Energy levels of scandium, Sc i through Sc xxi

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The energy levels of the scandium atom in all of its stages of ionization, as derived from the analyses of atomic spectra, have been critically compiled. In cases where only line classifications are reported in the literature, level values have been derived. Electron configurations, term designations, J-values, experimental g-values, and ionization energies are included. Calculated percentages of the two leading components of the eigenvectors of the levels are given, where available.

Key words: Atomic energy levels; atomic spectra; scandium energy levels.

Introduction

At the time of the first compilation of atomic energy levels by Bacher and Goudsmit in 1932, only the first 3 of the 21 spectra of scandium had been studied. By 1949, Moore was able to compile energy levels for the first 12 spectra of scandium. At that time, oxygen was the heaviest atom for which some levels of all stages of ionization were known.

A great amount of new experimental work has been carried out since then, particularly in the higher stages of ionization. Today, experimental results are available for every stage of ionization of scandium. This is the result of the development of more energetic light sources, which was stimulated by the need to interpret new spectroscopic observations of the sun at short wavelengths from rocket- and satellite-borne spectrographs. A new impetus for the interpretation of spectra of highly ionized atoms has arisen from the investigation of hot laboratory plasmas generated to achieve controlled nuclear fusion.

These activities have produced a substantial increase in spectroscopic information, particularly for elements of the iron period, making the earlier compilations of energy levels inadequate. The NBS Atomic Energy Levels Data Center has undertaken to provide new compilations of energy levels, including the elements of the iron period. The material on each atom and its ions is being published as a separate paper. A collection of these compilations, with revisions, is planned as one volume for the iron period. Already completed are the compilation for iron by Reader and Sugar (1975), chromium, vanadium, and calcium by Sugar and Corliss (1977, 1978, 1979), and manganese, titanium, and potassium by Corliss and Sugar (1977, 1979a, 1979b). The present work on scandium will be followed by a compilation of the energy levels of nickel.

The present compilation comprises the energy levels of the scandium atom and all of its ions, as derived from analyses of atomic spectra. For many of the ions the original papers do not give energy level values, but only classifications of observed lines. In these cases we have derived the level values. Although generally we used only published papers as sources of data, unpublished data have been included when they constituted a substantial improvement over material in the literature.

Ionization energies found in the literature are usually given in eV or in cm⁻¹. The latest conversion factor 8065.479±0.021 cm⁻¹/eV is given by Cohen and Taylor (1973).

In a few cases where Rydberg series were available but the ionization energy was not derived, we carried out the calculation. For a large number of ions, no suitable series are...
known. In these cases we have quoted values obtained by extrapolation along isoelectronic sequences. Although uncertainties are not usually provided with these extrapolated values, they are probably accurate to a few units of the last significant figure given.

Nearly all of the data are the result of observations of various types of laboratory light sources. However, they are sometimes supplemented by data obtained from solar observations. This is particularly true where spin-forbidden lines are needed to establish the absolute energy of a system of excited levels and also where parity-forbidden transitions between levels of a ground configuration are used to obtain accurate relative energies for the low levels. Whenever both solar data and equivalent laboratory data are available preference is generally given to the laboratory measurements in order to avoid the problem of blended lines of various elements in the solar spectrum.

For a convenient source of wavelengths of scandium lines below 2000 Å we refer the reader to the compilation by Kelly and Palumbo (1973). The strong scandium lines above 2000 Å are in the tables of spectral lines by Meggers, Corliss, and Scribner (1975).

When no observations are available to connect independent systems of levels, an estimate of the connecting energy is frequently made. Those levels affected by the estimate are denoted by "+x" following the level values. The value of x is the systematic error of the estimate. For Sc XX and XXI, which are isoelectronic with He I and H I, respectively, we give only calculated level values since they are much more accurate than experimental x-ray wavelengths from which level values may be obtained.

We have included the results of calculations, under the heading "Leading percentages," that express the percentage composition of levels in terms of the basis states of a single configuration, or more than one configuration where configuration interaction has been included. Where these results contradict an author's designation, we have accepted the theoretical term and configuration labeling of a level to conform with its calculated leading percentages. In some cases these are low and the labeling has less physical meaning.

In the columns of the present tables headed "Leading percentages" we give first the percentage of the basis state corresponding to the level's name; next the second largest percentage together with the related basis state.

