DENSITY DEPENDENT FORCES AND OXYGEN ISOTOPES

A STUDY OF OXYGEN ISOTOPES USING DENSITY DEPENDENT FORCES

by

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SCOPE AND CONTENTS:

This work is concerned with the use of different "effective" nucleon-nucleon interactions in the calculation of binding energies and spectra of some of the oxygen isotopes.

The variational procedure consists of using a complete set of Slater determinant wave functions, having the same total M value for the projection of the angular momentum, in order to minimize the ground states of various nucleonic configurations in the 2s-1d nuclei. The parameters obtained are used in the subsequent diagonalization of the Hamiltonian and its eigenvalues are interpreted as energy eigenvalues. The calculations performed in this work led to the conclusion that the density dependence of the effective force is extremely important and should not be neglected, at least in the calculation of binding energies.

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CHAPTER I

INTRODUCTION

The usual trend in performing nuclear structure calculations in order to fit the spectrum of nuclei is to neglect the binding energies of the systems under investigation. Furthermore, if the harmonic oscillator approximation is used, separate variations of the oscillator radii for the various orbitals (s, p, etc.) are usually not allowed in the sense that such a variation is assumed not to be critical.

Work performed by Volkov [Vo 64], [Vo 65], Volkov and Hughes [V.H. 66], and Volkov and Manning [Ma 67] pointed out the importance that such a variation could have on the deformation characteristics of nuclei. In particular, the equilibrium deformations for nuclei were found to be less than those predicted by Nilsson.

Such investigations showed also the possibility that calculations performed at zero deformation with an appropriate nuclear interaction could yield level ordering and spacing of nuclear spectra, in agreement with experimental data and that the binding energy so calculated could be close to the experimental ones.

The extensive work done using the shell model approach, or the Nilsson model, clearly indicates the validity of the

independent particle potential as a first approximation to the nuclear problem. One is led to the search for possible two body nuclear interactions which should approximately reproduce the scattering data and which could be used at the same time to calculate the properties of nuclear structure.

In order to avoid the difficulties posed by the presence of a hard core which appears in most "realistic" interactions, one often uses phenomenological potentials in nuclear spectroscopy to explain configuration mixing and the observed spectra. One has to solve the Schroedinger equation for an A particle system (A = N + Z) in general, or a V (valence particle) system in the usual shell model approach by using an appropriate phenomenological interaction. It is well known that the solution of such a differential equation is equivalent to finding functions which make the integral

$$(\Psi|H|\Psi) \qquad (1.1)$$

stationary subject to the condition that the normalization of the wave function is maintained in the process.

Such variational calculations can be performed in different ways. In the most general case the wave functions should be determined without imposing any functional "constraint" on them. More often a restricted version is used in the sense

that a particular set of single particle wave functions is chosen and the variation is performed on some parameters appearing in them. One can then obtain the best approximation to the true nuclear wave function corresponding to the given functional form. This is the approach used in the present investigation of the spectra of the isotopes of oxygen.

In contrast to the usual form of the Hartree Fock approximation, the variations are made with respect to a complete basis of Slater determinants, i.e. we include all possible configurations in the 2s - 1d shell compatible with a given nucleus.

The procedure consists essentially in the following: the complete set of Slater determinant wave functions having the same total M value are generated and the Hamiltonian matrix in this representation is diagonalized.

The ground state so obtained is then minimized with respect to the orbital parameters which in the more general case should include orbital sizes and deformations.

The eigenvalues of the Hamiltonian corresponding to this minimum value of the ground state are then interpreted as energy levels and the eigenvectors as nuclear wave functions.

The use of Slater determinants is necessary in the deformed cases where the angular momentum is not conserved and

and the usual techniques of the irreducible representations of the rotation group can no longer be applied, if one desires to keep the representation small and avoid lengthy projection calculations.

It must be noted further that the use of Slater determinants is convenient in the sense that the corresponding matrix can be diagonalized fairly rapidly with present day computers.

CHAPTER II

MANY BODY FORMULATION OF THE PROBLEM

The nuclear many body problem that we must solve is a very restricted one, in the sense that two basic assumptions are made. The first one is that only nuclear coordinates are introduced into the relevant equations and the second is that only two body interactions are considered to be important.

The first condition which actually prevents the production of virtual mesons is a low energy approximation and further suggests that the motion of nucleons inside the nucleus should be treated non "relativistically".

The basic question of the validity of such assumptions has not been answered yet, and the simplifications that follow are accepted rather on the basis of the absence of a clear indication of their breakdown in the usual energy ranges.

As a first approximation we are then led to consider the following model Hamiltonian

$$H_{mod} = \sum_{j=1}^{A} \left[\frac{p_j^2}{2m_j} + V(r_j)\right] \qquad (2.1)$$

where $V(r_j)$ is a suitable potential, which for the moment is left undetermined.

It is well known that in such a case eigenfunctions of the Hamiltonian of eq. (2.1) can be constructed as products of the eigenfunctions $\phi_\alpha(\vec{r})$ of the single particle Schroedinger equation.

$$H\phi_\alpha(\vec{r}) \equiv [\frac{p^2}{2m} + V(r)]\ \phi_\alpha(\vec{r}) = \varepsilon_\alpha \phi_\alpha(\vec{r}) \qquad (2.2)$$

where α stands for the set of quantum numbers which are needed to label the single particle states.

If we insist on the antisymmetry properties which a system of fermions must obey, then an initial set of eigenfunctions of equation (2.1) which is complete, orthogonal and antisymmetric consists of Slater determinants of the order A, i.e.

$$\Psi_\nu = \frac{1}{(A!)^{\frac{1}{2}}} \begin{vmatrix} \phi_{\alpha_1}(\vec{r}_i) & \cdots & \phi_{\alpha_1}(\vec{r}_A) \\ \vdots & & \vdots \\ \phi_{\alpha_A}(\vec{r}_i) & & \phi_{\alpha_A}(\vec{r}_A) \end{vmatrix} \qquad (2.3)$$

where α_i represents the set of quantum numbers of the ith nucleon, i.e. position, spin and isospin coordinates, and ν stands for the set of α_N quantum numbers $(\alpha_1\alpha_2 - \alpha_N)$. The eigenvalues of eq. (2.1) corresponding to the eigenfunctions defined in (2.3) are naturally determined by the eigenvalues of eq. (2.2) and by the set of quantum numbers represented by ν i.e.

$$E_\nu = \sum_{j=1}^{A} \varepsilon_{\alpha_j} \qquad (2.4)$$

If we are dealing with a closed shell nucleus, the ground state is represented by a single Ψ_ν with the set of α_i with lowest energy.

Otherwise, there will be degeneracy corresponding to the alternative mutual orientations of the nuclear orbits. Construction of linear combinations of Ψ_ν by well known methods is then required to single out ground and excited state wave functions with definite values of angular momentum and other constants of motion.

The central field approximation considered so far is certainly too crude an approximation to be able to predict satisfactorily most of the physical properties of a complex system like a nucleus.

The fact that the eigenfunctions (2,3) are a complete set, suggests the introduction of a more general Hamiltonian of the form

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m_i} + \sum_{i>j} V(r_{ij}) + C \sum_i \vec{\ell}_i \cdot \vec{s}_i - T_{cm} \qquad (2.5)$$

where $V(r_{ij})$ is some phenomenological potential which includes in the general case the various exchange operators and where T_{cm}, the centre-of-mass kinetic energy is subtracted in order to make H depend only on the intrinsic coordinates. Starting from the eigenfunctions Ψ_ν of the model Hamiltonian, we face

the following situation.

Let us consider the matrix element of H between two states Ψ_ν and $\Psi_{\nu'}$, written as

$$(\nu'|H|\nu) \qquad (2.6)$$

The diagonal elements $(\nu|H|\nu)$ give expectation values of the energy corresponding to the approximate Ψ_ν. The magnitude of the off diagonal terms, which would vanish if the Ψ_ν were exact wave functions, indicates the degree of approximation reached at this point and the relevant approximation indices for two configurations ν' and ν'' are given by [FA]

$$(\nu'|H|\nu'') = [(\nu'|H|\nu') - (\nu''|H|\nu'')]$$

It should be mentioned "en passant", that among the wave functions with structure (2.3), the best approximation to an energy eigenstate is constructed with single particle wave functions, which obey the Hartree Fock system of equations rather than the model equation (2.1).

We did not follow the Hartree Fock approach, at least in its usual form, because it is not too practical to form a complete orthogonal set of eigenstates and eigenvalues in this manner.

Improved wave functions Ψ_μ of (2.5) can be constructed by taking linear combinations of the original Ψ_ν i.e.

$$\Psi_\mu = \sum_\nu \Psi_\nu U_{\mu\nu} \qquad (2.7)$$

where in order for the Ψ_μ to be orthogonal, the matrix of the coefficients $U_{\mu\nu}$ has to be **unitary.**

The coefficients $U_{\mu\nu}$ which reduce the Hamiltonian matrix to its diagonal form obey the infinite system of equations

$$\sum_{\nu'} (\nu|H|\nu') \, U_{\nu'\mu} = U_{\nu\mu} \, E_\mu \qquad (2.8)$$

providing, at least in principle, the required energy levels and wave functions of the system. In practice one does not consider the infinite set of equations (2.8), but instead a finite, truncated, set of states are used in order to obtain an approximate solution of (2.8).

CHAPTER III

SINGLE PARTICLE POTENTIAL

Still not defined is the form of the central potential of eq. (2.1) which defines completely the set of single particle wave functions in the Slater determinants (2.3).

As mentioned before, the correct method of obtaining the set of single particle wave functions should be through a self consistent process, such as to determine the ϕ_{α_i} by the variational principle itself, without any further restrictions. Very often this principle is replaced by a more restricted one in which the initial states are determined "a priori" at least in their functional forms. In this context, since the development of the shell model extensive use has been made of the infinite square well potential and the infinite harmonic oscillator potential well.

In these two cases one can obtain an exact solution and they provide two contrasting viewpoints.

The square well has an infinitely sharp edge whereas the harmonic oscillator potential increases smoothly at the edges.

The main reason for the use of the Harmonic Oscillator potential well is due essentially to the analytic properties of its solution, which simplify the calculations of matrix

elements and to the fact that the harmonic oscillator well reproduces fairly well the shell closures occuring at the so-called magic numbers, if an appropriate spin orbit coupling is introduced.

The fact that such wave functions are not self consistent is not a very serious drawback, in the sense that it has been possible to prove that harmonic oscillator wave functions are indeed very close to being self consistent (Ne 59) and also that eigenvalues and eigenvectors of a cut off oscillator well are very close to the corresponding ones of an infinite well.

Actually, a potential which is intermediate between the square well and the harmonic oscillator well and which also has an experimental basis is the Wood Saxon potential obtained by fitting the data on nucleon-nucleus scattering. This potential which is flat at the center and falls off smoothly to zero at the edge of the nucleus is given by

$$V(r) = - V_0/[1 + \exp \mu(r - R)]$$

where

$$\mu^{-1} \simeq 0.5 \times 10^{-13} \text{ cm.}$$

and

$$R \simeq 1.33\, A^{1/3} \times 10^{-13} \text{ cm,}$$

A being the mass number of the nucleus and $V_o \gtrsim 50 \div 60$ MeV.

For $\mu \to \infty$, $V(r) = - V_o$ for $r < R$

and $V(r) = 0$ for $r > R$ and the potential corresponds to the square well.

For the Wood-Saxon potential, an exact solution cannot be obtained and numerical methods must be employed. In fact even in the square well and the harmonic oscillator well solutions in terms of known mathematical functions are only possible provided the former falls off infinitely sharply and the latter extends to infinity. However, for the consideration of low lying bound states, it is not of great importance whether the wells are cutoff or not. This being the case, and the fact that, at least for light nuclei, the levels of a Wood-Saxon potential are very close to those of an harmonic oscillator potential, one can safely assume that the single particle orbitals are eigenfunctions of a Schrodinger equation with a potential of the form

$$V(r) = \frac{1}{2} m\omega^2 \ (x^2 + y^2 + z^2) \qquad (3.1)$$

One usually treats the harmonic oscillator energy $\hbar\omega$ related to the nuclear radius parameter b by $b^2 = \frac{\hbar}{m\omega}$ as a variational parameter, in order to minimize the energy in the expression

$$\delta \int \Psi^* \ H \ \Psi \ \ d\tau = 0 \qquad (3.2)$$

The Schroedinger equation with the potential given in (3.1) can be solved in various coordinate systems.

If one uses Cartesian coordinates, the above

equation separates in the x,y,z directions, with the three quantum numbers n_x, n_y, n_z describing the physical state of the system and representing the number of quanta in the x,y,z directions respectively.

The total oscillator quantum number N is then

$$N = n_x + n_y + n_z$$

and the oscillator energy is

$$\varepsilon = (N + \frac{3}{2})\ \hbar\omega$$

Using a spherical representation, the wave equation is separable in the r,θ,ϕ directions with corresponding quantum number n,ℓ,m and energy given by

$$\varepsilon = (2n + \ell - \frac{1}{2})\hbar\omega$$

It has also become evident in the past years that some nuclei are best described by a deformed single particle potential with possibly different energies $\hbar\omega$ in the x,y and z directions. The relevant Schroedinger equation in this case is then

$$(\frac{p^2}{2m} + \frac{1}{2}\, m[\omega_x{}^2 x^2 + \omega_y{}^2 y^2 + \omega_z{}^2 z^2] - \varepsilon_i)\phi_{\alpha_i} = 0 \quad (3.3)$$

where ω_x, ω_y and ω_z can be treated as variational parameters.

In particular if $\omega_x = \omega_y \neq \omega_z$ one obtains the eigensolutions of an harmonic oscillator well with axial symmetry, with corresponding quantum numbers n,m,n_z and energy given by

$$\varepsilon = (2m+|m|+1)\ \hbar\omega_\rho + (m_z + \tfrac{1}{2})\hbar\omega_z \qquad (3.4)$$

Although originally applied to those regions of the nuclide chart where nuclei are clearly deformed, more recent investigations by Volkov, Hughes and Manning indicate the interest of such approach to light nuclei as well.

Extensive calculations performed in the 1p (Hu 69) region have shown that most nuclei are indeed deformed justifying the use of an axially symmetric oscillator potential as a natural representation for such nuclei. In the present work we use such approach in the 2s-1d region in an attempt to fit the spectrum of the oxygen isotopes with different phenomenological potentials.

The wave functions used have the virtue of maintaining the cylindrical symmetry of the problem, conserving the z component of the total angular momentum as a good quantum number, and thus simplifying the construction and diagonalization of the energy matrix.

