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Relativistic Many-Body Calculations of Energies for $n = 3$ States in Aluminiumlike Ions

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Abstract. Energies of the 148 ($3l3l'3l''$) states for aluminiumlike ions with Z =14–100 are evaluated to second order in relativistic many-body perturbation theory. Second-order Coulomb and Breit-Coulomb interactions are included. Corrections are made to lowest order for the frequency-dependent Breit interaction and for the Lamb shift. A detailed discussion of the various contributions to the energy levels is given for aluminiumlike germanium (Z=32). Comparisons of the calculated energy levels with available experimental data are made for the entire sequence.

Key words:atomic database - Excitation energies, correlation, relativistic and QED effects

I. INTRODUCTION

Correlation, relativistic, and radiative effects each play an important role for a fundamental atomic theory. Various computer programs have been created to calculate atomic characteristics; the most well-known are: MCHF (Froese Fischer [1]), MCHFP (Cowan [2]), MCDF (Grant [3], Desclaux [4], YODA Code [5]), SUPERSTRUCTURE (Eisner [6]), AUTOLSJ (Dubau [7]), MODEL POTENTIAL (Klapish [8], Ivanova [9]), MZ Code [10], and MBPT code [11]. Numerous papers were published by using these methods. Below, we review some papers based on fully relativistic calculations (MCDF, MBPT).

A many-body perturbation theory with a relativistic Hartree-Fock basis allows to obtain results for any atomic characteristics of atoms and ions with reliable accuracy. The first order perturbation theory is identical to multiconfiguration Dirac-Fock (MCDF) calculations with including quasi-degenerate states (for example, ns^2 $+np^2$). The second order perturbation theory describes the correlation effects by including virtual excitation. Partly this contribution can be taken into account by a CI (configuration interaction) method. CI calculations give very accurate result for a two-electron system. Unfortunately, the number of configuration increases very rapidly with an increasing number of electrons in a system. Using Dirac-Fock functions as a basis set, it is possible to consider any system as a core and a valence electron. In this case, the Be- and Mg-like systems can be represented as systems with a $1s^2$ and $1s^22s^22p^6$ cores and two valence electrons accordingly. The correlation contribution should be separated for three parts: correlation of core ($1s^2$, $1s^22s^22p^6$) electrons, correlation between a core and valence electrons, and correlation of two valence electrons. The second order perturbation theory with a Dirac-Fock basis allows to consider correlation effects directly by summing over virtual states. Recently, a MBPT method was used to obtain excitation energies and transition rates in a Be-like system [12–17] and in a Mg-like system [18] in a large scale of Z. It was shown that an agreement with experiment improves substantially with as nuclear charge increases.

The MBPT method was applied to calculate energies and transitions rates for a system with three valence electrons [19–22]. Boronlike ions are simple atomic systems for which both three-electron interactions and interactions with an atomic core are important. Three-electron interactions play a dominant role, of course, for ($1s2lnl'$) autoionizing levels of lithiumlike ions; however, for such ions there are no core interaction [23–25].

The aluminum isoelectronic sequence has three valence electrons outside a closed n=2 core, and is thus a model for studying strong correlation in close lying levels of heavy atoms. There are many examples in this sequence of level-crossings of states having the same parity and angular momentum; such examples occur for both low and high values of the nuclear charge Z. Notably, the $3s3p^2$, the $3s3p3d$, and the $3p^3$ levels cross the $3s^2nl$ (l=0 to 4) levels, becoming relatively more tightly bound as the nuclear charge Z increases. Such crossings provide severe tests of atomic structure calculations. Comparisons with measurements of energies, transition rates, and fine-structure intervals also provide useful tests of the quality of different theoretical models. Many experimental energy levels and fine-structure intervals are now available up to very high nuclear charge (Z=40) for the $3l3l'3l''$ levels; additionally, experimental rates for some transitions between these levels are available. The objective of this paper is to present a comprehensive set of calculations for $3l3l'3l''$ energies , and to compare them with previous calculations and experiments for the entire Al isoelectronic sequence. Most earlier measurements and calculations focused on the $3s^23p$ ^2P states and the low-lying $3s3p^2$ ^4P_J levels. Very few results exist for other $3s^23d$, $3s3p3d$ and $3p^3$ states. The large number of possible transitions have made experimental identification difficult. With this new, more accurate, set of calculations, experimental verifications should become simpler and more reliable.

Several early theoretical calculations for Al-like ions were based on the Hartree-Fock method: excitation energies and line strengths for the low-lying states of ions in the sequence were studied using multiconfiguration Dirac-Fock (MCDF) wave functions by Huang [26] and oscillator strengths were evaluated using multiconfiguration Hartree-Fock wave function by Fawcett [27]. Wavelengths, oscillator strengths and transition probabilities for the E1 transitions between levers of low-lying levels of the Al-like ions were calculated using relativistic parametric potential method by Farrag *et al.* in Ref. [28].

In the present paper, we use relativistic many-body perturbation theory (MBPT) to determine energies of $n = 3$ states for aluminiumlike ions with nuclear charges in the range $Z = 14$–100. We illustrate our calculation with detailed studies of the cases $Z = 32$. Our calculations are carried out to second order in perturbation theory and include the second-order Coulomb interaction. Correction for the frequency-dependent Breit interaction are taken in account in the lowest order. The screened self-energy and vacuum polarization data given by Blundell [29] are used to determine the QED correction $E^{(\mathrm{Lamb})}$. The three-electron contributions to the energy are compared with the one- and two-electron contributions. They are found to contribute about 10-20% of the total second-order energy.

Our perturbation theory calculations are carried out using single-particle orbitals calculated in the HF potential of the $1s^2 2s^2 2p^6$ neonlike core. As a first step, we determine and store the single-particle contributions to the energy for the five n=3 states ($3s, 3p_{1/2}, 3p_{3/2}, 3d_{3/2}$, and $3d_{5/2}$) in lowest, first and second orders. These contributions are precisely those needed to calculate energies of n=3 states of sodiumlike ions. Next, we evaluate and store the 155 two-particle matrix elements of the effective Hamiltonian, $\langle 3l3l'\, J|H^{\mathrm{eff}}|3l''3l'''\, J\rangle$, in the first and second orders. The one- and two-particle matrix elements were used previously to evaluate energies of the $(3l3l')$ levels for magnesiumlike ions [18]. Finally, second-order three-particle matrix elements are evaluated. Combining this data using the method described below, we calculate one-, two-, and three-particle contributions to the energies of aluminiumlike ions.

The present calculations are compared with predicted results from Refs. [30–45]. Comparisons of multiplet splitting along the isoelectronic sequence with available experimental data are also given.

II. METHOD

The evaluation of the second-order energies for Al-like ions follows the pattern of the corresponding calculation for Mg-like ions given in Ref. [18]. In particular, we use the second-order one- and two-particle matrix elements for Mg-like ions calculated in [18], but recoupled as described below, to obtain the contributions from all diagrams of the type shown in Fig. 1a. We will discuss how these matrix elements are combined to obtain the one- and two-particle contributions to energies of Al-like ions. We refer the reader to Ref. [18] for a discussion of the how the basic one- and two-particle matrix elements were evaluated. Intrinsically three-particle diagrams of the type shown in Fig. 1b also contribute to the second-order energy for Al-like ions. We discuss the evaluation of these three-particle diagrams in detail. It should be noted that the three-particle matrix elements calculated here can also be used in calculations of energies of ions with four or more valence electrons.

The model space state vector for an ion with three valence electrons outside a closed core can be represented as [19]:

$$\Psi(QJM) = N(Q) \sum \langle \beta_1\beta_2|K_{12}\rangle\langle K_{12}\beta_3|K\rangle a^\dagger_{\beta_1} a^\dagger_{\beta_2} a^\dagger_{\beta_3}|0\rangle \tag{2.1}$$

where $|0\rangle$ is the state vector for the core ($1s^2 2s^2 2p^6$, in our case), Q describes a three-particle state with quantum numbers $n_1^0\kappa_1^0 n_2^0\kappa_2^0[J_{12}]n_3^0\kappa_3^0$, and intermediate momentum J_{12}. We use the notation $K_i = \{J_i, M_i\}$ and $\beta_i = \{j_i, m_i\}$. The sum in Eq.(2.1) is over magnetic quantum numbers m_1, m_2, m_3 and M_{12}. The quantity $\langle K_1K_2|K_3\rangle$ is a Clebsch-Gordan coefficient:

$$\langle K_1K_2|K_3\rangle = (-1)^{J_1-J_2+M_3}\sqrt{2J_3+1}\begin{pmatrix} J_1 & J_2 & J_3 \\ M_1 & M_2 & -M_3 \end{pmatrix} \tag{2.2}$$

The above representation of the state vector is somewhat inconvenient; for example, it leads to an expression containing 36 terms for the three-particle diagram in Fig. 1b, differing only in the order of the initial and final indices. It is more efficient to express the state vector in a manifestly symmetric form. To this end, we rewrite Eq.(2.1) in six equivalent ways, mearly permuting the indices β_1, β_2 and β_3. The resulting state vector is

$$\begin{aligned}\Psi(QJM) = \frac{1}{6}N(Q)a^\dagger_{\beta_1} a^\dagger_{\beta_2} a^\dagger_{\beta_3}|0\rangle \\ \times \sum_{M_{12}\{\beta\}} [&\langle\beta_1\beta_2|K_{12}\rangle\langle K_{12}\beta_3|K\rangle\delta_{123} \\ &-\langle\beta_2\beta_1|K_{12}\rangle\langle K_{12}\beta_3|K\rangle\delta_{213} \\ &+\langle\beta_2\beta_3|K_{12}\rangle\langle K_{12}\beta_1|K\rangle\delta_{231} \\ &-\langle\beta_3\beta_2|K_{12}\rangle\langle K_{12}\beta_1|K\rangle\delta_{321} \\ &+\langle\beta_3\beta_1|K_{12}\rangle\langle K_{12}\beta_2|K\rangle\delta_{312} \\ &-\langle\beta_1\beta_3|K_{12}\rangle\langle K_{12}\beta_2|K\rangle\delta_{132}]\end{aligned} \tag{2.3}$$

where $\{\beta\}$ ranges over the 3! permutations of the single-particle indices, and where

$$\delta_{123} = \delta(1, 1^0)\delta(2, 2^0)\delta(3, 3^0)\,.$$

Using the following angular momentum identity [19]:

$$\sum_{M_{12}} \langle \beta_1 \beta_3 | K_{12} \rangle \langle K_{12} \beta_2 | K \rangle$$
$$= \sum_{J_{12} M_{12}} (-1)^{J_{12}+J''_{12}+j_3+j_2} \langle \beta_1 \beta_2 | K''_{12} \rangle \langle K''_{12} \beta_3 | K \rangle$$
$$\times \sqrt{(2J_{12}+1)(2J''_{12}+1)} \left\{ \begin{array}{ccc} j_2 & j_3 & J''_{12} \\ J_1 & J & J_{12} \end{array} \right\}, \qquad (2.4)$$

the three-particle state vector can be represented in a form:

$$\Psi(QJM) = \sum_{\beta_1 \beta_2 \beta_3} C^{QJM}_{\beta_1 \beta_2 \beta_3} a^\dagger_{\beta_1} a^\dagger_{\beta_2} a^\dagger_{\beta_3} |0\rangle \,. \qquad (2.5)$$

The factor $C^{QJM}_{\beta_1 \beta_2 \beta_3}$ provides the orthonormality and antisymmetry of the state vector in all one-electron (β_1, β_2 and β_3) indices. We may write

$$C^{QJM}_{\beta_1 \beta_2 \beta_3} \qquad (2.6)$$
$$= \sum_{K''_{12}} \langle \beta_1 \beta_2 | K''_{12} \rangle \langle K''{}_{12} \beta_3 | K \rangle C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J),$$

where the indices $(1,2,3)$ and $(1^0,2^0,3^0)$ designate $(n_1\kappa_1, n_2\kappa_2, n_3\kappa_3)$ and $(n_1^0\kappa_1^0, n_2^0\kappa_2^0, n_3^0\kappa_3^0)$ accordingly. We note that the dependence on magnetic quantum numbers is included in the two Clebsch-Gordan coefficients, and all permutations of the three indices are in the factor $C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J)$, which is independent of magnetic quantum numbers. One finds:

$$C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J) \qquad (2.7)$$
$$= N(1^0,2^0,3^0) \left[\delta(3,3^0) \delta(J_{12}, J''_{12}) P_{J_{12}}(11^0, 22^0) \right.$$
$$+ \sqrt{(2J_{12}+1)(2J''_{12}+1)}$$
$$\times \left(\delta(3,1^0) P_{J''_{12}}(13^0, 22^0) \left\{ \begin{array}{ccc} j_3^0 & j_2^0 & J''_{12} \\ j_1^0 & J & J_{12} \end{array} \right\} \right.$$
$$\left. \left. + \delta(3,2^0) P_{J''_{12}}(13^0, 21^0) \left\{ \begin{array}{ccc} j_3^0 & j_1^0 & J''_{12} \\ j_2^0 & J & J_{12} \end{array} \right\} (-1)^{j_1^0+j_2^0+J_{12}} \right) \right],$$

where

$$P_{J_{12}}(11^0, 22^0) = \delta(1,1^0)\delta(2,2^0) +$$
$$(-1)^{j_1^0+j_2^0+J_{12}+1} \delta(1,2^0)\delta(2,1^0) \,. \qquad (2.8)$$

Here, we have used $N(1^0,2^0,3^0)$ instead of $N(Q)$ to designate the normalization factor, which can be obtained from

$$\sum_{1,2,3,J''_{12}} (C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J))^2 = 6 \,. \qquad (2.9)$$

Using this representation it is possible to express contributions of diagrams of the type shown in Fig.1a in terms of the energy matrix elements for two-electron (magnesiumlike) ions. Moreover, with this representation, only one expression is needed to evaluate the contributions from the diagram in Fig.1b.

The model space for $n = 3$ states of aluminiumlike ions includes 75 odd-parity states consisting of 13 J=1/2 states, 22 J=3/2 states, 19 J=5/2 states, 13 J=7/2 states, 6 J=9/2 states, and two J=11/2 states. Additionally, there are 73 even-parity states consisting of 13 J=1/2 states, 21 J=3/2 states, 20 J=5/2 states, 11 J=7/2 states, 7 J=9/2 states, and one J=11/2 states. The distribution of the 36 states in the model space is summarized in Table I.

Let us now consider the coefficients $C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J)$ for aluminiumlike ions. To simplify the formulae the following notation used:

$$C_J(1^0 2^0 J_{12} 3^0) \equiv C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J)$$
$$Q_J(1^0 2^0 3^0) \equiv C_{11^0 22^0}(J) \delta(3,3^0)$$
$$C_{11^0 22^0}(J) = \eta_{12} P_{J_{12}}(11^0, 22^0) \,, \qquad (2.10)$$

where η is equal to 1 for non-equivalent electrons and $1/\sqrt{2}$ for equivalent ones. We then obtain from Eq.2.7:
$3s^2 3p$ configuration:

$$C_{1/2}(3s_{1/2}3s_{1/2}[0]3p_{1/2}) = Q_0(3s_{1/2}3s_{1/2}3p_{1/2}) \qquad (2.11)$$
$$-\frac{1}{\sqrt{2}} Q_0(3p_{1/2}3s_{1/2}3s_{1/2}) + \sqrt{\frac{3}{2}} Q_1(3p_{1/2}3s_{1/2}3s_{1/2})$$

$$C_{3/2}(3s_{1/2}3s_{1/2}[0]3p_{1/2}) = Q_0(3s_{1/2}3s_{1/2}3p_{1/2}) \qquad (2.12)$$
$$-\frac{\sqrt{3}}{2} Q_0(3p_{1/2}3s_{1/2}3s_{1/2}) + \frac{\sqrt{5}}{2} Q_1(3p_{1/2}3s_{1/2}3s_{1/2})$$

$3p^3$ configuration:

$$C_{1/2}(3p_{3/2}3p_{3/2}[0]3p_{1/2}) = Q_0(3p_{3/2}3p_{3/2}3p_{1/2}) \qquad (2.13)$$
$$-\frac{\sqrt{3}}{2} Q_1(3p_{1/2}3p_{3/2}3p_{3/2}) + \frac{\sqrt{5}}{2} Q_2(3p_{1/2}3p_{3/2}3p_{3/2})$$

$$C_{5/2}(3p_{3/2}3p_{3/2}[2]3p_{1/2}) = Q_2(3p_{3/2}3p_{3/2}3p_{1/2}) \qquad (2.14)$$
$$-\frac{1}{2} Q_1(3p_{1/2}3p_{3/2}3p_{3/2}) + \frac{\sqrt{7}}{2} Q_2(3p_{1/2}3p_{3/2}3p_{3/2})$$

$$C_{3/2}(3p_{3/2}3p_{3/2}[0]3p_{1/2}) = Q_2(3p_{3/2}3p_{3/2}3p_{1/2}) \qquad (2.15)$$
$$-\sqrt{\frac{3}{2}} Q_1(3p_{1/2}3p_{3/2}3p_{3/2}) - \frac{1}{\sqrt{2}} Q_2(3p_{1/2}3p_{3/2}3p_{3/2})$$

$$C_{3/2}(3p_{1/2}3p_{1/2}[0]3p_{3/2}) = Q_0(3p_{1/2}3p_{1/2}3p_{3/2}) \qquad (2.16)$$
$$-\frac{\sqrt{3}}{2} Q_1(3p_{1/2}3p_{3/2}3p_{1/2}) + \frac{\sqrt{5}}{2} Q_2(3p_{1/2}3p_{3/2}3p_{1/2})$$

$$C_{3/2}(3p_{3/2}3p_{3/2}[0]3p_{3/2}) \qquad (2.17)$$
$$= \frac{1}{\sqrt{2}} Q_0(3p_{3/2}3p_{3/2}3p_{3/2}) - \sqrt{\frac{5}{2}} Q_2(3p_{3/2}3p_{3/2}3p_{3/2})$$

$3s3p^2$ configuration:

$$C_{1/2}(3p_{1/2}3p_{1/2}[0]3s_{1/2}) = Q_0(3p_{1/2}3p_{1/2}3s_{1/2}) - \frac{1}{\sqrt{2}}Q_0(3s_{1/2}3p_{1/2}3p_{1/2}) + \sqrt{\frac{3}{2}}Q_1(3s_{1/2}3p_{1/2}3p_{1/2}) \tag{2.18}$$

$$C_{1/2}(3p_{3/2}3p_{3/2}[0]3s_{1/2}) = Q_0(3p_{3/2}3p_{3/2}3s_{1/2}) - \frac{\sqrt{3}}{2}Q_1(3s_{1/2}3p_{3/2}3p_{3/2}) + \frac{\sqrt{5}}{2}Q_2(3s_{1/2}3p_{3/2}3p_{3/2}) \tag{2.19}$$

$$C_{1/2}(3p_{1/2}3p_{3/2}[1]3s_{1/2}) = Q_1(3p_{1/2}3p_{3/2}3s_{1/2}) - Q_1(3s_{1/2}3p_{3/2}3p_{1/2}) - Q_1(3s_{1/2}3p_{1/2}3p_{3/2}) \tag{2.20}$$

$$C_{3/2}(3p_{1/2}3p_{3/2}[1]3s_{1/2}) = Q_1(3p_{1/2}3p_{3/2}3s_{1/2}) - \frac{1}{4}Q_1(3s_{1/2}3p_{3/2}3p_{1/2}) - \frac{\sqrt{15}}{4}Q_2(3s_{1/2}3p_{3/2}3p_{1/2}) - \sqrt{\frac{3}{8}}Q_0(3s_{1/2}3p_{1/2}3p_{3/2}) + \sqrt{\frac{5}{8}}Q_1(3s_{1/2}3p_{1/2}3p_{3/2}) \tag{2.21}$$

$$C_{3/2}(3p_{1/2}3p_{3/2}[2]3s_{1/2}) = Q_2(3p_{1/2}3p_{3/2}3s_{1/2}) + \frac{\sqrt{15}}{4}Q_1(3s_{1/2}3p_{3/2}3p_{1/2}) + \frac{1}{4}Q_2(3s_{1/2}3p_{3/2}3p_{1/2}) - \sqrt{\frac{5}{8}}Q_0(3s_{1/2}3p_{1/2}3p_{3/2}) - \sqrt{\frac{3}{8}}Q_1(3s_{1/2}3p_{1/2}3p_{3/2}) \tag{2.22}$$

$$C_{3/2}(3p_{3/2}3p_{3/2}[2]3s_{1/2}) = Q_2(3p_{3/2}3p_{3/2}3s_{1/2}) - \sqrt{\frac{3}{2}}Q_1(3s_{1/2}3p_{3/2}3p_{3/2}) - \frac{1}{\sqrt{2}}Q_2(3s_{1/2}3p_{3/2}3p_{3/2}) \tag{2.23}$$

$$C_{5/2}(3p_{1/2}3p_{3/2}[2]3s_{1/2}) = Q_2(3p_{1/2}3p_{3/2}3s_{1/2}) - Q_2(3s_{1/2}3p_{3/2}3p_{1/2}) + Q_1(3s_{1/2}3p_{1/2}3p_{3/2}) \tag{2.24}$$

$$C_{5/2}(3p_{3/2}3p_{3/2}[2]3s_{1/2}) = Q_2(3p_{3/2}3p_{3/2}3s_{1/2}) - \frac{1}{2}Q_1(3s_{1/2}3p_{3/2}3p_{3/2}) + \frac{\sqrt{7}}{2}Q_2(3s_{1/2}3p_{3/2}3p_{3/2}) \tag{2.25}$$

Using this representation, the expression for the energy matrix element for diagrams of the type Fig.1a (which we designate by R) can be written:

$$\begin{aligned} & E^R(1^0 2^0[J_{12}]3^0 J, 1'^0 2'^0[J'_{12}]J) \\ &= \sum_{1,2,1',2'} \sum_{J''_{12}} E^R_a(12, 2'1', J) N(12) N(1'2') \\ &\times \sum_3 C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J) C_{1'1'^0 2'2'^0 33'^0}(J'_{12}, J''_{12}, J) , \end{aligned} \tag{2.26}$$

where $E^R(12, 1'2', J)$ is the two-particle contribution to the $n_1\kappa_1 n_2\kappa_2 n_{1'}\kappa_{1'} n_{2'}\kappa_{2'}$ J matrix element for magnesiumlike ions. Here, $N(12) = 1/\sqrt{2}$ if electrons 1 and 2 are equivalent and 1/2 they are not equivalent. This choice accounts for the fact that $E^R(12, 1'2', J)$ contains both direct and exchange contributions.

The three-electron coefficients given by Eqs.(2.6, 2.7) allow us to obtain the expression for the diagram of Fig.1b, designated by G. The contribution of this diagram to the second-order matrix elements take the form:

$$\begin{aligned} & E^G(1^0 2^0[J_{12}]3^0 J, 1'^0 2'^0[J'_{12}]J) \\ &= \sum_{1,2,3,1',2',3'} \sum_n \frac{v_{123'n} v_{1'2'3n}}{\epsilon_n + \epsilon_{3'} - \epsilon_1 - \epsilon_2} \times C^{QJM}_{123} C^{Q'JM}_{1'2'3'} , \end{aligned} \tag{2.27}$$

where $v_{ijkl} = g_{ijkl} + b_{ijkl}$ is the sum of two-particle Coulomb matrix element g_{ijkl}, and the two-particle matrix element of instantaneous Breit interaction, b_{ijkl} . Carrying out angular reduction we obtain for Coulomb interaction (from the gg term in Eq.(2.27))

$$\begin{aligned} & E^G(1^0 2^0[J_{12}]3^0 J, 1'^0 2'^0[J'_{12}]J) \\ &= - \sum_{1,2,3,1',2',3'} \sum_{J''_{12}, J''^{\prime}_{12}} \sum_{kk'} (-1)^{j_2 + j_{2'} - j_3 - j_{3'} + J''_{12} + J''^{\prime}_{12} + k + k'} \\ &\times \sum_n \frac{X_k(123'n) X_k(1'2'3n)}{\epsilon_n + \epsilon_{3'} - \epsilon_1 - \epsilon_2} \sqrt{(2J''_{12} + 1)(2J'''_{12} + 1)} \\ &\times \left\{ \begin{array}{ccc} j_n & j_{3'} & J''_{12} \\ j_1 & j_2 & k \end{array} \right\} \left\{ \begin{array}{ccc} j_n & j_3 & J \\ j_{1'} & j_{2'} & k' \end{array} \right\} \left\{ \begin{array}{ccc} J''^{\prime}_{12} & j_{3'} & J \\ J''_{12} & j_3 & j_n \end{array} \right\} \\ &\times C_{11^0 22^0 33^0}(J_{12}, J''_{12}, J) C_{1'1'^0 2'2'^0 3'3'^0}(J'_{12}, J'''_{12}, J) \end{aligned} \tag{2.28}$$

where

$$X_k(abcd) = (-1)^k \langle a||C_k||c\rangle \langle b||C_k||d\rangle R_k(abcd) \tag{2.29}$$

(see for detail [12]). We obtain similar term for Breit contribution from linear terms ($gb + bg$) of the Eq.(2.27) by changing $X_k(123'n)X_k(1'2'3n)$ to $X^B_k(123'n)X_k(1'2'3n) + X_k(123'n)X^B_k(1'2'3n)$ in Eq.(2.28) and expression for $X^B_k(abcd)$ is given in [46]. We see that the contribution of the G diagram is determined by a sum n over the single-particle spectrum (with restrictions for states with principal quantum number 3).

III. ENERGY MATRIX FOR GE^{19+}

In Tables II-V, we give details of our calculations of the first- and second-order contributions to the energy matrices for the special case of Al-like germanium, Z=32. We list results for the one-electron energy $E[3lj]$= $E_0 + E_1 + B_1 + E_2$ in Table II, the diagonal and non-diagonal matrix elements for two-electron energy $E[3l_1j_1 3l_2j_2(J), 3l_3j_3 3l_4j_4(J)]$= $E_1 + B_1 + E_2$ in Table III, and the diagonal matrix elements to the three-electron energy $E[3l_1j_1 3l_2j_2[J_{12}]3l_3(J), 3l_1j_1 3l_2 3j_2[J_{12}]3l_3(J)]$= $E_0 + E_1 + B_1 + E_2$ in Table IV. The columns headed E_0, E_1, B_1, and E_2 contain the zeroth-, first-, and second-order contributions from the Coulomb and Breit operators, respectively. Details of the evaluation of the E_i and B_i contributions given in Tables II and III follow the pattern of the corresponding calculation for Mg-like ions given in Ref. [18]. In particular, we use the second-order one- and two-particle matrix elements for Mg-like ions presented in Tables II and III, but recoupled as described below, to obtain the contributions from all diagrams of the type shown in Fig. 1a. We will discuss how these matrix elements are combined to obtain the one- and two-particle contributions to energies of Al-like ions.