Of course, the percentage compositions cannot be considered to be as reliable as experimental quantities inasmuch as a new calculation using a different approximation, such as the introduction of configuration interaction where none had been used before, might yield a different set of percentages. For some levels the percentages may change drastically in a new calculation. In the present tables, the percentages are taken mostly from published least squares level-fitting calculations. When only ab initio calculations are found in the literature, we have used them if there appears to be a reasonable correspondence with the experimental data. For higher ionization stages there have been fewer publications relating quantitatively the theoretical results to the observations by means of least-squares calculations.

For configurations of equivalent d electrons, repeating terms of the same LS type sometimes occur. These are theoretically distinguished by their seniority number. In the present compilations they are designated in the notation of Nielson and Koster (1963). For example, in the 3d⁶ configuration there are three 3d terms with seniorities of 1, 3, and 5. These terms are denoted as 3d¹, 3d², and 3d³, respectively, by Nielson and Koster. Martin, Zalubas, and Hagan (1978) give a complete summary of the coupling notations used here.

In assembling the data for each spectrum, we referred to the following bibliographies:

i. papers cited by Moore (1949)
ii. C. E. Moore (1968)
iii. L. Hagan and W. C. Martin (1972)
iv. L. Hagan (1977)
v. card file of publications since June 1975 maintained by the NBS Atomic Energy Levels Data Center.

A selection of data was made that, in our judgment, represents the most accurate and reliable available. The text for each ion is not always a complete review of the literature but is intended to credit the major contributions. This compilation is intended to include all material available as of March 1, 1979.

Acknowledgments

Throughout this work we have made extensive use of the bibliographical files and reprint collection maintained in the Atomic Energy Levels Data Center by Dr. Romuald Zalubas. Our thanks are extended to him for generous cooperation. The compilation has also benefited greatly from the preprints that were provided by many of our colleagues.

We thank Dr. W. C. Martin for a critical reading of the manuscript.

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References for Introduction


Nielson, C. W., and Koster, G. F. (1963), Spectroscopic Coefficients for the \( p^1, d^1, \) and \( f^1 \) Configurations (The M.I.T. Press, Cambridge).


Z = 21

Ground state: 1s²2s²2p⁶3s²3p⁶3d⁴s² 2D₉/₂

Ionization energy = 52 922.0 ± 0.5 cm⁻¹ (6.56154 ± 0.00006 eV)

The first extensive analysis of Sc I was carried out by Russell and Meggers (1927), who classified about 350 lines between 2690 and 8250 Å as combinations among 128 energy levels of nine configurations. The analysis was extended by Neufeld (1970) and Neufeld and Schrenk (1975), who added 150 newly classified lines and 22 new levels and measured g-values for 98 levels.

Observations of the absorption spectrum of Sc in the range 1200–3200 Å were made by Garton, Reeves, Tomkins, and Ercoli (1973) with a measurement accuracy of ±0.01 Å. They identified eight series arising from the 2D ground term in combination with 3d⁴s² 2p ¹D, 3d⁴s(3D)np ¹P, 3d⁴s(3F)np ¹L, and 3d²(3F)np ¹L’ (where L may be D, F, or G). By far the strongest series arises from the 3d⁴s² 2D–4s² ⁵F transitions. The three series 3d⁴s² ²D—3d⁴s(3P)np ¹P were observed to much higher n and were used to derive the ionization energy. Two more series found to converge to the 3d⁴s(1D) limit were identified tentatively as 3d⁴s² ²D—3d⁴s(1P)np ¹D* with unresolved ²D* splitting. A final series labeled 3d⁴s²—3d²(3F)np ¹L’ observed from n = 7 to 15 and much stronger than the ²D* series was reported. Since L may represent D*, F*, or G* terms, the most likely candidate for a strong series is ²F* and we have used this designation for the series. Many additional absorption features not compiled here were reported with no identification of the upper levels.

A new analysis of Sc I based on new observations between 2000 and 34 000 Å has been published by Ben Ahmed and Verges (1977) together with a theoretical interpretation by Ben Ahmed (1977). They established 108 additional levels and derived the complete system of known levels up to 49 000 cm⁻¹ from their new measurements, classifying 1230 lines.

Our compilation is from the papers of Ben Ahmed and Verges, Ben Ahmed, and Garton et al. The ionization energy is from the latter authors, who derived their value from the 3d⁴s(1D)np ¹P₁/₂ series.

The g-values are from Ben Ahmed and Verges, except for those of the ground term, which are taken from the report of the magnetic resonance experiments by Childs (1971).