Ideally one would like to perform these calculations in the whole 2s-1d shell. Unfortunately the number of configurations which are involved gets very rapidly out of hand and limits the method to but a few of all possible nuclei.

CHAPTER IV

MODEL SPACE

As mentioned, the aim of explaining the properties of complex nuclei is furthered by separating the potential into two parts, one of which is, or at least is hoped to be, a good first approximation to the true potential felt by a nucleon inside a nucleus.

This leads, as we have seen, to a matrix equation of the form

$$\sum_{\nu'} (\nu|H|\nu') \; U_{\nu'\mu} = U_{\nu\mu} \; E_{\mu} \qquad (4.1)$$

i.e. to an infinite system of equations in the representation spanned by a "complete" set of Slater determinants, whose constituent wave functions span the complete Hilbert space H' of the system. The dimensions of H' exceed all bounds and the many body problem involved cannot be solved by simply choosing a particular basis in this space: this would involve the solution of a Shroedinger equation, whose Hamiltonian is acting on an infinite dimensional space. We are faced with the necessity of defining a Hamiltonian acting on a finite dimensional space "h", which would be small enough to carry out the numerical analysis of the problem, and at the same time be "wide" enough so as to contain

all the interesting features of the low lying nuclear levels.

Methods of performing this act of truncation are based essentially on the fact that the single particle wave functions are chosen to be as close as possible self consistent. Since the extreme single particle model is so successful in explaining ground state spins and other properties, it appears reasonable to keep our functional space as close to this model as possible.

The A particles in the nucleus are thus divided into two classes: the first A - V particles remain undisturbed in completely filled orbits to form an inert core, while the remaining v particles (the so called valence particles) are allowed to occupy as few of the possible single particle orbits available as possible.

In the case of μ allowed orbitals, which are labelled by a set of quantum numbers $\alpha_1 \ldots\ldots \alpha_\mu$ then the model space h is the finite vector space which is spanned by a complete set of Slater determinants which are the mathematical "realization" of the n particle configurations.

The presence of a constant of motion can be used to further simplify the numerical analysis. The corresponding operators split the finite vector space h into subspaces which are disjoint and are labelled by the possible values that the resultant operators can assume. Having defined the model space, the Hamiltonian matrix can then be evaluated.

Its subsequent diagonalization, which corresponds to a solution of the Schroedinger equation within this model space, can then be performed separately in each subspace of the model space h.

CHAPTER V

NUCLEAR INTERACTIONS

The assumptions of chapter II thus lead to the general form of the phenomenological potentials used, as a two body interaction, i.e. as

$$\sum_{i<j} V(|\vec{r}_i - \vec{r}_j|) \qquad (5.1)$$

The first condition that the potentials must satisfy is due to the use of harmonic oscillator wave functions as basis states. One then requires that such an interaction has well defined matrix elements between such states.

The desirability of using "realistic interactions" is ruled out by the fact that most of them possess a hard core, such that the corresponding matrix elements are not finite.

One is thus led to the search of effective potentials, which have a simple analytical form and which contain few parameters that can be adjusted in order to reproduce the most important experimental features of the interaction.

The first type of force used and which satisfies the requirement of easy evaluation of matrix elements (and referred to as force 1) is the Volkov force [see Table I]

$$V(r) = [w+mP_x+bP_\sigma+hP_\tau] * V_A \exp(-\frac{r^2}{\lambda_a^2}) + V_R \exp(-\frac{r^2}{\lambda_r^2}) \qquad (5.2)$$

where P_x, P_σ, P_τ are the space, spin, isospin exchange operators respectively and where the radial dependence (the sum of two gaussians) gives a shape which is similar to the Moszkowski-Scott form for v_e (the effective long range part of the interaction).

The parameters V_A V_R λ_a λ_r which have been used, were evaluated by M. Manning and D. J. Hughes, in order to fit the binding energy of O^{16} and approximately fit the low energy scattering data. The same calculations gave values for m, b, h, parameters (w = 1-m) with one exchange parameter still undetermined.

In the calculation performed for the oxygen isotopes, a moderate spin-orbit force was included.

The value 2.0 for the constant c in the epxression

$$V_{s.o} = - C \vec{\ell} \cdot \vec{s}$$

was chosen in order to give the experimental splitting between the $d_{5/2}$ and $d_{3/2}$ levels, which are observed in stripping reactions on O^{16}.

This type of force has been used extensively in 1p shell nuclei calculations, and gives fairly good agreement for binding energies and energy spectra for nuclei in this region.

Unfortunately, it has been found that such a potential for nuclei larger than O^{16} leads to too small sizes and progressive collapse. This phenomenon increases with the number

of nucleons. This is due to the fact that the forces of this type did not saturate nuclear matter.

Another type of force has also been used in this work: it has a density dependent character and was obtained by imposing the requirements that

1) it reproduces approximately the correct phase shift for free nucleon-nucleon scattering up to 250 MeV.,
2) it has approximately the same long range as realistic potentials and
3) it gives the correct saturation properties in nuclear matter. In particular, condition 3) is important for application to a wide range of nuclei.

The more general nuclear interaction is then of the same functional form as given in 5.2 but with

$$\lambda_r = \lambda_r(k) = \lambda_r^{o} \left[1 + c_1 (k-c_2)^2\right]$$

$$V_a = V_A \left[1 - c_3 \rho^{m_1/3}(\vec{R})\right]$$

$$V_r = V_R \left[1 + c_4^{m_2/3} (\vec{R})\right]$$

where k is the average relative wave number between interacting particles and ρ is the average density of the nucleus evaluated at $\vec{R} = \frac{1}{2}(\vec{r}_1+\vec{r}_2)$ the center of mass of the interacting particles [see Table II].

Again the parameters V_A V_R λ_a λ_r c_1 c_2 are obtained by approximately fitting the singlet and triplet wave phase shifts to 250 MeV, with the difference between the singlet even and triplet even states so giving a value as for b - h and saturating nuclear matter in a first order Hartree-Fock

calculation [Ma 67]. It is possible to prove that all matrix elements between many particle states of the [4,4,4,-----4] supermultiplet symmetry are unchanged by variation in w, m, b, h as long as the quantity = 10[w+m] - 8[b+h] remains unchanged.

Various values of n_1 and n_2 can be used with the above potential, in order to fit the data

$$\frac{E}{A} = 16 \text{ MeV}$$

$$k_F = 1.36 \text{ fm}^{-1}$$

for nuclear matter, allowing the determination of the constants c_3, c_4 for given ν.

Four different forces of this form have been used in this work,whose characteristic parameters are given in Tables I and II and which will be referred to as force 2, 3, 4, 5 respectively.

CHAPTER VI

ENERGY MINIMIZATION

The deformation ε can be defined as the ratio of the two oscillator constants α and β corresponding to the ρ dependent part and to the z dependent part of the wave functions of a cylindrically symmetric harmonic oscillator.

Their ratio is given in Appendix A of Nilsson paper [N 55] by

$$\frac{\alpha}{\beta} = (1 + \frac{\varepsilon}{3}) \; / \; (1 - \frac{2\varepsilon}{3})$$

where positive values of ε represent a prolate deformation, while negative values of ε represent an oblate shape.

As mentioned in Chapter I, investigations performed on the 1p shell nuclei have shown the usefulness of allowing the variation of the oscillator constants of the different single particle orbitals of the approximate wave function. The main reason for such an approach is the possibility that it offers to provide a closer approximation to the more "realistic" Wood Saxon potential, while avoiding the worst mathematical difficulties of the more realistic single particle potential. In order to further simplify the calculations, it is required that the ratio of α's and β's for the different orbitals involved be the same.

This is equivalent to demanding that the deformation ε be the same for all orbits, which is in the spirit of a Hartree Fock potential which should be similar for all the orbitals.

Furthermore, the extension to the 2s-1d shell nuclei poses another constrainton such parameters in the sense that in order to maintain orthogonality between the $1s_o$, $1d_o$ and $2s_o$ states, the same oscillator constant must be assigned to them.

Actually, one could assign different orbital size parameters to all single particle levels, but in this case, one would have to renormalize the corresponding Slater determinants, in order to regain orthogonality which is not easy.

In calculating spectra with the total angular momentum a good quantum number, it is necessary to use a set of functions which form an appropriate basis of the rotational group.

This constraint allows only two possible variational parameters, which are the oscillator constants for the 1s (α_o) and the 1p (α_1) shells.

The energy matrix is then calculated for a given force and determines a ground state energy $E(\alpha_o,\alpha_1)$, which depends on the value of α_o and α_1.

One can define an auxiliary parameter

$$\frac{\alpha_1}{\alpha_o} = \sigma$$

and then minimize $E(\alpha_o,\sigma)$ with respect to α_o and σ. This is done in our computation by applying a parabolic fit to

$$E(\alpha_o,\sigma) \quad , \quad E(\alpha_o+\delta\sigma_o,\sigma) \quad , \quad E(\ _o+2\delta\alpha_o,\sigma)$$

to yield:

$$E(\alpha'_o,\sigma) \tag{6.1}$$

and then another parabolic fit to

$$E(\alpha_o,\sigma+\delta\sigma) \ , \ E(\alpha_o+\delta\alpha_o,\sigma+\delta\sigma) \ , \ E(\alpha_o+2\delta\alpha_o,\sigma+2\delta\sigma)$$

to yield:

$$E(\alpha_o'' \ , \ \sigma + \delta\sigma) \tag{6.2}$$

and finally another parabolic fit to

$$E(\alpha_o,\sigma+2\delta\sigma) \ , \ E(\alpha_o+\delta\sigma_o,\sigma+2\delta\sigma) \ , \ E(\alpha_o+2\delta\alpha_o,\sigma+2\delta\sigma)$$

to yield:

$$E(\alpha_o'',\sigma + 2\delta\sigma). \tag{6.3}$$

From (6.1), (6.2) and (6.3)

$$E(\alpha_o,\sigma_m) \quad , \quad E(\alpha_o+\delta\alpha_o,\sigma_m) \quad , \quad E(\alpha_o+2\delta\alpha_o,\sigma_m)$$

is fit to yield

$$E(\alpha_{om},\sigma_m)$$

where the parameters' values are the ones corresponding to the minimum energy corresponding to zero deformation. The process can be continued by repeating each step and starting with the best fit value obtained in the previous calculation.

Once the values of the parameters for the best ground state energy are obtained, their value is used for the complete diagonalization of the Hamiltonian matrix in all the different subspaces, in order to obtain the spectra of the nuclei considered.

CHAPTER VII

RESULTS FOR O^{17} O^{18} O^{19} AND O^{20}

As mentioned, the calculations were performed by using a representation whose result at zero deformation could be compared with the conventional intermediate coupling results.

This was done by using a Slater determinant representation characterized by the z projection of the total angular momentum of the system. In this case the Hamiltonian is reducible with respect to J_z and the various matrices can be diagonalized separately.

The sizes of the matrices involved are generally larger than the corresponding matrices used in the conventional spherical representation, but on the other hand the simpler representation has some compensating features as long as the system does not require too many states, which is the case for the positive parity states of the oxygen isotopes.

First, it is fairly easy to construct the representation which is uniquely defined by the number of neutrons in the 2s-1d shell, and the z projection of the total angular momentum.

Second, the calculation of matrix elements in this representation has become a "standard routine" due to the

presence of computer subroutines, developed by Manning (MA 67).

The number of configurations for the various nuclei and values is given in Table III.

The worst case is O^{20} which has 81 possible configurations in the case of $J_z = 0$.

Due to the great number of diagonalizations involved in the minimization of the ground state energies, a restriction has been put on the number of configurations considered important for O^{19} and O^{20}. In particular, for O^{19} only the configurations in which 2 particles are in the [0,0,2] and/or [001] states were taken into consideration (see Table VI).

This gives a Hamiltonian matrix of size 4 × 4 instead of the original 37 × 37 matrix.

In the case of O^{20} the configurations are restricted to the ones corresponding to the presence of two particles in the [002] states only (see Table VII).

This approximation was taken into account in the hope that the limitation of the number of determinant wave functions would not be too critical in the minimization procedure, and was based on the results obtained by Volkov in his work on the equilibrium energies of nuclei in the 1p shell [Vo 65].

The full diagonalization was then employed with the parameters so determined, for the calculation of the spectra.

The poor fit to the energy levels obtained can be in part attributed to the restriction on the oscillator constants which has been imposed in order to maintain orthoganality of the eigenvectors.

This is dramatically observed in the case of O^{17} for the $J = \frac{1}{2}$ states, which in the case of force number 3 lies at more than 4 MeV above the experimental level.

The restriction on the oscillator constant is then such as to bring the 2s particle inside the orbits of the 1p particle in such a way that the valence particles feel the repulsive part of the potential more than they should.

In particular, the matrix elements between the 2s states are in general larger than the matrix elements between s and d states. It is then expected that a decrease of the coefficient C_4 appearing in the density dependent part of the repulsive part of the potential will increase the matrix elements between the s states leading to the lowering of the $\frac{1}{2}$ levels [Hu 67]. This is in fact what is observed as a general trend with the use of forces 4 and 5.

The energy interval between experimental and calculated $\frac{1}{2}$ levels in the case of calculation with force 5 is reduced to 3 MeV only and one expects that the relaxation of the restriction on the oscillator constants, if possible, would lower still further the level. The case of force number 2 shows the same tendency, although the different type of density

dependence in this case prevents a direct comparison. Furthermore, the lowering of this level in this case is not as one would expect, due to the presence of a higher density dependence attractive part in the potential.

It should be noted also that the observed deviations from the experimental levels could be explained by allowing an admixture of core excitation to the single particle motion, whose evidence is found in the splitting of the $1/2^+$ and $3/2^+$ levels in O^{17}, the occurrence of low lying negative parity states in this nucleus and the E2 admixture for the neutron hole transition $3/2^- \rightarrow 1/2^-$ in O^{15}. The same phenomenon appears in the case of O^{18} where the difference in energy between the calculated and experimental 0^+ excited state drops from about 7 MeV to about 5 from force 3 to force 5. In an analogous way the 2^+ excited state comes down to about 0.8 MeV in the case of force 5.

It must be further noted that in the particular case of O^{18} some of the levels such as 0^+, 2^+ can be identified as rotational levels. This brings further doubts on the validity of the approach used here in the sense that the action of truncation of the Hilbert space has been too drastic and has no "life" left in it to describe such rotational levels.

In O^{19} this general trend is once more indicated by the behaviour of the $1/2^+$ level found experimentally at 1.46 MeV, and when calculated lies at 4.43 for force 3 and goes down to 3.15 MeV for force 5. Similar behaviour is shown by

the second 3/2 level, which comes down from 4.3 Mev to 3.94 Mev although in this case no comparison with experiment can be done, due to the lack of spin and parity assignments in this level.