Let us describe in more detail the calculation of E_0, E_1, E_2, and B_1 for three-electron system given in Table IV. Consider, as an example, the (simplest) case of the $E[3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2), 3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2)]$ diagonal matrix element. In this case only two one-particle ($E^{(1)}[3s_{1/2}]$ and $E^{(1)}[3p_{1/2}]$) and three two-particle contributions ($E^{(2)}[3s_{1/2}3s_{1/2}(0), 3s_{1/2}3s_{1/2}(0)]$, $E^{(2)}[3s_{1/2}3p_{1/2}(0), 3s_{1/2}3p_{1/2}(0)]$ and $E^{(2)}[3s_{1/2}3p_{1/2}(1), 3s_{1/2}3p_{1/2}(1)]$) are necessary. Using the following table:

	E_0	E_1	B_1	E_2
$3s_{1/2}$	-32.345102	0.0	0.012104	-0.027696
$3p_{1/2}$	-30.595853	0.0	0.019052	-0.033384

it is possible to calculate the one-particle contributions, $E^{(1)}$, as

$$E^{(1)}[3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2),\ 3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2)]$$
$$= 2E^{(1)}[3s_{1/2}] + E^{(1)}[3p_{1/2}]$$

Using Eq.(2.26), the expression for the corresponding $C_{1 1^0 2 2^0 3 3^0}(J_{12}, J''_{12}, J) = C_J(1^0 2^0 J_{12} 3^0)$ coefficient

$$C_{1/2}(3s_{1/2}3s_{1/2}[0]3p_{1/2}) = Q_0(3s_{1/2}3s_{1/2}3p_{1/2})$$
$$-\frac{1}{\sqrt{2}}Q_0(3p_{1/2}3s_{1/2}3s_{1/2}) + \sqrt{\frac{3}{2}}Q_1(3p_{1/2}3s_{1/2}3s_{1/2})$$

and values for the two-particle matrix elements,

		E_1	B_1	E_2
$3s_{1/2}3s_{1/2}$	$3s_{1/2}3s_{1/2}(0)$	1.743788	0.000400	-0.021984
$3s_{1/2}3p_{1/2}$	$3s_{1/2}3p_{1/2}(0)$	1.800984	0.000769	-0.029776
$3s_{1/2}3p_{1/2}$	$3s_{1/2}3p_{1/2}(1)$	1.963896	0.001492	-0.041080

we can calculate the two-particle contributions, E^2:

$$E^{(2)}[3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2), 3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2)] =$$
$$E^{(2)}[3s_{1/2}3s_{1/2}(0), 3s_{1/2}3s_{1/2}(0)]$$
$$+\frac{1}{2}E^{(2)}[3s_{1/2}3p_{1/2}(0), 3s_{1/2}3p_{1/2}(0)]$$
$$+\frac{3}{2}E^{(2)}[3s_{1/2}3p_{1/2}(1), 3s_{1/2}3p_{1/2}(1)].$$

Non-zero value of the three-particle contribution gives the second-order diagram, G shown in Fig. 1b. The value of this diagram E^G for the matrix element $[3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2), 3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2)]$ is equal to -0.026506 (see the last column headed E^G in Table IV)). In summary, we obtain for the $E[3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2), 3s_{1/2}3s_{1/2}[0]3p_{1/2}(1/2)]$ diagonal matrix element:

$E^{(i)}$	E_0	E_1	B_1	E_2
$E^{(1)}$	-95.286057	0.000000	0.043260	-0.088776
$E^{(2)}$	0.000000	4.897918	0.000692	-0.052528
$E^{(3)}$	0.000000	0.000000	0.000000	-0.026506
$E^{(\mathrm{tot})}$	-95.286057	4.897918	0.043952	-0.167810

which gives E = -90.511997 for the total energy. Results of similar calculations for the 148 diagonal matrix elements are given in Table IV. It should be noted that the whole number of diagonal and non-diagonal matrix elements is equal to 2404. We illustrate the values of the zeroth-, first-, and second order contributions (E_0, E_1, B_1, and E_2) for the Al-like sequence by the diagonal matrix elements only. In the last column of Table IV, the contribution of the three-particle interaction, E^G is presented. As can be seen from comparison of E_2=$E_2^{(1)}$ + $E_2^{(2)}$ + $E_2^{(3)}$ and E^G=$E_2^{(3)}$, the three-particle contributions gives 10-20% into the whole second-order values.

Carrying out the recoupling by this method does not require significant computer time, provided the one- and two-particle contributions are known (as they are in the present case). The only contribution that must be calculated anew is the three-particle diagram. This contribution, however, contains only a single sum over intermediate states, and does not require a lengthy calculation. It should be noted that no additional calculations are necessary to evaluate matrix elements for four-particle systems; it is only necessary to determine the recoupling coefficients C and combine the known one- two- and three-particle matrix-elements.

After evaluating the energy matrices, we calculate eigenvalues and eigenvectors for states with given values of J and parity. There are two possible methods to carry out the diagonalization: (a) diagonalize the sum of zeroth- and first-order matrices, then calculate the second-order contributions using the resulting eigenvectors; or (b) diagonalize the sum of the zeroth-, first- and second-order matrices together. Following Ref. [19], we choose the second method here.

In Table V, we list the following contributions to the energies of 148 excited states in Ge^{19+}: $E^{(0+1)}$ = E_0 +E_1+B_1, the second-order Coulomb energy E_2, the QED correction E_{LAMB}, and the total theoretical energy E_{tot}. The QED correction is approximated as the sum of the one-electron self energy and the first-order vacuum-polarization energy. The screened self-energy and vacuum polarization data given by Blundell [29] are used to determine the QED correction E_{LAMB} (see, for detail Ref. [18]). We also present in Table V the separate contributions: $E^{(0+1)}$, E_2, and E_{LAMB}, together with the total theoretical energy E_{tot} counted from the ground level. As can be seen, the second order contribution is about 2% of the total excitation energy. This table shows clearly the importance of including second-order contributions. As can be seen from Table V, the excitation energies are increases with increasing the number of $3d$ one-particle states. The levels in this table could be divided in two groups: less than 5.7a.u and larger than 9a.u. for odd-parity states and less than 3.2a.u and larger than 6a.u. for even-parity states. The first group includes $3s_{1/2}3s_{1/2}[0]3p_j(J)$, $3s_{1/2}3p_j[J_{12}]3d_{j'}(J)$, $3s_{1/2}3s_{1/2}[0]3d_j(J)$, and $3s_{1/2}3p_j[J_{12}]3p_{j'}(J)$ levels (together 40 levels) and the second group includes all other 108 levels ($3d_j3d_{j'}[J_{12}]3p_{j''}(J)$, $3p_j3p_{j'}[J_{12}]3d_{j''}(J)$, and $3d_j3d_{j'}[J_{12}]3d_{j''}(J)$ levels). The first group of levels is studied experimentally, however it is not any experimental data for the second group of levels. Below, we discuss about the first group of levels only. For these 40 levels, we use not only jj designations but also LS designations. When starting calculations from relativistic Dirac-Fock wavefunctions, it is natural to use jj designations for uncoupled energy matrix elements; however, neither jj nor LS coupling describes the *physical* states properly, except for the single-configuration state $3d_{5/2}3d_{5/2}(4)3d_{3/2} \equiv 3d^3\ {}^3G_{11/2}$. Both designations are given in Table VI for 40 levels in Al-like ions.

IV. Z-DEPENDENCES OF EIGENVECTORS AND EIGENVALUES IN AL-LIKE IONS

In Figs. 2-27, we illustrate the Z-dependence of the eigenvectors and eigenvalues of the $3lj3l'j'[J_{12}]3l''j''(J))$ three-particle states. Strong mixing between states inside of even-parity complex with J=3/2, 5/2 discussed by Ekberg *et al.* in Ref. [30] and Jupén *et al.* in Ref. [31]. Additionally, we found strong mixing inside of the odd-parity complex with J=1/2-5/2 and even-parity complex with J=1/2. In Figs. 2-4, the mixing between even-parity $[3p_{1/2}3p_{1/2}[0]3s_{1/2}]$+$[3p_{3/2}3p_{3/2}[0]3s_{1/2}]$+ $[3p_{1/2}3p_{3/2}[1]3s_{1/2}]$ states with J=1/2 for small-Z ions is illustrated. Strong mixing in even parity complex with J=3/2 between $[3p_{3/2}3p_{3/2}[2]3s_{1/2}]$+ $[3s_{1/2}3s_{1/2}[0]3d_{3/2}]$ states for Z=41-42 and between $[3p_{3/2}3p_{3/2}[2]3s_{1/2}]$+ $[3p_{1/2}3p_{1/2}[0]3d_{3/2}]$ states for Z=73-74 is presented in Figs. 5, 6. In Figs. 7- 9, the strong mixing in even parity complex with J=5/2 between $[3p_{1/2}3p_{3/2}[2]3s_{1/2}]$+ $[3p_{3/2}3p_{3/2}[2]3s_{1/2}]$ states for Z=27-28, between $[3p_{3/2}3p_{3/2}[2]3s_{1/2}]$+ $[3s_{1/2}3s_{1/2}[0]3d_{3/2}]$ states for Z=53-54 and between $[3p_{3/2}3p_{3/2}[2]3s_{1/2}]$+ $[3p_{1/2}3p_{1/2}[0]3d_{3/2}]$ states for Z=83-84 is demonstrated.

The six levels of odd-parity complex with J=1/2 are described by the 36 mixing coefficients $C^{(i)}[3s_{1/2}3s_{1/2}[0]3p_{1/2}]$, $C^{(i)}[3p_{1/2}3p_{1/2}[0]3p_{1/2}]$, $C^{(i)}[3s_{1/2}3p_{1/2}[1]3d_{3/2}]$, $C^{(i)}[3s_{1/2}3p_{3/2}[1]3d_{3/2}]$, $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{3/2}]$, and $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{5/2}]$, where index i is the label of the six levels: $3s^23p\ {}^2P_{1/2}$, $3p^3\ {}^2P_{1/2}$, $3s3p[{}^3P]3d\ {}^4P_{1/2}$, $3s3p[{}^3P]3d\ {}^4D_{1/2}$, $3s3p[{}^3P]3d\ {}^2P_{1/2}$, and $3s3p[{}^1P]3d\ {}^2P_{1/2}$. It should be noted that, we omit the i index in Figs. 2-27. The mixing coefficient $C^{(i)}[3s_{1/2}3s_{1/2}[0]3p_{1/2}]$, is almost equal to 1.0 when index i belongs to the ground level $3s^23p\ {}^2P_{1/2}$. The other five levels of this complex are described at least by two or three mixing coefficients, as can be seen from Figs. 10-14. There are two largest mixing coefficients when index i=$3p^3\ 2P_{1/2}$: $C^{(i)}[3p_{1/2}3p_{1/2}[0]3p_{1/2}]$ (Z=14-39) and $C^{(i)}[3s_{1/2}3p_{1/2}[1]3d_{3/2}]$ (Z=40-100). As can be seen from Fig. 10, it is possible to use for this level jj designations: $3p_{1/2}3p_{1/2}[0]3p_{1/2}$ for Z=14-39 and $3s_{1/2}3p_{1/2}[1]3d_{3/2}$ for Z=40-100. The similar situation for levels shown in Figs. 13 and 14. The levels with indexes i= $3s3p[{}^3P]3d\ {}^2P_{1/2}$, and $3s3p[{}^1P]3d\ {}^2P_{1/2}$ can be described by $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{5/2}]$, and $C^{(i)}[3s_{1/2}3p_{3/2}[1]3d_{3/2}]$ mixing coefficients. As can be seen from Fig. 12, the level $3s3p[{}^3P]3d\ {}^4D_{1/2}$ is possible to describe by $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{s/2}]$ mixing coefficient with index i=$3s3p[{}^3P]3d\ {}^4D_{1/2}$. It is more complicated situation for the level shown in Fig. 11. The four mixing coefficients: $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{3/2}]$ (Z=14-20), $C^{(i)}[3s_{1/2}3p_{1/2}[1]3d_{3/2}]$ (Z=21-39), $C^{(i)}[3p_{3/2}3p_{3/2}[0]3p_{1/2}]$ (Z=40-89), and $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{3/2}]$ (Z=90-100) describe the level when i=$3s3p[{}^3P]3d\ {}^4P_{1/2}$. It should be noted the energy of this level, $3s3p[{}^3P]3d\ {}^4P_{1/2}$, is almost equal to the energy of the $3p^3\ {}^2P_{1/2}$ level for Z=39. The difference is 6620 cm^{-1} when the energies of $3s3p[{}^3P]3d\ {}^4P_{1/2}$ and $3p^3\ {}^2P_{1/2}$ levels are equal to 1417317 cm^{-1} and 1423937 cm^{-1}, respectively. We can see the very sharp change in mixing coefficients $C^{(i)}[3p_{3/2}3p_{3/2}[0]3p_{1/2}]$ and $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{3/2}]$ for Z=39 when i=$3s3p[{}^3P]3d\ {}^4P_{1/2}$ (Fig. 11) and i=$3p^3\ {}^2P_{1/2}$ (Fig. 10).

The similar sharp change of the mixing coefficients is shown in Fig. 6 (for Z=74 ΔE= 0.017 % of the energy levels) and Fig. 9 (for$Z$=83 ΔE= 0.11 % of the energy levels).

In Figs. 15 and 16, we illustrate the Z-dependence of mixing coefficients for $3s3p[{}^3P]3d\ {}^2D_{3/2}$ and $3p^3\ {}^4S_{3/2}$ levels. As can seen from Fig. 15, the jj coupling scheme is not appropriate for small-Z ions since the four mixing coefficients ($C^{(i)}[3p_{3/2}3p_{3/2}[2]3p_{1/2}]$, $C^{(i)}[3p_{1/2}3p_{1/2}[0]3p_{3/2}]$, $C^{(i)}[3p_{3/2}3p_{3/2}[0]3p_{3/2}]$, and $C^{(i)}[3s_{1/2}3p_{1/2}[0]3d_{3/2}]$) give the similar contributions when index i=$3s3p[{}^3P]3d\ {}^2D_{3/2}$. The mixing coefficient $C^{(i)}[3p_{3/2}3p_{3/2}[2]3p_{1/2}]$ is about 0.75-0.85 for small-Z ions when i=$3p^3\ {}^4S_{3/2}$ (see Fig. 16). The mixing of three states in jj coupling scheme is involved to describe the $3s3p[{}^3P]3d\ {}^2D_{5/2}$ level, as can be seen from Fig. 17. The largest contribution gives the $C^{(i)}[3p_{3/2}3p_{3/2}[2]3p_{1/2}]$ coefficient for Z=14-40 and the $C^{(i)}[3s_{1/2}3p_{1/2}[1]3d_{3/2}]$ coefficient for Z=41-100. The similar behavior is demonstrated for the $3s3p[{}^1P]3d\ {}^2F_{5/2}$ level shown in Fig. 18; the largest contribution gives the $C^{(i)}[3s_{1/2}3p_{3/2}[1]3d_{3/2}]$ coefficient for Z=14-62 and the $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{5/2}]$ coefficient for Z=63-100. As can be seen from Figs. 19, 20, the LS coupling scheme is appropriate for small-Z ions, however the jj coupling scheme is more reasonable for high-Z ions. The $C^{(i)}[3s_{1/2}3p_{3/2}[2]3d_{3/2}]$ coefficient is about 0.8-1.0 when index i=$3s3p[^3P]3d\ ^4D_{7/2}$ for $Z > 60$, and The $C^{(i)}[3s_{1/2}3p_{3/2}[1]3d_{5/2}]$ coefficient is about 0.8-1.0 when index i=$3s3p[^1P]3d\ ^2F_{7/2}$ for $Z > 50$.

The energy diagrams are illustrated in Figs. 21-27. We show LS designations for small Z and jj for large Z in these figures. Usually, either LS or jj designations are used to label the resulting eigenvectors rather than simply enumerating with an index N. As can be seen from Figs. 22, 23 a such numeration leads to change of level labels. As can be seen from Fig. 22, the $3s^23d\ ^2D_{3/2}$ level has the largest value of energy for small-Z ions among the four even-parity levels with J=3/2. This order is changed for high-Z ions when we use jj designations ; the $3s_{1/2}3s_{1/2}[0]3d_{3/2}$ level is situated between three $3pj3pj'[J_{1/2}]3s_{1/2}$ levels . It was included additional $3p_{1/2}3p_{1/2}[0]3d_{3/2}$ level among the $3pj3pj'[J_{1/2}]3s_{1/2}$ and $3s_{1/2}3s_{1/2}[0]3d_{3/2}$ levels presented for small-Z ions. The E-value of the $3p_{1/2}3p_{1/2}[0]3d_{3/2}$ level becomes smaller than the E-value of the $3p_{3/2}3p_{3/2}[2]3s_{1/2}$ level for ions with $Z > 75$. We can see not smooth Z-dependence of the fourth curve in Fig. 22. The similar behavior of the curve labeled as the $3s^23d\ ^2D_{5/2}$ is demonstrated in Fig. 23. Using the same designations for the whole energy interval could be lead to the crossing energy levels inside of one complex that is forbidden by Wigner and Neumann theorem (see, for example in Ref. [47].

It is more complicated situation with odd-parity states shown in Figs. 24-27. It should be noted that we present in figures energy relative to the ground $3s^23p\ ^2P_{1/2}$ level. Only one $3s^23p\ ^2P_{3/2}$ level is not involved in the change of its label among the other 27 odd-parity levels as can be seen from Figs. 24-27. The labels of the second level, $3p^3\ ^2P_{1/2}$ in Fig. 24 is changed into $3s_{1/2}3p_{1/2}[1]3d_{3/2}$ for high-Z ions. The similar situation is for the $3p^3\ ^4S_{3/2},^2P_{3/2},^2D_{3/2}$ levels shown in Fig. 25 and the $3p^3\ ^2D_{5/2}$ level shown in Fig. 26.

V. COMPARISON OF RESULTS WITH OTHER THEORY AND EXPERIMENT

We calculate energies of the 75 odd-parity states
$(3s_{1/2}3s_{1/2}[0]3p_j(J)$, $3s_{1/2}3p_j[J_{1/2}]3d_{j'}(J)$,
$3p_j3p_{j'}[J_{1/2}]3p_{j''}(J)$, and $3d_j3d_{j'}[J_{1/2}]3p_{j''}(J))$
and the 73 even-parity excited states
$(3p_j3p_{j'}[J_{1/2}]3s_{1/2}(J)$, $3s_{1/2}3s_{1/2}[0]3d_j(J)$,
$3p_j3p_{j'}[J_{1/2}]3d_{j''}(J)$, and $3d_j3d_{j'}[J_{1/2}]3d_{j''}(J))$
for Al-like ions with nuclear charges ranging from Z=14-100. In Table VII, we illustrate our theoretical results for energies of the 30 odd-parity $3s_{1/2}3s_{1/2}[0]3p_j(J)$, $3s_{1/2}3p_j[J_{1/2}]3d_{j'}(J)$, and $3p_j3p_{j'}[J_{1/2}]3p_{j''}(J)$ states in jj coupling or $3s^23p\ ^2P_J$, $3s3p3d\ ^{2S+1}L_J$, and $3p^3\ ^{2S+1}L_J$ states in LS coupling and the ten even-parity $3p_j3p_{j'}[J_{1/2}]3s_{1/2}(J)$ and $3s_{1/2}3s_{1/2}[0]3d_j(J)$ states in jj coupling or $3s3p^2\ ^{2S+1}L_J$ and $3s^23d\ ^2D_J$ states in LS coupling for Al-like ions with nuclear charges ranging from Z=15-40. We limited the number of states and ions to compare with other results and experimental data. Our comparison is presented in two parts: transition energies and fine-structure energy differences.

A. Transition energies

In Tables VIII-X, our theoretical results of $3s^23p\ ^2P_J$, $3s3p3d\ ^{2S+1}L_J$, $3s3p^2\ ^{2S+1}L_J$, and $3s^23d\ ^2D_J$ states for Al-like ions with nuclear charges ranging from Z=15-40 are compared with other calculations and with experiments. We compare in Table VIII our MBPT results with NIST data for P^{2+} given by Martin *et al.* in Ref. [33], for S^{3+} given by Martin *et al.* in Ref. [34], and for Fe^{13+} given by Shirai *et al.* in Ref. [39]. As can be seen from Table VIII, our results are in good agreement with experimental NIST data. The difference between NIST and MBPT data is about 0.3-0.5% for many cases. It should be noted that relativistic MBPT calculations are more accurate for high-Z ions and good agreement with experimental data obtained for low-Z gives as possibility to conclude that the MBPT method can provide us for the accurate data for all-Z ions.

In Table IX, the MBPT energies of $3s^23p\ ^2P_J$, $3s3p3d\ ^{2S+1}L_J$, $3s3p^2\ ^{2S+1}L_J$, and $3s^23d\ ^2D_J$ states for Al-like ions with nuclear charges ranging from Z=32-40 are compared with adopted level energies presented by Ekberg *et al.* in Ref. [30]. The adopted values in [30] were determined from the observed transitions in a stepwise fitting procedure. The differences between the observed energies and the theoretically calculated values using the Grant codes were fitted by a polynomial representation in order to obtain smoothed energies. As can be seen from Table IX, our results are in excellent agreement with adopted data (heading Fit in Table IX) from Ref. [30]. The difference between the MBPT data and adopted data is about 0.01-0.1% for many cases. We can conclude that with this accuracy of our MBPT calculations it will be very simple to fill out the empty places for adopted data in Table IX.

Isoelectronic sequence of the Al-like $3s^23p\ ^2P$-$3s3p^2\ ^4P$ transitions in the ions P^{2+}-Mo^{29+} were investigated in recently published paper by Jupén and Curtis in Ref. [31]. We use the base of observed data from [31] to compare with our MBPT results in Table X. We did not find the smooth Z-dependence between MBPT (a) and observed (b) data. The difference for the $3s^23p\ ^2P_{1/2}$-$3s3p^2\ ^4P_{1/2}$ transition between a and b data is about 45-164 cm^{-1} for most of ions shown in Table X except the cases of ions with Z=15, 29, 32, 34, 35, 38-40, and 42 when this difference is about 360-1300 cm^{-1}. We found a little bit better agreement between a and b data for the $3s^23p\ ^2P_{3/2}$-$3s3p^2\ ^4P_{5/2}$ transition: 1, 7, and 12 cm^{-1} for ions with Z=16, 24, and 25. Even for high-Z ions, the difference between a and b data is very small for this transition (22, 50, 31, 50, and 77 cm^{-1} for ions with Z=35, 36, 38, 39, and 40 accordingly).

B. Fine structure of the ^2L and ^4L terms in Al-like ions

No measurements of fine-structure intervals were made by observing the wavelength differences between transitions within the doublet or quartet states. The intervals of both upper and lower states are over-determined if all allowed ($3s^23p\ ^2P$ – $3s3p^2\ ^2S$, ^2P, ^2D) or intercombination $3s^23p\ ^2P$ – $3s3p^2\ ^4P$ transitions are observed [30,31]. These fine structures are quite regular throughout the isoelectronic sequence, following the Landé interval rules reasonably well that can be seen from Table XI. In this table, we present the fine-structure splitting for the eleven doublet terms ($3s^23p\ ^2P$, $3s3p^2\ ^2P$, $3s3p^2\ ^2D$, $3s^23d\ ^2D$, $3p^3\ ^2P$, $3p^3\ ^2D$, $3s3p[^3P]3d\ ^2P$, $3s3p[^1P]3d\ ^2P$, $3s3p[^3P]3d\ ^2D$, $3s3p[^1P]3d\ ^2D$, $3s3p[^3P]3d\ ^2F$, and $3s3p[^1P]3d\ ^2F$) and the four quartet terms ($3s3p^2\ ^4P$, $3s3p[^3P]3d\ ^4P$, $3s3p[^3P]3d\ ^4D$, and $3s3p[^3P]3d\ ^4F$). On the other hand, our calculations show that the fine structures of the $3s3p3d$ levels do not follow the Landé rules for all Z. The ^2D terms are inverted, the ^4P, ^4D, ^2D, and ^2F terms are partially inverted, while the ^4F terms show regular ordering of the fine-structure splitting. The unusual splitting are due principally to changes from LS to jj coupling, with mixing from other doublet and quartet states. States with different J states mix differently. Further experimental confirmation would be very helpful in verifying the correctness of these occasionally sensitive mixing parameters.

In Table XII, we compare results for the three fine-structure intervals: $3s^23p\ ^2P_{3/2}$ – $^2P_{1/2}$, $3s3p^2\ ^4P_{3/2}$ – $^4P_{1/2}$, and $3s3p^2\ ^4P_{5/2}$ – $^4P_{3/2}$ in Al-like ions with Z=15-42. Our MBPT values are compared with predicted data by Jupén and Curtis in Ref. [31], by Ekberg *et al.* in Ref. [30] and NIST group in Refs. [33–45]. As can be seen from Table XII, there is disagreement between the MBPT values and predicted values by Jupén and Curtis in Ref. [31] for $3s3p^2\ ^4P_{3/2}$ – $^4P_{1/2}$ and $3s3p^2\ ^4P_{5/2}$ – $^4P_{3/2}$ intervals. On the other hand, the MBPT values agree very well with NIST values [33–45] for these above mentioned intervals and for $3s^23p\ ^2P_{3/2}$ – $^2P_{1/2}$ interval. In two last columns of Table XII, we compare the MBPT results and results from Ref. [31] for the $3s3p^2\ ^4P_{5/2}$ – $^4P_{1/2}$ interval. We can see from this table, that two results for the $3s3p^2\ ^4P_{5/2}$ – $^4P_{1/2}$ interval agree much better than results $3s3p^2\ ^4P_{3/2}$ – $^4P_{1/2}$ and $3s3p^2\ ^4P_{5/2}$ – $^4P_{3/2}$ intervals. In summary, we can conclude that the middle $3s3p^2\ ^4P_{3/2}$ level could be shifted in Ref. [31], to obtain reasonable agreement with our theoretical results and NIST predictions in [35–44].

VI. CONCLUSION

In summary, a systematic second-order MBPT study of the energies of the n = 3 states of Al-like ions has been presented. In conclusion, we find that MBPT gives excellent agreement with experimental data and adopted results. It would be beneficial if experimental data for other highly-charged Al-like ions were available. At the present time, there are no experimental data between Z=43 and Z=100 for the aluminium isoelectronic sequence. Availability of such data could lead to an improved understanding of the relative importance of different contributions to the energies of highly-charge ions. These calculations are presented as a theoretical benchmark for comparison with experiment and theory. The results could be further improved by including third-order correlation corrections.

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TABLE I. Possible three-particle states in the n=3 complex; jj-coupling scheme.

Odd-parity states

J=0.5	J=1.5	J=2.5	J=3.5-5.5
$3s_{1/2}3s_{1/2}[0]3p_{1/2}$	$3s_{1/2}3s_{1/2}[0]3p_{3/2}$	$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$
$3p_{3/2}3p_{3/2}[0]3p_{1/2}$	$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	$3s_{1/2}3p_{1/2}[0]3d_{5/2}$	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3p_{1/2}3p_{1/2}[0]3p_{3/2}$	$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3p_{3/2}3p_{3/2}[0]3p_{3/2}$	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s_{1/2}3p_{1/2}[0]3d_{3/2}$	$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3d_{3/2}3d_{3/2}[2]3p_{3/2}$
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3d_{5/2}3d_{5/2}[2]3p_{3/2}$
$3d_{3/2}3d_{3/2}[0]3p_{1/2}$	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[4]3p_{1/2}$
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3d_{5/2}3d_{5/2}[4]3p_{3/2}$
$3d_{5/2}3d_{5/2}[0]3p_{1/2}$	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	$3d_{3/2}3d_{5/2}[2]3p_{3/2}$
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[3]3p_{1/2}$
$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$
$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	$3d_{3/2}3d_{3/2}[0]3p_{3/2}$	$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[4]3p_{1/2}$
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	$3d_{3/2}3d_{5/2}[4]3p_{3/2}$
	$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	
	$3d_{5/2}3d_{5/2}[0]3p_{3/2}$	$3d_{3/2}3d_{5/2}[2]3p_{1/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$
	$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	$3d_{5/2}3d_{5/2}[4]3p_{1/2}$
	$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[3]3p_{1/2}$	$3d_{5/2}3d_{5/2}[4]3p_{3/2}$
	$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$
	$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	$3d_{3/2}3d_{5/2}[4]3p_{1/2}$
	$3d_{3/2}3d_{5/2}[2]3p_{1/2}$		$3d_{3/2}3d_{5/2}[4]3p_{3/2}$
	$3d_{3/2}3d_{5/2}[2]3p_{3/2}$		
	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$		$3d_{5/2}3d_{5/2}[4]3p_{3/2}$
			$3d_{3/2}3d_{5/2}[4]3p_{3/2}$

Even-parity states

J=0.5	J=1.5	J=2.5	J=3.5-5.5
$3p_{1/2}3p_{1/2}[0]3s_{1/2}$	$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	$3p_{3/2}3p_{3/2}[2]3d_{3/2}$
$3p_{3/2}3p_{3/2}[0]3s_{1/2}$	$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$
$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	$3s_{1/2}3s_{1/2}[0]3d_{5/2}$	$3p_{1/2}3p_{3/2}[1]3d_{5/2}$
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	$3s_{1/2}3s_{1/2}[0]3d_{3/2}$	$3p_{1/2}3p_{1/2}[0]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{3/2}$
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{1/2}[0]3d_{3/2}$	$3p_{3/2}3p_{3/2}[0]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$
$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	$3p_{3/2}3p_{3/2}[0]3d_{3/2}$	$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[4]3s_{1/2}$
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{5/2}[3]3s_{1/2}$
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	$3d_{3/2}3d_{5/2}[4]3s_{1/2}$
$3d_{3/2}3d_{3/2}[0]3s_{1/2}$	$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$
$3d_{5/2}3d_{5/2}[0]3s_{1/2}$	$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[2]3d_{3/2}$
$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3d_{5/2}3d_{5/2}[4]3d_{3/2}$
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$
	$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$
	$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	$3d_{3/2}3d_{5/2}[3]3s_{1/2}$	$3d_{5/2}3d_{5/2}[4]3s_{1/2}$
	$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	$3d_{3/2}3d_{3/2}[0]3d_{5/2}$	$3d_{3/2}3d_{5/2}[4]3s_{1/2}$
	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$
	$3d_{5/2}3d_{5/2}[0]3d_{3/2}$	$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[4]3d_{3/2}$
	$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	$3d_{5/2}3d_{5/2}[2]3d_{5/2}$
	$3d_{3/2}3d_{3/2}[0]3d_{3/2}$	$3d_{5/2}3d_{5/2}[0]3d_{5/2}$	
	$3d_{5/2}3d_{5/2}[2]3d_{5/2}$		$3d_{5/2}3d_{5/2}[4]3d_{3/2}$

TABLE II. Contribution to the one-electron energy $E[3lj]= E_0 + E_1 + B_1 + E_2$ for the case of germanium, Z=32 in a.u.