References

### Sc I

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### Configuration Term \( J \) \( \text{Level (cm}^{-1}\) \( g \) Leading percentages

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| \( Sc\,\, II\, 3d4s^1(D) \) | Limit | 55 463 | \[
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ENERGY LEVELS OF SCANDIUM

Z = 21

Ca I isoelectronic sequence

Ground state: 1s²2s²2p⁶3s²3p⁶3d⁴4s 3D₁

Ionization energy = 103 237.1 ± 2 cm⁻¹ (12.79987 ± 0.0002 eV)

The first extensive analysis of Sc II was reported by Russell and Meggers (1927). They classified 142 lines in the range 2540 to 6600 Å as combinations among 53 energy levels of eight configurations. Many of these levels were determined to better accuracy by Neufeld (1970). Neufeld also provided g-values for 18 levels.

Johansson and Litzén (1979) have reobserved the spectrum from 1100 to 10 000 Å with a pulsed hollow cathode. They extended the analysis and redetermined the level values. Their results are quoted below.

Roth (1969) calculated the composition of the 3d⁴4p configuration. Wyart has calculated 3d⁴4p, 3d⁵p, 3d⁴f, 3d⁵f, and 4s⁴p with configuration interaction. His results, as reported by Johansson and Litzén, are given here.

The ionization energy was derived by Johansson and Litzén from a polarization formula.

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### ENERGY LEVELS OF SCANDIUM

#### Sc II

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Z = 21

K I isoelectronic sequence

Ground state: \(1s^22s^22p^63s^23p^63d^2\) \(^2D_{3/2}\)

Ionization energy = 199 677.37 ± 0.1 cm\(^{-1}\) (24.75704 ± 0.00005 eV)

The early work on Sc III was reported by Gibbs and White (1926), Smith (1927), and Russell and Lang (1927).

Two modern analyses of Sc III were published by Holmstrom (1972) and Van Deurzen, Conway, and Davis (1973). Holmstrom lists 64 observed lines between 557 and 8882 Å. He states the accuracy of his level values to be ±0.4 cm\(^{-1}\). Van Deurzen, Conway, and Davis observed 93 lines between 557 and 9371 Å. Their level values are stated to be accurate to less than 0.1 cm\(^{-1}\). This compilation is taken from Van Deurzen et al. except for the \(^2H\) terms given only by Holmstrom. They are derived here from Holmstrom's lines and the levels of Van Deurzen et al.

Van Deurzen et al. calculated the ionization energy from four members (\(n = 5-8\)) of the \(ng\) series. Their value agrees with the value calculated by Holmstrom with a polarization formula. The uncertainty in eV is determined by the uncertainty in the conversion factor.

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ENERGY LEVELS OF SCANDIUM

Sc IV

Z = 21

Ar I isoelectronic sequence

Ground state: \(1s^22s^22p^63s^23p^6\) \(^1S\)

Ionization energy = 592 732±3 cm\(^{-1}\) (73.4900±0.0004 eV)

Four resonance lines were classified by Kruger, Weissberg, and Phillips (1937). Smitt (1973) has carried out the extensive analysis quoted here, which confirmed only two of the four resonance lines. The uncertainty of his level values is estimated to be ±2 cm\(^{-1}\). He calculated the ionization energy with a polarization formula.

The \(3s3p^53p\) \(^1P^+\) term was observed by Kastner, Crooker, Behring, and Cohen (1977) in absorption in a high voltage spark.

### References


### Sc IV

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Sc v (3P$_{3/2}$) Limit 592 732
ENERGY LEVELS OF SCANDIUM

Sc V

Z = 21

Cl 1 isoelectronic sequence

Ground state: 1s²2s²2p⁶3s²3p⁵2P⁵/₂

Ionization energy = 741 000 cm⁻¹ (91.9 eV)

Measurements by Beckman (1937) (± 10 cm⁻¹) and by Kruger and Phillips (1937) (± 5 cm⁻¹) between 220 and 590 Å in Sc v established the 3s³P, 3s3p, and 3s³p⁴4s configurations. The level values given here for the 3s³p⁴4s configuration are averages of their determinations. For the ¹P₁/₂ and ³P₁/₂ levels, the values of Kruger and Phillips are not in accord with the isoelectronic sequence and are not used.

The values for 3s³p⁵ ²P⁰ and 3s3p⁵ ²S are from Smitt (1973) (± 0.8 cm⁻¹). The 3p⁻¹(1P)3d terms are taken from Svensson and Ekberg (1968) (± 10 cm⁻¹) and the 3p⁻¹(1D)3d terms from Fawcett and Gabriel (1966) (± 20 cm⁻¹). The 3p⁵S terms were identified by Fawcett, Peacock, and Cowan (1968), whose measurements at 180 Å are stated to be accurate to 0.03 Å (± 90 cm⁻¹).

