# 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 en-

ergies 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 $1s^22s^22p^6$ 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 ($1s^22s^22p^6$, 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 $\beta_1, \beta_2$ and $\beta_3$. 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 ($\beta_1, \beta_2$ and $\beta_3$) 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 $\eta$ 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:

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

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

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

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

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

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

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

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

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:

$$E^R(1^02^0[J_{12}]3^0J, 1'^02'^0[J'_{12}]J) \quad (2.26)$$
$$= \sum_{1,2,1',2'} \sum_{J''_{12}} E^R_a(12, 2'1', J)N(12)N(1'2')$$
$$\times \sum_3 C_{11^022^033^0}(J_{12}, J''_{12}, J)C_{1'1'^02'2'^033'^0}(J'_{12}, J''_{12}, J)\,,$$

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:

$$E^G(1^02^0[J_{12}]3^0J, 1'^02'^0[J'_{12}]J) \quad (2.27)$$
$$= \sum_{1,2,3,1',2',3'} \sum_n \frac{v_{123'n}v_{1'2'3n}}{\epsilon_n + \epsilon_{3'} - \epsilon_1 - \epsilon_2} \times C^{QJM}_{123}C^{Q'JM}_{1'2'3'}\,,$$

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))

$$E^G(1^02^0[J_{12}]3^0J, 1'^02'^0[J'_{12}]J) \quad (2.28)$$
$$= -\sum_{1,2,3,1',2',3'} \sum_{J''_{12},J''_{12}} \sum_{kk'} (-1)^{j_2+j_{2'}-j_3-j_{3'}+J''_{12}+J''^{'}_{12}+k+k'}$$
$$\times \sum_n \frac{X_k(123'n)X_k(1'2'3n)}{\epsilon_n + \epsilon_{3'} - \epsilon_1 - \epsilon_2} \sqrt{(2J''_{12}+1)(2J'''_{12}+1)}$$
$$\times \left\{ \begin{array}{ccc} j_n & j_{3'} & J''_{12} \\ j_1 & j_2 & k \end{array} \right\} \left\{ \begin{array}{ccc} j_n & j_3 & J \\ j_{1'} & j_{2'} & k' \end{array} \right\} \left\{ \begin{array}{ccc} J''^{'}_{12} & j_{3'} & J \\ J''_{12} & j_3 & j_n \end{array} \right\}$$
$$\times C_{11^022^033^0}(J_{12}, J''_{12}, J)C_{1'1'^02'2'^03'3'^0}(J'_{12}, J''^{'}_{12}, J)$$

where

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

(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 $C_{11^0 22^0 33^0}(J_{12}, J'_{12}, J) = C_J(1^0 2^0 J_{12} 3^0)$ 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 $E_{\mathrm{LAMB}}$, and the total theoretical energy $E_{\mathrm{tot}}$. 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 $E_{\mathrm{LAMB}}$ (see, for detail Ref. [18]). We also present in Table V the separate contributions: $E^{(0+1)}$, $E_2$, and $E_{\mathrm{LAMB}}$, together with the total theoretical energy $E_{\mathrm{tot}}$ 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 $i$=$3s3p[^3P]3d\ \ ^4P_{1/2}$.