$3lj$	E_0	E_1	B_1	E_2
$3s_{1/2}$	-32.345102	0.0	0.012104	-0.027696
$3p_{1/2}$	-30.595853	0.0	0.019052	-0.033384
$3p_{3/2}$	-30.321706	0.0	0.012724	-0.032427
$3d_{3/2}$	-27.969556	0.0	0.008577	-0.036968
$3d_{5/2}$	-27.919778	0.0	0.004638	-0.036198

TABLE III. Contribution to the two-electron energy $E[3l_1j_13l_2j_2(J),3l_3j_33l_4j_4(J)]= E_1+B_1+E_2$ for the case of germanium, Z=32 in a.u.

$3l_1j_13l_2j_2$	$3l_3j_33l_4j_4$	E_1	B_1	E_2
		Even-parity states, J=0		
$3s_{1/2}3s_{1/2}$	$3s_{1/2}3s_{1/2}$	1.743788	0.000400	-0.021984
$3p_{1/2}3p_{1/2}$	$3p_{1/2}3p_{1/2}$	1.800984	0.000769	-0.029776
$3p_{3/2}3p_{3/2}$	$3p_{3/2}3p_{3/2}$	1.963896	0.001492	-0.041080
$3d_{3/2}3d_{3/2}$	$3d_{3/2}3d_{3/2}$	2.221077	0.002327	-0.064125
$3d_{5/2}3d_{5/2}$	$3d_{5/2}3d_{5/2}$	2.309021	0.003467	-0.073600
$3s_{1/2}3s_{1/2}$	$3p_{1/2}3p_{1/2}$	-0.384671	-0.000293	0.024783
$3p_{1/2}3p_{1/2}$	$3s_{1/2}3s_{1/2}$	-0.384671	-0.000293	0.022612
$3s_{1/2}3s_{1/2}$	$3p_{3/2}3p_{3/2}$	-0.544408	-0.000662	0.035437
$3p_{3/2}3p_{3/2}$	$3s_{1/2}3s_{1/2}$	-0.544408	-0.000662	0.031835
$3s_{1/2}3s_{1/2}$	$3d_{3/2}3d_{3/2}$	0.209638	0.000372	-0.014315
$3d_{3/2}3d_{3/2}$	$3s_{1/2}3s_{1/2}$	0.209638	0.000372	-0.010282
$3s_{1/2}3s_{1/2}$	$3d_{5/2}3d_{5/2}$	0.257272	0.000659	-0.017636
$3d_{5/2}3d_{5/2}$	$3s_{1/2}3s_{1/2}$	0.257272	0.000659	-0.012570
$3p_{1/2}3p_{1/2}$	$3p_{3/2}3p_{3/2}$	0.256856	0.000406	-0.016807
$3p_{3/2}3p_{3/2}$	$3p_{1/2}3p_{1/2}$	0.256856	0.000406	-0.016499
$3p_{1/2}3p_{1/2}$	$3d_{3/2}3d_{3/2}$	-0.467870	-0.000751	0.031161
$3d_{3/2}3d_{3/2}$	$3p_{1/2}3p_{1/2}$	-0.467870	-0.000751	0.026375
$3p_{1/2}3p_{1/2}$	$3d_{5/2}3d_{5/2}$	-0.164000	-0.000501	0.014969
$3d_{5/2}3d_{5/2}$	$3p_{1/2}3p_{1/2}$	-0.164000	-0.000501	0.011960
$3p_{3/2}3p_{3/2}$	$3d_{3/2}3d_{3/2}$	-0.232469	-0.000433	0.019197
$3d_{3/2}3d_{3/2}$	$3p_{3/2}3p_{3/2}$	-0.232469	-0.000433	0.015987
$3p_{3/2}3p_{3/2}$	$3d_{5/2}3d_{5/2}$	-0.569116	-0.001312	0.039209
$3d_{5/2}3d_{5/2}$	$3p_{3/2}3p_{3/2}$	-0.569116	-0.001312	0.033385
$3d_{3/2}3d_{3/2}$	$3d_{5/2}3d_{5/2}$	0.229976	0.000751	-0.024406
$3d_{5/2}3d_{5/2}$	$3d_{3/2}3d_{3/2}$	0.229976	0.000751	-0.024279
		Even-parity states, J=1		
$3s_{1/2}3d_{3/2}$	$3s_{1/2}3d_{3/2}$	1.696132	0.000483	-0.026901
$3p_{1/2}3p_{3/2}$	$3p_{1/2}3p_{3/2}$	1.610158	0.000745	-0.017749
$3d_{3/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	2.030107	0.002331	-0.043992
$3s_{1/2}3d_{3/2}$	$3p_{1/2}3p_{3/2}$	0.001099	0.000122	-0.000102
$3p_{1/2}3p_{3/2}$	$3s_{1/2}3d_{3/2}$	0.001099	0.000122	-0.000104
$3s_{1/2}3d_{3/2}$	$3d_{3/2}3d_{5/2}$	-0.000067	0.000028	0.000022
$3d_{3/2}3d_{5/2}$	$3s_{1/2}3d_{3/2}$	-0.000067	0.000028	0.000019
$3p_{1/2}3p_{3/2}$	$3d_{3/2}3d_{5/2}$	-0.313910	-0.000555	0.017544
$3d_{3/2}3d_{5/2}$	$3p_{1/2}3p_{3/2}$	-0.313910	-0.000555	0.015441
		Even-parity states, J=2		
$3s_{1/2}3d_{3/2}$	$3s_{1/2}3d_{3/2}$	1.814721	-0.000079	-0.038559
$3s_{1/2}3d_{5/2}$	$3s_{1/2}3d_{5/2}$	1.871995	0.000494	-0.044243
$3p_{1/2}3p_{3/2}$	$3p_{1/2}3p_{3/2}$	1.755458	-0.000217	-0.031426
$3p_{3/2}3p_{3/2}$	$3p_{3/2}3p_{3/2}$	1.674117	0.000298	-0.024387
$3d_{3/2}3d_{3/2}$	$3d_{3/2}3d_{3/2}$	1.887145	0.000465	-0.040629
$3d_{5/2}3d_{5/2}$	$3d_{5/2}3d_{5/2}$	1.998222	0.001470	-0.047955
$3d_{3/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	1.970509	0.000716	-0.043917
$3s_{1/2}3d_{3/2}$	$3s_{1/2}3d_{5/2}$	-0.145388	-0.000061	0.014270
$3s_{1/2}3d_{5/2}$	$3s_{1/2}3d_{3/2}$	-0.145388	-0.000061	0.014240
$3s_{1/2}3d_{3/2}$	$3p_{1/2}3p_{3/2}$	-0.277747	0.000104	0.022130
$3p_{1/2}3p_{3/2}$	$3s_{1/2}3d_{3/2}$	-0.277747	0.000104	0.022593
$3s_{1/2}3d_{3/2}$	$3p_{3/2}3p_{3/2}$	-0.193972	0.000031	0.015528
$3p_{3/2}3p_{3/2}$	$3s_{1/2}3d_{3/2}$	-0.193972	0.000031	0.015704
$3s_{1/2}3d_{3/2}$	$3d_{3/2}3d_{3/2}$	0.089449	0.000276	-0.010631
$3d_{3/2}3d_{3/2}$	$3s_{1/2}3d_{3/2}$	0.089449	0.000276	-0.008509
$3s_{1/2}3d_{3/2}$	$3d_{5/2}3d_{5/2}$	0.117158	0.000303	-0.013744
$3d_{5/2}3d_{5/2}$	$3s_{1/2}3d_{3/2}$	0.117158	0.000303	-0.010966
$3s_{1/2}3d_{3/2}$	$3d_{3/2}3d_{5/2}$	0.082927	-0.000006	-0.009694
$3d_{3/2}3d_{5/2}$	$3s_{1/2}3d_{3/2}$	0.082927	-0.000006	-0.007778

$3l_1j_13l_2j_2$	$3l_3j_33l_4j_4$	E_1	B_1	E_2
		Even-parity states, J=2		
$3s_{1/2}3d_{5/2}$	$3p_{1/2}3p_{3/2}$	0.336537	0.000120	-0.026682
$3p_{1/2}3p_{3/2}$	$3s_{1/2}3d_{5/2}$	0.336537	0.000120	-0.027275
$3s_{1/2}3d_{5/2}$	$3p_{3/2}3p_{3/2}$	0.237853	0.000045	-0.018984
$3p_{3/2}3p_{3/2}$	$3s_{1/2}3d_{5/2}$	0.237853	0.000045	-0.019231
$3s_{1/2}3d_{5/2}$	$3d_{3/2}3d_{3/2}$	-0.109520	0.000019	0.012827
$3d_{3/2}3d_{3/2}$	$3s_{1/2}3d_{5/2}$	-0.109520	0.000019	0.010316
$3s_{1/2}3d_{5/2}$	$3d_{5/2}3d_{5/2}$	-0.143734	-0.000195	0.016805
$3d_{5/2}3d_{5/2}$	$3s_{1/2}3d_{5/2}$	-0.143734	-0.000195	0.013449
$3s_{1/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	-0.101605	0.000083	0.011840
$3d_{3/2}3d_{5/2}$	$3s_{1/2}3d_{5/2}$	-0.101605	0.000083	0.009508
$3p_{1/2}3p_{3/2}$	$3p_{3/2}3p_{3/2}$	0.102593	0.000171	-0.009763
$3p_{3/2}3p_{3/2}$	$3p_{1/2}3p_{3/2}$	0.102593	0.000171	-0.009655
$3p_{1/2}3p_{3/2}$	$3d_{3/2}3d_{3/2}$	-0.185261	-0.000190	0.015350
$3d_{3/2}3d_{3/2}$	$3p_{1/2}3p_{3/2}$	-0.185261	-0.000190	0.012679
$3p_{1/2}3p_{3/2}$	$3d_{5/2}3d_{5/2}$	-0.069622	-0.000232	0.010388
$3d_{5/2}3d_{5/2}$	$3p_{1/2}3p_{3/2}$	-0.069622	-0.000232	0.008011
$3p_{1/2}3p_{3/2}$	$3d_{3/2}3d_{5/2}$	-0.263613	-0.000094	0.019279
$3d_{3/2}3d_{5/2}$	$3p_{1/2}3p_{3/2}$	-0.263613	-0.000094	0.016195
$3p_{3/2}3p_{3/2}$	$3d_{3/2}3d_{3/2}$	-0.046494	-0.000087	0.006090
$3d_{3/2}3d_{3/2}$	$3p_{3/2}3p_{3/2}$	-0.046494	-0.000087	0.004831
$3p_{3/2}3p_{3/2}$	$3d_{5/2}3d_{5/2}$	-0.303668	-0.000422	0.021278
$3d_{5/2}3d_{5/2}$	$3p_{3/2}3p_{3/2}$	-0.303668	-0.000422	0.018092
$3p_{3/2}3p_{3/2}$	$3d_{3/2}3d_{5/2}$	0.085444	-0.000018	-0.001473
$3d_{3/2}3d_{5/2}$	$3p_{3/2}3p_{3/2}$	0.085444	-0.000018	-0.001838
$3d_{3/2}3d_{3/2}$	$3d_{5/2}3d_{5/2}$	0.034235	0.000132	-0.005873
$3d_{5/2}3d_{5/2}$	$3d_{3/2}3d_{3/2}$	0.034235	0.000132	-0.005840
$3d_{3/2}3d_{3/2}$	$3d_{3/2}3d_{5/2}$	0.077152	-0.000050	-0.006587
$3d_{3/2}3d_{5/2}$	$3d_{3/2}3d_{3/2}$	0.077152	-0.000050	-0.006573
$3d_{5/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	-0.037480	0.000176	-0.002172
$3d_{3/2}3d_{5/2}$	$3d_{5/2}3d_{5/2}$	-0.037480	0.000176	-0.002182
		Even-parity states, J=3		
$3s_{1/2}3d_{5/2}$	$3s_{1/2}3d_{5/2}$	1.693752	-0.000027	-0.026871
$3d_{3/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	1.825575	0.000394	-0.034478
$3s_{1/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	0.000086	0.000413	-0.000101
$3d_{3/2}3d_{5/2}$	$3s_{1/2}3d_{5/2}$	0.000086	0.000413	-0.000065
		Even-parity states, J=4		
$3d_{5/2}3d_{5/2}$	$3d_{5/2}3d_{5/2}$	1.876771	-0.000046	-0.042563
$3d_{3/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	2.042046	-0.001073	-0.067936
$3d_{5/2}3d_{5/2}$	$3d_{3/2}3d_{5/2}$	0.108080	0.000208	-0.016559
$3d_{3/2}3d_{5/2}$	$3d_{5/2}3d_{5/2}$	0.108080	0.000208	-0.016612
		Odd-parity states, J=0		
$3s_{1/2}3p_{1/2}$	$3s_{1/2}3p_{1/2}$	1.384729	0.000555	-0.002000
$3p_{3/2}3d_{3/2}$	$3p_{3/2}3d_{3/2}$	1.817350	0.001679	-0.034980
$3s_{1/2}3p_{1/2}$	$3p_{3/2}3d_{3/2}$	-0.269113	-0.000396	0.018829
$3p_{3/2}3d_{3/2}$	$3s_{1/2}3p_{1/2}$	-0.269113	-0.000396	0.016641
		Odd-parity states, J=1		
$3s_{1/2}3p_{1/2}$	$3s_{1/2}3p_{1/2}$	1.641177	0.000010	-0.019696
$3s_{1/2}3p_{3/2}$	$3s_{1/2}3p_{3/2}$	1.889309	0.000485	-0.037332
$3p_{1/2}3d_{3/2}$	$3p_{1/2}3d_{3/2}$	1.989496	0.000841	-0.053052
$3p_{3/2}3d_{3/2}$	$3p_{3/2}3d_{3/2}$	1.851465	0.000591	-0.038482
$3p_{3/2}3d_{5/2}$	$3p_{3/2}3d_{5/2}$	2.095120	0.001580	-0.066242
$3s_{1/2}3p_{1/2}$	$3s_{1/2}3p_{3/2}$	-0.362796	-0.000090	0.025168
$3s_{1/2}3p_{3/2}$	$3s_{1/2}3p_{1/2}$	-0.362796	-0.000090	0.024974
$3s_{1/2}3p_{1/2}$	$3p_{1/2}3d_{3/2}$	0.326726	0.000173	-0.026027
$3p_{1/2}3d_{3/2}$	$3s_{1/2}3p_{1/2}$	0.326726	0.000173	-0.022624
$3s_{1/2}3p_{1/2}$	$3p_{3/2}3d_{3/2}$	-0.266389	-0.000127	0.020133
$3p_{3/2}3d_{3/2}$	$3s_{1/2}3p_{1/2}$	-0.266389	-0.000127	0.017522

$3l_1j_13l_2j_2$	$3l_3j_33l_4j_4$	E_1	B_1	E_2
		Odd-parity states, J=1		
$3s_{1/2}3p_{1/2}$	$3p_{3/2}3d_{5/2}$	0.197673	0.000237	-0.018377
$3p_{3/2}3d_{5/2}$	$3s_{1/2}3p_{1/2}$	0.197673	0.000237	-0.015382
$3s_{1/2}3p_{3/2}$	$3p_{1/2}3d_{3/2}$	-0.270423	-0.000141	0.023352
$3p_{1/2}3d_{3/2}$	$3s_{1/2}3p_{3/2}$	-0.270423	-0.000141	0.020195
$3s_{1/2}3p_{3/2}$	$3p_{3/2}3d_{3/2}$	0.037043	-0.000041	-0.004736
$3p_{3/2}3d_{3/2}$	$3s_{1/2}3p_{3/2}$	0.037043	-0.000041	-0.003847
$3s_{1/2}3p_{3/2}$	$3p_{3/2}3d_{5/2}$	-0.530331	-0.000544	0.043226
$3p_{3/2}3d_{5/2}$	$3s_{1/2}3p_{3/2}$	-0.530331	-0.000544	0.037307
$3p_{1/2}3d_{3/2}$	$3p_{3/2}3d_{3/2}$	-0.065486	-0.000058	0.007774
$3p_{3/2}3d_{3/2}$	$3p_{1/2}3d_{3/2}$	-0.065486	-0.000058	0.007657
$3p_{1/2}3d_{3/2}$	$3p_{3/2}3d_{5/2}$	0.207448	0.000291	-0.023566
$3p_{3/2}3d_{5/2}$	$3p_{1/2}3d_{3/2}$	0.207448	0.000291	-0.023218
$3p_{3/2}3d_{3/2}$	$3p_{3/2}3d_{5/2}$	-0.094815	-0.000087	0.010512
$3p_{3/2}3d_{5/2}$	$3p_{3/2}3d_{3/2}$	-0.094815	-0.000087	0.010491
		Odd-parity states, J=2		
$3s_{1/2}3p_{3/2}$	$3s_{1/2}3p_{3/2}$	1.376037	0.000083	-0.001815
$3p_{1/2}3d_{3/2}$	$3p_{1/2}3d_{3/2}$	1.548383	-0.000080	-0.018296
$3p_{1/2}3d_{5/2}$	$3p_{1/2}3d_{5/2}$	1.782245	0.000880	-0.032385
$3p_{3/2}3d_{3/2}$	$3p_{3/2}3d_{3/2}$	1.712641	0.000336	-0.028238
$3p_{3/2}3d_{5/2}$	$3p_{3/2}3d_{5/2}$	1.679051	0.000566	-0.026017
$3s_{1/2}3p_{3/2}$	$3p_{1/2}3d_{3/2}$	0.037399	0.000037	-0.002570
$3p_{1/2}3d_{3/2}$	$3s_{1/2}3p_{3/2}$	0.037399	0.000037	-0.002309
$3s_{1/2}3p_{3/2}$	$3p_{1/2}3d_{5/2}$	0.183420	0.000064	-0.012604
$3p_{1/2}3d_{5/2}$	$3s_{1/2}3p_{3/2}$	0.183420	0.000064	-0.011306
$3s_{1/2}3p_{3/2}$	$3p_{3/2}3d_{3/2}$	-0.074873	0.000011	0.005171
$3p_{3/2}3d_{3/2}$	$3s_{1/2}3p_{3/2}$	-0.074873	0.000011	0.004607
$3s_{1/2}3p_{3/2}$	$3p_{3/2}3d_{5/2}$	-0.171746	-0.000125	0.011859
$3p_{3/2}3d_{5/2}$	$3s_{1/2}3p_{3/2}$	-0.171746	-0.000125	0.010548
$3p_{1/2}3d_{3/2}$	$3p_{1/2}3d_{5/2}$	0.000000	-0.000012	0.000217
$3p_{1/2}3d_{5/2}$	$3p_{1/2}3d_{3/2}$	0.000000	-0.000012	0.000216
$3p_{1/2}3d_{3/2}$	$3p_{3/2}3d_{3/2}$	-0.058047	0.000191	0.003072
$3p_{3/2}3d_{3/2}$	$3p_{1/2}3d_{3/2}$	-0.058047	0.000191	0.003071
$3p_{1/2}3d_{3/2}$	$3p_{3/2}3d_{5/2}$	-0.034689	-0.000050	0.002553
$3p_{3/2}3d_{5/2}$	$3p_{1/2}3d_{3/2}$	-0.034689	-0.000050	0.002506
$3p_{1/2}3d_{5/2}$	$3p_{3/2}3d_{3/2}$	0.071360	0.000190	-0.004392
$3p_{3/2}3d_{3/2}$	$3p_{1/2}3d_{5/2}$	0.071360	0.000190	-0.004373
$3p_{1/2}3d_{5/2}$	$3p_{3/2}3d_{5/2}$	-0.075660	-0.000050	0.004978
$3p_{3/2}3d_{5/2}$	$3p_{1/2}3d_{5/2}$	-0.075660	-0.000050	0.004913
$3p_{3/2}3d_{3/2}$	$3p_{3/2}3d_{5/2}$	0.107946	-0.000049	-0.006809
$3p_{3/2}3d_{5/2}$	$3p_{3/2}3d_{3/2}$	0.107946	-0.000049	-0.006798
		Odd-parity states, J=3		
$3p_{1/2}3d_{5/2}$	$3p_{1/2}3d_{5/2}$	1.863404	-0.000381	-0.047636
$3p_{3/2}3d_{3/2}$	$3p_{3/2}3d_{3/2}$	1.860776	-0.000486	-0.050051
$3p_{3/2}3d_{5/2}$	$3p_{3/2}3d_{5/2}$	1.947776	0.000145	-0.050798
$3p_{1/2}3d_{5/2}$	$3p_{3/2}3d_{3/2}$	-0.330643	0.000204	0.031024
$3p_{3/2}3d_{3/2}$	$3p_{1/2}3d_{5/2}$	-0.330643	0.000204	0.030728
$3p_{1/2}3d_{5/2}$	$3p_{3/2}3d_{5/2}$	0.117281	0.000180	-0.016451
$3p_{3/2}3d_{5/2}$	$3p_{1/2}3d_{5/2}$	0.117281	0.000180	-0.016196
$3p_{3/2}3d_{3/2}$	$3p_{3/2}3d_{5/2}$	-0.193699	-0.000103	0.021765
$3p_{3/2}3d_{5/2}$	$3p_{3/2}3d_{3/2}$	-0.193699	-0.000103	0.021711
		Odd-parity states, J=4		
$3p_{3/2}3d_{5/2}$	$3p_{3/2}3d_{5/2}$	1.519828	-0.000240	-0.017487

TABLE IV. Diagonal contributions to the three-electron energy $E[3l_1j_13l_2j_2[J_{12}]3l_3(J), 3l_1j_13l_23j_2[J_{12}]3l_3(J)] = E_0 + E_1 + B_1 + E_2$ for the case of germanium, Z=32 in a.u.

$3l_1j_13l_2j_2[J_{12}]3l_3$	$3l_1j_13l_2j_2[J_{12}]3l_3$	E_0	E_1	B_1	E_2	E^G
Odd-parity states, J=1/2						
$3s_{1/2}3s_{1/2}[0]3p_{1/2}$	$3s_{1/2}3s_{1/2}[0]3p_{1/2}$	-95.286056	4.897918	0.043952	-0.167811	-0.026506
$3p_{3/2}3p_{3/2}[0]3p_{1/2}$	$3p_{3/2}3p_{3/2}[0]3p_{1/2}$	-91.239265	5.365837	0.046278	-0.225383	-0.033470
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	-90.910510	5.326804	0.041066	-0.233031	-0.035334
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	-90.636363	5.535290	0.034844	-0.252306	-0.042884
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-90.636363	4.909723	0.035206	-0.188381	-0.025553
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-90.586586	5.343152	0.031624	-0.229276	-0.020656
$3d_{3/2}3d_{3/2}[0]3p_{1/2}$	$3d_{3/2}3d_{3/2}[0]3p_{1/2}$	-86.534964	5.648678	0.039064	-0.272410	-0.038306
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-86.260817	5.520663	0.031397	-0.265319	-0.046485
$3d_{5/2}3d_{5/2}[0]3p_{1/2}$	$3d_{5/2}3d_{5/2}[0]3p_{1/2}$	-86.435409	5.968196	0.032085	-0.317041	-0.055097
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-86.161262	5.535474	0.024322	-0.257509	-0.036177
$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	-86.485186	5.360735	0.035399	-0.240544	-0.039321
$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	-86.211039	5.785456	0.029024	-0.295486	-0.049935
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-86.211039	5.562748	0.027898	-0.272622	-0.048532
Odd-parity states, J=3/2						
$3s_{1/2}3s_{1/2}[0]3p_{3/2}$	$3s_{1/2}3s_{1/2}[0]3p_{3/2}$	-95.011909	4.880816	0.037799	-0.166400	-0.026329
$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	-91.239265	4.967083	0.045806	-0.195879	-0.030916
$3p_{1/2}3p_{1/2}[0]3p_{3/2}$	$3p_{1/2}3p_{1/2}[0]3p_{3/2}$	-91.513412	5.202925	0.051883	-0.213971	-0.032404
$3p_{3/2}3p_{3/2}[0]3p_{3/2}$	$3p_{3/2}3p_{3/2}[0]3p_{3/2}$	-90.965118	5.167240	0.039663	-0.210870	-0.032081
$3s_{1/2}3p_{1/2}[0]3d_{3/2}$	$3s_{1/2}3p_{1/2}[0]3d_{3/2}$	-90.910510	4.868780	0.040684	-0.191621	-0.026057
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	-90.910510	5.205858	0.040510	-0.220302	-0.031267
$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	-90.860733	5.295416	0.037179	-0.227447	-0.033844
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	-90.636363	5.421730	0.034350	-0.237697	-0.036831
$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	-90.586586	5.518431	0.031126	-0.253356	-0.042017
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-90.636363	4.918575	0.034357	-0.190926	-0.026284
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-90.586586	5.086832	0.030988	-0.207090	-0.023268
$3d_{3/2}3d_{3/2}[0]3p_{3/2}$	$3d_{3/2}3d_{3/2}[0]3p_{3/2}$	-86.260817	5.841124	0.032421	-0.303159	-0.052426
$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	-86.534964	5.645580	0.037892	-0.277160	-0.040486
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-86.260817	5.414205	0.031729	-0.256053	-0.043787
$3d_{5/2}3d_{5/2}[0]3p_{3/2}$	$3d_{5/2}3d_{5/2}[0]3p_{3/2}$	-86.161262	5.808479	0.026004	-0.293207	-0.044636
$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	-86.435409	5.616817	0.030719	-0.276690	-0.048017
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-86.161262	5.875888	0.024673	-0.315947	-0.060276
$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	-86.485186	5.679875	0.034813	-0.282519	-0.048402
$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	-86.211039	5.705181	0.028591	-0.287893	-0.053419
$3d_{3/2}3d_{5/2}[2]3p_{1/2}$	$3d_{3/2}3d_{5/2}[2]3p_{1/2}$	-86.485186	5.504268	0.034029	-0.267935	-0.049675
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-86.211039	5.723157	0.027504	-0.284199	-0.044133
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-86.211039	5.544682	0.027896	-0.269385	-0.044933
Odd-parity states, J=5/2						
$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	-91.239265	5.148708	0.044604	-0.214090	-0.032031
$3s_{1/2}3p_{1/2}[0]3d_{5/2}$	$3s_{1/2}3p_{1/2}[0]3d_{5/2}$	-90.860733	4.982337	0.036683	-0.199309	-0.024641
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	-90.910510	5.004281	0.039584	-0.207184	-0.032585
$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	-90.860733	5.254964	0.036436	-0.221998	-0.029279
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	-90.636363	5.479583	0.033743	-0.253553	-0.039805
$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	-90.586586	5.500676	0.030383	-0.244394	-0.035542
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-90.636363	4.870032	0.033887	-0.189868	-0.026540
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-90.586586	4.957243	0.030295	-0.195780	-0.024915
$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	-86.534964	5.094190	0.036742	-0.234153	-0.040923
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-86.260817	5.528111	0.030536	-0.275225	-0.047136
$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	-86.435409	5.684450	0.029668	-0.290497	-0.049116
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-86.161262	5.375785	0.024174	-0.252127	-0.039234
$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	-86.161262	5.647463	0.023857	-0.284714	-0.045593
$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	-86.211039	5.447781	0.028558	-0.253629	-0.042232
$3d_{3/2}3d_{5/2}[2]3p_{1/2}$	$3d_{3/2}3d_{5/2}[2]3p_{1/2}$	-86.485186	5.520315	0.032970	-0.267686	-0.041397
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-86.211039	5.589520	0.027089	-0.280842	-0.051037