In O^{20} the spacings between the 2^+ and 4^+ levels found tend to indicate their nature as rotational levels.

The mechanism which has been assumed in explaining the bad fit of the spectra obtained is confirmed in the calculations performed with the so called density approximation 2 (DA2) performed for O^{17} with forces 3,4,5.

In this approximation the particles in 2s-1d shells are with a bigger weighting factor than the corresponding particles in the density approximation used so far.

The physical explanation is that such particles can be thought of as being less restricted by the condition on the oscillator constants.

They tend to assume the value of the parameters corresponding to no constraint and the lowering of the 1/2 level is particularly clear in the case of force 5.

The variation of the energy levels corresponding to changes in the spin-orbit coefficients, as illustrated by the graphs of Tables 19, 20, are typical.

In this context it is seen that the 2^+ and 4^+ level in O^{18} are of a nature (predominantly L - S coupling with S = 0) which leads to practically no dependence on the spin-orbit term.

It is important to note, finally, that the best fit to the levels has been obtained by the use of force 1, in which no density dependence has been included, although this force in this particular region tends to overbind the nuclei.

The reason for this behaviour is essentially the fact that in obtaining such a force the emphasis was put on the fit of energy levels in Li^6.

CHAPTER VIII

CONCLUSIONS

The use of different types of nucleon-nucleon interactions in the region of 2s-1d shell nuclei has proved the validity of harmonic oscillator wave functions in cylindrical coordinates in the study of binding energies and spectra of such nucleonic configurations. While some formal difficulties still remain to be solved, such as the independent variation of all the oscillator constants, several new areas appear for future investigations. In particular one should attempt to extend the calculation presented to other nuclei in this region.

The major difficulty of having Hamiltonians whose dimensions are extremely large, could be overcome by avoiding the full diagonalization procedure and looking at a few of the low lying excited states by using approximate methods for the evaluation of the required eigenvalues (MM 64). Investigations performed earlier have shown that except for possible excited states resulting from particle-levels states O^{17} and O^{18} are essentially spherical nuclei, thus providing further justification to the approach used in this work.

On the other hand, nuclei such as F^{19} and Ne^{20} have been found to have strong prolate deformations [Co 65] due to the progressive influence of the $1d_o$ orbitals constant some doubts on the possibility of evaluating the spectra of sucn nuclei at zero deformation.

An important conclusion reached is that forces which are density and energy (state) dependent are extremely important and should not be neglected at least in the calculations of the binding energies of such nuclei [Ma 67].

The reason why such forces give a poor fit to the energy levels with respect to a force not density dependent as force 1, is not clear yet and this problem should be further investigated.

CAPTIONS FOR TABLES AND FIGURES

Tables I, II: The analytic form of the forces used is given with the numerical values of the parameters as determined by M. Manning and D. J. Hughes.

Table III: Sizes of the Hamiltonians for the different nuclei and corresponding to the disjoint subspaces where the diagonalizations were performed.

Table IV to VII: Results for the relevant quantities as obtained in the minimization of the ground state.

Table VIII: Calculated Binding energies vs. experimental for the different forces.

Figs. 1 to 8: Energy levels obtained in this work compared with the experimental data.

Figs. 9-11: The effect of two different "density" approximations are shown for the case of O^{17}. The occupation matrices indicate the weighting factors assigned to the core particles in the two cases.

Fig. 12-13: Effect of different spin orbit coefficient "c" on the levels of O^{17} and O^{18}.

Fig. 14: Influence of the variation of the Majorama component in the nuclear interaction on the levels of O^{18}.

Fig. 16: Binding Energies per particle with different forces vs. experimental values.

FORCES # 1, 2

Analytic form:

$$V(r, R) = (1 - c_3 \rho^{2/3}(R))\,(w + m P_x + b P_\sigma + h P_\tau)\,(V_A \exp(-r^2/\lambda_a^2) + V_R \exp(-r^2/\lambda_r (k)^2))$$

where $\lambda_r(k) = \lambda_r^o (1 + c_1 (k - c_2)^2)$

Force Parameters

Force #	V_A	V_R	λ_a	λ_r^o	c_1	c_2	c_3	w	m	b	h
1	-78.03	82.8	1.5	0.8	0.0	0.0	0.0	0.24	0.71	0.20	-0.05

Force #	w + m	ν*	b - h
2	1.00	-1.228	0.4

* $\nu = 10 (w - m) + 8 (b + h)$

TABLE I

Forces # 3, 4, 5

Analytic form:

$$V(r, R) = (w + m P_x + b P_\sigma + h P_\tau) \left[V_a \exp (\right.$$

where

$$V_a = V_A \left[1 - c_3 \rho^{1/3} \right]$$

$$V_r = V_R \left[1 + c_4 \rho^{2/3} \right]$$

$$\lambda_r = \lambda_r^o (1 + c_1 (k - c_2)^2)$$

Force #	V_A	V_R	λ_a	λ_r^o	c_1
3	-250	255	1.5	1.247	0.15
4	"	"	"	"	"
5	"	"	"	"	"

TABLE

$- r^2/\lambda_a^2) + V_r \exp (- r^2/\lambda_r(k)^2)\Big]$

c_2	c_3	c_4	w	m	h	b
0.836	-0.12731	0.76868	0.5	0.5	-0.375	0.075
"	-0.0436	0.7223	0.5	0.5	-0.2675	0.1375
"	0.04149	0.6427	0.5	0.5	-0.2	0.2

II

CONFIGURATIONS

Nucleus	MZ Value	Hamiltonian
O^{17}	1/2	3 x 3
	3/2	2 x 2
	5/2	1 x 1
O^{18}	0	14 x 14
	1	11 x 11
	2	9 x 9
	3	4 x 4
	4	2 x 2
O^{19}	1/2	37 x 37
	3/2	32 x 32
	5/2	22 x 22
	7/2	12 x 12
	9/2	6 x 6
	11/2	1 x 1
O^{20}	0	81 x 81
	1	72 x 72
	2	60 x 60
	3	39 x 39
	4	24 x 24
	5	9 x 9
	6	3 x 3

TABLE III

Calculations for O^{17}

Occupation matrix $\left[2.0000\right]^{8}$

Restrictions on minimization "none"

For minimum energy

Force	Radius	ρ^2
1	2.131	3.027
2	2.915	5.665
3	2.890	5.567
4	2.963	5.854
5	3.025	6.099

$\left[0.\ 08333\right]^{12}$

z^2	$\alpha(1)$	$\alpha(2)$	B.E. (mev)
1.514	.46418	.52877	-125.432
2.833	.23250	.29054	-123.135
2.784	.25227	.28762	-151.580
2.927	.24153	.27289	-131.262
3.05	.23193	.26184	-114.198

TABLE IV

Calculations for O^{18}

Occupation matrix $\left[2.000\right]^8$

Restrictions on minimization "none"

For minimum energy

Force	Radius	ρ^2
1	2.205	3.240
2	2.996	5.984
3	2.961	5.846
4	3.032	6.13
5	3.091	6.371

$$\left[0.\ 16666\right]^{12}$$

z^2	$\alpha(1)$	$\alpha(2)$	B.E. (mev)
1.620	.46418	.52877	-125.433
2.992	.22692	.28769	-128.180
2.923	.24599	.28567	-157.630
3.065	.23572	.27183	-137.108
3.185	.22630	.26187	-119.866

TABLE V

Calculations for O^{19}

Occupation matrix $\left[2.000\right]^{8}$ $\left[.24999\right]^{12}$

Minimization of the ground state performed in a model space spanned by the basis states

$(0\ 0\ 2)^2\ (0\ 1\ 1)^1$; $(0\ 0\ 2)^2\ (1\ 0\ 0)^1$; $(0\ 1\ 1)^2\ (0\ -1\ 1)^1$; $(0\ 1\ 1)^2\ (0\ -2\ 0)^1$;

For minimum energy

Force	Radius	ρ^2	z^2	$\alpha(1)$	$\alpha(2)$	B.E. (mev)
1	2.278	3.459	1.729	.42380	.50296	-123.273
2	3.071	6.287	3.144	.22362	.28463	-131.099
3	3.028	6.112	3.056	.24162	.28331	-161.250
4	3.095	6.387	3.194	.73146	.27087	-140.976
5	3.151	6.621	3.310	.22244	.26198	-123.847

TABLE VI

Calculations for O^{20}

Occupation matrix $\left[2.0000\right]^{8}$ $\left[0.33333\right]^{12}$

Minimization of the ground state performed in a model space spanned by the basis states

$(0\ 0\ 2)^2\ (1\ 0\ 0)^2$; $(0\ 0\ 2)^2\ (0\ 1\ 1)^1\ (0\ -1\ 1)^1$; $(0\ 0\ 2)^2\ (0\ 1\ 1)^1\ (0\ -2\ 0)^1$; $(0\ 0\ 2)^2\ (0\ 1\ 1)^1\ (0\ -1\ 1)^1$;
$(0\ 0\ 2)^2\ (0\ 1\ 1)^1\ (1\ 0\ 0)^1$; $(0\ 0\ 2)\ (0\ -1\ 1)^1\ (1\ 0\ 0)^1$; $(0\ 0\ 2)^2\ (0\ -1\ 1)^1\ (0\ 2\ 0)^1$; $(0\ 0\ 2)^2\ (0\ 2\ 0)^1\ (0\ -2\ 0)^1$
$(0\ 0\ 2)^2\ (0\ 2\ 0)^1\ (0\ -2\ 0)^1$

For minimum energy

Force	Radius	ρ^2	z^2	$\alpha(1)$	$\alpha(2)$	B.E. (mev)
1	2.351	3.685	1.843	.40578	.48966	-124.044
2	3.151	6.618	3.309	.21870	.28009	-135.570
3	3.107	6.436	3.218	.23303	.27971	-166.515
4	3.170	6.701	3.350	.22408	.26838	-146.354
5	3.223	6.923	3.462	.21623	.26041	-129.244

TABLE VII

BINDING ENERGIES

	1	2	3	4	5	exp
O^{17}	125.432	123.135	151.58	131.262	114.198	131.762
O^{18}	126.007	128.180	157.630	137.108	119.866	139.808
O^{19}	123.273	131.099	161.250	140.976	123.847	143.765
O^{20}	124.044	135.576	166.515	146.354	129.244	151.370