The similar situation we found for the eleven, eight, and four levels of odd-parity complex with $J$=3/2, 5/2, and 7/2 accordingly. 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 $^4P\ ^2D$, 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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[1] C. Froese Fischer, *The Hartree-Fock method for atoms* (N. Y., John Wiley) (1977).
[2] R. D. Cowan, *The theory of atomic structure and spectra*, (Berkeley-Los Angeles: Univ.of California Press) (1981).
[3] I. P. Grant, B. J. McKenzie, P. H. Norrington , D. F. Mayers, and N. C.Pyper, Comput. Phys. Commun. **21**, 207 (1980).
[4] J. P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975).
[5] J. Nilsen, At. Data Nucl. Data Tables **37**, 191 (1987).
[6] W. Eissner, M. Jones, and H. Nussbaumer, Comput. Phys. Commun. **8**, 270 (1974).
[7] J. Dubau and M. Loulergue, Phys. Scr. **23**, 136 (1981).
[8] M. Klapisch, Comp. Phys. Commun. **2**, 239 (1971).
[9] E. P. Ivanova and A. V. Glushkov, Journ. Quant. Spectr. Rad. Transf. **36**, 127 (1986).
[10] L. A. Vainshtein and U. I. Safronova, Phys. Scr. **31**, 519 (1985).
[11] W. R. Johnson, M. Idress, and J. Sapirstein, Phys. Rev. A **35**, 3218 (1987).
[12] M. S. Safronova, W. R. Johnson, and U. I. Safronova, Phys. Rev. A **53**, 4036 (1996).
[13] M. S. Safronova, W. R. Johnson, and U. I. Safronova, J. Phys. B **30**, 2375 (1997).
[14] M. S. Safronova, W. R. Johnson, and U. I. Safronova, Phys. Scr. T **73**, 48 (1997).
[15] U. I. Safronova, W. R. Johnson, M. S. Safronova, and A. Derevianko, Phys. Scr. **59**, 286 (1999).
[16] U. I. Safronova, A. Derevianko, M. S. Safronova, and W. R. Johnson, J. Phys. B **32**, 3527 (1999).
[17] U. I. Safronova, W. R. Johnson, and A. Derevianko, Phys. Scr. **60**, 46 (1999).

[18] U. I. Safronova, W. R. Johnson, and H. G. Berry, Phys. Rev. A **61**, 052503 (2000).
[19] M. S. Safronova, W. R. Johnson, and U. I. Safronova, Phys. Rev. A **54** 2850 (1996).
[20] W.R Johnson, M.S Safronova, and U.I. Safronova, Phys. Scr. **56**, 252 (1997).
[21] U.I Safronova, W.R Johnson, and M.S. Safronova, At. Data Nucl. Data Tables **69**, 183 (1998).
[22] U.I Safronova, W.R Johnson, and A.E. Livingston Phys. Rev. A **60**, 996 (1999).
[23] L.A. Vainshtein and U.I. Safronova, At. Data Nucl. Data Tables **21**, 49 (1978); **25**, 311 (1980).
[24] U.I. Safronova and R. Bruch, Phys. Scr. **50**, 45 (1994).
[25] M.J. Connely, L. Lipsky and A. Russek, Phys. Rev. A **46**, 4012 (1992).
[26] K.-N. Huang, At. Data Nucl. Data Tables **34**, 1 (1986).
[27] B. C. Fawcett, At. Data Nucl. Data Tables **28**, 557 (1983).
[28] A. Farrag, E. Luc-Koenig, and J. Sinzelle, At. Data Nucl. Data Tables **27**, 539 (1982).
[29] S. A Blundell, Phys. Rev. A **47**, 1790 (1993).
[30] J. O. Ekberg, A. Redfors, M. Brown, U. Feldman, and J. F. Seely, Phys. Scr. **44**, 539 (1991).
[31] C. Jupén and J. Curtis, Phys. Scr. **53**, 312 (1996).
[32] W.C. Martin and R. Zalubas J. Phys. Chem. Ref. Data **12**, 323 (1983)
[33] W.C. Martin, R. Zalubas and A. Musgrove J. Phys. Chem. Ref. Data bf 14, 751 (1985).
[34] W.C. Martin, R. Zalubas and A. Musgrove J. Phys. Chem. Ref. Data bf 19, 821 (1990)
[35] J. Shugar and Ch. Corliss, J. Phys. Chem. Ref. Data **14**, Suppl. 2 (1985)
[36] T. Shirai, T. Nakagaki, J. Sugar, and W. L. Wiese, J. Phys. Chem. Ref. Data **21**, 273 (1992).
[37] T. Shirai, Y. Nakai, T. Nakagaki , J. Sugar, and W. L. Wiese, J. Phys. Chem. Ref. Data **22**, 1279 (1993).
[38] T. Shirai, T. Nakagaki, K. Okazaki, J. Sugar, and W. L. Wiese, J. Phys. Chem. Ref. Data **23**, 179 (1994).
[39] T. Shirai, Y. Funatake, K. Mori, J. Sugar, W. L. Wiese, and Y. Nakai, J. Phys. Chem. Ref. Data **19**, 127 (1990).
[40] T. Shirai, A. Mengoni, Y. Nakai, K. Mori, J. Sugar, W. L. Wiese, K. Mori, and N. Sakai, J. Phys. Chem. Ref. Data **21**, 23 (1992).
[41] J. Sugar, and A. Musgrove J. Phys. Chem. Ref. Data **19**, 527 (1990).
[42] J. Sugar, and A. Musgrove J. Phys. Chem. Ref. Data **24**, 1803 (1995).
[43] J. Sugar, and A. Musgrove J. Phys. Chem. Ref. Data **22**, 1213 (1993).
[44] T. Shirai, K. Okazaki, and J. Sugar, J. Phys. Chem. Ref. Data **24**, 1577 (1995)
[45] J. Sugar, and A. Musgrove J. Phys. Chem. Ref. Data **17**, 155 (1988).
[46] W.R. Johnson, S.A. Blundell and J. Sapirstein, Phys. Rev. A**37**, 2764 (1988).
[47] L. D. Landau and E. M. Lifshitz, p. 281 *Quantum Mechanics-Non-Relativistic Theory*, Pergamon Press, London (1963)