$3l_1j_13l_2j_2[J_{12}]3l_3$	$3l_1j_13l_2j_2[J_{12}]3l_3$	E_0	E_1	B_1	E_2	E^G
Odd-parity states, J=5/2						
$3d_{3/2}3d_{5/2}[3]3p_{1/2}$	$3d_{3/2}3d_{5/2}[3]3p_{1/2}$	-86.485186	5.459295	0.033936	-0.259175	-0.042601
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-86.211039	5.456284	0.027511	-0.262776	-0.045099
$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	-86.211039	5.858660	0.027139	-0.317930	-0.051821
Odd-parity states, J=7/2						
$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	-90.860733	5.198332	0.035396	-0.224642	-0.033160
$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	-90.586586	5.281158	0.030070	-0.234377	-0.040304
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-90.636363	5.051534	0.032923	-0.209352	-0.021837
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-90.586586	5.017538	0.029803	-0.201823	-0.024709
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-86.260817	5.534629	0.029782	-0.278806	-0.042620
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-86.161262	5.390550	0.023469	-0.253841	-0.039365
$3d_{5/2}3d_{5/2}[4]3p_{1/2}$	$3d_{5/2}3d_{5/2}[4]3p_{1/2}$	-86.435409	5.468314	0.029623	-0.263501	-0.045304
$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	-86.161262	5.646508	0.023112	-0.288839	-0.049788
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-86.211039	5.381248	0.026535	-0.253705	-0.040346
$3d_{3/2}3d_{5/2}[3]3p_{1/2}$	$3d_{3/2}3d_{5/2}[3]3p_{1/2}$	-86.485186	5.301213	0.032424	-0.253926	-0.042489
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-86.211039	5.459010	0.026504	-0.262297	-0.041189
$3d_{3/2}3d_{5/2}[4]3p_{1/2}$	$3d_{3/2}3d_{5/2}[4]3p_{1/2}$	-86.485186	5.749935	0.032693	-0.306816	-0.051371
$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	-86.211039	5.569408	0.025729	-0.287231	-0.047516
Odd-parity states, J=9/2						
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-90.586586	4.589616	0.029282	-0.169941	-0.027447
$3d_{5/2}3d_{5/2}[4]3p_{1/2}$	$3d_{5/2}3d_{5/2}[4]3p_{1/2}$	-86.435409	5.590052	0.027731	-0.286627	-0.045554
$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	-86.161262	5.356453	0.022218	-0.251264	-0.036677
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-86.211039	5.220067	0.025919	-0.247143	-0.041667
$3d_{3/2}3d_{5/2}[4]3p_{1/2}$	$3d_{3/2}3d_{5/2}[4]3p_{1/2}$	-86.485186	5.453833	0.030733	-0.276760	-0.036342
$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	-86.211039	5.688575	0.025036	-0.304694	-0.049998
Even-parity states, J=1/2						
$3p_{1/2}3p_{1/2}[0]3s_{1/2}$	$3p_{1/2}3p_{1/2}[0]3s_{1/2}$	-93.536808	4.955114	0.051269	-0.183102	-0.028316
$3p_{3/2}3p_{3/2}[0]3s_{1/2}$	$3p_{3/2}3p_{3/2}[0]3s_{1/2}$	-92.988514	5.100923	0.039511	-0.192740	-0.028843
$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	-93.262661	5.140644	0.045119	-0.199043	-0.030758
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-88.612968	5.307635	0.035376	-0.237422	-0.039371
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-88.563190	5.136236	0.031769	-0.224224	-0.036696
$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	-88.887115	5.024783	0.042073	-0.215023	-0.036859
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-88.887115	5.547527	0.042189	-0.265053	-0.043675
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-88.837337	5.632823	0.038657	-0.274843	-0.042780
$3d_{3/2}3d_{3/2}[0]3s_{1/2}$	$3d_{3/2}3d_{3/2}[0]3s_{1/2}$	-88.284213	5.761577	0.031847	-0.281607	-0.047476
$3d_{5/2}3d_{5/2}[0]3s_{1/2}$	$3d_{5/2}3d_{5/2}[0]3s_{1/2}$	-88.184657	5.845060	0.025229	-0.290468	-0.048557
$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	-88.234435	5.716823	0.028066	-0.273236	-0.045581
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-83.858889	5.843061	0.024094	-0.297868	-0.059253
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-83.809111	5.842617	0.020542	-0.298090	-0.059230
Even-parity states, J=3/2						
$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	-93.262661	4.563283	0.044947	-0.153842	-0.025491
$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	-93.262661	5.093585	0.044473	-0.198420	-0.029738
$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	-92.988514	5.196099	0.038619	-0.204789	-0.030946
$3s_{1/2}3s_{1/2}[0]3d_{3/2}$	$3s_{1/2}3s_{1/2}[0]3d_{3/2}$	-92.659759	5.284289	0.033447	-0.216520	-0.033802
$3p_{1/2}3p_{1/2}[0]3d_{3/2}$	$3p_{1/2}3p_{1/2}[0]3d_{3/2}$	-89.161262	5.228585	0.047980	-0.235175	-0.039004
$3p_{3/2}3p_{3/2}[0]3d_{3/2}$	$3p_{3/2}3p_{3/2}[0]3d_{3/2}$	-88.612968	5.583944	0.035733	-0.265983	-0.042836
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-88.612968	5.201177	0.035709	-0.229514	-0.038030
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-88.563190	5.538447	0.031890	-0.268807	-0.043353
$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	-88.887115	5.016166	0.041647	-0.214421	-0.036109
$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	-88.837337	5.376507	0.038071	-0.252618	-0.038487
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-88.887115	5.451435	0.041273	-0.253285	-0.038795
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-88.837337	5.408929	0.037929	-0.252767	-0.041424
$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	-88.284213	5.338703	0.030407	-0.243923	-0.042031
$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	-88.184657	5.623383	0.023492	-0.269453	-0.044502
$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	-88.234435	5.494154	0.027925	-0.250390	-0.044493
$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	-88.234435	5.583062	0.026631	-0.264449	-0.044140
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-83.858889	5.753934	0.024563	-0.287737	-0.056639
$3d_{5/2}3d_{5/2}[0]3d_{3/2}$	$3d_{5/2}3d_{5/2}[0]3d_{3/2}$	-83.809111	6.234046	0.021628	-0.351520	-0.068196

$3l_1j_13l_2j_2[J_{12}]3l_3$	$3l_1j_13l_2j_2[J_{12}]3l_3$	E_0	E_1	B_1	E_2	E^G
Even-parity states, $J=3/2$						
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-83.809111	5.853979	0.021084	-0.300933	-0.058812
$3d_{3/2}3d_{3/2}[0]3d_{3/2}$	$3d_{3/2}3d_{3/2}[0]3d_{3/2}$	-83.908667	5.828400	0.028058	-0.301817	-0.057278
$3d_{5/2}3d_{5/2}[2]3d_{5/2}$	$3d_{5/2}3d_{5/2}[2]3d_{5/2}$	-83.759334	5.890566	0.017027	-0.307745	-0.059909
Even-parity states, $J=5/2$						
$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	-93.262661	4.772671	0.043756	-0.173192	-0.026747
$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	-92.988514	4.554508	0.038116	-0.154498	-0.025052
$3s_{1/2}3s_{1/2}[0]3d_{5/2}$	$3s_{1/2}3s_{1/2}[0]3d_{5/2}$	-92.609981	5.279828	0.029626	-0.215534	-0.033741
$3p_{1/2}3p_{1/2}[0]3d_{5/2}$	$3p_{1/2}3p_{1/2}[0]3d_{5/2}$	-89.111484	5.460159	0.043800	-0.255933	-0.040627
$3p_{3/2}3p_{3/2}[0]3d_{5/2}$	$3p_{3/2}3p_{3/2}[0]3d_{5/2}$	-88.563190	5.463354	0.032114	-0.254044	-0.041764
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-88.612968	5.315084	0.034515	-0.246045	-0.038739
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-88.563190	5.551783	0.031586	-0.264273	-0.035940
$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	-88.887115	5.248926	0.041152	-0.243277	-0.037579
$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	-88.837337	5.304710	0.037483	-0.242413	-0.037565
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-88.887115	5.227985	0.040691	-0.236417	-0.037746
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-88.837337	5.333381	0.037082	-0.243392	-0.038211
$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	-88.284213	5.486939	0.029705	-0.258842	-0.042379
$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	-88.184657	5.474847	0.023058	-0.254208	-0.043734
$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	-88.234435	5.459256	0.026174	-0.251645	-0.043393
$3d_{3/2}3d_{5/2}[3]3s_{1/2}$	$3d_{3/2}3d_{5/2}[3]3s_{1/2}$	-88.234435	5.413427	0.026445	-0.249804	-0.041365
$3d_{3/2}3d_{3/2}[0]3d_{5/2}$	$3d_{3/2}3d_{3/2}[0]3d_{5/2}$	-83.858889	6.146102	0.024426	-0.340894	-0.066275
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-83.858889	5.742901	0.024017	-0.291229	-0.055664
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-83.809111	6.012948	0.019640	-0.329272	-0.062844
$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	-83.809111	5.838545	0.020537	-0.296816	-0.058768
$3d_{5/2}3d_{5/2}[0]3d_{5/2}$	$3d_{5/2}3d_{5/2}[0]3d_{5/2}$	-83.759334	6.019689	0.017383	-0.323850	-0.062382
Even-parity states, $J=7/2$						
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-88.612968	5.321601	0.033762	-0.253678	-0.038275
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-88.563190	4.957237	0.030691	-0.213728	-0.037676
$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	-88.837337	5.009532	0.037386	-0.217016	-0.036461
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-88.887115	5.164617	0.039570	-0.241543	-0.038992
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-88.837337	5.469336	0.036374	-0.260475	-0.039529
$3d_{5/2}3d_{5/2}[4]3s_{1/2}$	$3d_{5/2}3d_{5/2}[4]3s_{1/2}$	-88.184657	5.561347	0.022149	-0.267701	-0.042352
$3d_{3/2}3d_{5/2}[3]3s_{1/2}$	$3d_{3/2}3d_{5/2}[3]3s_{1/2}$	-88.234435	5.326658	0.025728	-0.241158	-0.041125
$3d_{3/2}3d_{5/2}[4]3s_{1/2}$	$3d_{3/2}3d_{5/2}[4]3s_{1/2}$	-88.234435	5.617563	0.025103	-0.285291	-0.044613
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-83.858889	5.855801	0.022012	-0.316020	-0.058338
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-83.809111	5.910764	0.018670	-0.323486	-0.059883
$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	-83.809111	5.730896	0.019516	-0.290367	-0.055656
Even-parity states, $J=9/2$						
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-88.563190	4.981240	0.030145	-0.217889	-0.036657
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-88.837337	5.138689	0.035576	-0.237121	-0.038563
$3d_{5/2}3d_{5/2}[4]3s_{1/2}$	$3d_{5/2}3d_{5/2}[4]3s_{1/2}$	-88.184657	5.293982	0.021367	-0.240923	-0.041630
$3d_{3/2}3d_{5/2}[4]3s_{1/2}$	$3d_{3/2}3d_{5/2}[4]3s_{1/2}$	-88.234435	5.550519	0.024140	-0.278653	-0.044426
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-83.858889	5.835942	0.021029	-0.323275	-0.057551
$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	-83.809111	5.742999	0.017822	-0.302781	-0.055445
$3d_{5/2}3d_{5/2}[2]3d_{5/2}$	$3d_{5/2}3d_{5/2}[2]3d_{5/2}$	-83.759334	5.708389	0.014752	-0.294093	-0.054344

TABLE V. Energies of Al-like germanium, Z=32 in a.u. $E^{(0+1)} \equiv E_0 + E_1 + B_1$.

jj-coupling	$E^{(0+1)}$	E_2	E_{LAMB}	E_{tot}	$E^{(0+1)}$	E_2	E_{LAMB}	E_{tot}
Odd-parity states, J=1/2								
$3s_{1/2}3s_{1/2}[0]3p_{1/2}$	-90.482233	-0.150878	0.011710	-90.621401	0.000000	0.000000	0.000000	0.000000
$3p_{3/2}3p_{3/2}[0]3p_{1/2}$	-86.079540	-0.200045	0.001639	-86.277946	4.402693	-0.049167	-0.010071	4.343455
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	-85.870751	-0.189035	0.005944	-86.053842	4.611482	-0.038157	-0.005766	4.567559
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	-85.723046	-0.184160	0.006253	-85.900953	4.759187	-0.033282	-0.005457	4.720448
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-84.978205	-0.253607	0.005793	-85.226019	5.504028	-0.102729	-0.005917	5.395382
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-84.832708	-0.275664	0.005708	-85.102665	5.649525	-0.124786	-0.006002	5.518736
$3d_{3/2}3d_{3/2}[0]3p_{1/2}$	-81.101794	-0.240344	-0.000083	-81.342222	9.380439	-0.089466	-0.011793	9.279179
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-81.083557	-0.239941	-0.000082	-81.323580	9.398676	-0.089063	-0.011792	9.297821
$3d_{5/2}3d_{5/2}[0]3p_{1/2}$	-80.843906	-0.239630	0.000343	-81.083194	9.638327	-0.088752	-0.011367	9.538207
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-80.734599	-0.260151	0.000179	-80.994571	9.747634	-0.109273	-0.011531	9.626830
$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	-80.583712	-0.272143	0.000327	-80.855528	9.898521	-0.121265	-0.011383	9.765872
$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	-80.330089	-0.313922	0.000183	-80.643828	10.152144	-0.163044	-0.011527	9.977573
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-79.738244	-0.397240	0.000320	-80.135164	10.743989	-0.246362	-0.011390	10.486236
Odd-parity states, J=3/2								
$3s_{1/2}3s_{1/2}[0]3p_{3/2}$	-90.236083	-0.149070	0.012129	-90.373024	0.246150	0.001808	0.000419	0.248376
$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	-86.590984	-0.173294	0.001599	-86.762678	3.891249	-0.022416	-0.010111	3.858722
$3p_{1/2}3p_{1/2}[0]3p_{3/2}$	-86.453897	-0.173721	0.001013	-86.626606	4.028336	-0.022843	-0.010697	3.994795
$3p_{3/2}3p_{3/2}[0]3p_{3/2}$	-86.225614	-0.172462	0.005779	-86.392296	4.256619	-0.021584	-0.005931	4.229104
$3s_{1/2}3p_{1/2}[0]3d_{3/2}$	-86.001770	-0.191312	0.002390	-86.190693	4.480463	-0.040434	-0.009320	4.430708
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	-85.880027	-0.188102	0.005873	-86.062256	4.602206	-0.037224	-0.005837	4.559144
$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	-85.721776	-0.185438	0.006189	-85.901024	4.760457	-0.034560	-0.005521	4.720376
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	-85.637995	-0.203576	0.005154	-85.836417	4.844238	-0.052698	-0.006556	4.784984
$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	-85.101332	-0.253021	0.005120	-85.349233	5.380901	-0.102143	-0.006590	5.272168
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-84.815500	-0.269681	0.005819	-85.079362	5.666733	-0.118803	-0.005891	5.542039
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-84.781698	-0.274071	0.005611	-85.050158	5.700535	-0.123193	-0.006099	5.571242
$3d_{3/2}3d_{3/2}[0]3p_{3/2}$	-81.176021	-0.242635	-0.000040	-81.418696	9.306212	-0.091756	-0.011750	9.202704
$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	-81.039255	-0.242280	-0.000031	-81.281566	9.442978	-0.091402	-0.011741	9.339835
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-81.005878	-0.244389	0.000153	-81.250114	9.476355	-0.093510	-0.011557	9.371287
$3d_{5/2}3d_{5/2}[0]3p_{3/2}$	-80.901299	-0.249874	0.000107	-81.151066	9.580934	-0.098996	-0.011603	9.470334
$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	-80.746691	-0.262764	0.000116	-81.009338	9.735542	-0.111886	-0.011594	9.612062
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-80.676129	-0.269799	0.000223	-80.945706	9.806104	-0.118921	-0.011487	9.675695
$3d_{3/2}3d_{5/2}[1]3p_{1/2}$	-80.517675	-0.285714	0.000254	-80.803135	9.964558	-0.134836	-0.011456	9.818266
$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	-80.369111	-0.305609	0.000309	-80.674411	10.113122	-0.154731	-0.011401	9.946990
$3d_{3/2}3d_{5/2}[2]3p_{1/2}$	-80.165540	-0.316161	0.000509	-80.481192	10.316693	-0.165283	-0.011201	10.140208
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-79.873809	-0.381204	0.000265	-80.254748	10.608424	-0.230326	-0.011445	10.366653
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-79.704374	-0.394892	0.000385	-80.098881	10.777859	-0.244014	-0.011325	10.522520
Odd-parity states, J=5/2								
$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	-86.505847	-0.163105	0.002391	-86.666562	3.976386	-0.012227	-0.009319	3.954839
$3s_{1/2}3p_{1/2}[0]3d_{5/2}$	-86.173523	-0.172354	0.005927	-86.339951	4.308710	-0.021476	-0.005783	4.281450
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	-85.901628	-0.187743	0.005856	-86.083515	4.580605	-0.036865	-0.005854	4.537886
$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	-85.727475	-0.187361	0.006110	-85.908727	4.754758	-0.036483	-0.005600	4.712674
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	-85.629913	-0.205270	0.005443	-85.829739	4.852320	-0.054392	-0.006267	4.791662
$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	-85.515275	-0.219168	0.006037	-85.728406	4.966958	-0.068290	-0.005673	4.892995
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-84.943005	-0.266915	0.006099	-85.203821	5.539228	-0.116037	-0.005611	5.417579
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-84.793283	-0.265732	0.005563	-85.053452	5.688950	-0.114854	-0.006147	5.567949
$3d_{3/2}3d_{3/2}[2]3p_{1/2}$	-81.461996	-0.225511	-0.000215	-81.687722	9.020237	-0.074633	-0.011925	8.933679
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-81.233229	-0.243707	-0.000053	-81.476990	9.249004	-0.092829	-0.011763	9.144411
$3d_{5/2}3d_{5/2}[2]3p_{1/2}$	-81.080407	-0.242593	0.000216	-81.322785	9.401826	-0.091715	-0.011494	9.298616
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-81.005232	-0.241508	0.000077	-81.246664	9.477001	-0.090630	-0.011633	9.374737
$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	-80.930474	-0.241044	0.000405	-81.171113	9.551759	-0.090166	-0.011305	9.450287
$3d_{3/2}3d_{5/2}[1]3p_{3/2}$	-80.801901	-0.248774	0.000322	-81.050353	9.680332	-0.097896	-0.011388	9.571047
$3d_{3/2}3d_{5/2}[2]3p_{1/2}$	-80.734759	-0.254052	0.000291	-80.988520	9.747474	-0.103174	-0.011419	9.632881
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-80.480250	-0.301075	0.000177	-80.781148	10.001983	-0.150197	-0.011533	9.840253
$3d_{3/2}3d_{5/2}[3]3p_{1/2}$	-80.296344	-0.312024	0.000419	-80.607949	10.185889	-0.161146	-0.011291	10.013451
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-80.126734	-0.348035	0.000381	-80.474388	10.355499	-0.197157	-0.011329	10.147013
$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	-79.876983	-0.378608	0.000355	-80.255236	10.605250	-0.227730	-0.011355	10.366164

jj-coupling	$E^{(0+1)}$	E_2	$E_{\rm LAMB}$	$E_{\rm tot}$	$E^{(0+1)}$	E_2	$E_{\rm LAMB}$	$E_{\rm tot}$
	Odd-parity states, J=7/2							
$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	-86.094753	-0.171841	0.006143	-86.260451	4.387480	-0.020963	-0.005567	4.360949
$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	-85.735333	-0.185399	0.006313	-85.914419	4.746900	-0.034521	-0.005397	4.706981
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	-85.329043	-0.224325	0.006334	-85.547034	5.153190	-0.073447	-0.005376	5.074367
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-84.971901	-0.265010	0.006180	-85.230730	5.510332	-0.114132	-0.005530	5.390671
$3d_{3/2}3d_{3/2}[2]3p_{3/2}$	-81.394260	-0.224080	-0.000037	-81.618377	9.087973	-0.073202	-0.011747	9.003023
$3d_{5/2}3d_{5/2}[2]3p_{3/2}$	-81.094981	-0.246627	0.000223	-81.341385	9.387252	-0.095749	-0.011487	9.280015
$3d_{5/2}3d_{5/2}[4]3p_{1/2}$	-80.986340	-0.249336	0.000162	-81.235514	9.495893	-0.098458	-0.011548	9.385886
$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	-80.907234	-0.259420	0.000240	-81.166414	9.574999	-0.108542	-0.011470	9.454987
$3d_{3/2}3d_{5/2}[2]3p_{3/2}$	-80.882477	-0.242306	0.000401	-81.124381	9.599756	-0.091428	-0.011309	9.497019
$3d_{3/2}3d_{5/2}[3]3p_{1/2}$	-80.736770	-0.252270	0.000303	-80.988737	9.745463	-0.101392	-0.011407	9.632664
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-80.425863	-0.306872	0.000304	-80.732430	10.056370	-0.155994	-0.011406	9.888971
$3d_{3/2}3d_{5/2}[4]3p_{1/2}$	-80.231539	-0.341804	0.000158	-80.573185	10.250694	-0.190926	-0.011552	10.048215
$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	-80.074780	-0.349662	0.000410	-80.424032	10.407453	-0.198784	-0.011300	10.197368
	Odd-parity states, J=9/2							
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	-85.973234	-0.169262	0.006430	-86.136066	4.508999	-0.018384	-0.005280	4.485335
$3d_{5/2}3d_{5/2}[4]3p_{1/2}$	-81.308445	-0.223674	0.000155	-81.531964	9.173788	-0.072796	-0.011555	9.089436
$3d_{5/2}3d_{5/2}[4]3p_{3/2}$	-80.976051	-0.268107	0.000010	-81.244147	9.506182	-0.117229	-0.011700	9.377253
$3d_{3/2}3d_{5/2}[3]3p_{3/2}$	-80.900306	-0.249926	0.000288	-81.149944	9.581927	-0.099048	-0.011422	9.471457
$3d_{3/2}3d_{5/2}[4]3p_{1/2}$	-80.745162	-0.272614	0.000408	-81.017369	9.737071	-0.121736	-0.011302	9.604032
$3d_{3/2}3d_{5/2}[4]3p_{3/2}$	-80.127951	-0.352703	0.000269	-80.480385	10.354282	-0.201825	-0.011441	10.141016
	Even-parity states, J=1/2							
$3p_{1/2}3p_{1/2}[0]3s_{1/2}$	-88.970451	-0.139512	0.005984	-89.103978	1.511782	0.011366	-0.005726	1.517422
$3p_{3/2}3p_{3/2}[0]3s_{1/2}$	-88.009846	-0.200780	0.006070	-88.204556	2.472387	-0.049902	-0.005640	2.416844
$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	-87.761253	-0.200413	0.006475	-87.955190	2.720980	-0.049535	-0.005235	2.666210
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-83.872268	-0.209535	0.000203	-84.081600	6.609965	-0.058657	-0.011507	6.539801
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-83.663936	-0.203863	0.000937	-83.866862	6.818297	-0.052985	-0.010773	6.754539
$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	-83.465209	-0.228283	0.000382	-83.693111	7.017024	-0.077405	-0.011328	6.928290
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-83.278062	-0.249833	0.001457	-83.526437	7.204171	-0.098955	-0.010253	7.094964
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-83.120236	-0.247279	0.001092	-83.366424	7.361997	-0.096401	-0.010618	7.254977
$3d_{3/2}3d_{3/2}[0]3s_{1/2}$	-82.776369	-0.244626	0.005971	-83.015023	7.705864	-0.093748	-0.005739	7.606378
$3d_{5/2}3d_{5/2}[0]3s_{1/2}$	-81.977520	-0.345303	0.004610	-82.318213	8.504713	-0.194425	-0.007100	8.303188
$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	-81.925178	-0.343395	0.005427	-82.263146	8.557055	-0.192517	-0.006283	8.358255
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-77.983823	-0.292299	-0.000034	-78.276156	12.498410	-0.141421	-0.011744	12.345245
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-77.832886	-0.327007	0.000085	-78.159808	12.649347	-0.176129	-0.011625	12.461592
	Even-parity states, J=3/2							
$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	-88.855254	-0.136228	0.006251	-88.985231	1.626979	0.014650	-0.005459	1.636170
$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	-88.395840	-0.164942	0.006901	-88.553881	2.086393	-0.014064	-0.004809	2.067520
$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	-87.704538	-0.203947	0.006491	-87.901994	2.777695	-0.053069	-0.005219	2.719407
$3s_{1/2}3s_{1/2}[0]3d_{3/2}$	-87.311306	-0.215997	0.010976	-87.516327	3.170927	-0.065119	-0.000734	3.105073
$3p_{1/2}3p_{1/2}[0]3d_{3/2}$	-84.076204	-0.208034	-0.000096	-84.284333	6.406029	-0.057156	-0.011806	6.337067
$3p_{3/2}3p_{3/2}[0]3d_{3/2}$	-83.909923	-0.206034	0.000310	-84.115647	6.572310	-0.055156	-0.011400	6.505754
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-83.786280	-0.209200	0.000443	-83.995038	6.695953	-0.058322	-0.011267	6.626363
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-83.543978	-0.226338	0.000670	-83.769646	6.938255	-0.075460	-0.011040	6.851754
$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	-83.423521	-0.220676	0.000924	-83.643272	7.058712	-0.069798	-0.010786	6.978128
$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	-83.261459	-0.262747	0.000857	-83.523349	7.220774	-0.111869	-0.010853	7.098051
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-83.122486	-0.251037	0.001578	-83.371945	7.359747	-0.100159	-0.010132	7.249456
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-83.017355	-0.230800	0.005888	-83.242268	7.464878	-0.079922	-0.005822	7.379133
$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	-82.767745	-0.244269	0.006015	-83.005999	7.714488	-0.093391	-0.005695	7.615402
$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	-82.658730	-0.300299	0.000872	-82.958157	7.823503	-0.149421	-0.010838	7.663243
$3d_{3/2}3d_{5/2}[1]3s_{1/2}$	-82.460864	-0.298794	0.004960	-82.754698	8.021369	-0.147916	-0.006750	7.866702
$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	-81.939864	-0.345210	0.004522	-82.280552	8.542369	-0.194332	-0.007188	8.340848
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-78.224973	-0.273368	-0.000119	-78.498460	12.257260	-0.122490	-0.011829	12.122940
$3d_{5/2}3d_{5/2}[0]3d_{3/2}$	-77.979381	-0.294789	-0.000052	-78.274222	12.502852	-0.143911	-0.011762	12.347178
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-77.861085	-0.322259	-0.000012	-78.183356	12.621148	-0.171381	-0.011722	12.438044
$3d_{3/2}3d_{3/2}[0]3d_{3/2}$	-77.791572	-0.324104	0.000257	-78.115419	12.690661	-0.173226	-0.011453	12.505981
$3d_{5/2}3d_{5/2}[2]3d_{5/2}$	-77.329026	-0.384185	0.000096	-77.713115	13.153207	-0.233307	-0.011614	12.908285

