ANNEXE I

ETUDE PARAMETRIQUE DE LA STRUCTURE HYPERFINE DES NIVEAUX DE LA CONFIGURATION $5p^5 8d$ DU XENON 129.

L'étude paramétrique des énergies des niveaux des configurations impaires montre que la configuration $5p^5 8d$ se mélange peu aux autres configurations.

En effet, l'écart quadratique moyen au sens de RACAH $\overline{\Delta E} = 22,3\ cm^{-1}$, obtenu dans une étude de cette configuration seule, est extrêmement satisfaisant ; il permet de penser que cette configuration subit peu d'influence de la part des autres.

Le tableau ci-dessous donne, à titre de comparaison, les valeurs des écarts quadratiques moyens obtenus pour les autres configurations.

Tableau I

Nom des configurations	$\overline{\Delta E}$ en cm^{-1}
$5p^5$ 6d	98,4
$5p^5$ 7d	90,6
$5p^5$ 6s et 5d (S. Liberman)	73
$5p^5$ 6s,5d et 6d	57,3
$5p^5$ 6s,5d et 7d	66,1
$5p^5$ 6s,5d,6d et 7d	32,1
$5p^5$ 6s,7s,5d,6d et 7d	31,6
$5p^5$ 6p et 7p (S. Liberman)	24,6
$5p^5$ 8d	22,3

Ce tableau montre bien la diminution de l'écart quadratique moyen au fur et à mesure que nous tenons compte des influences réciproques des configurations $5p^5$(6s,7s,5d,6d et 7d) ; c'est pourquoi nous les avons traitées ensemble, alors que la configuration $5p^5$8d a été traitée séparément.

Il est impossible de déterminer les paramètres de structure hyperfine de la configuration $5p^5$8d avec les 2 seules valeurs de constantes hyperfines connues. Cela est d'ailleurs inutile ; en effet l'étude des configurations $5p^5$(6s,5d,6d et 7d) nous a fourni tous les paramètres utiles, car l'influence de l'électron "d" extérieur est absolument négligeable devant l'électron 5p , dont les paramètres sont : a_{5p} = 16,41 mK ; b_{5p} = -126 mK et c_{5p} = -165,9 mK .

Connaissant ces paramètres et leurs coefficients pour chaque niveau, fournis par le calcul paramétrique des énergies, nous calculons facilement les constantes A .

Le tableau II donne les valeurs calculées des constantes A .

Si pour le niveau 8d 3/2 2 l'accord avec la valeur mesurée est satisfaisant, il n'en est rien pour le niveau 8d 1/2 1 , où l'écart est d'une dizaine de millikaysers.

On peut remarquer que la série nd 1/2 1 est extrêmement perturbée car l'évolution des valeurs des constantes A est très irrégulière

	5d 1/2	6d 1/2	7d 1/2	8d 1/2
A mesuré en mK	-80,7	-1,7	$+23,9_5$	-24,8

Cette irrégularité est due à deux phénomènes.

Le premier est le couplage propre de chaque configuration $5p^5nd$ qui est loin de tout couplage extrême et varie d'une configuration à l'autre. A titre d'indication, en couplage j-ℓ la constante A du niveau nd 1/2 1 vaudrait +28,2 mK .

Le deuxième est l'influence de niveaux de même J d'autres configurations.

La figure I montre les différents niveaux qui perturbent la série nd 1/2 1 .

Tableau II

Constantes de structure hyperfine des niveaux de la configuration $5p^5 8d$, en mK.

Niveaux	Calcul	Mesures
8d 1/2 1	-14,5	-24,8 ± 0,8
8d 3/2 1	+ 28,6	
8d 3/2 2	- 7,8	-6,5 ± 0,5
8d 5/2 2	- 24,6	
8d 5/2 3	- 16,5	
8d 7/2 3	- 28,2	
8d 7/2 4	- 21,2	
8d'3/2 1	+ 98,7	
8d' [3/2] 2	- 92,7	
8d' [5/2] 2	+ 59,7	
8d'5/2 3	- 65,7	