TABLE VIII

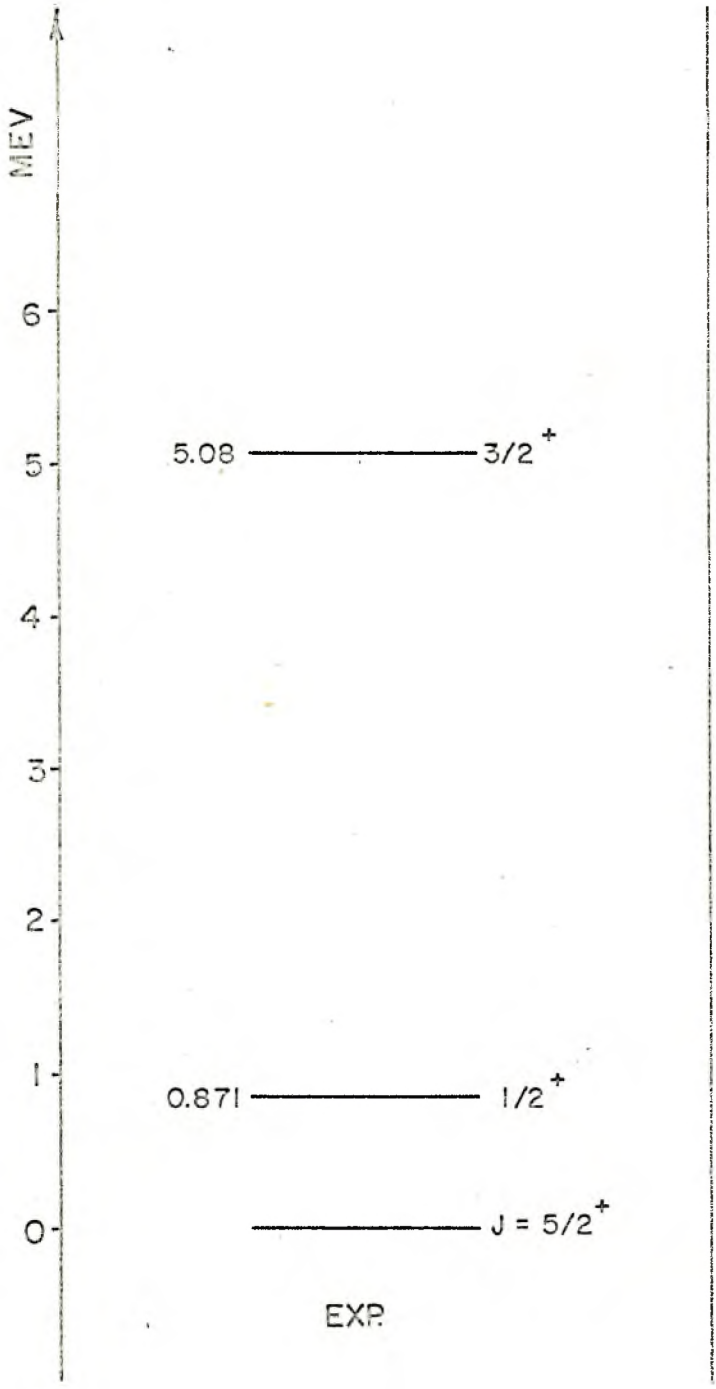
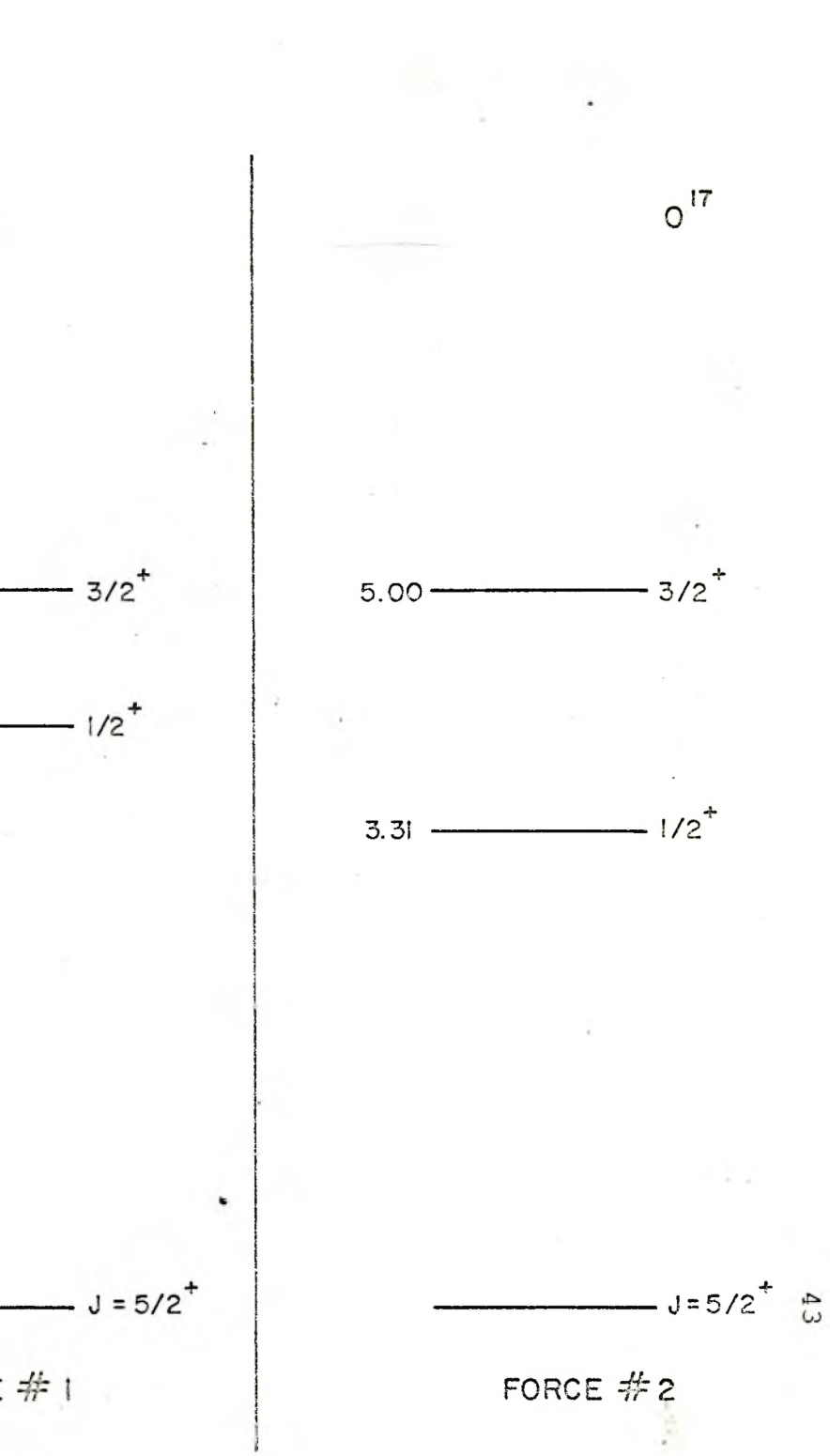
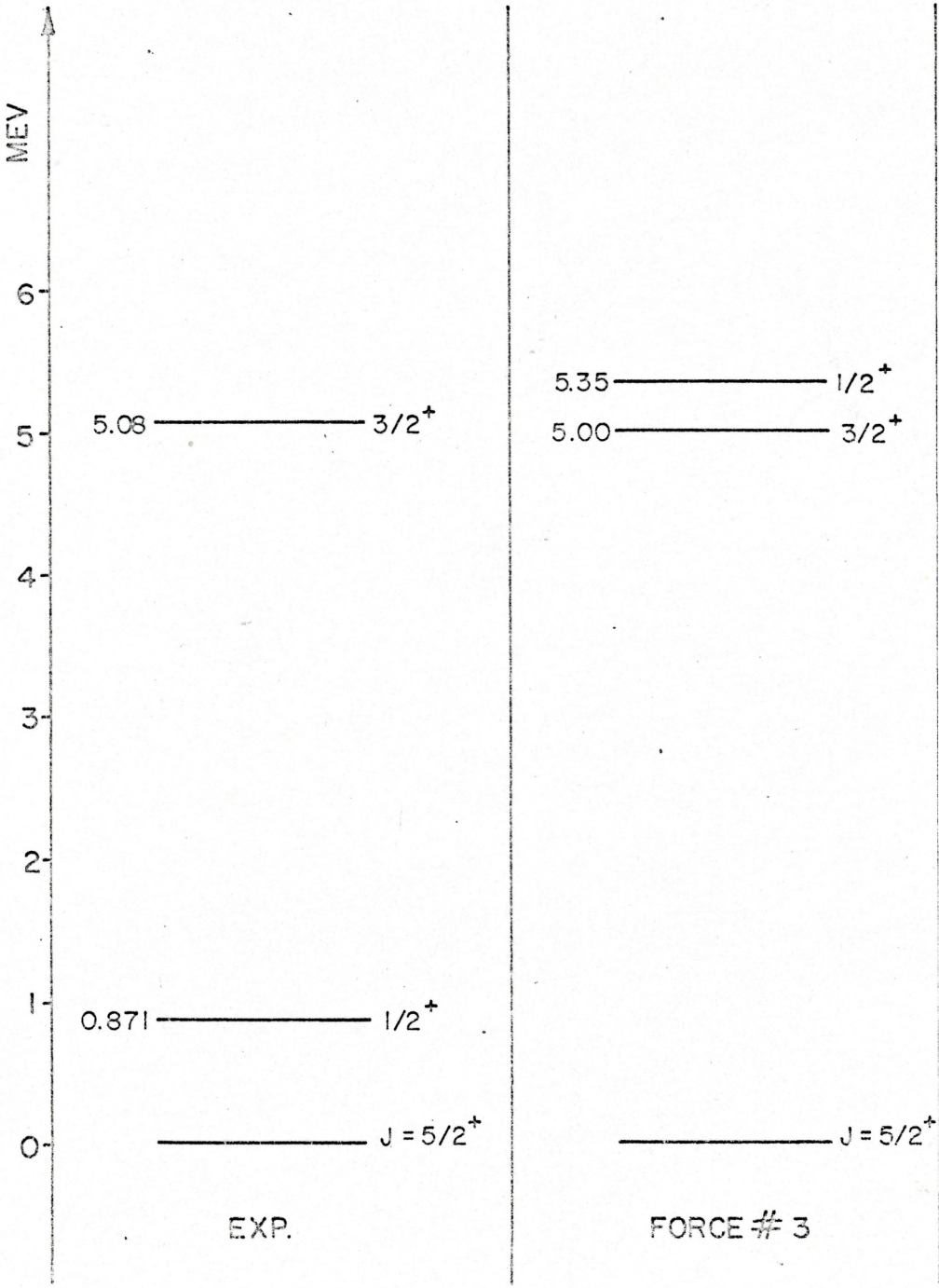


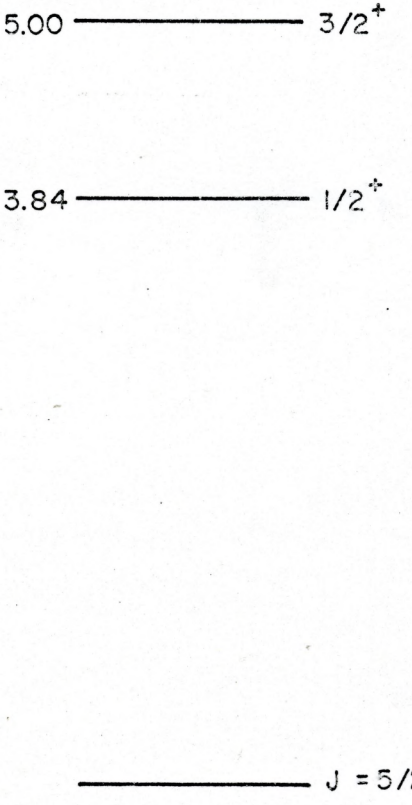
FIGURE 1


O^{17}
$3/2^+$
$1/2^+$
$J = 5/2^+$
1
5.00
$3/2^+$
3.31
$1/2^+$
$J = 5/2^+$
FORCE # 2



FIGUR

FORCE # 4



FORCE #5

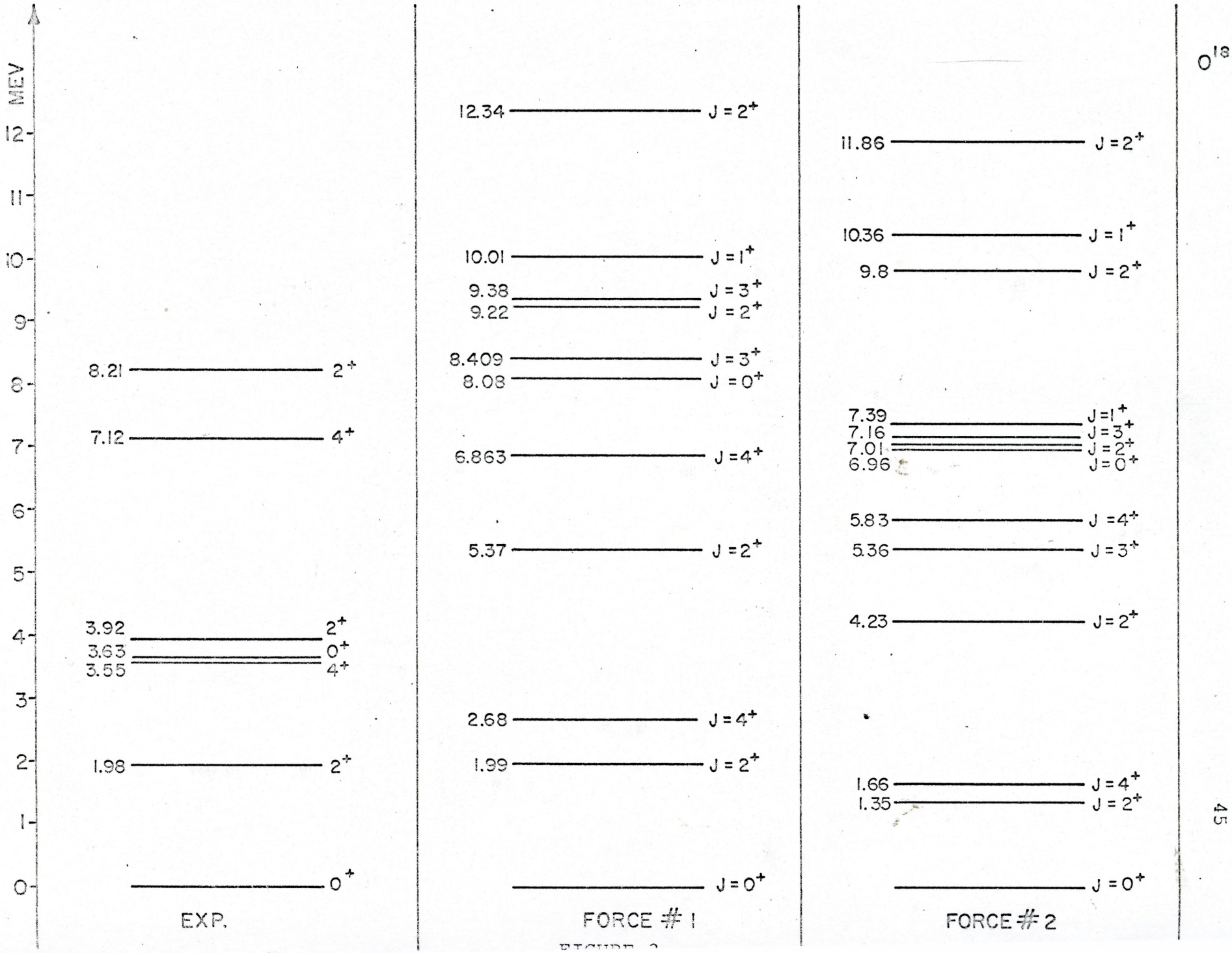
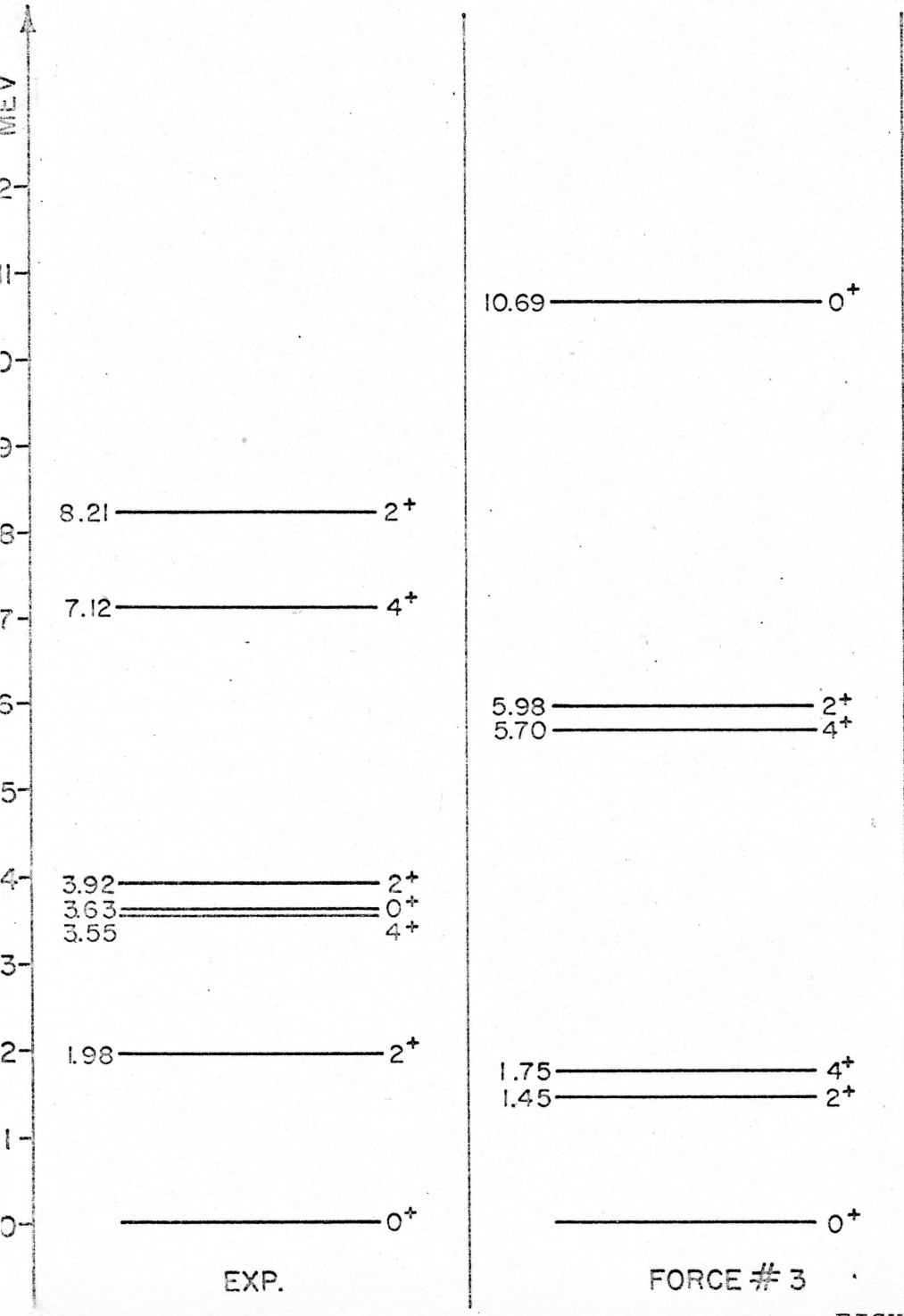
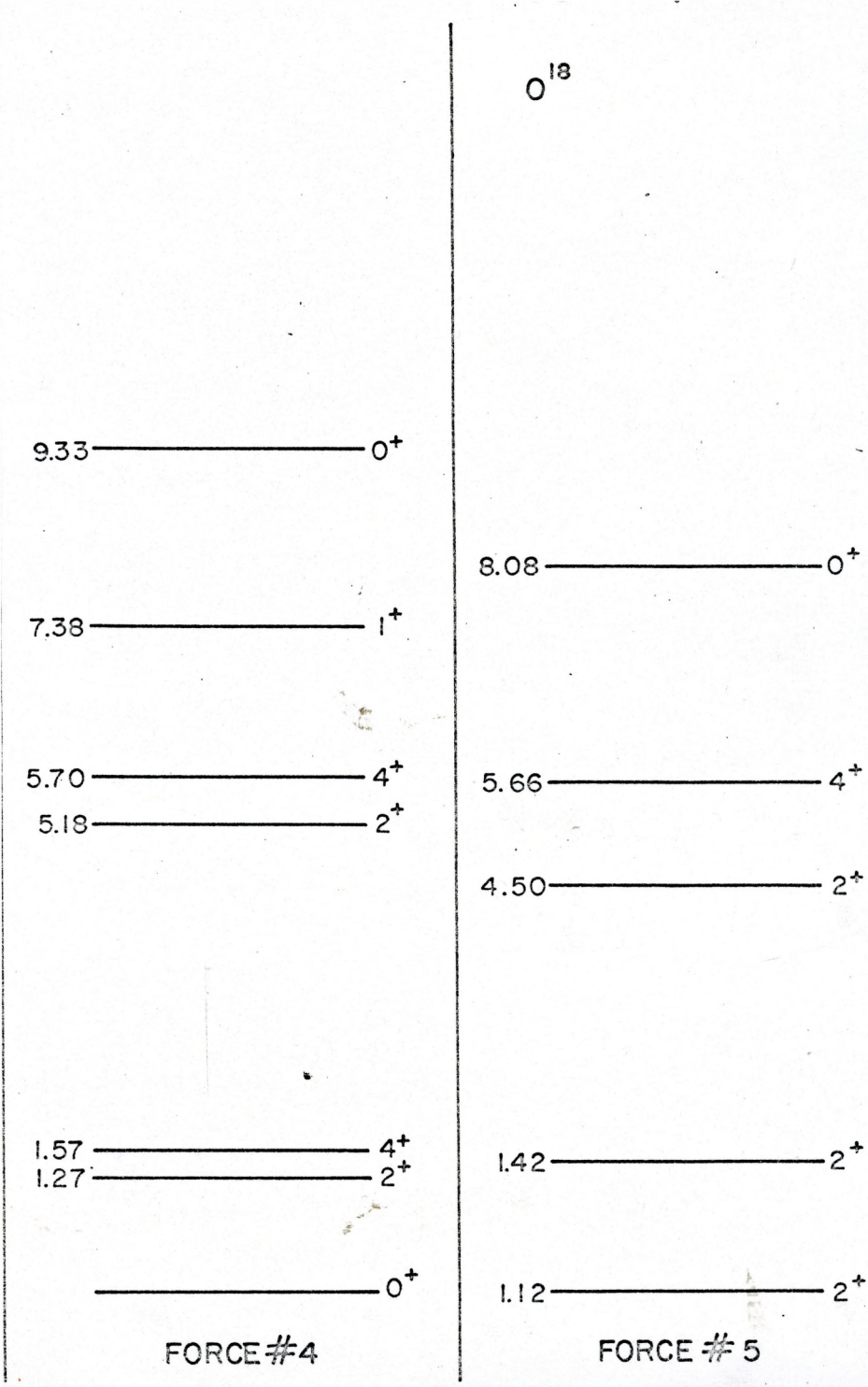