The ionization energy was determined by extrapolation by Lotz (1967).

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Sc vi (³P₂) Limit 741 000
Z = 21

Sc I isoelectronic sequence

Ground state: \( 1s^2 2s^2 2p^6 3s^2 3p^1 3p_2 \)

Ionization energy = 892 700 ± 400 cm\(^{-1}\) (110.68 ± 0.05 eV)

The analysis of Sc VI was initiated by Beckman (1937) and by Kruger and Pattin (1937), who reported terms of the \( 3s^2 3p^1, 3s3p^5, \) and \( 3s^2 3p^4 3s \) configurations. The \( 3s^2 3p^1 1p^1 \) term was found by Edlén (1942).

The \( 3s^2 3p^3 3d \) configuration was observed by Svensson and Ekberg (1968) and the level values given here (with an uncertainty of about ± 5 cm\(^{-1}\)) are derived from their observations.

The values for the two lower configurations (\( 3s^2 3p^4 \) and \( 3s^2 3p^5 \)) are from the more accurate observations of Smitt, Svensson and Oulred (1976).

The \( 3p^4 4s \) levels are derived from Beckman (± 5 cm\(^{-1}\)) and the \( 3p^4 4d \) and \( 5s \) levels are from Fawcett, Peacock, and Cowan (1968) (± 100 cm\(^{-1}\)). Fawcett, Cowan, and Hayes (1972) have observed transitions in the \( 3p^3 d - 3p^4 f \) array, but they are not connected with the present system.

We derived the ionization energy from the \( 3s^2 3p^1 (3S^1) 4s \) and \( 5s \) \( (S^1) \) terms, adopting a value for the change in the effective quantum number between them of 1.0247 obtained from the \( 3s^2 3p^1 \) terms of Cr VI from the analysis of Ekberg (1973).

The analysis of Sc VI was initiated by Beckman (1937) and by Kruger and Pattin (1937), who reported terms of the \( 3s^2 3p^1, 3s3p^5, \) and \( 3s^2 3p^4 3s \) configurations. The \( 3s^2 3p^1 1p^1 \) term was found by Edlén (1942).

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ENERGY LEVELS OF SCANDIUM

Sc VII

Z = 21

P I isoelectronic sequence

Ground state: 1s²2s²2p⁶3s²3p³ ¹S₀;

Ionization energy = 1 113 000 cm⁻¹ (138.0 eV)

The levels are from the work of Ekberg and Svensson (1970) and Smitt, Svensson, and Outred (1976). The levels for the 3s²3p¹ and 3s3p¹ configurations are taken from the latter paper and have an uncertainty of about ±2 cm⁻¹. We have combined these values with the measurements and classifications given by Ekberg and Svensson in the wavelength range of 182-598 Å to derive new level values for the 3p³3d and 4s configurations. Most of the wavelengths used by Ekberg and Svensson are taken from Beckman (1937), Kruger and Pattin (1937), and Fawcett (1970). The uncertainty of these upper levels is about ±10 cm⁻¹.

Since no intersystem transitions have been observed, all of the doublets have an added systematic error “x,” relative to the ground term ¹S₀. The value of “x” depends on the accuracy of calculations by Smitt, Svensson and Outred and is expected to be less than ±20 cm⁻¹.

The ionization energy is from an extrapolation by Lotz (1967).

References


Z = 21

Si I isoelectronic sequence

Ground state: $1s^2 2s^2 2p^6 3s^2 3p^2 \cdot 1S^0$

Ionization energy = 1 275 000 cm$^{-1}$ (158.1 eV)

The study of this spectrum was initiated by Kruger and Phillips (1937), who classified fifteen lines as transitions between the ground term and three odd terms $3s^2 3p^2 \cdot 1S^0$, $3s^2 3p^3 \cdot 1P^0$ and $3s^2 3p^4 \cdot 1P^0$. Phillips (1939) found $3s^2 3p^2 \cdot 1D$ and $3s^2 3p^3 \cdot 1P^0$. Fawcett, Gabriel, and Saunders (1967) extended the $3p^2 - 3p3d$ array; Fawcett (1970) added to the $3s^2 3p^2 - 3s3p$ array. Fawcett, Cowan, and Hayes (1972) identified lines in $3p3d - 3p4f$ which are not connected with the other levels.