jj-coupling	$E^{(0+1)}$	E_2	E_{LAMB}	E_{tot}	$E^{(0+1)}$	E_2	E_{LAMB}	E_{tot}
Even-parity states, J=5/2								
$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	-88.744587	-0.138388	0.006415	-88.876560	1.737646	0.012490	-0.005295	1.744841
$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	-88.343187	-0.160729	0.007073	-88.496843	2.139046	-0.009851	-0.004637	2.124558
$3s_{1/2}3s_{1/2}[0]3d_{5/2}$	-87.280516	-0.214153	0.011234	-87.483435	3.201717	-0.063275	-0.000476	3.137965
$3p_{1/2}3p_{1/2}[0]3d_{5/2}$	-84.051023	-0.194995	0.000751	-84.245268	6.431210	-0.044117	-0.010959	6.376133
$3p_{3/2}3p_{3/2}[0]3d_{5/2}$	-84.005867	-0.205030	0.000097	-84.210799	6.476366	-0.054152	-0.011613	6.410601
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-83.780322	-0.210628	0.000396	-83.990554	6.701911	-0.059750	-0.011314	6.630847
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-83.580655	-0.222652	0.000563	-83.802744	6.901578	-0.071774	-0.011147	6.818656
$3p_{1/2}3p_{3/2}[1]3d_{3/2}$	-83.421530	-0.222843	0.000979	-83.643394	7.060703	-0.071965	-0.010731	6.978007
$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	-83.132923	-0.272727	0.001005	-83.404645	7.349310	-0.121849	-0.010705	7.216756
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-83.025988	-0.266051	0.001121	-83.290919	7.456245	-0.115173	-0.010589	7.330482
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-83.003016	-0.230720	0.005911	-83.227825	7.479217	-0.079842	-0.005799	7.393575
$3d_{3/2}3d_{3/2}[2]3s_{1/2}$	-82.714277	-0.290146	0.001863	-83.002560	7.767956	-0.139268	-0.009847	7.618841
$3d_{5/2}3d_{5/2}[2]3s_{1/2}$	-82.745772	-0.254624	0.005094	-82.995302	7.736461	-0.103746	-0.006616	7.626099
$3d_{3/2}3d_{5/2}[2]3s_{1/2}$	-82.463000	-0.295022	0.005050	-82.752972	8.019233	-0.144144	-0.006660	7.868429
$3d_{3/2}3d_{5/2}[3]3s_{1/2}$	-82.179512	-0.325839	0.004328	-82.501023	8.302721	-0.174961	-0.007382	8.120378
$3d_{3/2}3d_{3/2}[0]3d_{5/2}$	-78.210445	-0.272482	-0.000043	-78.482970	12.271788	-0.121604	-0.011753	12.138431
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-77.960948	-0.290841	0.000071	-78.251718	12.521285	-0.139963	-0.011639	12.369683
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-77.821444	-0.322052	0.000116	-78.143381	12.660789	-0.171174	-0.011594	12.478020
$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	-77.665000	-0.351987	0.000071	-78.016916	12.817233	-0.201109	-0.011639	12.604485
$3d_{5/2}3d_{5/2}[0]3d_{5/2}$	-77.335836	-0.383431	0.000088	-77.719179	13.146397	-0.232553	-0.011622	12.902221
Even-parity states, J=7/2								
$3p_{3/2}3p_{3/2}[2]3d_{3/2}$	-83.976225	-0.195359	0.000849	-84.170734	6.506008	-0.044481	-0.010861	6.450666
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-83.911280	-0.202914	0.000362	-84.113832	6.570953	-0.052036	-0.011348	6.507569
$3p_{1/2}3p_{3/2}[1]3d_{5/2}$	-83.651082	-0.214666	0.000746	-83.865002	6.831151	-0.063788	-0.010964	6.756399
$3p_{1/2}3p_{3/2}[2]3d_{3/2}$	-83.627354	-0.224093	0.001018	-83.850428	6.854879	-0.073215	-0.010692	6.770972
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-83.031828	-0.271129	0.001201	-83.301756	7.450405	-0.120251	-0.010509	7.319644
$3d_{5/2}3d_{5/2}[4]3s_{1/2}$	-82.984943	-0.229928	0.006032	-83.208839	7.497290	-0.079050	-0.005678	7.412562
$3d_{3/2}3d_{5/2}[3]3s_{1/2}$	-82.443224	-0.305752	0.005429	-82.743547	8.039009	-0.154874	-0.006281	7.877854
$3d_{3/2}3d_{5/2}[4]3s_{1/2}$	-82.162719	-0.323295	0.004651	-82.481362	8.319514	-0.172417	-0.007059	8.140038
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-78.192143	-0.272040	0.000040	-78.464143	12.290090	-0.121162	-0.011670	12.157257
$3d_{5/2}3d_{5/2}[2]3d_{3/2}$	-77.977424	-0.319387	0.000010	-78.296802	12.504809	-0.168509	-0.011700	12.324598
$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	-77.674188	-0.351763	0.000057	-78.025895	12.808045	-0.200885	-0.011653	12.595506
Even-parity states, J=9/2								
$3p_{3/2}3p_{3/2}[2]3d_{5/2}$	-83.834423	-0.208186	0.000499	-84.042109	6.647810	-0.057308	-0.011211	6.579291
$3p_{1/2}3p_{3/2}[2]3d_{5/2}$	-83.540715	-0.226672	0.001182	-83.766206	6.941518	-0.075794	-0.010528	6.855195
$3d_{5/2}3d_{5/2}[4]3s_{1/2}$	-82.961931	-0.229187	0.006146	-83.184972	7.520302	-0.078309	-0.005564	7.436428
$3d_{3/2}3d_{5/2}[4]3s_{1/2}$	-82.439038	-0.306245	0.005432	-82.739851	8.043195	-0.155367	-0.006278	7.881550
$3d_{3/2}3d_{3/2}[2]3d_{5/2}$	-78.171324	-0.272401	0.000119	-78.443606	12.310909	-0.121523	-0.011591	12.177794
$3d_{5/2}3d_{5/2}[4]3d_{3/2}$	-77.969339	-0.325648	-0.000025	-78.295013	12.512894	-0.174770	-0.011735	12.326388
$3d_{5/2}3d_{5/2}[2]3d_{5/2}$	-77.913718	-0.326269	0.000174	-78.239813	12.568515	-0.175391	-0.011536	12.381588

TABLE VI. Comparison of the jj- and LS-coupling schemes for three-particle states in the n=3 complex.

jj scheme	LS scheme	J	jj scheme	LS scheme	J
$3p_{1/2}3p_{1/2}[0]3s_{1/2}$	$3p^2[^3P]3s\ ^4P$	1/2	$3s_{1/2}3s_{1/2}[0]3p_{1/2}$	$3s^2[^1S]3p\ ^2P$	1/2
$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	$3p^2[^1S]3s\ ^2P$	1/2	$3p_{3/2}3p_{3/2}[0]3p_{1/2}$	$3p^2[^3P]3p\ ^2P$	1/2
$3p_{3/2}3p_{3/2}[0]3s_{1/2}$	$3p^2[^3P]3s\ ^2P$	1/2	$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s3p[^3P]3d\ ^4P$	1/2
$3p_{1/2}3p_{3/2}[1]3s_{1/2}$	$3p^2[^3P]3s\ ^4P$	3/2	$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3s3p[^3P]3d\ ^4D$	1/2
$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	$3p^2[^1D]3s\ ^2D$	3/2	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s3p[^3P]3d\ ^2P$	1/2
$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	$3p^2[^3P]3s\ ^2P$	3/2	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s3p[^1P]3d\ ^2P$	1/2
$3s_{1/2}3s_{1/2}[0]3d_{3/2}$	$3s^2[^1S]3d\ ^2D$	3/2	$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	$3p^2[^3P]3p\ ^2D$	5/2
$3p_{1/2}3p_{3/2}[2]3s_{1/2}$	$3p^2[^3P]3s\ ^4P$	5/2	$3s_{1/2}3p_{1/2}[0]3d_{5/2}$	$3s3p[^3P]3d\ ^2D$	5/2
$3p_{3/2}3p_{3/2}[2]3s_{1/2}$	$3p^2[^1D]3s\ ^2D$	5/2	$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s3p[^3P]3d\ ^4F$	5/2
$3s_{1/2}3s_{1/2}[0]3d_{5/2}$	$3s^2[^1S]3d\ ^2D$	5/2	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s3p[^3P]3d\ ^4P$	5/2
$3s_{1/2}3s_{1/2}[0]3p_{3/2}$	$3s^2[^1S]3p\ ^2P$	3/2	$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3s3p[^3P]3d\ ^4D$	5/2
$3p_{1/2}3p_{1/2}[0]3p_{3/2}$	$3p^2[^3P]3p\ ^4S$	3/2	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3s3p[^3P]3d\ ^2F$	5/2
$3p_{3/2}3p_{3/2}[2]3p_{1/2}$	$3p^2[^3P]3p\ ^2P$	3/2	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s3p[^1P]3d\ ^2F$	5/2
$3p_{3/2}3p_{3/2}[0]3p_{3/2}$	$3p^2[^3P]3p\ ^2D$	3/2	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s3p[^1P]3d\ ^2D$	5/2
$3s_{1/2}3p_{1/2}[0]3d_{3/2}$	$3s3p[^3P]3d\ ^2D$	3/2	$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s3p[^3P]3d\ ^4F$	7/2
$3s_{1/2}3p_{1/2}[1]3d_{3/2}$	$3s3p[^3P]3d\ ^4F$	3/2	$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3s3p[^3P]3d\ ^4D$	7/2
$3s_{1/2}3p_{1/2}[1]3d_{5/2}$	$3s3p[^3P]3d\ ^4P$	3/2	$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s3p[^3P]3d\ ^2F$	7/2
$3s_{1/2}3p_{3/2}[1]3d_{3/2}$	$3s3p[^3P]3d\ ^4D$	3/2	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s3p[^1P]3d\ ^2F$	7/2
$3s_{1/2}3p_{3/2}[1]3d_{5/2}$	$3s3p[^3P]3d\ ^2P$	3/2	$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s3p[^3P]3d\ ^4F$	9/2
$3s_{1/2}3p_{3/2}[2]3d_{3/2}$	$3s3p[^1P]3d\ ^2P$	3/2			
$3s_{1/2}3p_{3/2}[2]3d_{5/2}$	$3s3p[^1P]3d\ ^2D$	3/2			

TABLE VII. Energies of Al-like ions relative to the ground state in cm^{-1} for ions with Z=15-40.

conf.	LSJ	Z=15	Z=16	Z=17	Z=18	Z=19	Z=20	Z=21	Z=22	Z=23
$3s^23p$	$^2P_{1/2}$	0	0	0	0	0	0	0	0	0
$3s^23p$	$^2P_{3/2}$	564	950	1493	2209	3134	4392	5755	7534	9682
$3s3p^2$	$^4P_{1/2}$	55614	71229	85672	100321	115273	135434	144666	160310	176094
$3s3p^2$	$^4P_{3/2}$	55812	71560	86208	101119	116414	137020	146812	163161	179821
$3s3p^2$	$^4P_{5/2}$	56132	72080	87045	102350	118144	139374	149932	167202	184955
$3s3p^2$	$^2D_{3/2}$	73902	93769	112980	132057	151700	176156	190802	211458	232470
$3s3p^2$	$^2D_{5/2}$	73930	93806	113045	132160	151861	176369	191170	212003	233261
$3s3p^2$	$^2S_{1/2}$	94942	126812	147165	169813	193012	220861	239656	263850	288351
$3s3p^2$	$^2P_{1/2}$	111187	133960	157814	181937	206367	236033	254904	280335	306170
$3s3p^2$	$^2P_{3/2}$	111525	134564	158768	183325	208291	238615	258213	284491	311247
$3s^23d$	$^2D_{3/2}$	117061	151542	184209	217980	249863	283270	312624	344199	375811
$3s^23d$	$^2D_{5/2}$	117022	151538	184222	218030	249974	283288	312964	344726	376584
$3s3p3d$	$^2D_{3/2}$	144918	184332	222030	259555	297543	340833	373445	412733	452507
$3s3p3d$	$^2D_{5/2}$	144983	184416	222171	259765	297854	341308	374107	413695	453886
$3p^3$	$^4S_{3/2}$	157234	197132	233275	270375	308055	351214	383843	423261	463298
$3s3p3d$	$^4F_{3/2}$	157495	202164	246378	290045	333631	382170	419612	463380	505889
$3s3p3d$	$^4F_{5/2}$	157607	202353	246675	290489	334268	383051	420794	464938	509294
$3s3p3d$	$^4F_{7/2}$	157767	202622	247100	291124	335181	384321	422514	467215	512251
$3s3p3d$	$^4F_{9/2}$	157978	202979	247662	291968	336398	386020	424828	470300	516290
$3p^3$	$^2P_{1/2}$	164149	212500	252576	293233	334629	379299	418389	461285	504940
$3p^3$	$^2P_{3/2}$	164163	212518	252529	293209	334663	379436	418680	461846	505889
$3s3p3d$	$^4P_{1/2}$	173310	221791	269643	316813	363841	415750	456413	503262	550183
$3s3p3d$	$^4P_{3/2}$	173191	221590	269324	316328	363135	414802	455283	502037	548896
$3s3p3d$	$^4P_{5/2}$	173007	221293	268879	315700	362295	413738	454005	500557	547217
$3s3p3d$	$^4D_{1/2}$	174854	223688	271635	318711	365555	417376	458328	505957	554076
$3s3p3d$	$^4D_{3/2}$	174904	223778	271789	318970	365960	417939	458978	506596	554658
$3s3p3d$	$^4D_{5/2}$	174965	223882	271951	319206	366275	418317	459380	506976	554972
$3s3p3d$	$^4D_{7/2}$	175016	223961	272060	319338	366412	418427	459423	506910	554760
$3p^3$	$^2D_{3/2}$	185975	233893	280343	328864	376018	428446	469980	518071	566564
$3p^3$	$^2D_{5/2}$	185978	233873	280313	328820	375982	428429	469997	518144	566719
$3s3p3d$	$^2F_{5/2}$	187623	240030	290653	343349	393262	448090	491682	541512	591427
$3s3p3d$	$^2F_{7/2}$	188088	240808	291851	345106	395747	451501	496245	547483	599096
$3s3p3d$	$^2P_{1/2}$	205581	265820	321031	376441	430723	489957	537483	591712	646225
$3s3p3d$	$^2P_{3/2}$	205596	265801	320697	375966	429882	488541	535637	589105	642673
$3s3p3d$	$^2F_{5/2}$	204543	240808	319929	375645	430885	490767	539417	594392	649593
$3s3p3d$	$^2F_{7/2}$	204379	240029	319584	375157	430219	489885	538279	592959	647824
$3s3p3d$	$^2P_{1/2}$	221682	278235	332770	390186	445332	505823	554791	610461	666366
$3s3p3d$	$^2P_{3/2}$	221508	278047	332741	390093	445358	505935	555089	610978	667119
$3s3p3d$	$^2D_{3/2}$	224185	282319	338153	395132	450356	510442	559408	614764	670443
$3s3p3d$	$^2D_{5/2}$	224255	282459	338358	395438	450792	511035	560155	615681	671511

conf.	LSJ	Z=24	Z=25	Z=26	Z=27	Z=28	Z=29	Z=30	Z=31	Z=32
$3s^23p$	$^2P_{1/2}$	0	0	0	0	0	0	0	0	0
$3s^23p$	$^2P_{3/2}$	12246	15278	18831	22962	27731	33201	39441	46520	54512
$3s3p^2$	$^4P_{1/2}$	192144	208499	225187	242224	259627	277405	295565	314110	333054
$3s3p^2$	$^4P_{3/2}$	196946	214613	232889	251638	271526	293023	313401	335733	359098
$3s3p^2$	$^4P_{5/2}$	203357	222498	242451	263287	285072	307870	331743	356750	382948
$3s3p^2$	$^2D_{3/2}$	253993	276113	298903	322435	346780	372011	398202	425429	453768
$3s3p^2$	$^2D_{5/2}$	255126	277711	301126	325489	350924	377567	405567	435083	466286
$3s3p^2$	$^2S_{1/2}$	313234	338530	364267	390476	417197	444483	472400	501023	530436
$3s3p^2$	$^2P_{1/2}$	332633	359878	388057	417320	447817	479698	513114	548217	585165
$3s3p^2$	$^2P_{3/2}$	338680	366910	396052	426221	457537	490124	524114	559641	596841
$3s^23d$	$^2D_{3/2}$	407623	439746	472279	505319	538960	573295	608425	644451	681245
$3s^23d$	$^2D_{5/2}$	408710	441226	474242	507862	542192	577334	613395	650481	688704
$3s3p3d$	$^2D_{3/2}$	492938	534105	576065	618861	662532	707116	752665	799234	846891
$3s3p3d$	$^2D_{5/2}$	494898	536864	579912	624163	669745	716786	765417	815773	867986
$3p^3$	$^4S_{3/2}$	504154	545959	588844	632943	678402	725366	773983	824400	876756
$3s3p3d$	$^4F_{3/2}$	550911	596018	641239	687039	733529	780798	828935	878031	928181
$3s3p3d$	$^4F_{5/2}$	554065	599371	645313	691987	739490	787913	837352	887904	939669
$3s3p3d$	$^4F_{7/2}$	557844	604128	651223	699244	748302	798508	849974	902807	957117
$3s3p3d$	$^4F_{9/2}$	563048	610745	659539	709587	761051	814092	868882	925597	984417
$3p^3$	$^2P_{1/2}$	549476	595019	641696	689638	738981	789864	842438	896857	953278
$3p^3$	$^2P_{3/2}$	551612	597514	645244	694612	745789	798967	854345	912111	972428
$3s3p3d$	$^4P_{1/2}$	597441	645191	693557	742648	792568	843414	895282	948268	1002463
$3s3p3d$	$^4P_{3/2}$	596093	643771	692051	741048	790868	841618	893409	946360	1000616
$3s3p3d$	$^4P_{5/2}$	594205	641653	689678	738388	787889	838288	889691	942208	995950
$3s3p3d$	$^4D_{1/2}$	602892	652552	703197	754970	808018	862489	918540	976328	1036018
$3s3p3d$	$^4D_{3/2}$	603407	653000	703580	755291	808276	862683	918667	976385	1036002
$3s3p3d$	$^4D_{5/2}$	603619	653080	703500	755023	807792	861953	917656	975057	1034312
$3s3p3d$	$^4D_{7/2}$	603232	652501	702727	754066	806675	860711	916341	973733	1033063
$3p^3$	$^2D_{3/2}$	615700	665641	716538	768535	821780	876418	932599	990472	1050182
$3p^3$	$^2D_{5/2}$	615972	666069	717163	769397	822910	877819	934224	992173	1051648
$3s3p3d$	$^2F_{5/2}$	641668	692391	743733	795834	848841	902921	958273	1015151	1073888
$3s3p3d$	$^2F_{7/2}$	651360	704460	758566	813845	870461	928580	988375	1050020	1113695
$3s3p3d$	$^2P_{1/2}$	701320	757193	814018	871960	931184	991849	1054121	1118165	1184149
$3s3p3d$	$^2P_{3/2}$	696596	751032	806112	861961	918700	976450	1035340	1095509	1157107
$3s3p3d$	$^2F_{5/2}$	705300	761697	818947	877205	936625	997358	1059562	1123395	1189021
$3s3p3d$	$^2F_{7/2}$	703154	759137	815939	873722	932647	992877	1054581	1117933	1183115
$3s3p3d$	$^2P_{1/2}$	722770	778843	837739	896611	956613	1017904	1080651	1145029	1222746
$3s3p3d$	$^2P_{3/2}$	723763	781062	839172	898285	958617	1020381	1083786	1149037	1222023
$3s3p3d$	$^2D_{3/2}$	726764	783960	842226	901718	962572	1024931	1088959	1154832	1211222
$3s3p3d$	$^2D_{5/2}$	727926	785121	843273	902552	963132	1025187	1088896	1154446	1216336

conf.	LSJ	Z=33	Z=34	Z=35	Z=36	Z=37	Z=38	Z=39	Z=40
$3s^23p$	$^2P_{1/2}$	0	0	0	0	0	0	0	0
$3s^23p$	$^2P_{3/2}$	63497	73555	84772	97281	111095	126350	143149	161599
$3s3p^2$	$^4P_{1/2}$	352340	372011	392039	411898	432550	453504	474742	496245
$3s3p^2$	$^4P_{3/2}$	383577	409255	436220	464088	493872	525232	558273	593104
$3s3p^2$	$^4P_{5/2}$	410395	439146	469262	500343	533352	567939	604189	642201
$3s3p^2$	$^2D_{3/2}$	483300	514104	546266	579451	614558	651292	689750	730036
$3s3p^2$	$^2D_{5/2}$	499360	534496	571893	611361	653872	699271	747767	799573
$3s3p^2$	$^2S_{1/2}$	560735	592018	624395	657480	692344	728653	766533	806117
$3s3p^2$	$^2P_{1/2}$	624125	665266	708771	754381	803156	854890	909798	967576
$3s3p^2$	$^2P_{3/2}$	635854	676814	719847	764631	812074	861783	913683	970168
$3s^23d$	$^2D_{3/2}$	719646	759071	799916	842274	886553	932979	981960	1034041
$3s^23d$	$^2D_{5/2}$	728178	769022	811362	855275	900994	948618	998298	1050197
$3s3p3d$	$^2D_{3/2}$	895719	945801	997233	1049206	1103566	1159586	1217382	1277073
$3s3p3d$	$^2D_{5/2}$	922194	978523	1037096	1097220	1160516	1226267	1294428	1364833
$3p^3$	$^4S_{3/2}$	931193	987840	1046810	1107265	1170891	1236427	1302661	1368260
$3s3p3d$	$^4F_{3/2}$	979491	1032077	1086086	1141165	1198700	1258882	1323211	1393312
$3s3p3d$	$^4F_{5/2}$	992755	1047274	1103354	1160608	1220221	1281924	1346003	1412846
$3s3p3d$	$^4F_{7/2}$	1013018	1070616	1130027	1190862	1254197	1319689	1387457	1457627
$3s3p3d$	$^4F_{9/2}$	1045534	1109144	1175451	1244203	1316517	1392195	1471474	1554606
$3p^3$	$^2P_{1/2}$	1011873	1072815	1136283	1201579	1270576	1342586	1417317	1488715
$3p^3$	$^2P_{3/2}$	1035367	1100565	1165572	1227316	1289606	1353270	1418701	1486094
$3s3p3d$	$^4P_{1/2}$	1057963	1114859	1173250	1232711	1294365	1357903	1423937	1498838
$3s3p3d$	$^4P_{3/2}$	1056420	1114437	1177416	1247406	1323368	1403439	1487260	1574356
$3s3p3d$	$^4P_{5/2}$	1051039	1107593	1165745	1225100	1286823	1350587	1416567	1484959
$3s3p3d$	$^4D_{1/2}$	1097783	1161799	1228250	1296841	1368706	1443604	1521748	1603365
$3s3p3d$	$^4D_{3/2}$	1097696	1161646	1228052	1296621	1368560	1443701	1522446	1605410
$3s3p3d$	$^4D_{5/2}$	1095581	1169009	1224706	1292121	1361774	1432172	1503363	1576297
$3s3p3d$	$^4D_{7/2}$	1094513	1158273	1224537	1293028	1364878	1439860	1518198	1600123
$3p^3$	$^2D_{3/2}$	1111880	1175705	1241797	1309701	1371134	1454317	1530793	1610367
$3p^3$	$^2D_{5/2}$	1112559	1174800	1238411	1303206	1373983	1443197	1519831	1600574
$3s3p3d$	$^2F_{5/2}$	1134914	1198695	1265621	1335418	1409202	1486632	1567864	1653088
$3s3p3d$	$^2F_{7/2}$	1179588	1247892	1318808	1392067	1468801	1548794	1632280	1719501
$3s3p3d$	$^2P_{1/2}$	1252246	1322627	1395470	1470443	1548708	1629978	1714439	1802294
$3s3p3d$	$^2P_{3/2}$	1220303	1285285	1352266	1420903	1492598	1567123	1644833	1726119
$3s3p3d$	$^2F_{5/2}$	1256614	1326350	1398416	1472503	1549780	1629995	1713368	1800133
$3s3p3d$	$^2F_{7/2}$	1250321	1319750	1391617	1465653	1543032	1623555	1707474	1795066
$3s3p3d$	$^2P_{1/2}$	1279431	1349862	1422744	1497768	1576236	1657918	1743095	1832063
$3s3p3d$	$^2P_{3/2}$	1285890	1357901	1432578	1509620	1590223	1674131	1761572	1852788
$3s3p3d$	$^2D_{3/2}$	1292915	1365567	1440952	1518779	1600417	1685672	1774884	1868422
$3s3p3d$	$^2D_{5/2}$	1291830	1364067	1438949	1516157	1596952	1681071	1768760	1860273

TABLE VIII. Energies of Al-like ions relative to the ground state in cm^{-1} for ions with Z=15,16, and 26. Comparison between MBPT and NIST data: *a* - W. C. Martin, R. Zalubas and A. Musgrove J. Phys. Chem. Ref. Data **14**, 751 (1985); *b* - W. C. Martin, R. Zalubas and A. Musgrove J. Phys. Chem. Ref. Data **19**, 821 (1990), *c* - T. Shirai, Y. Funatake, K. Mori, J. Sugar, W. L. Wiese and Y. Nakai, J. Phys. Chem. Ref. Data **19**, 127 (1990).

conf.	LSJ	Z=15		Z=16		Z=26	
		MBPT	NIST[a]	MBPT	NIST[b]	MBPT	NIST[c]
$3s^23p$	$^2P_{1/2}$	0	0	0	0	0	0
$3s^23p$	$^2P_{3/2}$	564	559	950	951	18831	18852
$3s3p^2$	$^4P_{1/2}$	55614	56922	71229	71184	225187	225095
$3s3p^2$	$^4P_{3/2}$	55812	57126	71560	71528	232889	232805
$3s3p^2$	$^4P_{5/2}$	56132	57454	72080	72074	242451	242401
$3s3p^2$	$^2D_{3/2}$	73902	74917	93769	94103	298903	299248
$3s3p^2$	$^2D_{5/2}$	73930	74945	93806	94150	301126	301472
$3s3p^2$	$^2S_{1/2}$	94942	100200	126812	123509	364267	363693
$3s3p^2$	$^2P_{1/2}$	111187	109037	133960	133620	388057	388510
$3s3p^2$	$^2P_{3/2}$	111525	109413	134564	134246	396052	396515
$3s^23d$	$^2D_{3/2}$	117061	116874	151542	152133	472279	473227
$3s^23d$	$^2D_{5/2}$	117022	116886	151538	152146	474242	475217
$3s3p3d$	$^2D_{3/2}$	144918	147323	184332	185055		
$3s3p3d$	$^2D_{5/2}$	144983	147385	184416	185143		
$3p^3$	$^4S_{3/2}$	157234	159719	197132	196455	588843	589080
$3s3p3d$	$^4F_{3/2}$	157495	159125	202164	203442		
$3s3p3d$	$^4F_{5/2}$	157607	159238	202353	203633		
$3s3p3d$	$^4F_{7/2}$	157767	159401	202622	203906		
$3s3p3d$	$^4F_{9/2}$	157978	159614	202979	204266		
$3p^3$	$^2P_{1/2}$	164149	170171	212500	211377		
$3p^3$	$^2P_{3/2}$	164163	170110	212518	211367		
$3s3p3d$	$^4P_{1/2}$	173310	174106	221791	222692		
$3s3p3d$	$^4P_{3/2}$	173191	173985	221590	222487		
$3s3p3d$	$^4P_{5/2}$	173007	173814	221293	222198		
$3s3p3d$	$^4D_{1/2}$	174854	175260	223688	224343		
$3s3p3d$	$^4D_{3/2}$	174904	175314	223778	224436		
$3s3p3d$	$^4D_{5/2}$	174965	175376	223882	224539		
$3s3p3d$	$^4D_{7/2}$	175016	175425	223961	224617		
$3p^3$	$^2D_{3/2}$	185975	185074	233893	233642		
$3p^3$	$^2D_{5/2}$	185978	185098	233873	233610		
$3s3p3d$	$^2F_{5/2}$	187623	188215	240030	241646		
$3s3p3d$	$^2F_{7/2}$	188088	188677	240808	242421		
$3s3p3d$	$^2P_{1/2}$	205581	206631	265820	265055		
$3s3p3d$	$^2P_{3/2}$	205596	206613	265801	264883		
$3s3p3d$	$^2F_{5/2}$	204543	210112	240808	242424		
$3s3p3d$	$^2F_{7/2}$	204379	210048	240029	241640		
$3s3p3d$	$^2P_{1/2}$	224185	219708	282319	281093		
$3s3p3d$	$^2P_{3/2}$	224255	219847	282459	281231		
$3s3p3d$	$^2D_{3/2}$	221682	220152	278235	278676		
$3s3p3d$	$^2D_{5/2}$	221508	220176	278047	278642		

TABLE IX. Energies of Al-like ions relative to the ground state in cm^{-1} for ions with Z=32-40. Comparison MBPT results with adopted level energies (Fit) by J. O. Ekberg, A. Redfors, M. Brown, U. Feldman, and J. F. Seely in Ref. Physica Scripta **44**, 539 (1991).