MEV
12
11
10
9
8
7
6
5
4
3
2
1
0
8.21
2+
7.12
4+
3.92
3.63
3.55
2+
0+
4+
1.98
2+
0+
EXP.
12.34
J = 2+
10.01
J = 1+
9.38
9.22
J = 3+
J = 2+
8.409
8.08
J = 3+
J = 0+
6.863
J = 4+
5.37
J = 2+
2.68
J = 4+
1.99
J = 2+
J = 0+
FORCE # 1
11.86
J = 2+
10.36
J = 1+
9.8
J = 2+
7.39
7.16
7.01
6.96
J = 1+
J = 3+
J = 2+
J = 0+
5.83
J = 4+
5.36
J = 3+
4.23
J = 2+
1.66
J = 4+
1.35
J = 2+
J = 0+
FORCE # 2
O18

FIGURE 2


MEV
10.69 0+
8.21 2+
7.12 4+
5.98 2+
5.70 4+
3.92 2+
3.63 0+
3.55 4+
1.98 2+
1.75 4+
1.45 2+
0+
0+
EXP.
FORCE # 3

FIGU


O^{18}
9.33 0^+
7.38 1^+
5.70 4^+
5.18 2^+
1.57 4^+
1.27 2^+
0^+
FORCE #4
8.08 0^+
5.66 4^+
4.50 2^+
1.42 2^+
1.12 2^+
FORCE # 5

RE 4

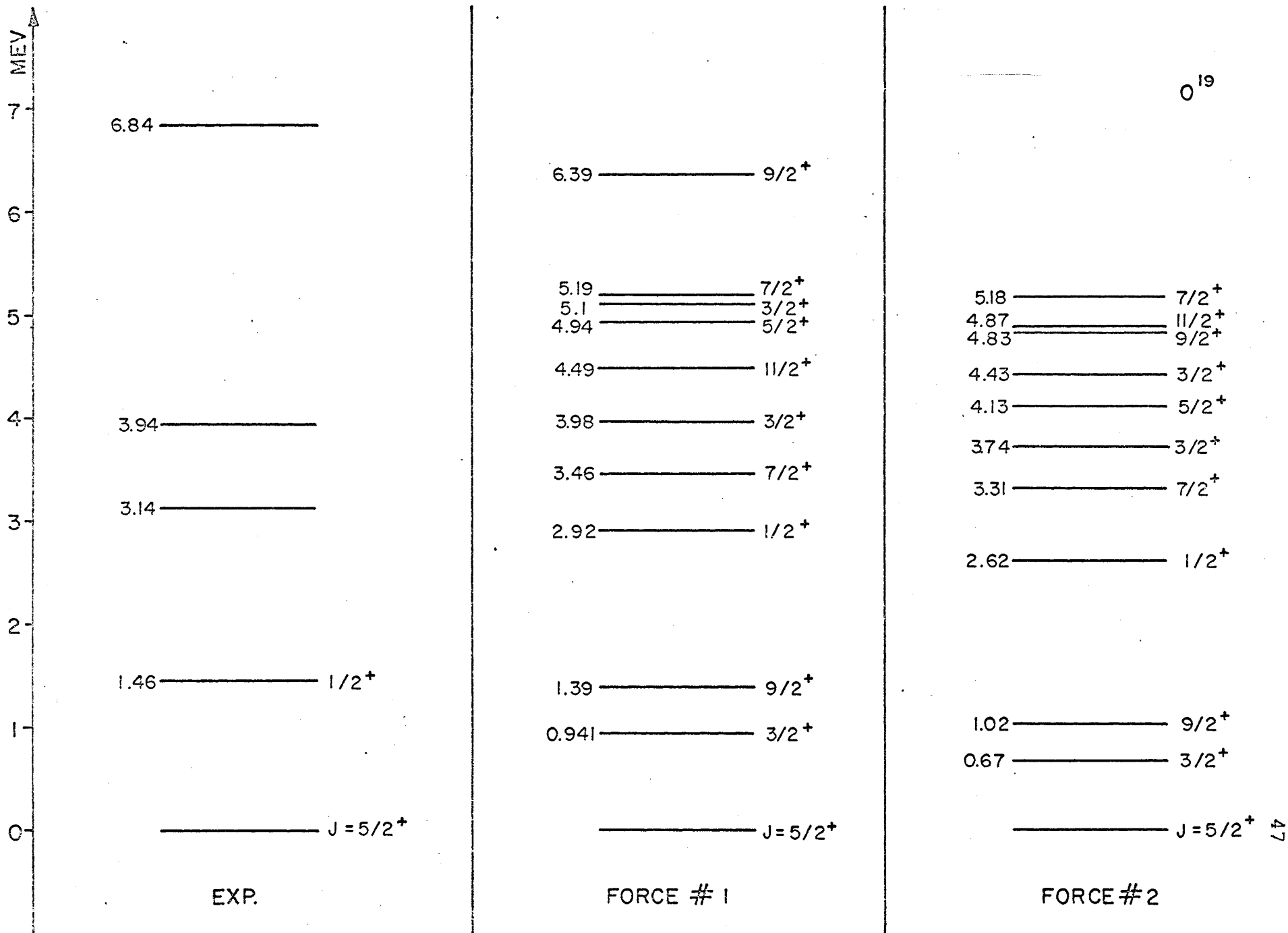
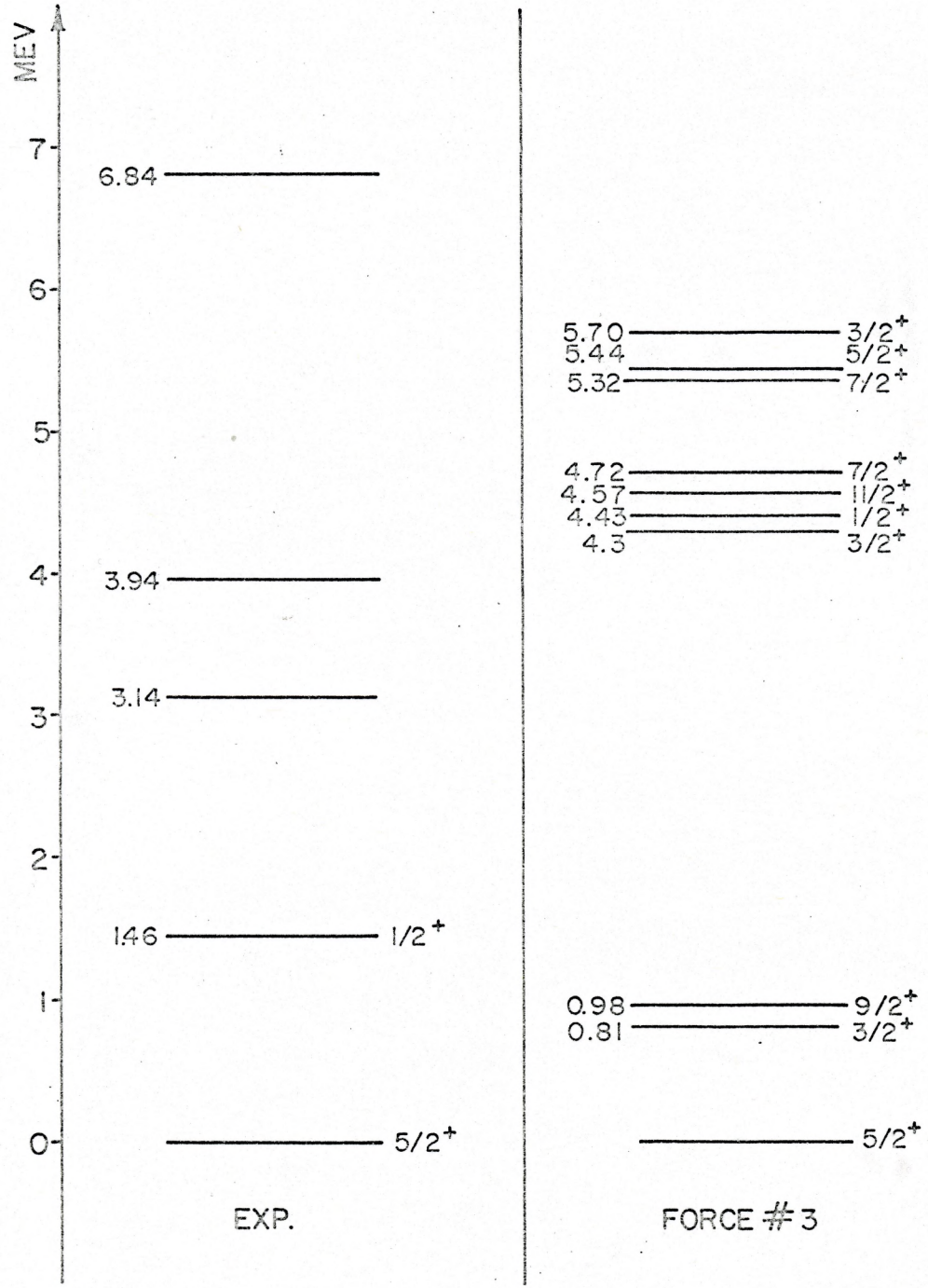
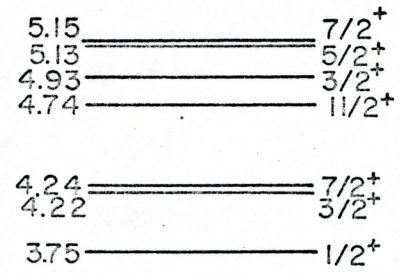
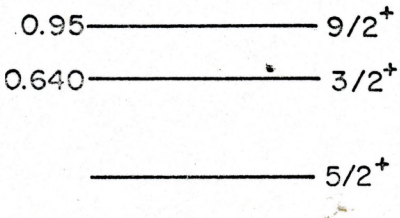