Ekberg and Svensson (1970) reanalyzed the spectrum using a compilation of wavelengths between 164 and 572 Å. Smitt, Svensson, and Outred (1976) made new observations between 362 and 640 Å. The level values for the $3s^2 3p^2$ and $3s^2 3p^3$ configurations are taken from the more accurate data of Smitt et al. and the values for $3s^2 3p3d$ and $3s^2 3p4s$ are derived by combining those values with the wavelengths in Ekberg and Svensson. The uncertainty of the level values from Smitt et al. is about ±5 cm$^{-1}$. Four intersystem transitions have been observed.

The ionization energy was obtained by Ekberg and Svensson from an extrapolation formula.

References


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|              |      | 1   | 2 271.9          | $3s^2 3p3d$  | $^3P^0$ | 2   | 319 569         |
|              |      | 2   | 5 507.7          | $3s^2 3p3d$  | $^3P^0$ | 1   | 322 541         |
|              |      | 0   | 25 026.9         | $3s^2 3p3d$  | $^3P^0$ | 0   | 323 673         |
| $3s^2 3p^2$  | $^1D$ | 1   | 179 662.3        | $3s^2 3p3d$  | $^3D^0$ | 1   | 329 862         |
|              |      | 2   | 180 032.7        | $3s^2 3p3d$  | $^3P^0$ | 2   | 330 716         |
|              |      | 3   | 180 592.6        | $3s^2 3p3d$  | $^3P^0$ | 3   | 333 153         |
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|              |      | 1   | 207 761.0        | $3s^2 3p3d$  | $^3P^0$ | 0   | 603 533         |
|              |      | 2   | 207 814.4        | $3s^2 3p4s$  | $^3P^0$ | 0   | 604 609         |
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| $3s3p^3$    | $^3S^0$ | 1  | 272 417.4        | $3s^2 3p4s$  | $^1P^0$ | 1   | 614 080         |

Sc IX ($^3P_{1/2}$) Limit 1 275 000
ENERGY LEVELS OF SCANDIUM

Sc ix

Z=21

Al isoelectronic sequence

Ground state: \( 1s^2 2s^2 2p^6 3s^2 3p^2 5p_{1/2} \)

Ionization energy = 1 452 000 ± 1000 cm\(^{-1}\) (180.03 ± 0.1 eV)

The initial work on the analysis of this spectrum was by Kruger and Phillips (1937) and by Beckman (1937). About a third of Beckman’s identifications were corrected by Fawcett (1970).

Using the earlier measurements, Ekberg and Svensson (1970) reanalyzed the spectrum between 90 and 540 Å and identified all the remaining terms given here. They extrapolated the position of \( 3s^2 3p^2 5p_{1/2} \) along the isoelectronic sequence. Since no intersystem transitions have been observed, we use their extrapolation to establish the energy of \( 5p_{1/2} \) relative to the ground level. The error is indicated by \( x \).

Smitt, Svensson, and Outred (1976) remeasured the \( 3s^2 3p^2 - 3s^2 3p^2 \) array between 380 and 540 Å and determined the doublet terms of those configurations with an uncertainty of ±4 cm\(^{-1}\). We used their term values in combination with the earlier measurements of Ekberg and Svensson to establish the higher doublet term values.

The ionization energy was obtained by Ekberg and Svensson from the \( nf \) series.

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Mg I isoelectronic sequence

Ground state: \(1s^22s^22p^63s^2^1S_0\)

Ionization energy = \(1815 \pm 1000 \text{ cm}^{-1} = 225.1 \pm 0.1 \text{ eV}\)

The initial work on the analysis was done by Beckman (1937) and Parker and Phillips (1940).

Ekberg (1971), using wavelengths between 76 and 470 Å, taken from the papers above, has redone the analysis and determined all the levels given in this compilation except the \(3p^2^1S\), the \(3p3d\), and the \(3p4f\) levels. These are taken from Fawcett (1970, 1976). The singlets and triplets have not been connected by observations. Ekberg has estimated the value for \(3s3p^3P\), used here by interpolation along the isoelectronic sequence. The uncertainty “\(x\)” is less than 1000 cm\(^{-1}\).

Ekberg derived the quoted value for the ionization energy by extrapolation.