conf.	LSJ	Z=32		Z=34		Z=38		Z=39		Z=40	
		MBPT	Fit	MBPT	Fit	MBPT	Fit	MBPT	Fit	MBPT	Fit
$3s^23p$	$^2P_{1/2}$	0	0	0	0	0	0	0	0	0	0
$3s^23p$	$^2P_{3/2}$	54512	54567	73555	73626	126350	126414	143149	143211	161599	161680
$3s3p^2$	$^4P_{1/2}$	333054	332671	372011	371506	453504	453144	474742	474266	496245	495631
$3s3p^2$	$^4P_{3/2}$	359098	358698	409255	408749	525232	525053	558273	558075	593104	592888
$3s3p^2$	$^4P_{5/2}$	382948	382673	439146	438805	567939	568034	604189	604311	642201	642359
$3s3p^2$	$^2D_{3/2}$	453768	453865	514104	514130	651292	651641	689750	690084	730036	730348
$3s3p^2$	$^2D_{5/2}$	466286	466384	534496	534499	699271	699542	747767	748038	799573	799856
$3s3p^2$	$^2S_{1/2}$	530436	530524	592018	591964	728653	728900	766533	766773	806117	806364
$3s3p^2$	$^2P_{1/2}$	585165	585304	665266	665272	854890	855008	909798	909806	967576	967981
$3s3p^2$	$^2P_{3/2}$	596841	597006	676814	676861	861783	862070	913683	913966	970168	967900
$3s^23d$	$^2D_{3/2}$	681245	682245	759071	759822	932979	933830	981960	982784	1034041	1034788
$3s^23d$	$^2D_{5/2}$	688704	689545	769022	769852	948618	949444	998298	999095	1050197	1050953
$3s3p3d$	$^2D_{3/2}$	846891		945801		1159586		1217382		1277073	
$3s3p3d$	$^2D_{5/2}$	867986		978523		1226267		1294428		1364833	
$3p^3$	$^4S_{3/2}$	876756	875849	987840	986426	1236427	1234516	1302661	1300100	1368260	1365109
$3s3p3d$	$^4F_{3/2}$	928181		1032077		1258882		1323211		1393312	
$3s3p3d$	$^4F_{5/2}$	939669		1047274		1281924		1346003		1412846	
$3s3p3d$	$^4F_{7/2}$	957117		1070616		1319689		1387457		1457627	
$3s3p3d$	$^4F_{9/2}$	984417		1109144		1392195		1471474		1554606	
$3p^3$	$^2P_{1/2}$	953278		1072815		1342586		1417317		1488715	
$3p^3$	$^2P_{3/2}$	972428		1100565		1353270		1418701		1486094	
$3s3p3d$	$^4P_{1/2}$	1002463	1002638	1114859	1114822	1357903	1358224	1423937	1424295	1498838	1498790
$3s3p3d$	$^4P_{3/2}$	1000616	1000786	1114437	1114488	1403439	1403779	1487260	1487490	1574356	1574594
$3s3p3d$	$^4P_{5/2}$	995950	996196	1107593	1107705	1350587	1350964	1416567	1419747	1484959	1485176
$3s3p3d$	$^4D_{1/2}$	1036018	1035634	1161799	1161207	1443604	1442932	1521748	1520895	1603365	1602303
$3s3p3d$	$^4D_{3/2}$	1036002		1161646		1443701		1522446		1605410	
$3s3p3d$	$^4D_{5/2}$	1034312		1169009		1432172		1503363		1576297	
$3s3p3d$	$^4D_{7/2}$	1033063	1033390	1158273	1158512	1439860	1440461	1518198	1518758	1600123	1600694
$3p^3$	$^2D_{3/2}$	1050182	1050591	1175705	1176005	1454317	1455087	1530793	1531513	1610367	1610930
$3p^3$	$^2D_{5/2}$	1051648		1174800		1443197		1519831		1600574	
$3s3p3d$	$^2F_{5/2}$	1073888		1198695		1486632		1567864		1653088	
$3s3p3d$	$^2F_{7/2}$	1113695	1114493	1247892	1248569	1548794	1549782	1632280	1633242	1719501	1720434
$3s3p3d$	$^2P_{1/2}$	1184149	1184751	1322627	1323199	1629978	1631372	1714439	1716006	1802294	1804058
$3s3p3d$	$^2P_{3/2}$	1157107	1157632	1285285	1285720	1567123	1567953	1644833	1645584	1726119	1726765
$3s3p3d$	$^2F_{5/2}$	1189021	1190045	1326350	1327218	1629995	1631258	1713368	1714657	1800133	1801463
$3s3p3d$	$^2F_{7/2}$	1183115	1184195	1319750	1320682	1623555	1624849	1707474	1708783	1795066	1796401
$3s3p3d$	$^2P_{1/2}$	1211222	1211959	1365567	1350143	1657918	1657492	1743095	1742273	1832063	1830802
$3s3p3d$	$^2P_{3/2}$	1216336	1217449	1364067	1358875	1674131	1675096	1761572	1762320	1852788	1853260
$3s3p3d$	$^2D_{3/2}$	1222746	1223701	1349862	1366441	1685672	1686922	1774884	1776005	1868422	1869332
$3s3p3d$	$^2D_{5/2}$	1222023	1222785	1357901	1364711	1681071	1682128	1768760	1769814	1860273	1861324

TABLE X. Energies of the $3s^23p\ ^2P_J$-$3s3p^2\ ^4P_{J'}$ transitions in cm^{-1} as function of Z. Comparison between MBPT (*a*) and experimental data (*b*) given in Ref. Physica Scripta, **53** 312 (1996) by C. Jupén and J. Curtis.

		$3s^23p\ ^2P_{1/2}$-$3s3p^2\ ^4P_{1/2}$	$3s^23p\ ^2P_{3/2}$-$3s3p^2\ ^4P_{3/2}$	$3s^23p\ ^2P_{3/2}$-$3s3p^2\ ^4P_{5/2}$
Z=15	*a*	55614	55248	55568
	b	56921.7±0.5	56566.9±0.5	56894.9±0.5
Z=16	*a*	71229	70610	71130
	b	71184.1±0.5	70574.7±0.5	71123.3±0.5
Z=17	*a*	85672	84716	85555
	b	85592.9±0.9	84638.3±1	85483±1
Z=18	*a*	100321	98910	100141
	b	100157.2±1	98748.9±1	99984±1
Z=22	*a*	160310	155627	159668
	b	160359±100	155836±120	
Z=24	*a*	192144	184700	191111
	b	192001±200	184843±170	191110±150
Z=25	*a*	208499	199335	207220
	b	208651±220	199521±200	207232±130
Z=26	*a*	225187	214058	223620
	b	225098±15	213948±8	223534±8
Z=27	*a*	242224	228876	240325
	b	242154±120	228765±45	240500±90
Z=28	*a*	259627	243795	257341
	b	259471±135	243546±120	257255±110
Z=29	*a*	277405	258822	274669
	b	276886±230	258398±330	274386±115
Z=30	*a*	295565	273960	292302
	b	295430±260	273673±300	291971±255
Z=32	*a*	333054	304586	328436
	b	332671±200	304131±200	328106±200
Z=34	*a*	372011	335700	365591
	b	371506±200	335123±200	365179±200
Z=35	*a*	392039	351448	384490
	b	391236±460	347947±1800	384468±450
Z=36	*a*	411898	366807	403062
	b	411760±50	366892±35	403112±40
Z=38	*a*	453504	398882	441589
	b	453144±200	398639±200	441620±200
Z=39	*a*	474742	415124	461040
	b	474266	414854±200	461090±200
Z=40	*a*	496245	431505	480602
	b	495631±200	431208±200	480679±200
Z=42	*a*	539966	464688	519215
	b	538993±70		520121±70

TABLE XI. Fine structure splitting (in cm^{-1}) of the ^2L and ^4L terms in Al-like ions with Z=15-100.

Z	$3s^23p$	$3s3p^2$		$3s3p^2$		$3s^23d$	$3s3p3d$		$3s3p3d$		
	^2P	^4P	^4P	^2D	^2P	^2D	^4P	^4P	^4D	^4D	^4D
	3/2-1/2	3/2-1/2	5/2-3/2	5/2-3/2	3/2-1/2	5/2-3/2	3/2-1/2	5/2-3/2	3/2-1/2	5/2-3/2	7/2-5/2
15	564	198	320	28	338	-39	-119	-184	50	61	51
16	950	331	526	37	604	-4	-201	-296	90	103	79
17	1493	536	840	64	954	13	-319	-445	155	162	109
18	2209	798	1231	103	1388	50	-485	-628	258	236	132
19	3134	1141	1730	161	1924	111	-706	-840	405	315	137
20	4392	1586	2354	214	2581	18	-948	-1064	563	378	110
21	5755	2146	3120	369	3310	340	-1129	-1277	650	402	43
22	7534	2852	4041	545	4156	527	-1225	-1480	639	380	-66
23	9682	3727	5134	791	5077	773	-1286	-1680	583	314	-213
24	12246	4802	6411	1133	6047	1087	-1348	-1889	515	212	-388
25	15278	6114	7884	1598	7032	1480	-1420	-2118	448	80	-579
26	18831	7702	9562	2224	7995	1962	-1506	-2374	384	-80	-773
27	22962	9613	11449	3054	8901	2543	-1601	-2660	321	-268	-957
28	27731	11899	13545	4144	9720	3232	-1700	-2978	258	-484	-1118
29	33201	14618	15846	5557	10426	4039	-1796	-3330	194	-731	-1242
30	39441	17835	18342	7365	11001	4970	-1873	-3718	127	-1010	-1316
31	46520	21624	21017	9654	11424	6030	-1908	-4152	57	-1328	-1324
32	54512	26062	23851	12518	11675	7219	-1847	-4666	-16	-1690	-1249
33	63497	31237	26818	16061	11729	8532	-1542	-5381	-88	-2115	-1067
34	73555	37244	29891	20392	11548	9952	-423	-6843	-152	-2638	-736
35	84772	44181	33042	25627	11076	11446	4166	-11671	-198	-3346	-170
36	97281	52190	36255	31911	10250	13001	14695	-22307	-220	-4500	907
37	111095	61323	39480	39315	8917	14441	29003	-36545	-146	-6786	3104
38	126350	71728	42706	47979	6893	15639	45536	-52852	97	-11530	7689
39	143149	83530	45917	58016	3886	16338	63323	-70693	698	-19083	14835
40	161599	96858	49098	69537	-530	16156	75517	-89397	2045	-29113	23826
41	181813	111845	52241	82644	-6906	14592	82500	-107786	3812	-40897	34273
42	203906	128628	55340	97434	-15831	11116	86184	-124413	1988	-50256	46011
43	228002	147349	58394	113990	-27774	5331	86182	-138562	63	-60576	58936
44	254224	168150	61403	132387	-42952	-2890	82856	-150443	-1324	-72384	72938
45	282716	191186	64369	152684	-61396	-13465	76836	-160554	-2279	-85439	87875
46	313608	216604	67295	174906	-83054	-26204	68655	-169312	-2975	-99357	103536
47	347010	244530	70184	199020	-107887	-40886	58727	-177119	-3528	-113718	119610
48	383122	275164	73042	225008	-135902	-57275	47412	-184546	-4007	-128152	135785
49	422077	308652	75873	252725	-167166	-75120	35062	-192406	-4443	-142217	151644
50	464039	345162	78681	281949	-201756	-94084	22073	-201688	-4856	-155529	166810
51	509174	384865	81471	312344	-239790	-113746	8850	-213391	-5254	-167793	180987
52	557657	427939	84247	343453	-281409	-133576	-4206	-228382	-5645	-178857	194016
53	609671	474568	87012	374725	-326802	-152997	-16753	-247345	-6030	-188679	205847
54	665402	524940	89770	405655	-376084	-171392	-28516	-270694	-6413	-197374	216585
55	725047	579252	92524	435830	-429495	-188350	-39352	-298736	-6795	-205031	226308
56	788812	637709	95276	465107	-487205	-203655	-49207	-331594	-7177	-211806	235161
57	856908	700521	98041	493557	-549402	-217291	-58106	-370363	-7559	-217891	241424
58	929555	767906	100786	521426	-616355	-229571	-66149	-411956	-7942	-223206	250719
59	1006984	840095	103548	548999	-688227	-240607	-73416	-459492	-8325	-228045	257619
60	1089010	916940	102726	585402	-757391	-243290	-65828	-518407	-8836	-243889	275418
61	1177150	999834	109091	604286	-847858	-260015	-86048	-569571	-9096	-236281	269907
62	1270394	1087889	111876	632530	-936060	-268757	-91598	-632204	-9484	-239842	275447
63	1369437	1181754	114671	661382	-1030258	-277050	-96736	-700101	-9873	-243043	280590
64	1474554	1281702	117476	691034	-1130690	-284991	-101525	-773364	-10263	-245951	285400
65	1586043	1388030	120302	721574	-1237687	-292636	-106012	-853038	-10656	-248576	288581
66	1704204	1501034	123130	753110	-1351574	-300095	-110236	-937649	-11050	-250894	292775
67	1829345	1621022	125962	785914	-1472483	-307403	-114248	-1027299	-11446	-253083	297967
68	1961821	1748341	128812	819709	-1601133	-314562	-118038	-1124226	-11843	-254862	301460
69	2101946	1883309	131677	854973	-1737446	-321604	-121669	-1227417	-12242	-256576	304842

Z	$3s^23p$	$3s3p^2$		$3s3p^2$		$3s^23d$	$3s3p3d$		$3s3p3d$		
	^2P	^4P	^4P	^2D	^2P	^2D	^4P	^4P	^4D	^4D	^4D
	3/2-1/2	3/2-1/2	5/2-3/2	5/2-3/2	3/2-1/2	5/2-3/2	3/2-1/2	5/2-3/2	3/2-1/2	5/2-3/2	7/2-5/2
70	2250093	2026295	134562	891597	-1881987	-328529	-125141	-1338065	-12641	-258074	306952
71	2406636	2177667	137442	929622	-2035181	-335389	-128462	-1454449	-13038	-259324	310774
72	2571960	2337812	140343	969244	-2197279	-342059	-131662	-1578795	-13434	-260452	313419
73	2746477	2507135	143255	1010406	-2368831	-348173	-134736	-1710904	-13824	-261352	315785
74	2930600	2686052	146180	1053349	-2550085	-341294	-137717	-1850920	-14206	-262175	318025
75	3124793	2875019	149114	1097902	-2741749	-194955	-140584	-1999518	-14573	-262725	319937
76	3329501	3074482	152069	1144347	-2944058	-53663	-143376	-2157369	-14918	-263173	320951
77	3545210	3284925	155019	1192696	-3157574	98275	-146098	-2323323	-15230	-263513	323300
78	3772436	3506858	157987	1242989	-3382833	261322	-148748	-2499980	-15497	-263688	324682
79	4011693	3740799	160964	1295342	-3620315	435950	-151379	-2685734	-15713	-263758	325910
80	4263540	3987302	163952	1349888	-3870527	622791	-153965	-2882458	-15871	-263768	327027
81	4528580	4246964	166949	1406527	-4134246	822190	-156476	-3090397	-15989	-263590	327897
82	4807386	4520358	169955	1465512	-4411873	1034868	-158886	-3309845	-16118	-263371	328675
83	5100604	4808131	172969	1526901	-4704078	1261031	-161088	-3541396	-16361	-263099	329348
84	5408925	5110965	175992	1590633	-5011694	1340225	-162879	-3785830	-16894	-262677	329809
85	5733008	5429526	179021	1657118	-5335057	1409855	-164179	-4043338	-17854	-262354	330328
86	6073588	5764545	182057	1726355	-5674988	1482447	-164824	-4314673	-19388	-262072	330841
87	6431511	6116853	185100	1798036	-6032719	1557938	-164527	-4601068	-21708	-261554	331047
88	6807519	6487202	188149	1872657	-6408594	1636422	-163436	-4902694	-24738	-261104	331274
89	7202516	6876485	191204	1950080	-6803737	1717990	-161438	-5220639	-28546	-260569	331351
90	7617319	7285531	194262	2030801	-7218574	1802731	-158906	-5555140	-32834	-260242	331595
91	8053011	7715397	197327	2114279	-7654805	1890737	-155411	-5907954	-37900	-259695	331531
92	8510383	8166910	200388	2201658	-8112207	1982108	-151968	-6278499	-42951	-259638	331939
93	8990765	8641351	203458	2291791	-8593301	2076914	-147536	-6669498	-48758	-259290	331920
94	9494947	9139558	206519	2386155	-9097558	2175276	-143525	-7079949	-54216	-259546	332468
95	10024453	9662995	209590	2483363	-9627940	2277281	-138545	-7513022	-60365	-259558	332521
96	10580225	10212657	212650	2584923	-10184029	2383029	-134109	-7967850	-66035	-260165	333078
97	11163823	10790061	215713	2689962	-10768331	2492619	-129294	-8447000	-71908	-260872	333452
98	11776391	11396386	218760	2799554	-11381057	2606155	-125190	-8950328	-77142	-262231	334315
99	12419556	12033240	221798	2913360	-12024273	2723743	-121361	-9479885	-82071	-263978	335345
100	13094833	12702138	224821	3031591	-12699397	2845485	-117969	-10036928	-86560	-266198	336615

Z	$3p^3$	$3s3p3d$		$3p^3$	$3s3p3d$		$3s3p3d$		$3s3p3d$		
	^2P	^2P	^2P	^2D	^2D	^2D	^2F	^2F	^4F	^4F	^4F
	3/2-1/2	3/2-1/2	3/2-1/2	5/2-3/2	5/2-3/2	5/2-3/2	7/2-5/2	7/2-5/2	5/2-3/2	7/2-5/2	9/2-7/2
15	14	15	-174	66	3	70	465	-164	112	160	211
16	18	-19	-187	84	-20	133	778	-230	189	269	356
17	-48	-335	-29	141	-30	204	1198	-345	297	425	562
18	-24	-475	-93	209	-44	307	1758	-488	444	636	844
19	34	-841	26	310	-36	436	2485	-666	637	913	1216
20	2871	-1416	111	475	-17	593	3411	-882	3614	1270	1700
21	1223	-1846	299	663	17	747	4562	-1137	2114	1720	2315
22	2095	-2607	518	961	73	918	5971	-1433	3092	2277	3085
23	2354	-3552	753	1379	156	1068	7670	-1770	3404	2958	4038
24	2136	-4724	994	1960	272	1162	9692	-2146	3154	3779	5204
25	2495	-6161	1219	2759	428	1162	12069	-2560	3353	4757	6617
26	3547	-7906	1432	3847	625	1046	14834	-3008	4074	5910	8316
27	4974	-9999	1674	5302	863	834	18011	-3483	4949	7256	10344
28	6808	-12484	2003	7213	1130	560	21619	-3978	5961	8812	12748
29	9103	-15399	2476	9669	1402	256	25659	-4481	7115	10596	15583
30	11906	-18781	3135	12753	1625	-62	30102	-4981	8417	12622	18909
31	15255	-22656	4008	16540	1702	-387	34869	-5462	9873	14903	22790
32	19150	-27042	5114	21095	1466	-723	39806	-5906	11488	17448	27300
33	23493	-31943	6460	26475	679	-1085	44674	-6293	13265	20262	32517
34	27750	-37342	8039	32721	-905	-1499	49197	-6599	15198	23342	38527
35	29289	-43204	9834	39863	-3386	-2003	53188	-6800	17268	26673	45424

Z	$3p^3$	$3s3p3d$		$3p^3$	$3s3p3d$		$3s3p3d$			$3s3p3d$	
	^2P	^2P	^2P	^2D	^2D	^2D	^2F	^2F	^4F	^4F	^4F
	3/2-1/2	3/2-1/2	3/2-1/2	5/2-3/2	5/2-3/2	5/2-3/2	7/2-5/2	7/2-5/2	5/2-3/2	7/2-5/2	9/2-7/2
36	25736	-49540	11852	48014	-6495	-2622	56649	-6850	19443	30254	53340
37	19030	-56111	13987	56950	-9542	-3465	59599	-6746	21522	33976	62320
38	10683	-62854	16214	66681	-11120	-4600	62162	-6440	23042	37764	72506
39	1384	-69607	18477	77046	-10962	-6125	64416	-5894	22793	41454	84017
40	-2621	-76176	20725	87760	-9793	-8150	66413	-5067	19534	44780	96980
41	-2865	-82352	22919	98392	-9236	-10801	68188	-3916	14042	47368	111524
42	-2670	-87924	25031	108421	-14617	-14221	69760	-2395	7743	48796	127786
43	-2306	-92687	27049	117418	-22916	-18575	71144	-455	1392	48808	145909
44	-1818	-96460	28975	125263	-32974	-24049	72346	1954	-4916	47535	166038
45	-1214	-99078	30819	132101	-44077	-30857	73375	4880	-11544	45458	188330
46	-499	-100390	32596	138160	-55684	-39235	74233	8376	-19014	43209	212939
47	314	-100248	34320	143612	-67361	-49438	74926	12492	-27784	41360	239995
48	8763	-98534	36012	148647	-78735	-61736	75462	17276	-30504	40298	269705
49	28673	-95167	37682	153323	-89517	-76411	75849	22777	-23264	40155	302221
50	49465	-90173	39347	157710	-99535	-93723	76099	29041	-16286	40877	337717
51	70852	-83681	41016	161842	-108766	-113926	76223	36111	-9381	42317	376371
52	92536	-75894	42698	165742	-117294	-137254	76236	44030	-2345	44309	418368
53	114280	-67014	44395	169394	-125256	-163943	76154	52836	5006	46712	463898
54	135877	-57235	46121	172859	-132789	-194136	75997	62569	12826	49414	513154
55	157284	-46658	47871	176093	-140002	-228049	75783	73262	21244	52329	566338
56	178515	-35349	49652	179123	-146973	-265821	75537	84948	30368	55396	623659
57	199683	-23312	51454	181544	-154562	-307222	79696	99583	39722	56315	692358
58	220912	-10550	53314	184588	-160376	-353544	75060	111402	51096	61812	751580
59	242392	3006	55198	187039	-166858	-403787	74926	126183	62855	65103	822633
60	265494	8930	47526	199169	-169387	-464121	74015	136083	73058	68866	899497
61	286781	32737	59057	191301	-179415	-517941	75667	158303	89509	71750	980124
62	309986	49045	61038	193177	-185501	-582136	78452	173844	104530	75083	1067069
63	334059	66415	63048	194845	-191453	-651380	87802	184146	120757	78411	1159837
64	359115	84917	65088	196347	-197274	-725831	103497	189486	138252	81728	1258702
65	385284	104627	67146	197444	-203782	-805328	123942	197199	156664	83418	1370270
66	412647	125611	69235	198576	-209325	-890961	144295	200722	176873	86771	1482151
67	441279	147942	71368	199851	-213931	-982771	164289	200612	198902	91578	1594871
68	471336	171684	73496	200590	-219193	-1080609	187837	204132	222016	94821	1721176
69	502847	196911	75659	201341	-224345	-1184697	213020	207683	246691	98041	1855151
70	535924	223683	77834	201815	-230172	-1295141	241789	214714	272635	99944	2003141
71	570624	252072	80030	202418	-234235	-1413535	268411	214906	300904	104414	2147587
72	607039	282142	82240	202851	-238988	-1538806	298730	218590	330566	107566	2306805
73	645248	313952	84458	203175	-243599	-1671865	330863	222322	361998	110697	2475228
74	685314	347583	86693	203538	-248098	-1812850	364888	226106	395280	113806	2653269
75	727329	383078	88927	203791	-252443	-1962421	400839	229935	430442	116894	2841387
76	771361	420518	91168	204024	-257455	-2120193	440560	237152	467305	118961	3045712
77	817468	459984	93419	204472	-260770	-2283653	478835	237739	506726	123010	3249685
78	865946	501527	95668	204481	-264726	-2301307	521000	241708	548134	125650	3470861
79	916266	545209	97916	205391	-268573	-2309065	565364	245722	591342	129051	3704077
80	969099	591127	100166	206034	-272296	-2315339	612007	249778	636950	132045	3949892
81	1024333	639323	102405	206739	-275864	-2319787	660978	253873	684823	135023	4208903
82	1082035	689891	104640	207598	-279315	-2322182	712366	258008	735054	137985	4481686
83	1142288	742907	106868	208601	-282645	-2322470	766244	262181	787713	140931	4768890
84	1205180	798418	109080	209698	-285814	-2320750	822666	266388	842839	143864	5071202
85	1270776	856562	111286	210999	-288910	-2316541	881757	270631	900572	146783	5389287
86	1339165	917405	113480	212460	-291912	-2309877	943583	274909	960970	149688	5723878
87	1410447	980946	115644	213958	-294707	-2301175	1008158	279214	1024021	152582	6075817
88	1484691	1047350	117792	215610	-297410	-2289836	1075630	283550	1089891	155464	6445853
89	1561993	1116648	119912	217349	-299953	-2276059	1146041	287913	1158601	158334	6834887
90	1642428	1189021	122014	219259	-302465	-2259233	1219552	292304	1230335	161194	7243745
91	1726108	1264404	124076	221192	-304742	-2240096	1296127	296716	1305009	164044	7673501

Z	$3p^3$	$3s3p3d$		$3p^3$	$3s3p3d$		$3s3p3d$		$3s3p3d$		
	^2P	^2P	^2P	^2D	^2D	^2D	^2F	^2F	^4F	^4F	^4F
	3/2-1/2	3/2-1/2	3/2-1/2	5/2-3/2	5/2-3/2	5/2-3/2	7/2-5/2	7/2-5/2	5/2-3/2	7/2-5/2	9/2-7/2
92	1813099	1343163	126123	223348	-307140	-2217173	1376075	301154	1383001	166883	8124967
93	1903509	1425044	128118	225485	-309240	-2191993	1459211	305609	1464031	169714	8599452
94	1997418	1510543	130092	227834	-311529	-2162607	1545944	310086	1548611	172534	9097774
95	2094955	1599315	132005	230145	-313469	-2130959	1636028	314573	1636360	175347	9621433
96	2196182	1691894	133886	232625	-315596	-2094961	1729895	319076	1727835	178151	10171401
97	2301222	1788077	135706	235127	-317545	-2055886	1827412	323588	1822804	180947	10749223
98	2410157	1888291	137483	237770	-319702	-2012236	1928927	328108	1921708	183734	11356064
99	2523103	1992521	139201	240486	-321908	-1964469	2034455	332633	2024514	186513	11993550
100	2640162	2100908	140855	243279	-324211	-1912402	2144127	337158	2131358	189283	12663202

TABLE XII. Fine structure splitting (in cm^{-1}) of the $3s^23p\ ^2P$ and $3s3p^2\ ^4P$ terms in Al-like ions with Z=15-42. Comparison of the MBPT and predicted data.