MEV
7
6
5
4
3
2
1
0
6.84
3.94
3.14
1.46
1/2+
J = 5/2+
EXP.
6.39
9/2+
5.19
7/2+
5.1
3/2+
4.94
5/2+
4.49
11/2+
3.98
3/2+
3.46
7/2+
2.92
1/2+
1.39
9/2+
0.941
3/2+
J=5/2+
FORCE # 1
O19
5.18
7/2+
4.87
11/2+
4.83
9/2+
4.43
3/2+
4.13
5/2+
3.74
3/2+
3.31
7/2+
2.62
1/2+
1.02
9/2+
0.67
3/2+
J = 5/2+
FORCE #2

FIGURE 5

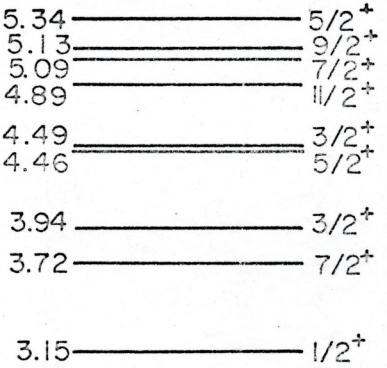

MEV
7
6
5
4
3
2
1
0
6.84
3.94
3.14
1.46
1/2+
5/2+
EXP.
5.70
3/2+
5.44
5/2+
5.32
7/2+
4.72
7/2+
4.57
11/2+
4.43
1/2+
4.3
3/2+
0.98
9/2+
0.81
3/2+
5/2+
FORCE #3

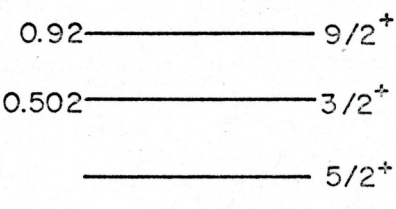
FIGU





FORCE # 4





FORCE # 5

RE 6

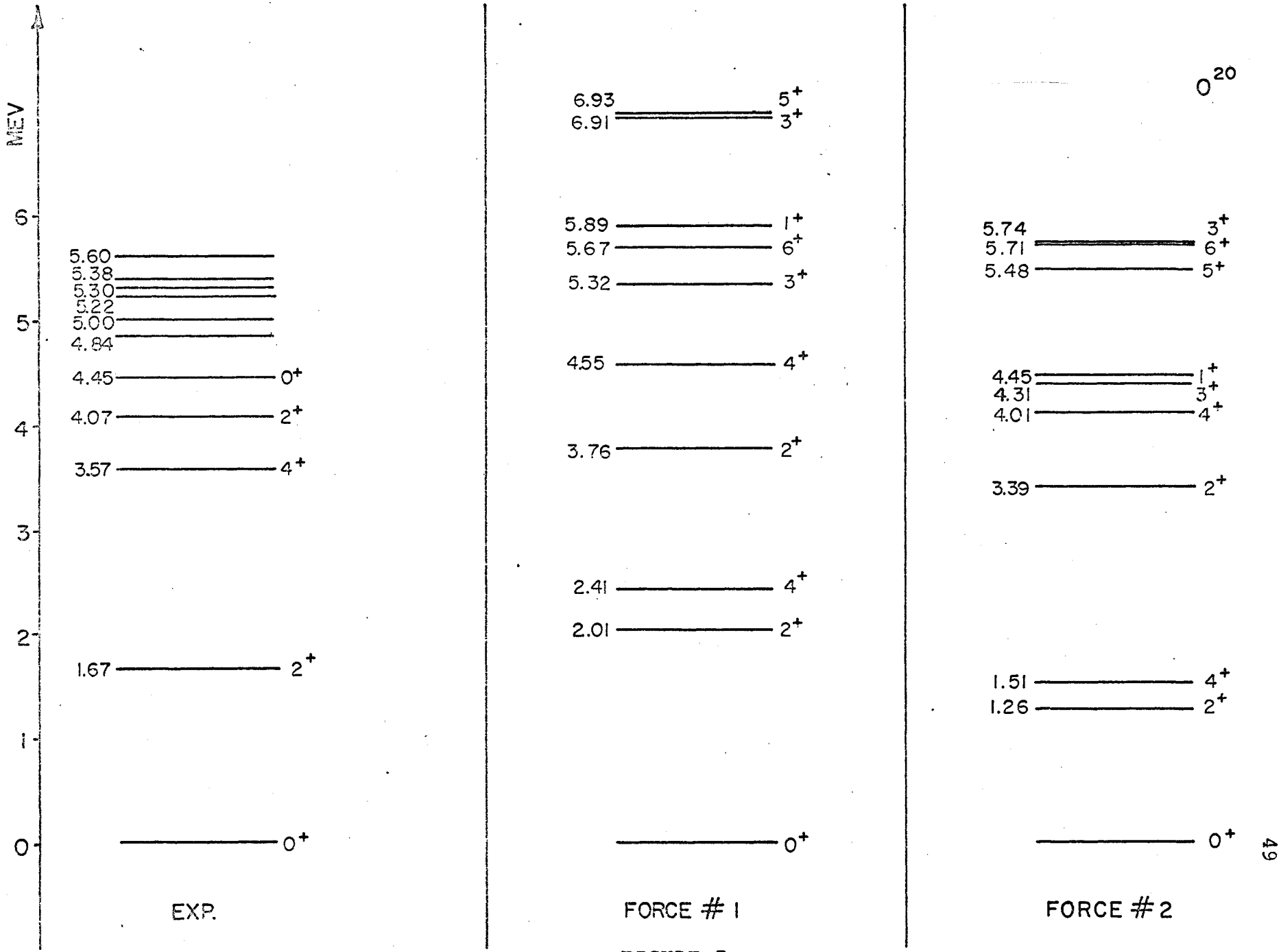
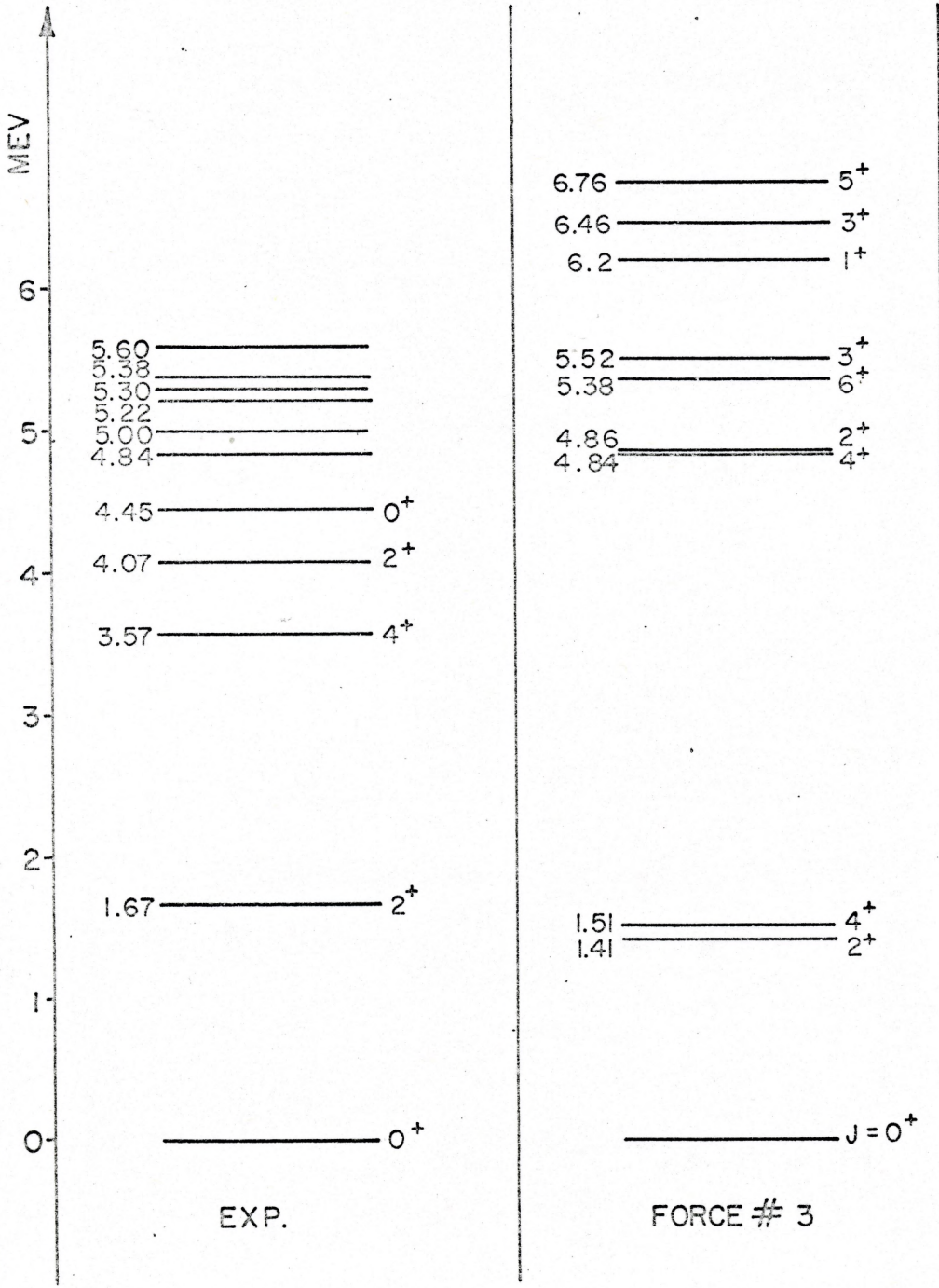
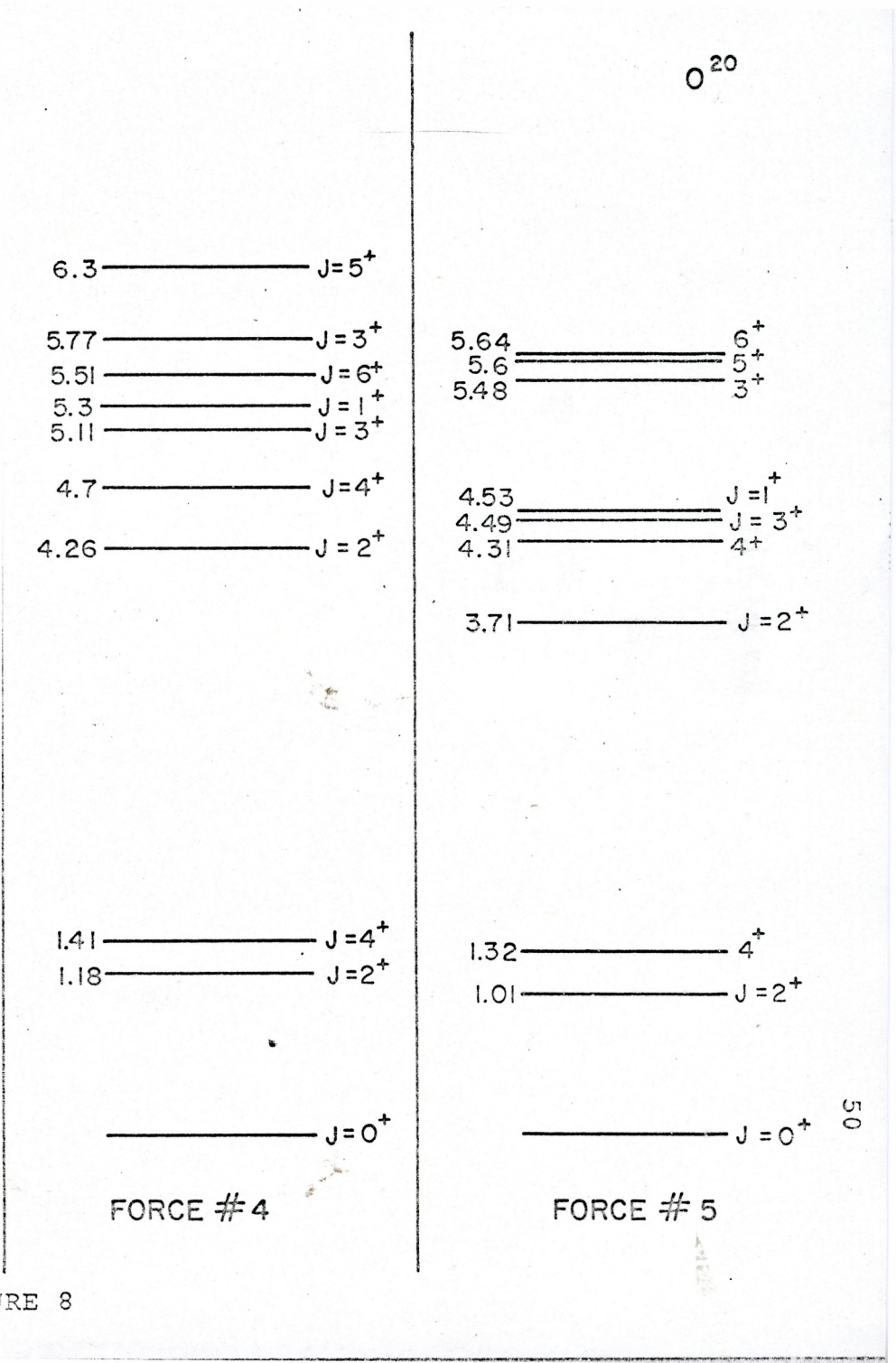

MEV
6
5
4
3
2
1
0
5.60
5.38
5.30
5.22
5.00
4.84
4.45 0+
4.07 2+
3.57 4+
1.67 2+
0+
EXP.
6.93 5+
6.91 3+
5.89 1+
5.67 6+
5.32 3+
4.55 4+
3.76 2+
2.41 4+
2.01 2+
0+
FORCE # 1
O20
5.74 3+
5.71 6+
5.48 5+
4.45 1+
4.31 3+
4.01 4+
3.39 2+
1.51 4+
1.26 2+
0+
FORCE # 2

FIGURE 7



FIGU


O 20
6.3
J=5+
5.77
J = 3+
5.51
J = 6+
5.3
J = 1+
5.11
J = 3+
4.7
J=4+
4.26
J = 2+
1.41
J =4+
1.18
J =2+
J=0+
FORCE #4
5.64
6+
5.6
5+
5.48
3+
4.53
J =1+
4.49
J = 3+
4.31
4+
3.71
J =2+
1.32
4+
1.01
J =2+
J = 0+
FORCE # 5