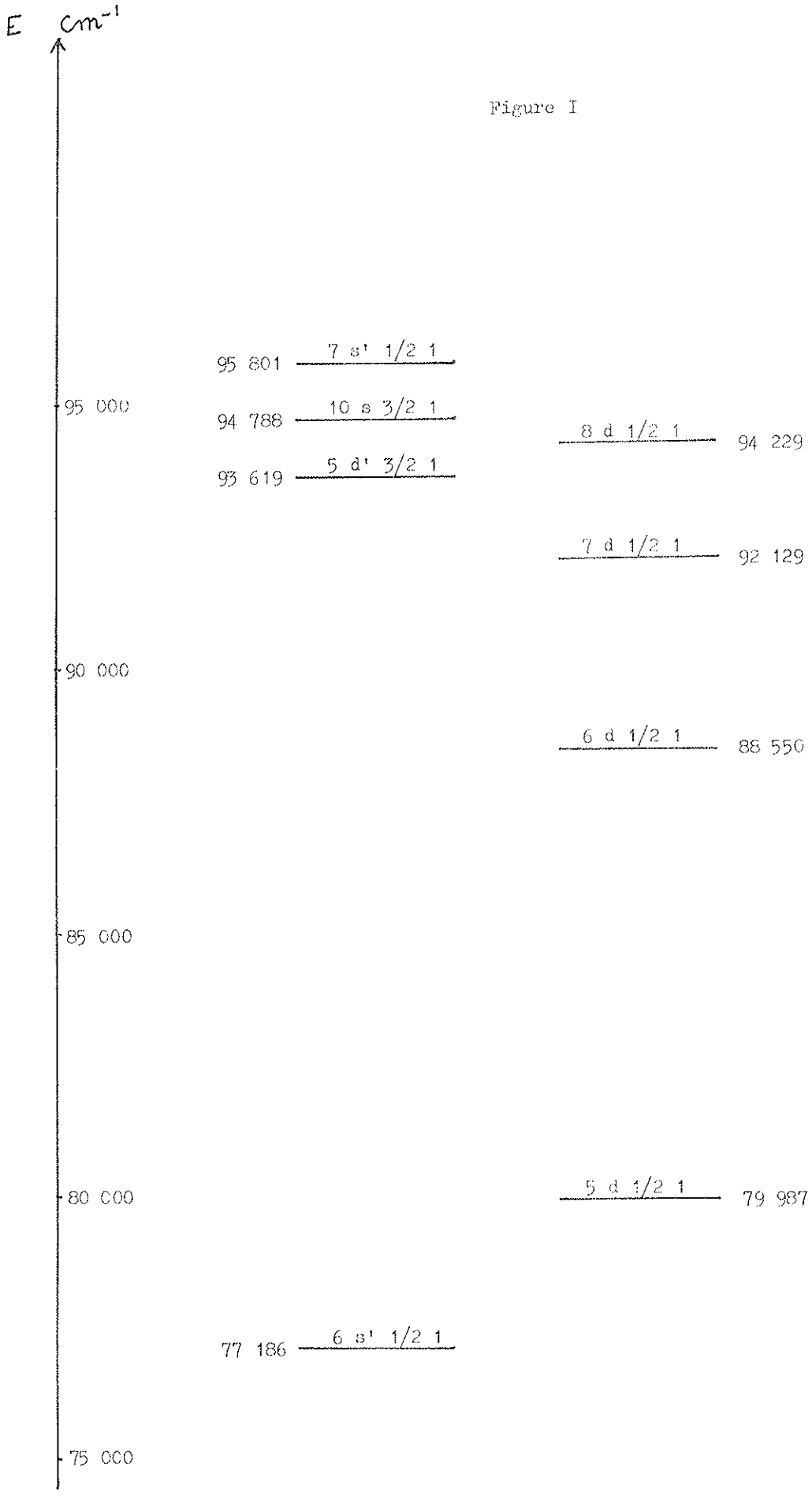
E cm⁻¹
95 000
90 000
85 000
80 000
75 000
95 801
7 s' 1/2 1
94 788
10 s 3/2 1
93 619
5 d' 3/2 1
77 186
6 s' 1/2 1
8 d 1/2 1
94 229
7 d 1/2 1
92 129
6 d 1/2 1
88 550
5 d 1/2 1
79 987

Figure I

Le calcul paramétrique des énergies nous apprend que 21% du niveau 5d' 3/2 1 participe à la configuration $5p^5 7d$ par l'intermédiaire des niveaux 7d 1/2 1 et 7d 3/2 1 , que 3,4% du niveau 5d' 3/2 1 participe à la configuration $5p^5 6d$ par l'intermédiaire des niveaux 6d 1/2 1 et 6d 3/2 1 et que pour environ 30% le niveau 6s' 1/2 1 se mélange au niveau 5d 1/2 1 .