Z	$3s^23p\ ^2P_{3/2} -\ ^2P_{1/2}$		$3s3p^2\ ^4P_{3/2} -\ ^4P_{1/2}$			$3s3p^2\ ^4P_{5/2} -\ ^4P_{3/2}$			$3s3p^2\ ^4P_{5/2} -\ ^4P_{1/2}$	
	MBPT	NIST	MBPT	NIST	Fit[a]	MBPT	NIST	Fit[a]	MBPT	Fit[a]
15	564	559[c]	198	204[c]	204	320	328[c]	328	518	532
16	950	951[d]	331	331[d]	343	526	520[d]	548	857	891
17	1493		536		537	840		845	1376	1382
18	2209		798		802	1231		1235	2029	2037
19	3134	3134[e]	1141	1136[e]	1053	1730	1737[e]	1829	2871	2882
20	4392	4309[e]	1586	1578[e]	1428	2354	2364[e]	2524	3940	3952
21	5755	5761[e]	2146	2122[e]	1919	3120	3157[e]	3364	5266	5283
22	7534	7543[e]	2852	2805[e]	2562	4041	4109[e]	4349	6893	6911
23	9682	9696[f]	3727	3711[f]	3392	5134	5151[f]	5485	8861	8877
24	12246	12261[g]	4802	4789[g]	4442	6411	6434[g]	6783	11213	11225
25	15278	15295[h]	6114	6107[h]	5758	7884	7913[h]	8241	13998	13999
26	18831	18852[i]	7702	7710[i]	7387	9562	9596[i]	9862	17264	17249
27	22962	22979[j]	9613	9571[j]	9373	11449	11471[j]	11654	21062	21027
28	27731	27770[e]	11899		11775	13545		13611	25444	25386
29	33201	33239[k]	14618	14579[k]	14645	15846	15898[k]	15738	30464	30383
30	39441	39483[l]	17835	17793[l]	18044	18342	18366[l]	18035	36177	36079
31	46520		21624		22035	21017		20502	42641	42537
32	54512	54567[b]	26062	26027[b]	26697	23851	23975[b]	23127	49913	49824
33	63497		31237		32073	26818		25935	58055	58008
34	73555	73626[b]	37244	37243[b]	38276	29891	30056[b]	28887	67135	67163
35	84772		44181		45348	33042		32016	77223	77364
36	97281	97312[m]	52190	51960[m]	53397	36255	36190[m]	35293	88445	88690
37	111095		61323		62511	39480		38714	100803	101225
38	126350	126414[b]	71728	71909[b]	72773	42706	42981[b]	42282	114434	115055
39	143149	143211[b]	83530	83809[b]	84279	45917	46236[b]	45990	129447	130269
40	161599	161680[b]	96858	97257[b]	97134	49098	49462[b]	49827	145956	146961
41	181813		111845		111471	52241		53757	164086	165228
42	203906	204020[n]	128628		127363	55340		57808	183968	185171

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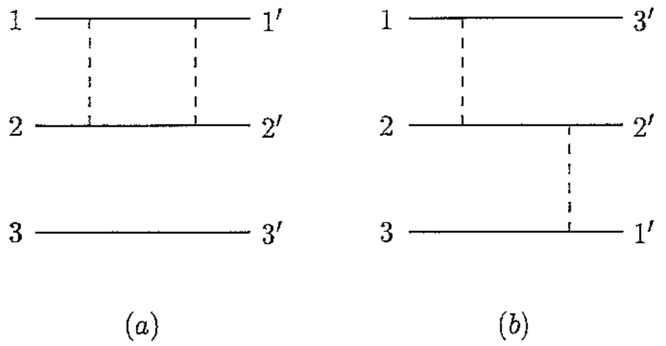

FIG.1. Second order diagrams

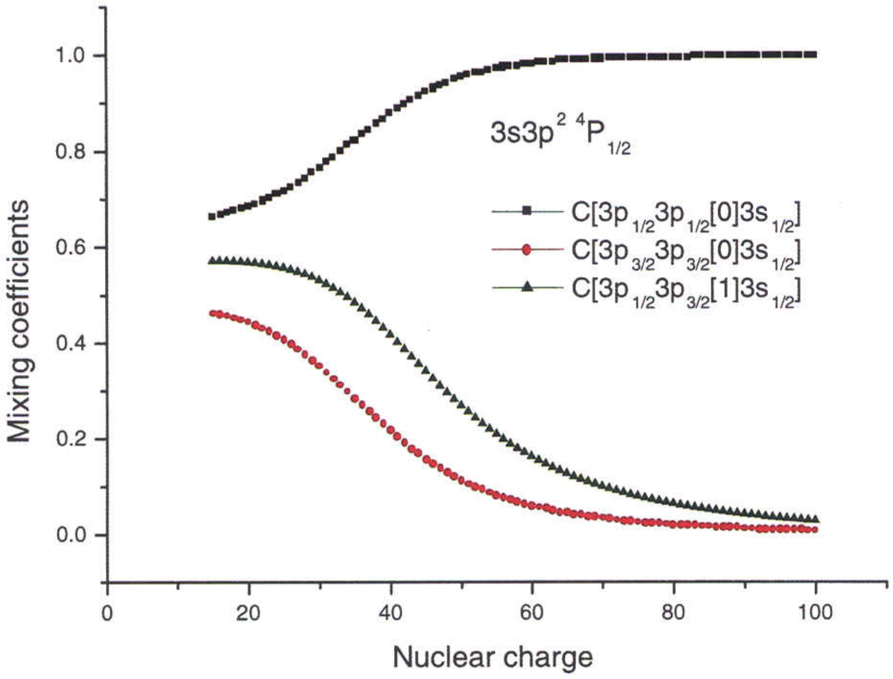

FIG. 2. Mixing coefficients for even-parity states with J=1/2 in Al-like ions as function of Z

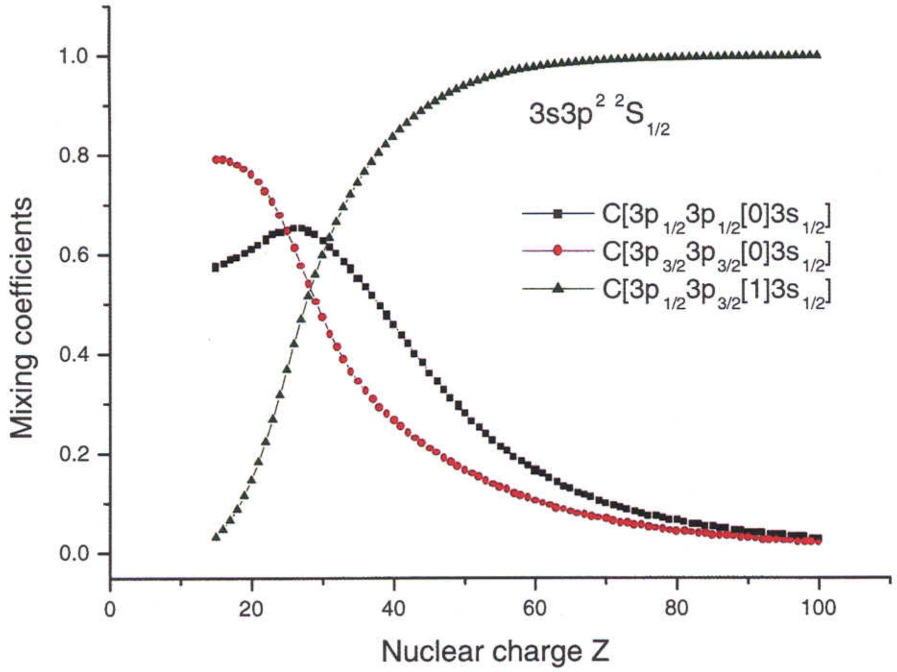

FIG. 3. Mixing coefficients for for even-parity states with J=1/2 in Al-like ions as function of Z

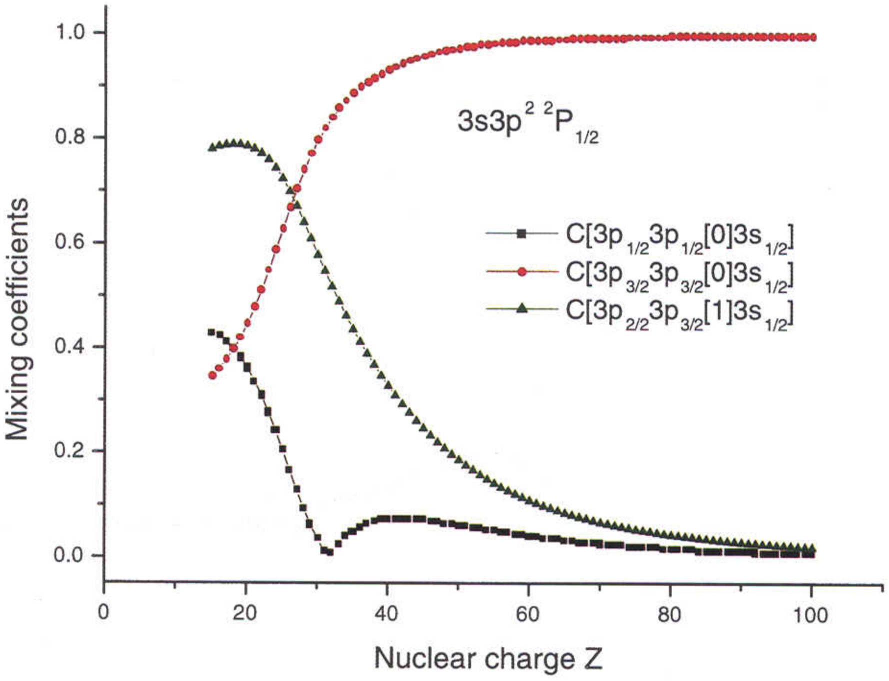

FIG. 4. Mixing coefficients for for even-parity states with $J=1/2$ in Al-like ions as function of Z

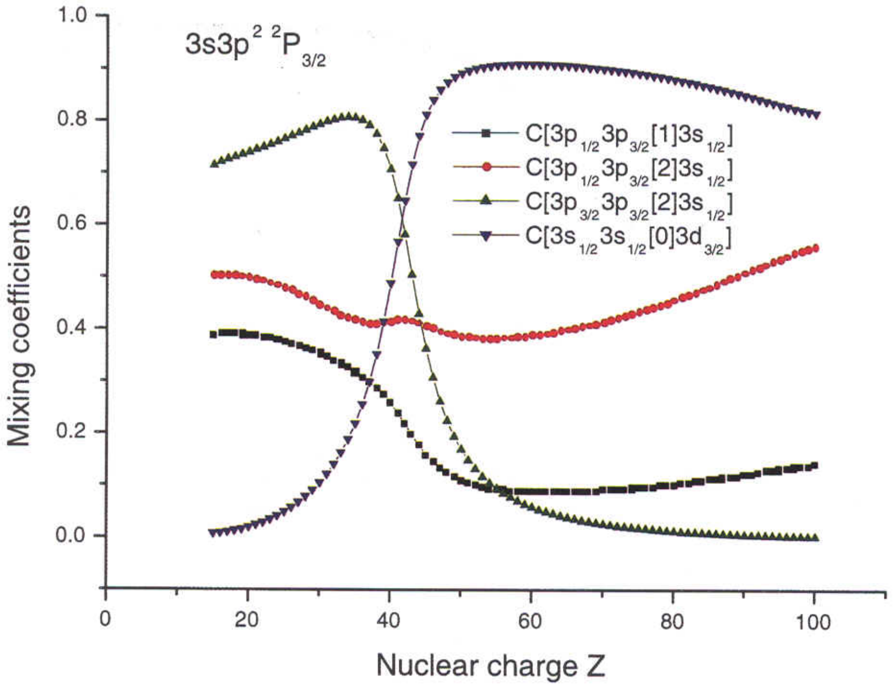

FIG. 5. Mixing coefficients for for even-parity states with $J=3/2$ in Al-like ions as function of Z

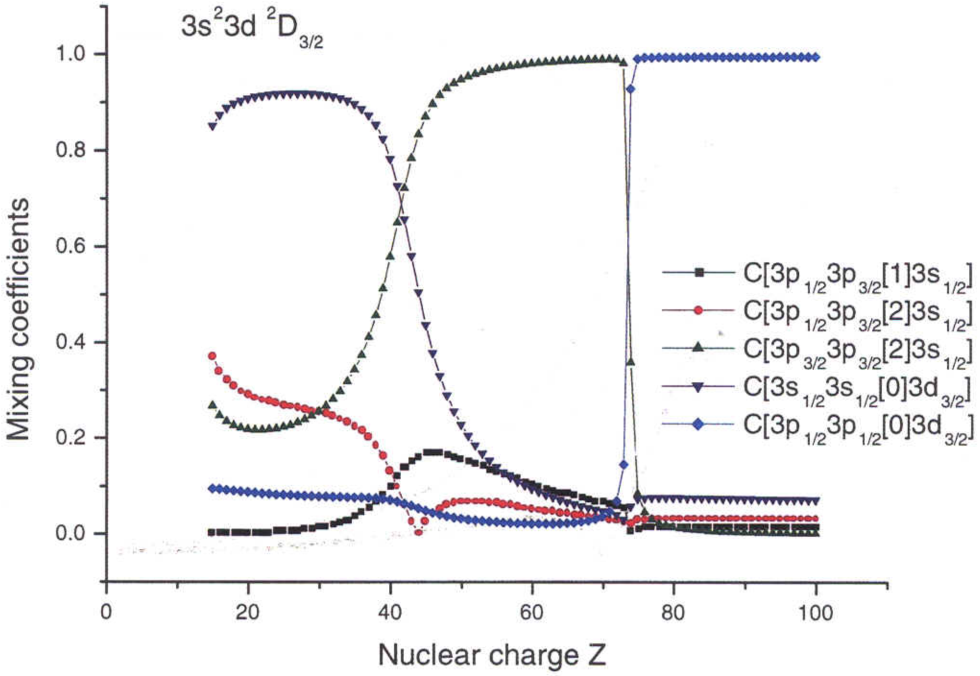

FIG. 6. Mixing coefficients for for even-parity states with J=3/2 in Al-like ions as function of Z

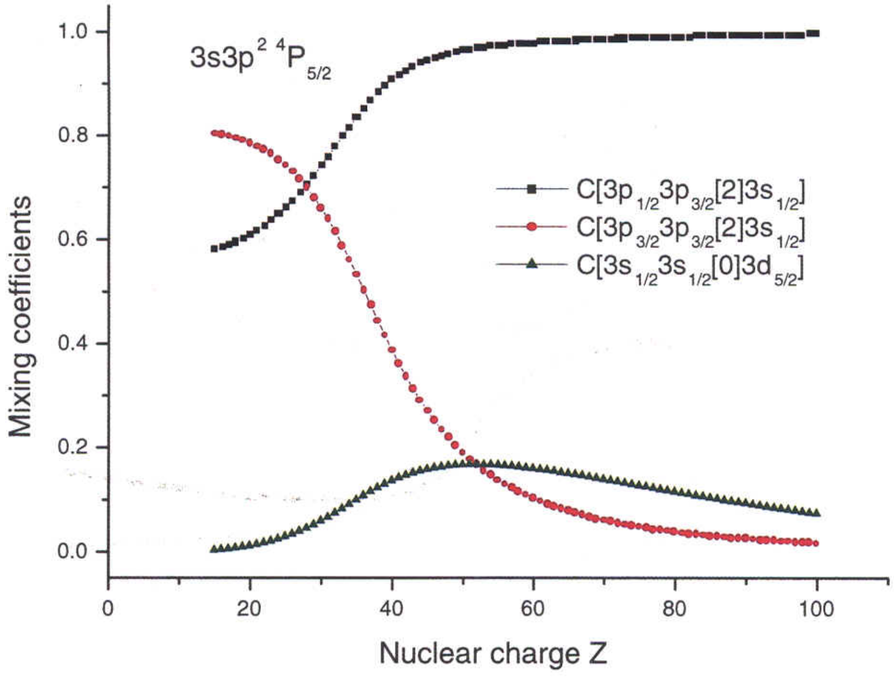

FIG. 7. Mixing coefficients for for even-parity states with J=5/2 in Al-like ions as function of Z

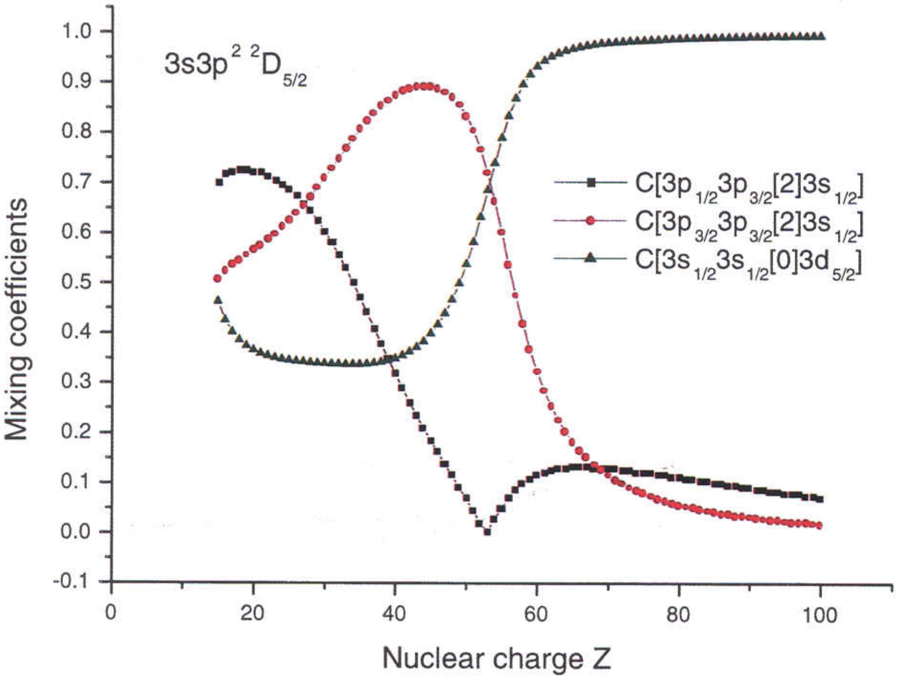

FIG. 8. Mixing coefficients for for even-parity states with J=5/2 in Al-like ions as function of Z

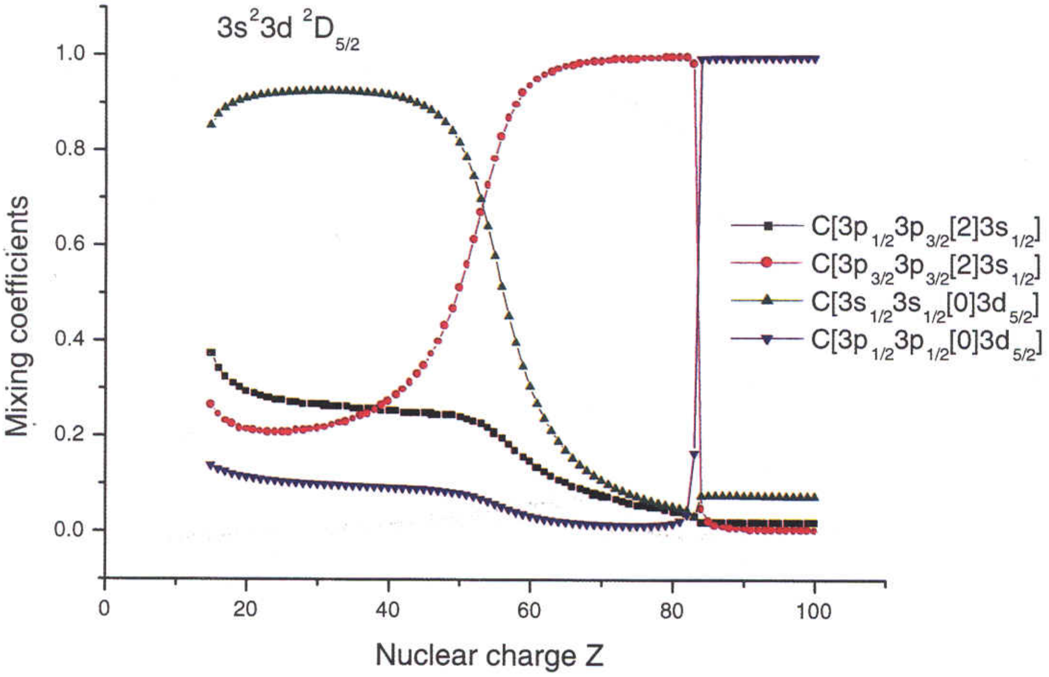

FIG. 9. Mixing coefficients for for even-parity states with J=5/2 in Al-like ions as function of Z

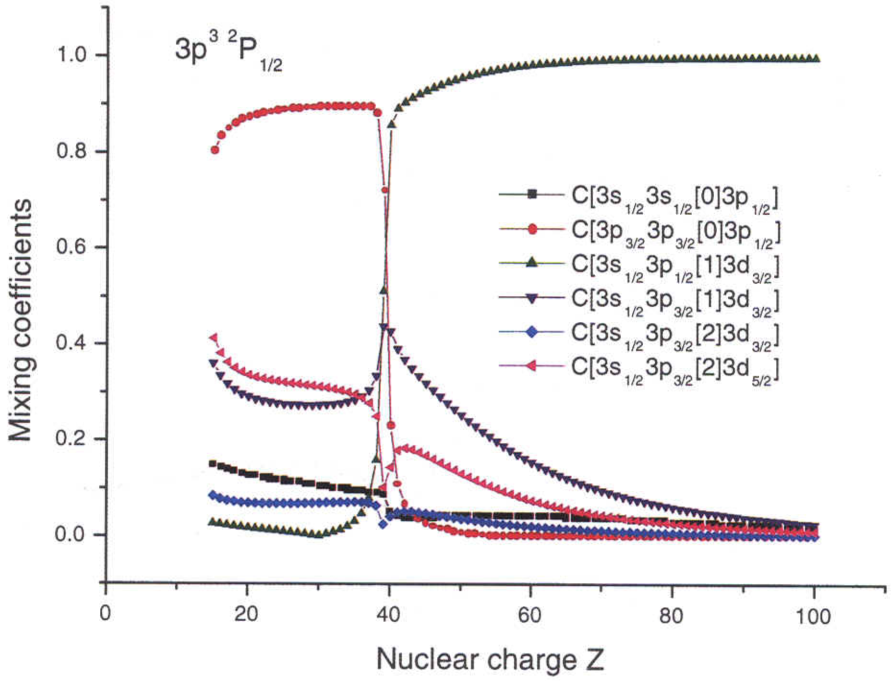

FIG. 10. Mixing coefficients for for odd-parity states with J=1/2 in Al-like ions as function of Z

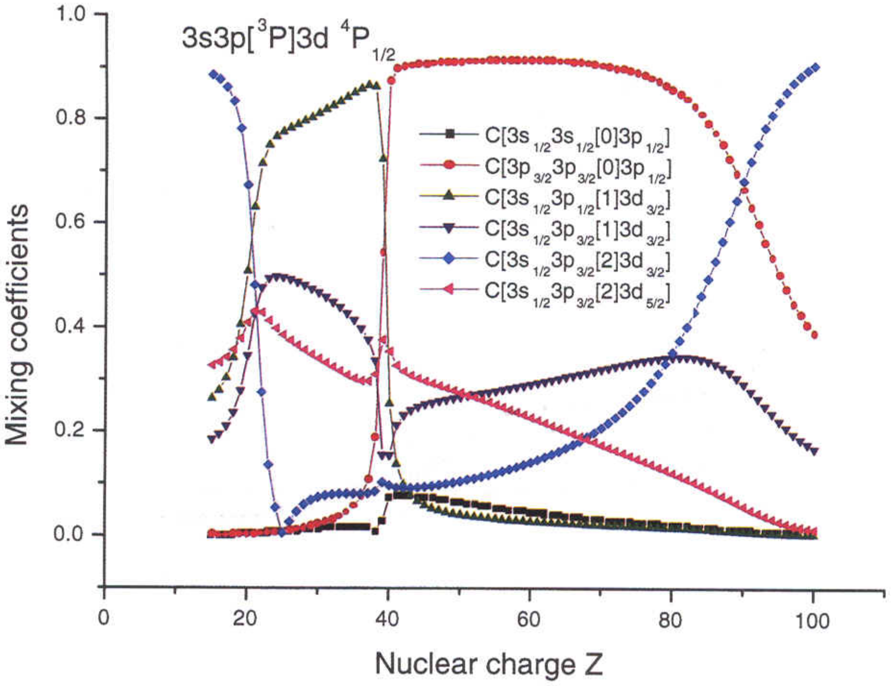

FIG. 11. Mixing coefficients for for odd-parity states with J=1/2 in Al-like ions as function of Z

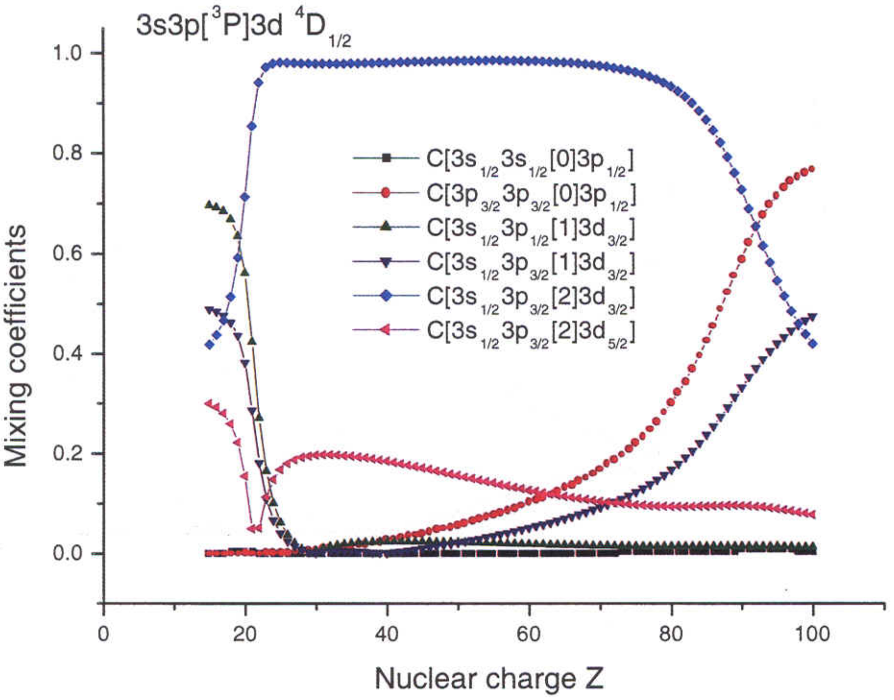

FIG. 12. Mixing coefficients for for odd-parity states with J=1/2 in Al-like ions as function of Z

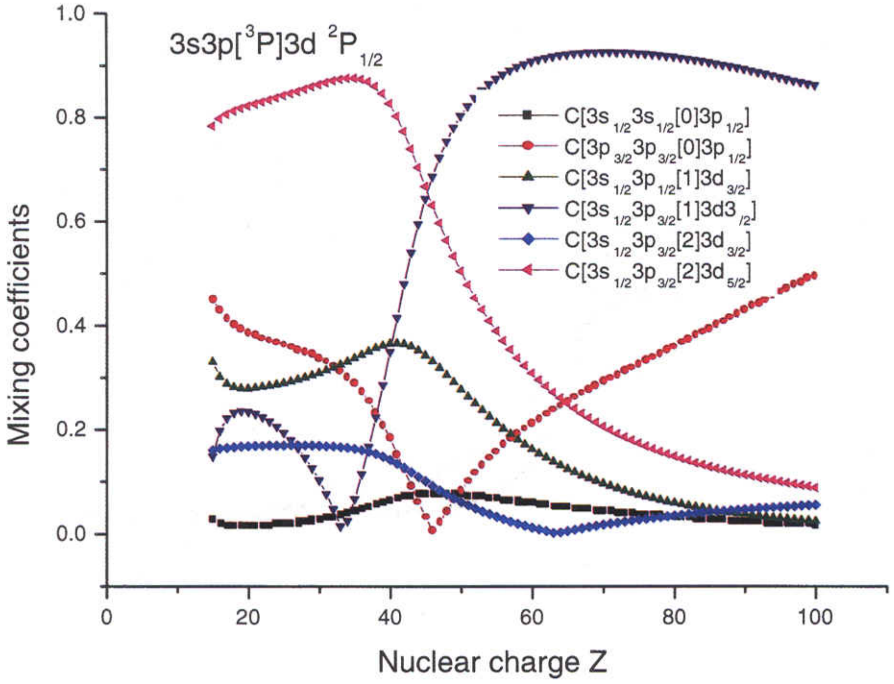

FIG. 13. Mixing coefficients for for odd-parity states with J=1/2 in Al-like ions as function of Z

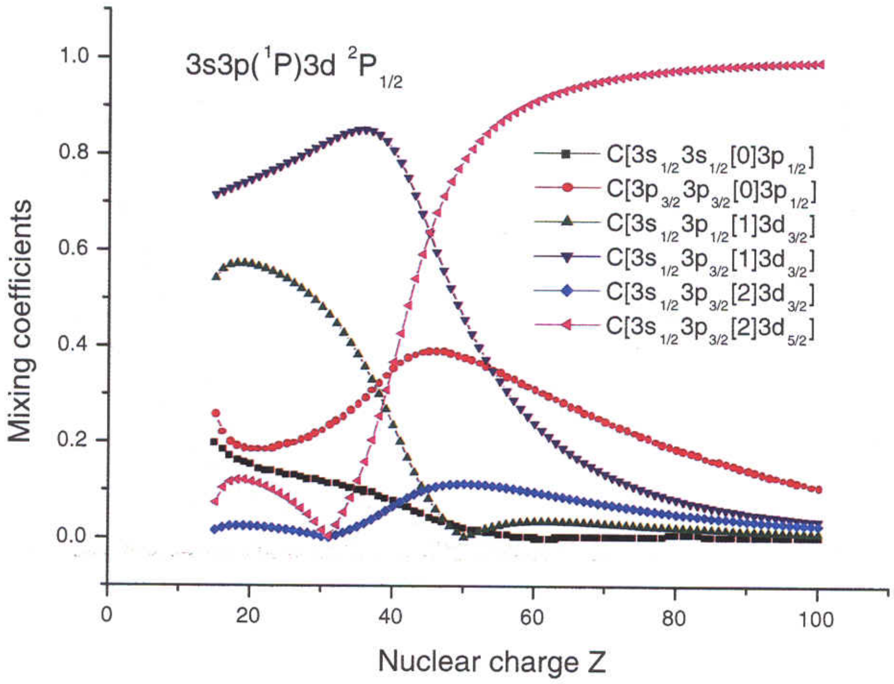

FIG. 14. Mixing coefficients for for odd-parity states with $J=1/2$ in Al-like ions as function of Z

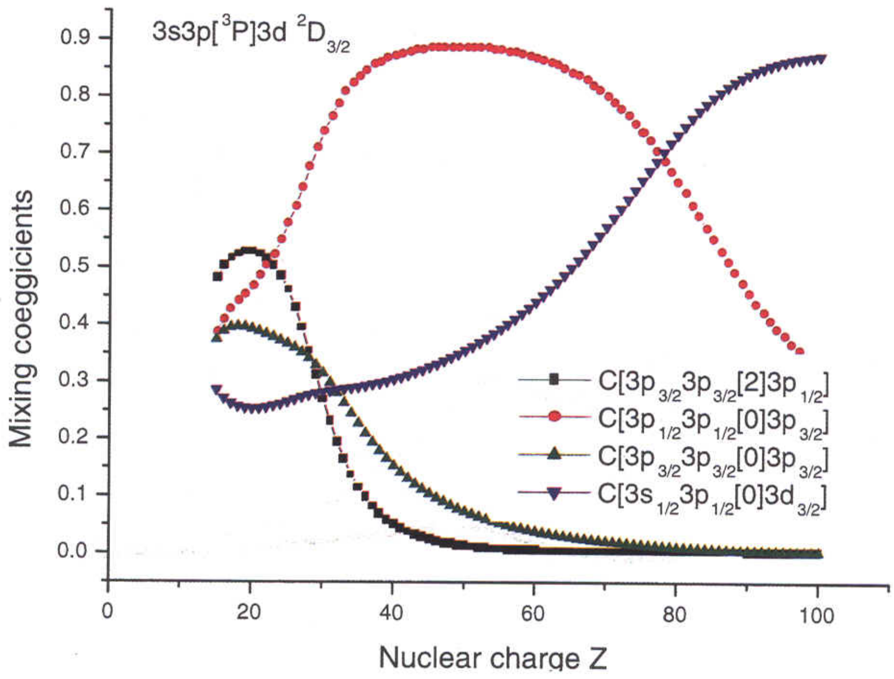

FIG. 15. Mixing coefficients for for odd-parity states with $J=3/2$ in Al-like ions as function of Z.