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### Energy Levels of Scandium

**Sc x**

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**Limit** | 1 815 600

Z = 21

Na I isoelectronic sequence

Ground state: 1s2 2s2 2p2 3s 2S1/2

Ionization energy = 2 015 050 ± 10 cm⁻¹ (249.837 ± 0.001 eV)

We have used the measurements and classifications of Kruger and Phillips (1939) between 97 and 523 Å to determine the 3p, 3d, 4d, and 5f levels and those of Edlen (1936) between 94 and 129 Å for the 4s, 4p, and 4f levels. The 5s, 5p, 5d, 6s, 6p, 6d, 6f, and 7d levels are from Beckman’s (1937) measurements. The p, d, and f terms for n = 8, 9 are from Fawcett (1976) and the 7p, 7f, and 7p are from Cohen and Behring (1976).

The limit is from Edlen (1978). It agrees with the determination of Crooker, which was reported by Cohen and Behring.

### References

Edlen, B. (1936), Z. Phys. 100, 621.

### Sc XI

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### Sc XII (1S0)

**Limit**

2 015 050
Z = 21

Ne I isoelectronic sequence

Ground state: \( 1s^2 2s^2 2p^6 1s_0 \)

Ionization energy = 5,543,900 ± 500 cm\(^{-1}\) (687.36 ± 0.06 eV)

Only resonance lines between 20 and 31 Å are classified by this system of energy levels. Edlén and Tyrén (1936) identified transitions from the \( 2p^3 3s \) and \( 3d \) configurations. We derived the ionization energy by application of a Ritz formula to the \( 2s^2 2p^6 (3P_{1/2})^m d (3/2)^n \) series for \( n = 3, 4, \) and 5. The result is in agreement with the value given by Edlén and Tyrén. Fawcett (1965) observed three transitions arising from \( 2p^5 4d \) and from \( 2s 2p^5 3p^4 1P^0 \). Feldman and Cohen (1967) observed eight transitions, including those reported by Fawcett. We have adopted the more accurate values of Feldman and Cohen.

In order to determine the coupling for the \( 2p^3 3s \) and \( 2p^5 3d \) levels, we calculated these configurations by using for the radial integrals, Hartree-Fock values scaled according to fitted values in \( Al^{IV} \) by Artru and Kaufman (1975). The result confirmed our use of \( J_J \)-coupling for \( 2p^3 3s \) and \( J_J \)-coupling for \( 2p^5 3d \) in this sequence. However, it also put in question the identification of the resonance lines assigned to the \( 2p^5 3d \) configuration. The total spread of the calculated levels of \( J = 1 \) is 53,120 cm\(^{-1}\) compared with the observed value of 98,900 cm\(^{-1}\). The percentages given for these levels are from this calculation.

Kastner, Behring, and Cohen (1975) identified transitions between \( 2p^5 3p \) and \( 2p^5 4d \), but there is no connection with the levels given here.

### References


<table>
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Z = 21

F isoelectronic sequence

Ground state: \(1s^22s^22p^52p_{3/2}^\circ\)

\[
\text{Ionization energy} = 6103\,000\,\text{cm}^{-1} \quad (756.7\,\text{eV})
\]

The first work on this spectrum was by Fawcett (1965), who classified lines of the \(2s^22p^5 - 2s^22p^6 3s\) and \(3d\) transition arrays between 24 and 28 Å. This work was revised and extended by Feldman, Doschek, Cowan, and Cohen (1973), from whose improved wavelengths the 3s and 3d levels are determined. Their estimated uncertainty of \(\pm 0.01\) Å gives a level uncertainty of \(\pm 500\,\text{cm}^{-1}\). The ground term interval is from Fawcett, Burgess, and Peacock (1967), who identified the \(2s^22p^5 - 2s^22p^6\) doublet at \(\sim 134\) Å. The uncertainty of these 3 levels is \(\sim 500\,\text{cm}^{-1}\).

The composition of the \(2p^43s\) and \(2p^43d\) levels is from Chapman and Shadmi (1973).

The \(2s2p^3 3s\) \(^2P^\circ\) term is from Feldman et al. (1973).

The ionization energy was obtained by extrapolation by Lotz (1967).

### References


### Sc XIII

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The observed spectrum of Sc XIV consists of the strong transition array \( 2s^22p^4 - 2s2p^5 \), which lies between 122 and 158 Å, and the arrays \( 2p^2 - 2p^33s \) at 25 Å and \( 2p^2 - 2p^33d \) at 23 Å. The \( 1S_0 \) due to \( 2p^2 \) combines with \( 2s2p^5 \) \( 1P_1 \) at 157 Å. The arrays at 25 Å and 23 Å were first observed by Goldsmith, Feldman, and Cohen (1971). The \( J=0 \) and 1 levels of the ground term could not be resolved at these wavelengths. Fawcett (1971) then observed the \( 2s^22p^4 - 2s2p^5 \) array at 150 Å and resolved the ground term. We have determined the levels of the \( 2s^22p^4 \) configurations from his measurements with an uncertainty of \( \pm 200 \) cm\(^{-1}\). The levels of \( 2s^22p^4 \) are adopted from Edlén’s (1972) re-evaluation of the data for this isoelectronic sequence. These are probably accurate to \( \pm 50 \) cm\(^{-1}\). Since no intersystem transitions have been observed, we based the singlet system on Edlen’s extrapolated value for \( 2p^4ld \). Its uncertainty is probably \( \pm 100 \) cm\(^{-1}\).