RE 8

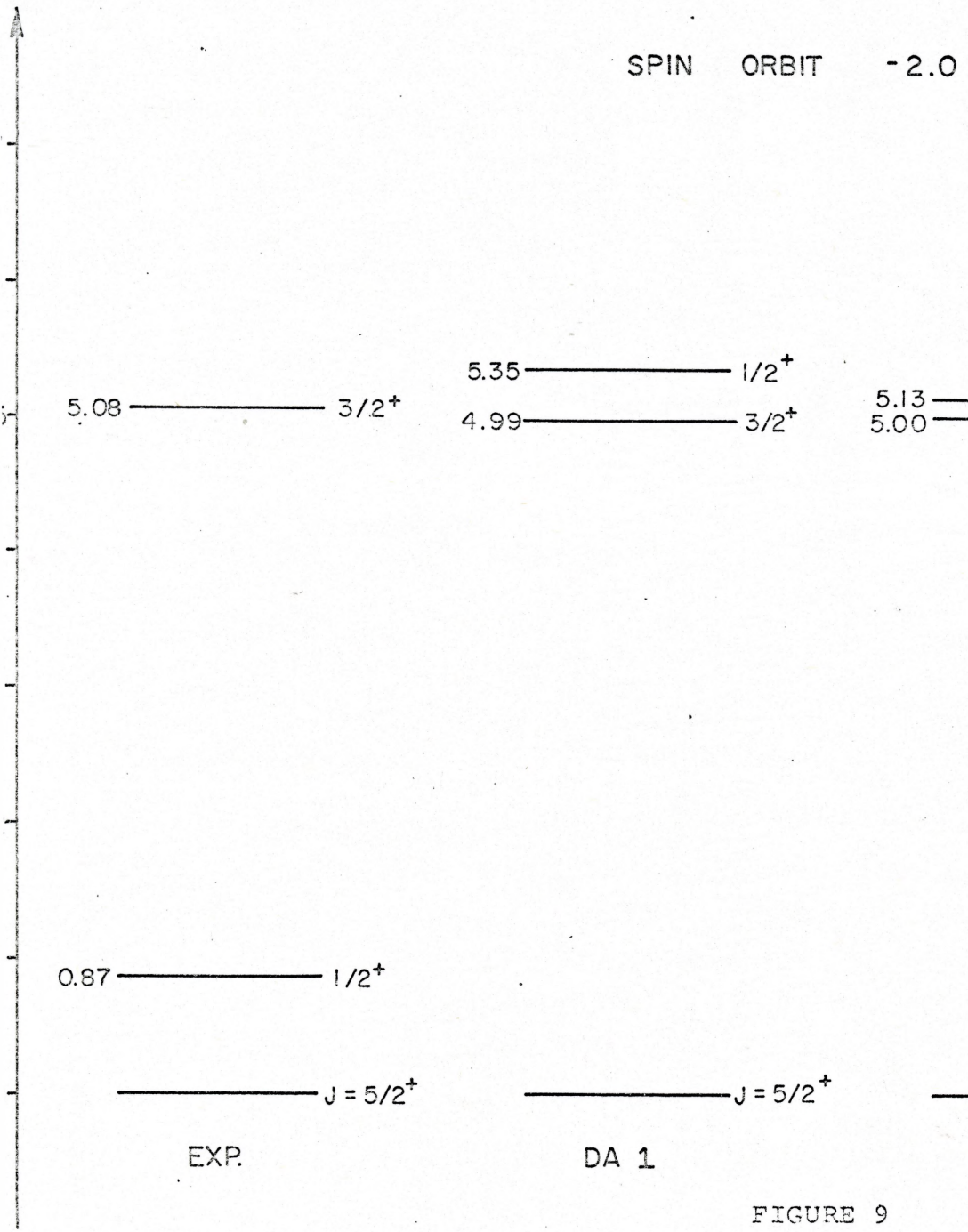


FIGURE 9

O^{17} FORCE #3

DA 1

OCCUPATION MATRIX

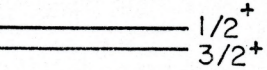
$[2]^{8}$ $[.08333]^{12}$

RADIUS = 2.8894

ρ^2 = 5.5658

Z^2 = 2.7829

B.E = 151.668



DA 2

OCCUPATION MATRIX

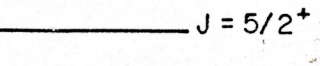
$[1.5]^{2}$ $[2]^{6}$ $[.16666]^{12}$

RADIUS = 2.9516

ρ^2 = 5.8082

Z^2 = 2.9041

B.E = 154.668



DA 2

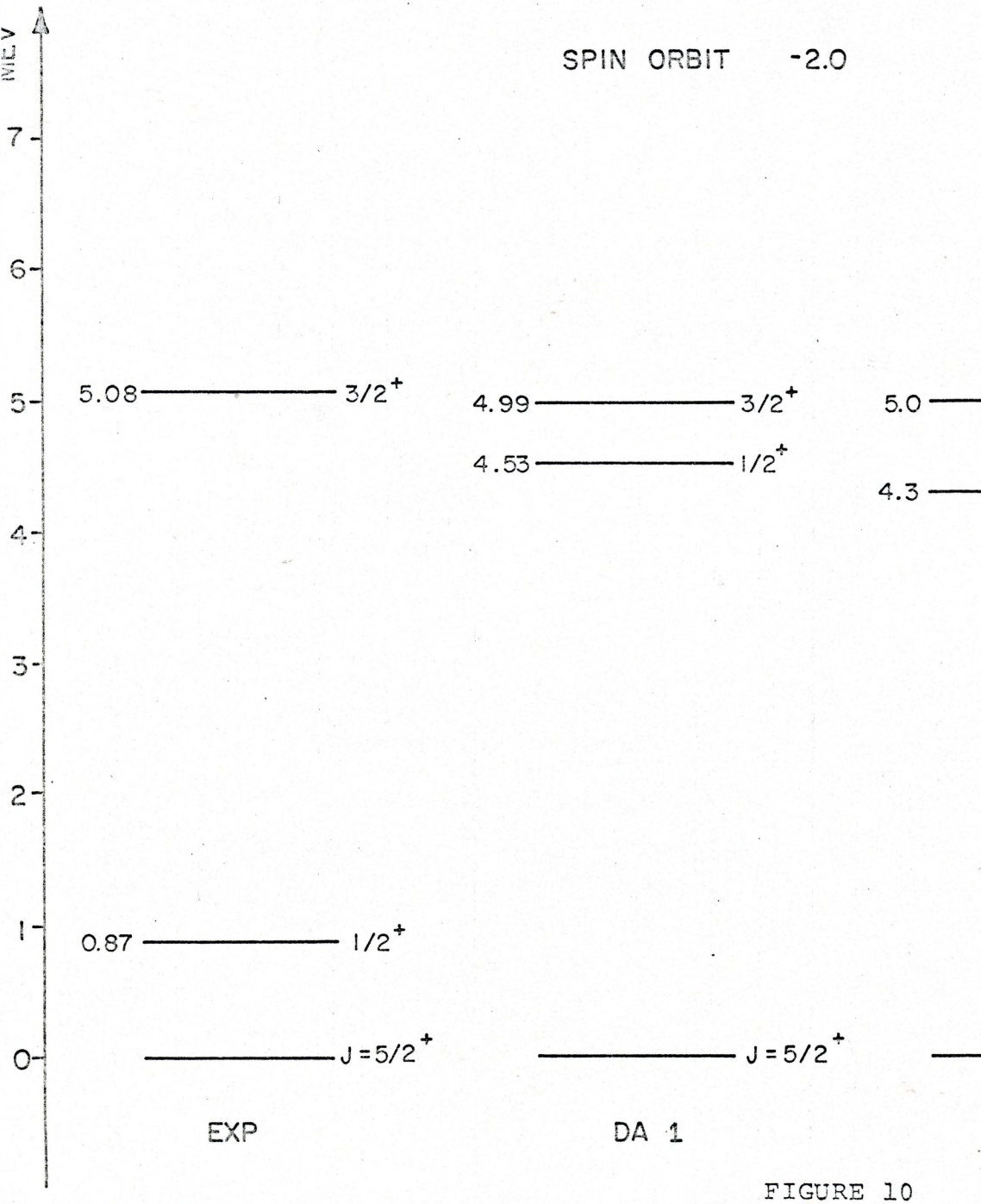

SPIN ORBIT -2.0
MEV
7
6
5
4
3
2
1
0
5.08
3/2+
0.87
1/2+
J=5/2+
EXP
4.99
3/2+
4.53
1/2+
J=5/2+
DA 1
5.0
4.3

FIGURE 10

O^{17} FORCE #4

DA 1

OCCUPATION MATRIX

$[2]^{8}$ $[0.08333]^{12}$

RADIUS = 2.96318

ρ^2 = 5.853

Z^2 = 2.9268

B.E = 131.262

$3/2^+$

$1/2^+$

DA 2

OCCUPATION MATRIX

$[1.5]^2$ $[2]^6$ $[0.6666]^{12}$

RADIUS = 3.0244

ρ^2 = 6.098

Z^2 = 3.049

B.E = 134.363

$J = 5/2^+$

DA 2

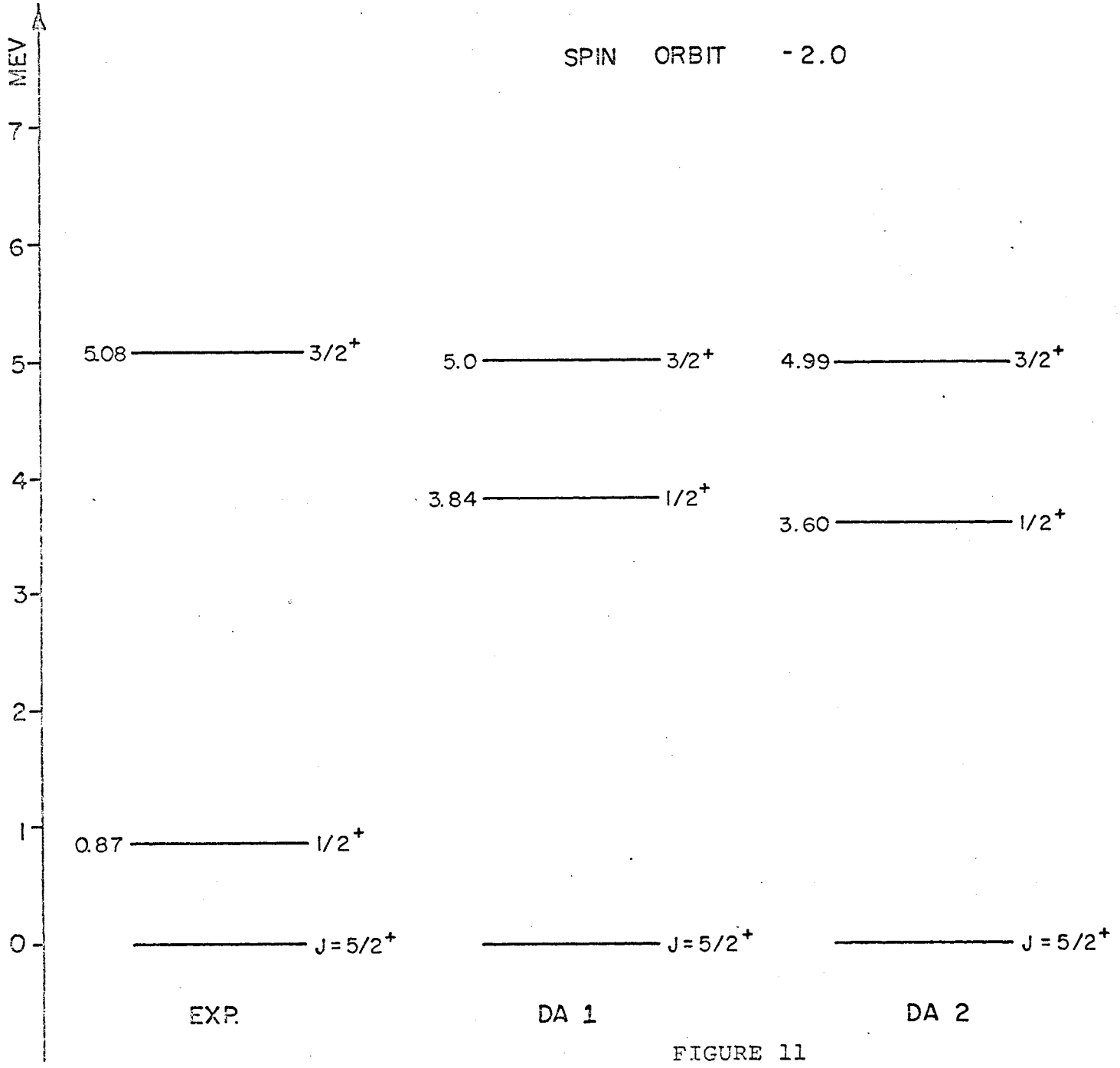


FIGURE 11

O^{17} FORCE#5

DA 1