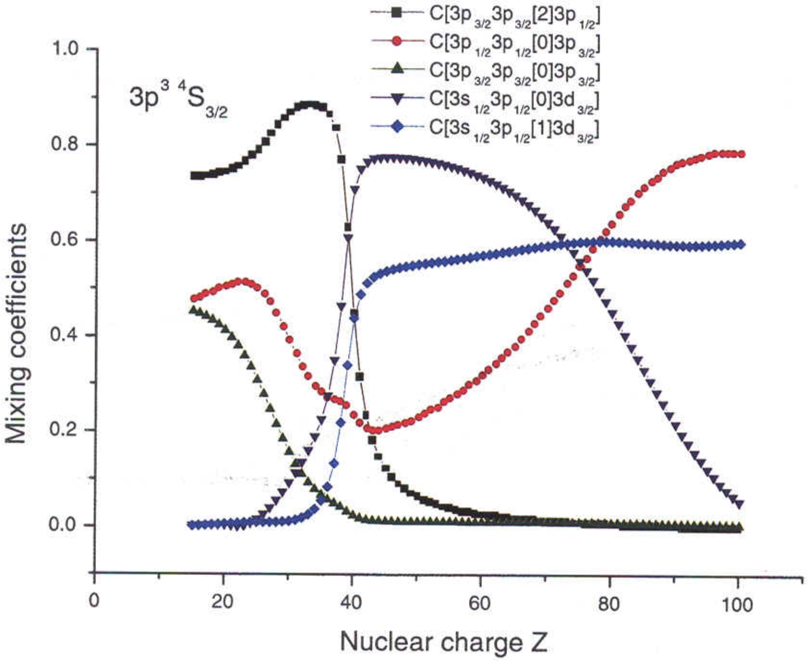

FIG. 16. Mixing coefficients for for odd-parity states with J=3/2 in Al-like ions as function of Z.

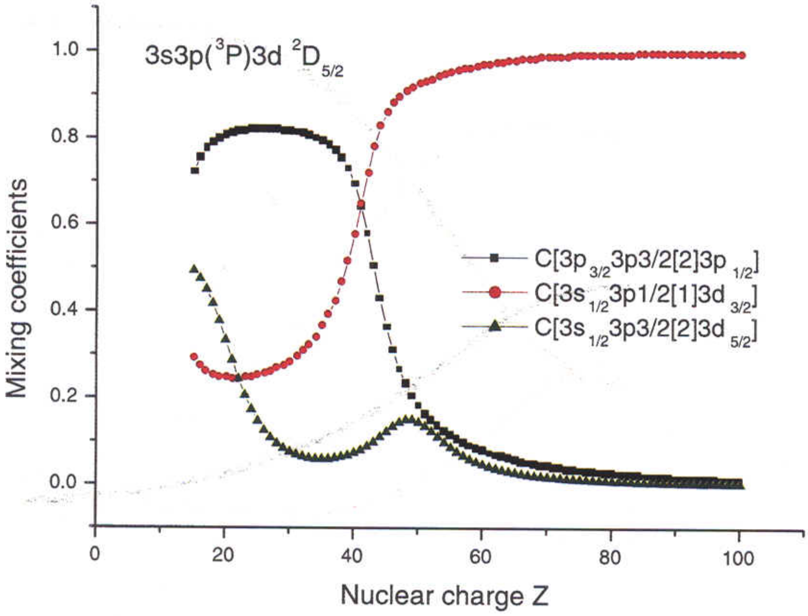

FIG. 17. Mixing coefficients for for odd-parity states with J=5/2 in Al-like ions as function of Z.

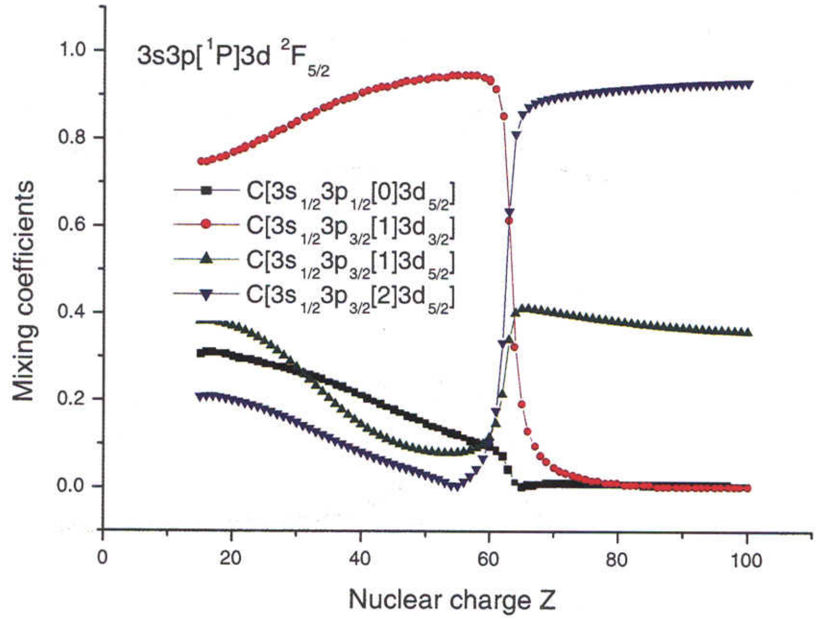

FIG. 18. Mixing coefficients for for odd-parity states with $J=5/2$ in Al-like ions as function of Z.

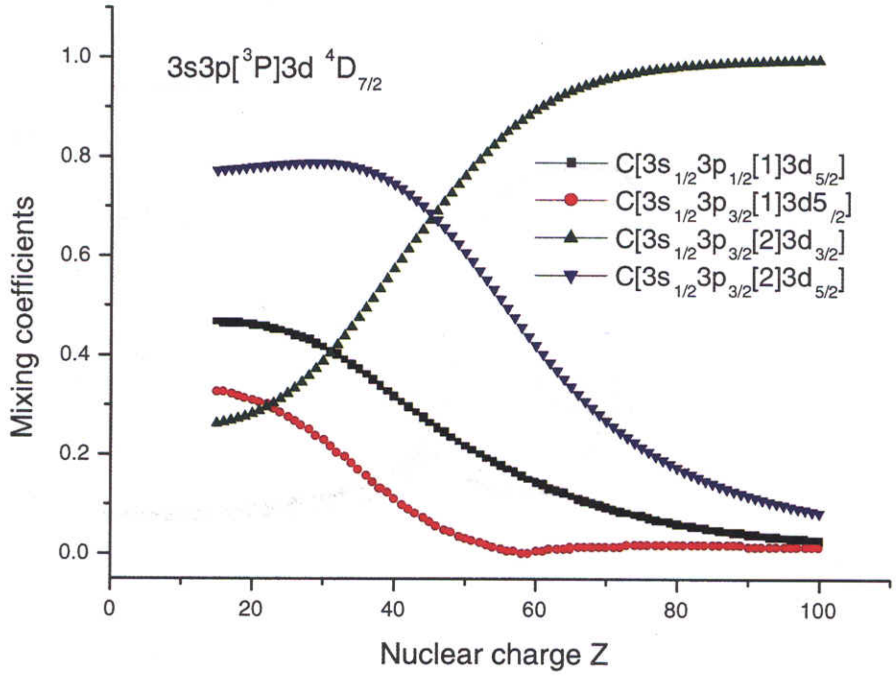

FIG. 19. Mixing coefficients for for odd-parity states with $J=7/2$ in Al-like ions as function of Z.

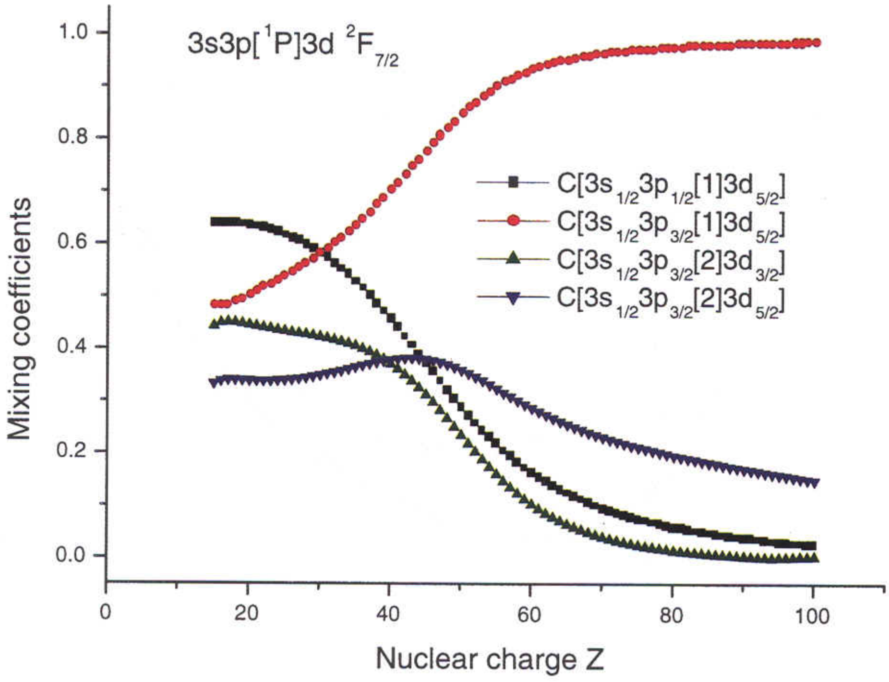

FIG. 20. Mixing coefficients for for odd-parity states with J=7/2 in Al-like ions as function of Z.

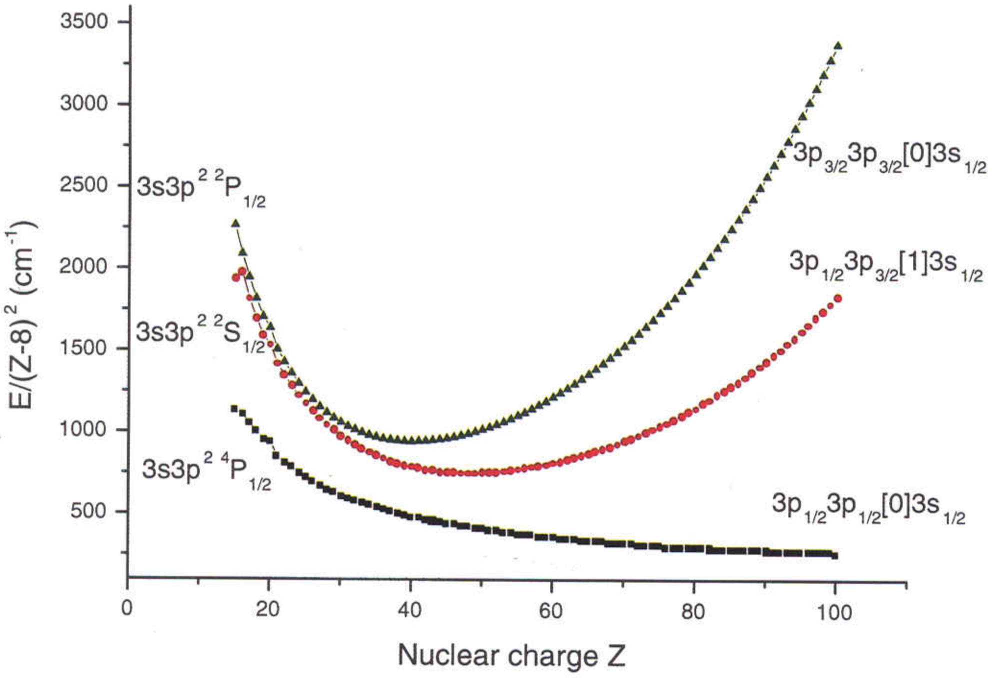

FIG. 21. Energies ($E/(Z-8)^2$ in cm^{-1}) of even-parity states with J=1/2 as functions of Z

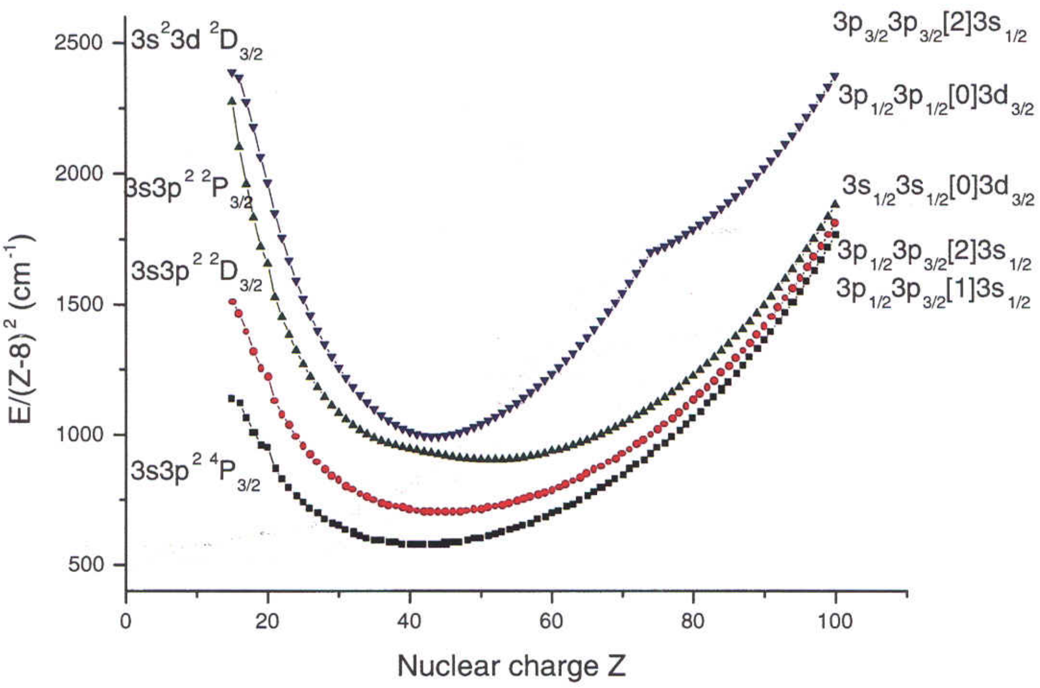

FIG. 22. Energies ($E/(Z-8)^2$ in cm^{-1}) of even-parity states with J=3/2 as functions of Z

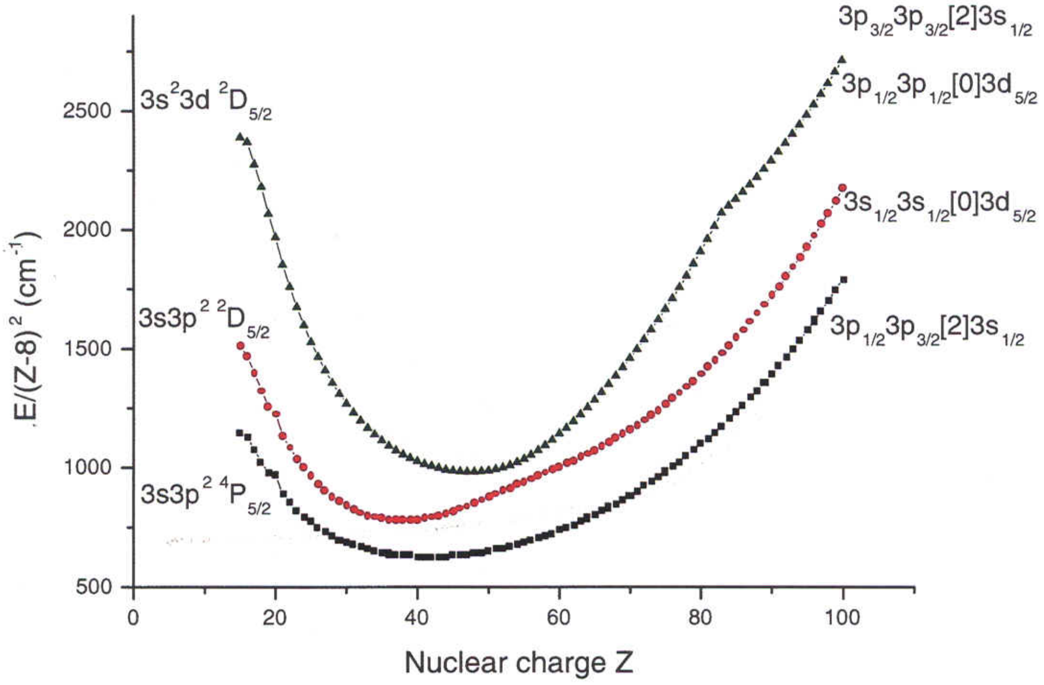

FIG. 23. Energies ($E/(Z-8)^2$ in cm^{-1}) of even-parity states with J=5/2 as functions of Z

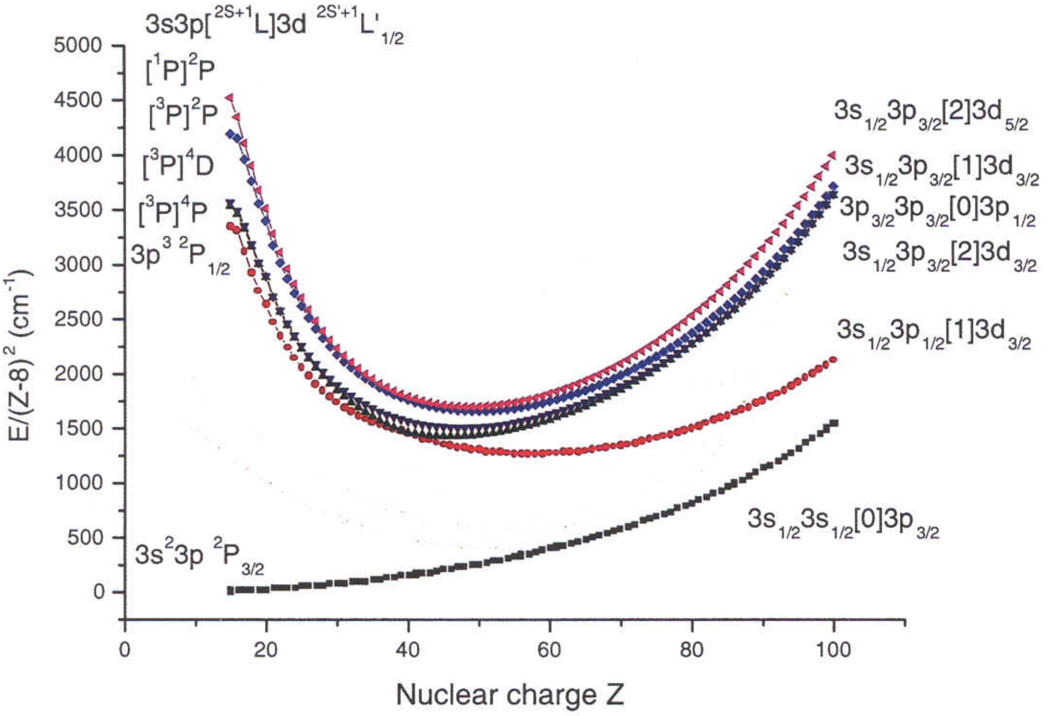

FIG. 24. Energies $(E/(Z-8)^2$ in $\mathrm{cm}^{-1})$ of odd-parity states with J=1/2 as functions of Z

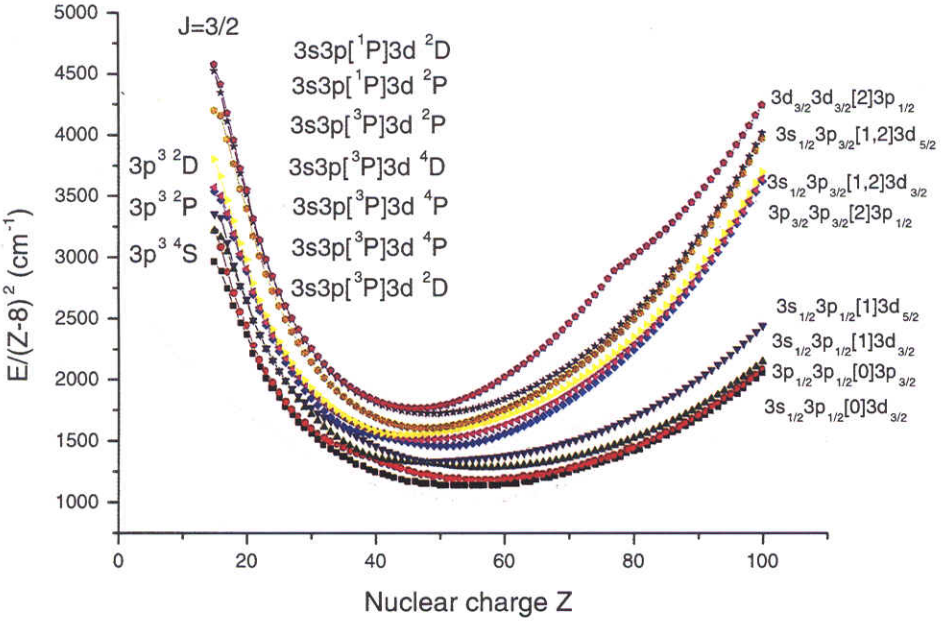

FIG. 25. Energies $(E/(Z-8)^2$ in $\mathrm{cm}^{-1})$ of odd-parity states with J=3/2 as functions of Z

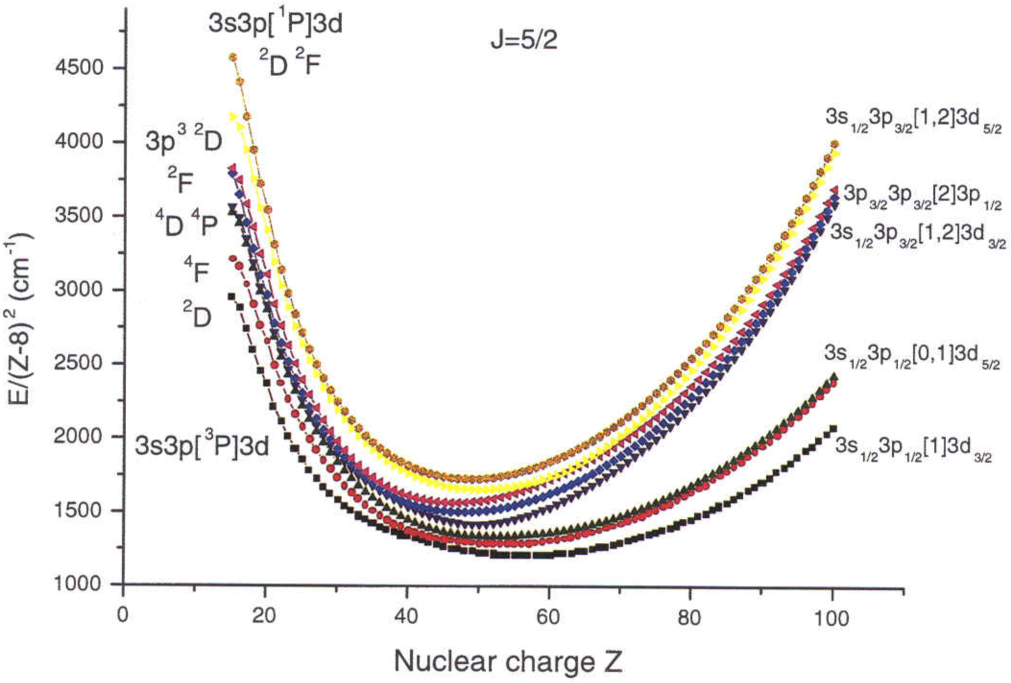

FIG. 26. Energies ($E/(Z-8)^2$ in cm^{-1}) of odd-parity states with J=5/2 as functions of Z

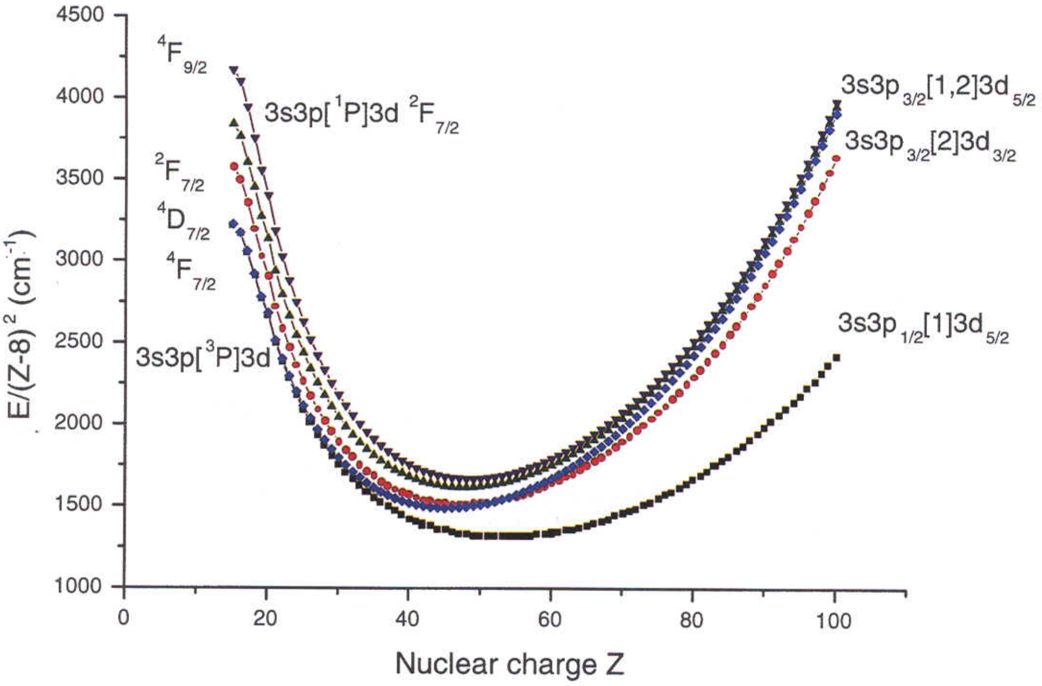

FIG. 27. Energies ($E/(Z-8)^2$ in cm^{-1}) of odd-parity states with J=7/2 as functions of Z

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