Improved measurements of the \( 2p^2 - 2p^33s \) array were obtained from Doschek, Feldman, and Cohen (1973). The \( 1S_0 \) due to \( 2p^2 \) combines with \( 2s2p^5 \) \( 1P_1 \) at 157 Å. The arrays at 25 Å and 23 Å were first observed by Goldsmith, Feldman, and Cohen (1971). The \( J=0 \) and 1 levels of the ground term could not be resolved at these wavelengths. Fawcett (1971) then observed the \( 2s^22p^4 - 2s2p^5 \) array at 150 Å and resolved the ground term. We have determined the levels of the \( 2s^22p^4 \) configurations from his measurements with an uncertainty of \( \pm 200 \) cm\(^{-1}\). The levels of \( 2s^22p^4 \) are adopted from Edlén’s (1972) re-evaluation of the data for this isoelectronic sequence. These are probably accurate to \( \pm 50 \) cm\(^{-1}\). Since no intersystem transitions have been observed, we based the singlet system on Edlen’s extrapolated value for \( 2p^4ld \). Its uncertainty is probably \( \pm 100 \) cm\(^{-1}\).

A revised analysis of \( 2p^4 - 2p^33d \) by Fawcett and Hayes (1975) is adopted here. A level uncertainty of \( \pm 3000 \) cm\(^{-1}\) is indicated. The subsequent revisions of this array proposed by Bromage and Fawcett (1977), following a new calculation, are regarded as tentative and the levels put in question are omitted pending further study.

The ionization energy was evaluated by Lotz (1967) by extrapolation.

### References


### Sc XIV

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Z = 21

N 1 isoelectronic sequence

Ground state: 1s²2s²2p⁵ ⁴S₉/₂

Ionization energy = 7 481 000 cm⁻¹ (927.5 eV)

The strong transition arrays 2s²2p₂⁻→2s2p⁰ and 2s²2p⁴⁻→2p⁵ were identified by Fawcett (1971) between 118 and 190 Å. The levels have an uncertainty of ±200 cm⁻¹. The position of the doublets relative to the ground state is based on the estimated position of 2s²2p³ ³D₂ by Edlén (1972).

The 2p³d terms are from observations by Fawcett and Hayes (1975) at 22 Å. They have an uncertainty of ±3000 cm⁻¹.

The ionization energy is from Lotz's (1967) extrapolation.

References


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Sc xv (²P₉)

Limit

7 481 000
Z = 21

C i isoelectronic sequence

Ground state: \(1s^22s^22p^2\) \(^3P_0\)

Ionization energy = 8 140 000 cm\(^{-1}\) (1009 eV)

The 2s\(^2\)2p\(^2\) --- 2s2p\(^3\) array was observed by Fawcett (1971) between 130 and 202 Å. New measurements and some revised classifications were given by Fawcett and Hayes (1975), who also identified 2s2p\(^3\) --- 2p\(^3\) lines in the same region. The levels of 2s\(^2\)2p\(^2\), 2s2p\(^3\), and 2p\(^3\) are derived from the data of Fawcett and of Fawcett and Hayes and have an uncertainty of ±100 cm\(^{-1}\). All levels of the higher configurations are from the measurements of Goldsmith, Feldman, Crooker and Cohen (1972) at 20--22 Å with an estimated uncertainty of ±0.005 Å, giving a level uncertainty of ±1000 cm\(^{-1}\).

No intersystem combinations have been observed. Goldsmith et al. extrapolated the position of \(2p^2\)D\(_2\) to 123 900 cm\(^{-1}\). Fawcett and Cowan (1975) obtained an extrapolated value of 123 400 cm\(^{-1}\). We have used the mean of these values as the reference value for the singlet system. Goldsmith et al. identified two quintet transitions but they are not connected to the triplet system.

The ionization energy is from the extrapolation by Lotz (1967).