OCCUPATION MATRIX

$[2]^{8}$ $[.08333]^{12}$

RADIUS = 3.0247

ρ^2 = 6.0993

Z^2 = 3.0496

B.E = 114.197

DA 2

OCCUPATION MATRIX

$[1.5]^{2}$ $[2]^{6}$ $[.16666]^{12}$

RADIUS = 3.0854

ρ^2 = 6.3465

Z^2 = 3.1732

B.E = 117.316

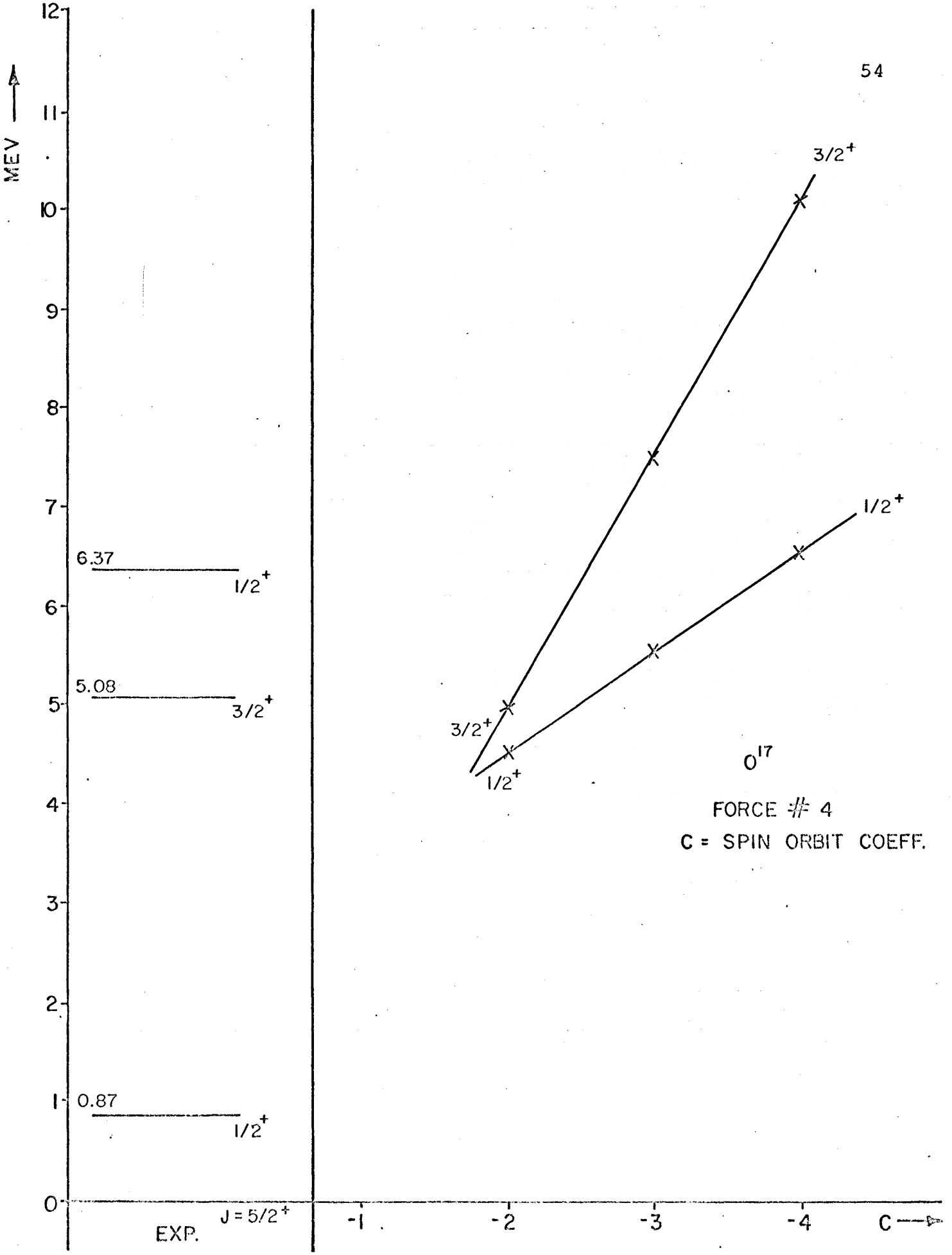

MEV
12
11
10
9
8
7
6
5
4
3
2
1
0
6.37
1/2+
5.08
3/2+
0.87
1/2+
EXP.
J = 5/2+
-1
-2
-3
-4
C
3/2+
1/2+
3/2+
1/2+
O17
FORCE # 4
C = SPIN ORBIT COEFF.

FIGURE 12

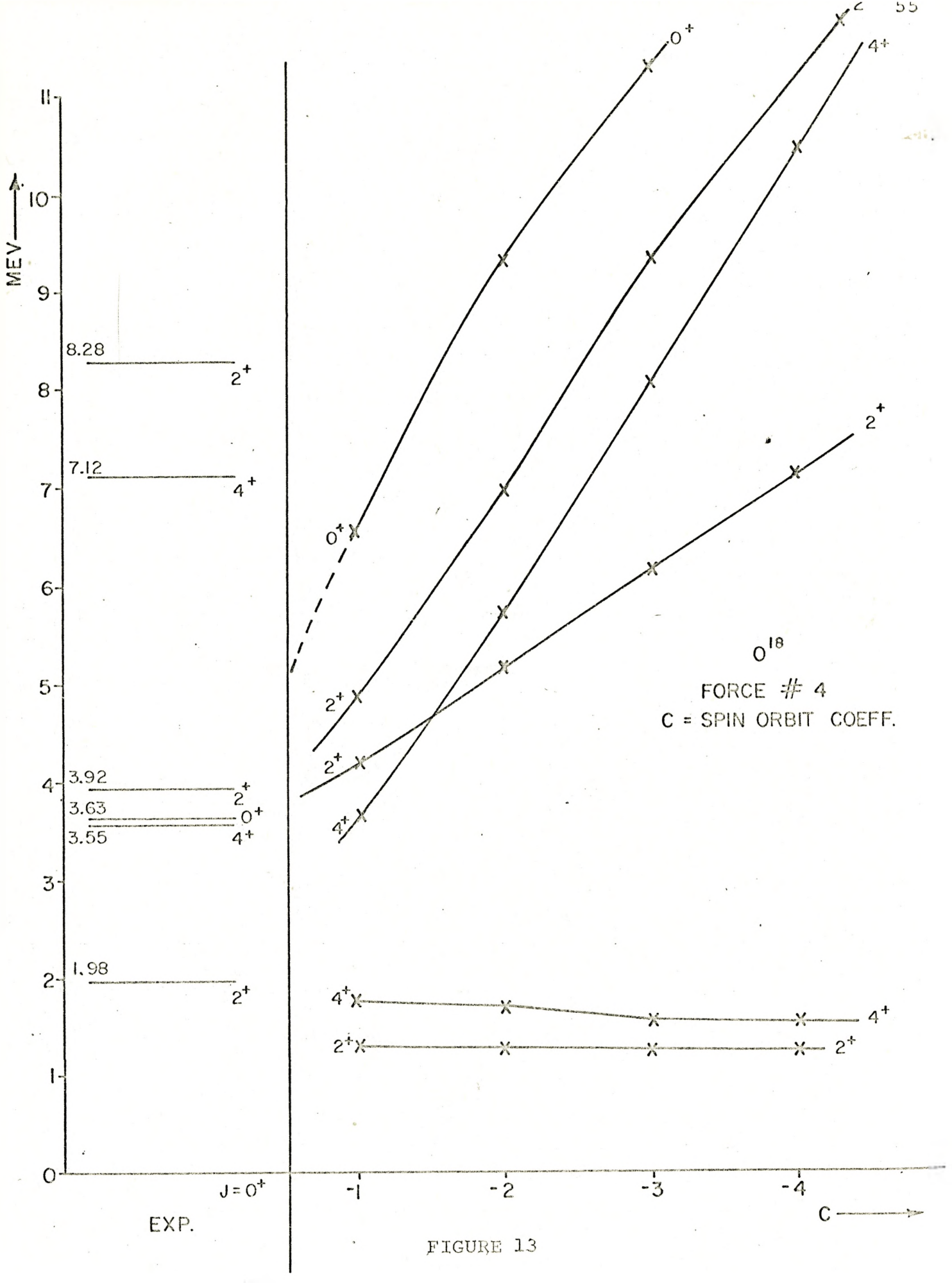

MEV
11
10
9
8
7
6
5
4
3
2
1
0
8.28
2+
7.12
4+
3.92
2+
3.63
0+
3.55
4+
1.98
2+
J=0+
EXP.
0+
2+
2+
4+
2+
4+
4+
2+
O18
FORCE # 4
C = SPIN ORBIT COEFF.
-1
-2
-3
-4
C

FIGURE 13

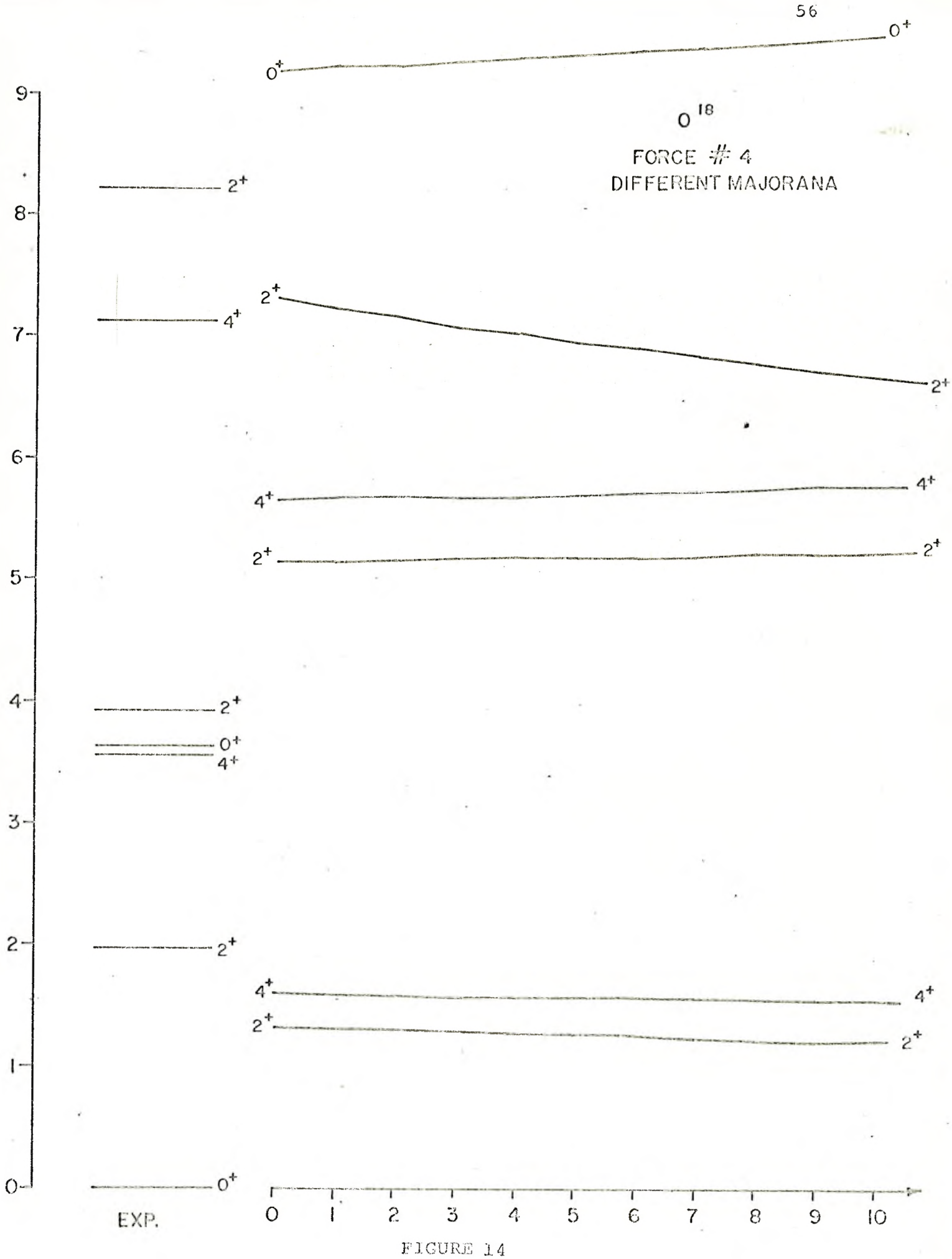

O 18
FORCE # 4
DIFFERENT MAJORANA
0+
0+
2+
4+
2+
2+
4+
4+
2+
2+
2+
0+
4+
2+
2+
4+
4+
2+
2+
0+
EXP.
0
1
2
3
4
5
6
7
8
9
10

FIGURE 14

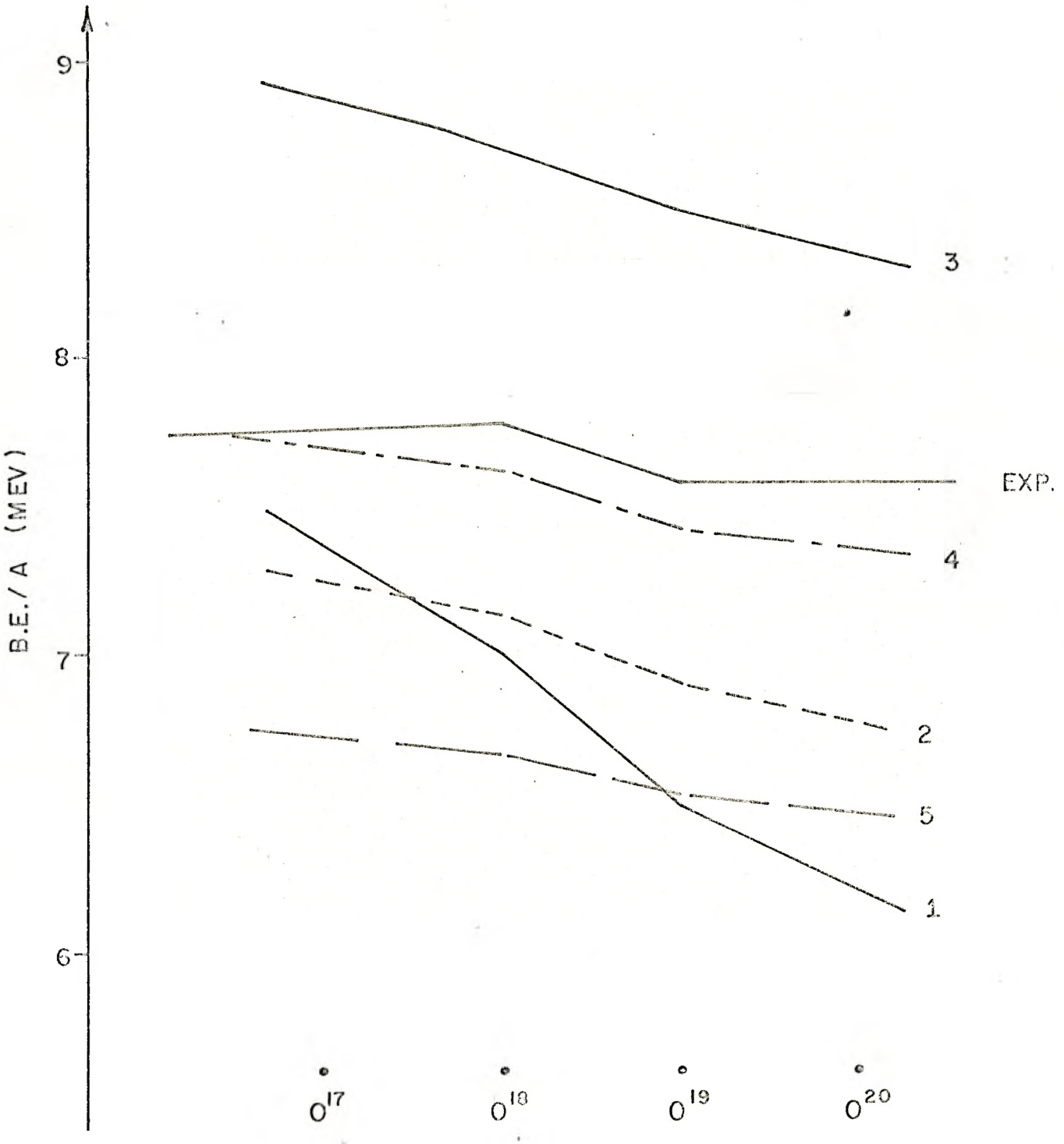


FIGURE 15

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MM (64)