Ces différentes perturbations permettent d'expliquer la variation apparemment aberrante des valeurs des constantes A .

Pour le niveau 8d 1/2 1 , nous n'avons pas identifié le niveau perturbateur. Nous pouvons penser au niveau 7s' 1/2 1 qui se mélangerait au niveau 8d 1/2 1 , en faisant un parallèle avec les niveaux 6s' 1/2 1 - 5d 1/2 1 ; ou au niveau 10s 3/2 1 qui est plus proche, ou encore, pour ne pas dire toujours, au niveau 5d' 3/2 1 . En effet le calcul paramétrique situe ce dernier niveau 15 cm^{-1} trop haut et l'influence du niveau 8d 1/2 1 , si elle était prise en compte, pourrait le ramener à sa place.

L'influence du mélange des niveaux, sur la structure hyperfine, se fait par l'intermédiaire du terme diagonal, c'est-à-dire que les niveaux 7s' 1/2 1 et 10s 3/2 1 , qui ont des constantes A négatives, vont tendre à diminuer la valeur de la constante A du niveau 8d 1/2 1 , alors que le niveau 5d' 3/2 1 aura une action inverse.

La réalité est probablement un mélange de ces trois actions, elle est malheureusement impossible à déterminer paramétriquement car les configurations $5p^5 ns$ n'ont que 4 niveaux.

ANNEXE II

COMPLEMENTS SUR L'ETUDE PARAMETRIQUE DES CONFIGURATIONS $5p^5(6s,7s,5d,6d \text{ et } 7d)$ ET DE LA CONFIGURATION $5p^5 8d$.

Dans cette annexe, figurent les résultats des calculs de la décomposition des niveaux, c'est-à-dire les carrés des coefficients du développement de la fonction d'onde associée à chaque niveau sur les vecteurs de base du couplage Russell-Saunders ; le signe - indique que le facteur de phase correspondant est égal à -1 .

Ces résultats, qui ne figurent pas dans l'article sur l'étude paramétrique de la structure hyperfine, ont été obtenus sur les calculatrices UNIVAC de la Faculté des Sciences d'ORSAY, en utilisant la chaîne des programmes * mis au point au Laboratoire Aimé Cotton.

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* A. CARLIER et Y. BORDARIER, Programmes du Laboratoire Aimé Cotton, non publiés.

Les vecteurs de base des différentes configurations sont notés de la façon suivante :

$^1P^*_1$
$^3P^*_0$
$^3P^*_1$
$^3P^*_2$

} configuration $5p^5 6s$

$^1P^{**}_1$
$^3P^{**}_0$
$^3P^{**}_1$
$^3P^{**}_2$

} configuration $5p^5 7s$

$^1P_1$
$^3P_0$
$^3P_1$
$^3P_2$
$^1D_2$
$^3D_1$
$^3D_2$
$^3D_3$
$^1F_3$
$^3F_2$
$^3F_3$
$^3F_4$

} configuration $5p^5 5d$.

Les vecteurs de base de la configuration $5p^5 6d$ sont indicés U et ceux de la configuration $5p^5 7d$ sont indices W .

Tableaux I

Vecteurs propres des configurations $5p^5(6s,7s,5d,6d \text{ et } 7d)$.