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 $E[3l_1j_1 3l_2j_2(J), 3l_3j_3 3l_4j_4(J)] = E_1 + B_1 + E_2$ for the case of germanium, $Z$=32 in a.u.

| $3l_1j_1 3l_2j_2$ | $3l_3j_3 3l_4j_4$ | $E_1$ | $B_1$ | $E_2$ |
|---|---|---|---|---|
| | | 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 |

| $3l_1j_1 3l_2j_2$ | $3l_3j_3 3l_4j_4$ | $E_1$ | $B_1$ | $E_2$ |
|---|---|---|---|---|
| | | 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 | $E^{(0+1)}$ | $E_2$ | $E_{\rm LAMB}$ | $E_{\rm tot}$ | $E^{(0+1)}$ | $E_2$ | $E_{\rm LAMB}$ | $E_{\rm tot}$ |
|---|---|---|---|---|---|---|---|---|
| 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 | $E^{(0+1)}$ | $E_2$ | $E_{\rm LAMB}$ | $E_{\rm tot}$ | $E^{(0+1)}$ | $E_2$ | $E_{\rm LAMB}$ | $E_{\rm tot}$ |
|---|---|---|---|---|---|---|---|---|
| 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 |
|---|---|---|---|---|---|---|---|---|---|---|
| $3s^2 3p$ | $^2P_{1/2}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $3s^2 3p$ | $^2P_{3/2}$ | 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 |
| $3s^2 3d$ | $^2D_{3/2}$ | 407623 | 439746 | 472279 | 505319 | 538960 | 573295 | 608425 | 644451 | 681245 |
| $3s^2 3d$ | $^2D_{5/2}$ | 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 |
|---|---|---|---|---|---|---|---|---|---|
| $3s^2 3p$ | $^2P_{1/2}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $3s^2 3p$ | $^2P_{3/2}$ | 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 |
| $3s^2 3d$ | $^2D_{3/2}$ | 719646 | 759071 | 799916 | 842274 | 886553 | 932979 | 981960 | 1034041 |
| $3s^2 3d$ | $^2D_{5/2}$ | 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 $3s^2 3p\ ^2P_J$-$3s3p^2\ ^4P_{J'}$ 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.

| | | $3s^2 3p\ ^2P_{1/2}$-$3s3p^2\ ^4P_{1/2}$ | $3s^2 3p\ ^2P_{3/2}$-$3s3p^2\ ^4P_{3/2}$ | $3s^2 3p\ ^2P_{3/2}$-$3s3p^2\ ^4P_{5/2}$ |
|---|---|---|---|---|
| $Z$=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 |

| $Z$ | $3s^2 3p$ | $3s3p^2$ | | $3s3p^2$ | | $3s^2 3d$ | $3s3p3d$ | | | $3s3p3d$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $^2P$ | $^4P$ | $^4P$ | $^2D$ | $^2P$ | $^2D$ | $^4P$ | $^4P$ | $^4D$ | $^4D$ | $^4D$ |
| | 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 $3s^2 3p\ ^2P$ and $3s3p^2\ ^4P$ terms in Al-like ions with $Z$=15-42. Comparison of the MBPT and predicted data.

| $Z$ | $3s^2 3p\ ^2P_{3/2} - {}^2P_{1/2}$ | | $3s3p^2\ ^4P_{3/2} - {}^4P_{1/2}$ | | | $3s3p^2\ ^4P_{5/2} - {}^4P_{3/2}$ | | | $3s3p^2\ ^4P_{5/2} - {}^4P_{1/2}$ | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 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 |

[a] C. Jupén and J. Curtis, Physica Scripta **53**, 312 (1996).