References


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Z = 21

B 1 isoelectronic sequence

Ground state: $1s^22s^22p\,^2P_{1/2}^o$

Ionization energy = 8 820 000 cm\(^{-1}\) (1094 eV)

Fawcett and Hayes (1975) analyzed the transition arrays $2s^22p - 2s2p^2$ and $2s2p^2 - 2p^3$ found between 143 and 211 Å. Their wavelength uncertainty is $\pm 0.02$ Å giving an uncertainty in the levels of $\pm 100$ cm\(^{-1}\). The quartet system is based on an interpolation between the predictions of the position of the $^3P_{1/2}^o$ level of $2s2p^2$ in Ti XVIII by Kasyanov et al. (1974) and in Ca XVI by Kononov, Koshelev, Podobedova, and Churilov (1975). The levels of $2p3p$ and $2p3d$ are also from the classifications made by Fawcett and Hayes of wavelengths at $\sim 19$ Å. The level uncertainty in this case is $\pm 3000$ cm\(^{-1}\).

The ionization energy is from an extrapolation by Lotz (1967).

**References**


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**Sc XVIII**

The level uncertainty in this case is $\pm 3000$ cm\(^{-1}\).

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Sc xviii

$Z = 21$

Be I isoelectronic sequence

Ground state: $1s^22s^21S_0$

Ionization energy = 9780 000 cm$^{-1}$ (1213 eV)

Fawcett and Hayes (1975) have identified the resonance transition $2s^2\,^1S_0-2s2p\,^1P^\prime$. The resonance transition from $2s2p\,^3P^\prime$ has not been observed. Edlén (1979) has made an extensive study of the Be I isoelectronic sequence and has proposed values for the $^3P^\prime$ term of $2s2p$ obtained by interpolation. We have adopted his values and combined them with the classifications of Fawcett and Hayes to obtain the higher-lying configurations. From their wavelength uncertainty of ±0.01 Å and an equal uncertainty assumed for Edlén’s interpolations, we estimate the level uncertainty to be ±3000 cm$^{-1}$.

The ionization energy was obtained by Lotz (1967) by extrapolation.

References


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ENERGY LEVELS OF SCANDIUM

Sc xix

Z = 21

Li I isoelectronic sequence

Ground state: 1s²2s ¹S₁/₂

Ionization energy = 10 388 200 ± 1600 cm⁻¹ (1287.98 ± 0.2 eV)

The first observations were reported by Goldsmith, Feldman, Oren, and Cohen (1972), who identified the transitions to 2s from 3p, 4p, and 5p and to 2p from 3s, 3d, 4d, and 5d in the range of 11-19 Å. These results were extended by Boiko, Faenov, and Pikuz (1978) to include transitions through 7p and 8d.

In a comprehensive review of all the available data for the Li I isoelectronic sequence Edlén (1979) derived smoothed-out values for all the wavelengths and new values for the energy levels through 4d. These are given below and combined with the classifications of Boiko et al. to obtain the higher-lying levels. The uncertainty for both sets of data is estimated to be about ±0.003 Å or ~1500 cm⁻¹.

Edlén derived the value for the ionization energy by means of a polarization formula applied to the 2p-nd series.

References


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Z = 21

He I isoelectronic sequence

Ground state: 1s² ¹S₀

Ionization energy = 45 773 660±200 cm⁻¹ (5675.26±0.03 eV)

The theoretical values calculated by Ermolaev and Jones (1974) for the singlet and triplet S and P terms of this two-electron ion are expected to be more accurate than the observed values, and we have quoted them up to n = 5. The uncertainty of the ionization energy and level values was estimated to be of the order of ±40 cm⁻¹, but this should probably be increased to several hundred cm⁻¹. For comparison, the 1s²–1s2p transition of this ion has been observed by Boiko et al. (1978) in a laser-produced plasma. They place 1s2p ³Pₚ at 34 660 000 cm⁻¹ and 1s2p ³P₀ at 34 820 000 cm⁻¹.

References


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Z = 21

H I isoelectronic sequence

Ground state: 1s $^2S_{1/2}$

Ionization energy = 48 665 240±90 cm$^{-1}$ (6033.769±0.016 eV)

No observations of this spectrum are available.

The theoretical values calculated by Erikson for terms of this hydrogen-like ion are given below through $n=5$. The binding energy of the 1s electron is reported with an uncertainty of ±90 cm$^{-1}$; the levels measured from the ground state taken as zero will also have this uncertainty. The uncertainty in the conversion factor determines the uncertainty in eV.

**References**


<table>
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