J = 0

	$^3P^*$	$^3P^{**}$	^3P	^3P_U	^3P_W
6s' 1/2 0	-0,6011	-0,0002	0,3964	0,0019	0,0003
7s' 1/2 0	0,0004	-0,9996			
5d 1/2 0	0,3983	0,0002	0,5949	0,0057	0,0009
6d 1/2 0	-0,0002		-0,0074	0,9923	-0,0001
7d 1/2 0			0,0013	-0,0001	-0,9987

Tableaux I (suite)

J = 1

	$^1P^*$	$^3P^*$	$^1P^{**}$	$^3P^{**}$	^1P	^3P	^3D	^1P_U	^3P_U	^3D_U	^1P_W	^3P_W	^3D_W
6s 3/2 1	0,5850	-0,4055	-0,0001		-0,0001	0,0090	0,0003						
6s'1/2 1	0,3180	0,3524	-0,0007	0,0005	-0,0089	-0,3042	-0,0138		-0,0013			-0,0002	
7s 3/2 1	-0,0011	-0,0012	-0,6507	0,3468	-0,0001	-0,0001							
7s'1/2 1		-0,0001	0,3478	0,6520									
5d 1/2 1	0,0938	0,2385	-0,0006	0,0006	0,0055	0,5917	0,0644	0,0001	0,0042			0,0007	
5d 3/2 1	0,0019	0,0017	-0,0001	0,0001	0,4920	0,0127	-0,4657	-0,0090	0,0006	0,0095	-0,0047		0,0020
5d' 3/2 1	-0,0001	0,0004			-0,3972	0,0641	-0,2994	-0,0008	-0,0209	0,0131	-0,1003	-0,0687	0,0349
6d 1/2 1					-0,0123	-0,0016	-0,0037	0,0281	0,8356	0,1185	-0,0001		
6d 3/2 1					0,0047		-0,0079	0,5607	0,0082	-0,3648	-0,0416	-0,0030	0,0090
6d'3/2 1					0,0048		0,0043	0,3739	-0,1274	0,4707	-0,0005	0,0044	-0,0139
7d 1/2 1					0,0514	-0,0064	0,0697	-0,0058	0,0006	0,0046	-0,1372	-0,6913	-0,0331
7d 3/2 1		-0,0001			0,0195	-0,0102	0,0692	-0,0125		0,0145	-0,3814	0,0820	0,4108
7d'3/2 1					0,0034		0,0017	0,0093	-0,0011	0,0042	0,3342	-0,1498	0,4964

Tableaux I (suite)

J = 2

	$^3P^*$	$^3P^{**}$	^3P	^1D	^3D	^3F	^3P_U	^1D_U	^3D_U	^3F_U	^3P_W	^1D_W	^3D_W	^3F_W
6s 3/2 2	-0,9859	-0,0004	0,0130	0,0003	0,0005									
7s 3/2 2	0,0004	-0,9996												
5d 3/2 2	0,0121	0,0001	0,6724	0,1152	0,1973	0,0001	0,0021	-0,0001	-0,0002		0,0004		-0,0001	
5d 5/2 2			0,0003	0,4124	-0,2600	-0,3204		-0,0035	0,0023	0,0002		-0,0006	0,0004	
5d' 3/2 2	0,0013		0,2433	-0,1897	-0,3332	0,0017	-0,0526	-0,0112	-0,0208		0,0737	0,0262	0,0463	
5d' 5/2 2			-0,0006	0,2008	-0,1002	0,5885	0,0002	0,0360	-0,0196	-0,0202	-0,0001	-0,0176	0,0088	0,0074
6d 3/2 2	-0,0002		-0,0223	0,0274	0,0406		-0,4934	-0,1576	-0,2572	-0,0001	-0,0006	-0,0003	-0,0004	
6d 5/2 2				0,0067	-0,0034	0,0717	-0,0001	-0,4236	0,2703	0,2239		-0,0001	0,0001	0,0001
6d' [3/2] 2			0,0002	0,0011	0,0002		-0,2290	0,3639	0,0374	0,3681				
6d' [5/2] 2			-0,0002		-0,0012		0,2179	-0,0029	-0,3906	0,3871				
7d 3/2 2				0,0100	-0,0063	0,0174		0,0004	-0,0003	-0,0004	0,0001	0,4498	-0,2892	-0,2261
7d 5/2 2	0,0002		0,0475	-0,0361	-0,0569		-0,0046	-0,0009	-0,0014		-0,4495	-0,1557	-0,2471	
7d' [3/2] 2				0,0001							-0,0019	0,1617	-0,0729	0,7634
7d' [5/2] 2			-0,0001	-0,0001	-0,0002						0,4737	-0,1879	-0,3248	0,0030