[b] J. O. Ekberg, A. Redfors, M. Brown, U. Feldman, and J. F. Seely, Physica Scripta **44**, 539 (1991).

[c] W.C. Martin, R. Zalubas, and A. Musgrove, J. Phys. Chem. Ref. Data bf 14, 751 (1985).

[d] W.C. Martin, R. Zalubas, and A. Musgrove, J. Phys. Chem. Ref. Data bf 19, 821 (1990).

[e] J. Shugar and Ch. Corliss, J. Phys. Chem. Ref. Data **14**, Suppl. 2 (1985).

[f] T. Shirai, T. Nakagaki, J. Sugar, and W. L. Wiese, J. Phys. Chem. Ref. Data **21**, 273 (1992).

[g] T. Shirai, Y. Nakai, T. Nakagaki , J. Sugar, and W. L. Wiese, J. Phys. Chem. Ref. Data **22**, 1279 (1993).

[h] T. Shirai, T. Nakagaki, K. Okazaki, J. Sugar, and W. L. Wiese, J. Phys. Chem. Ref. Data **23**, 179 (1994).

[i] T. Shirai, Y. Funatake, K. Mori, J. Sugar, W. L. Wiese, and Y. Nakai, J. Phys. Chem. Ref. Data **19**, 127 (1990).

[j] T. Shirai, A. Mengoni, Y. Nakai, K. Mori, J. Sugar, W. L. Wiese, K. Mori, and N. Sakai, J. Phys. Chem. Ref. Data **21**, 23 (1992).

[k] J. Sugar and A. Musgrove, J. Phys. Chem. Ref. Data bf 19, 527 (1990).

[l] J. Sugar and A. Musgrove, J. Phys. Chem. Ref. Data bf 24, 1803 (1995).

[m] T. Shirai, K. Okazaki, and J. Sugar, J. Phys. Chem. Ref. Data **24**, 1577 (1995).

[n] J. Sugar and A. Musgrove, J. Phys. Chem. Ref. Data bf 17, 155 (1988).

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 $Z$. Notations: 2=$C[3p_{3/2}3p_{3/2}[2]3p_{1/2}]$, 3=$C[3p_{1/2}3p_{1/2}[2]3p_{1/2}]$, 4=$C[3p_{3/2}3p_{3/2}[0]3p_{3/2}]$, 5=$C[3s_{1/2}3p_{1/2}[0]3d_{3/2}]$.

FIG. 16. Mixing coefficients for for odd-parity states with $J$=3/2 in Al-like ions as function of $Z$. Notations: 2=$C[3p_{3/2}3p_{3/2}[2]3p_{1/2}]$, 3=$C[3p_{1/2}3p_{1/2}[2]3p_{1/2}]$, 4=$C[3p_{3/2}3p_{3/2}[0]3p_{3/2}]$, 5=$C[3s_{1/2}3p_{1/2}[0]3d_{3/2}]$, 6=$C[3s_{1/2}3p_{1/2}[1]3d_{3/2}]$.

FIG. 17. Mixing coefficients for for odd-parity states with $J$=5/2 in Al-like ions as function of $Z$. Notations: 1=$C[3p_{3/2}3p_{3/2}[2]3p_{1/2}]$, 3=$C[3s_{1/2}3p_{1/2}[1]3d_{3/2}]$, 8=$C[3s_{1/2}3p_{3/2}[2]3d_{5/2}]$.

FIG. 18. Mixing coefficients for for odd-parity states with $J$=5/2 in Al-like ions as function of $Z$. Notations: 2=$C[3s_{1/2}3p_{1/2}[0]3d_{5/2}]$, 5=$C[3s_{1/2}3p_{3/2}[1]3d_{3/2}]$, 6=$C[3s_{1/2}3p_{3/2}[1]3d_{5/2}]$, 8=$C[3s_{1/2}3p_{3/2}[2]3d_{5/2}]$.

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 cm$^{-1}$) of odd-parity states with $J$=1/2 as functions of $Z$

FIG. 25. Energies ($E/(Z-8)^2$ in 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 $Z$