Tableaux I (suite)

J = 3

	^3D	^1F	^3F	^3D_U	^1F_U	^3F_U	^3D_W	^1F_W	^3F_W
5d 5/2 3	0,6336	0,3392	0,0125	-0,0084	-0,0042		-0,0013	-0,0007	
5d 7/2 3	0,0766	-0,2817	0,6405	-0,0002	0,0008			0,0002	
5d'5/2 3	0,2360	-0,3025	-0,2865	0,0076	-0,0009	0,0231	-0,0242	0,0454	-0,0739
6d 5/2 3	-0,0035	-0,0096	-0,0014	-0,6292	-0,3484	-0,0035	0,0005	0,0033	-0,0005
6d 7/2 3	-0,0084	0,0099	0,0143	0,1176	-0,2985	0,5504	0,0003	0,0007	
6d'5/2 3	-0,0013	0,0015	0,0001	-0,2356	0,3439	0,4158	0,0006		-0,0012
7d 5/2 3	-0,0118	0,0031	0,0058	-0,0010	-0,0004		-0,7410	-0,1568	-0,0800
7d 7/2 3	0,0285	-0,0521	-0,0389	-0,0002	-0,0019	0,0070	0,0022	-0,4557	0,4135
7d'5/2 3	0,0003	-0,0004		0,0002	-0,0009	-0,0003	0,2299	-0,3372	-0,4309

J = 4

	^3F	^3F_U	^3F_W
5d 7/2 4	-0,9991	-0,0008	-0,0001
6d 7/2 4	-0,0008	0,9992	
7d 7/2 4	-0,0001		0,9999

L'ensemble des Tableaux I montre la complexité du mélange entre ces 5 configurations. Nous voyons que de nombreux niveaux participent de façon non négligeable à 2 ou 3 configurations différentes. Ce n'est que par une connaissance précise de ce couplage intermédiaire que nous avons pu calculer la structure hyperfine et en expliquer les valeurs expérimentales, qui semblaient varier de façon aléatoire, pour un niveau de nombres quantiques donnés, d'une configuration $5p^5nd$ à l'autre.

La configuration $5p^58d$ ayant été traitée toute seule, nous avons adopté pour ses vecteurs de base la même notation que pour la configuration $5p^55d$.

Parmi les 4 niveaux bâtis sur le terme parent $^2P_{1/2}$, des configurations $5p^5nd$, seul le niveau nd' 3/2 1 est connu à partir de n=6 , car ils se situent au-dessus du premier potentiel d'ionisation. Les niveaux nd' 3/2 1 et nd' 5/2 3 peuvent être identifiés sans ambiguïté, mais il est impossible de dénommer avec certitude, dans

chaque configuration, les deux niveaux nd' 3/2 2 et nd' 5/2 2 . En effet, le couplage varie beaucoup d'une configuration $5p^5nd$ à l'autre, si bien que l'ordre des niveaux n'est pas toujours le même.

Tableaux II

Vecteurs propres de la configuration $5p^5 8d$

J = 0 et J = 1

	$^3P_0$	$^1P_1$	$^3P_1$	$^3D_1$
8d 1/2 0	1,00			
8d 1/2 1		0,0094	-0,8097	0,1809
8d 3/2 1		0,6341	-0,0346	-0,3313
8d'3/2 1		-0,3565	-0,1556	-0,4879

J = 2

	$^3P_2$	$^1D_2$	$^3D_2$	$^3F_2$
8d 3/2 2	0,5112	0,1955	-0,2933	
8d 5/2 2		0,4636	0,3091	-0,2273
8d' [3/2] 2		0,1365	0,0908	0,7727
8d' [5/2] 2	0,4888	-0,2044	0,3068	

J = 3 et J = 4

	$^3D_3$	$^1F_3$	$^3F_3$	$^3F_4$
8d 5/2 3	0,6881	0,2982	-0,0137	
8d 7/2 3	-0,0863	0,3658	0,5479	
8d' 5/2 3	0,2256	-0,3359	0,4384	
8d 7/2 4				1,00

Pour indiquer cet état de chose , nous avons mis dans les tableaux des crochets autour des nombres quantiques 3/2 et 5/2 , afin de montrer que l'identification en était incertaine.