On a group-theoretical approach to the periodic table of chemical elements
Maurice R. Kibler

To cite this version:
Maurice R. Kibler. On a group-theoretical approach to the periodic table of chemical elements. Jun 2004, Prague. hal-00002554

HAL Id: hal-00002554
https://hal.science/hal-00002554
Submitted on 16 Aug 2004
On a group-theoretical approach to the periodic table of chemical elements

MAURICE R. KIBLER

Institut de Physique Nucléaire de Lyon
IN2P3-CNRS et Université Claude Bernard
43 Bd du 11 Novembre 1918, F-69622 Villeurbanne Cedex, France

This paper is concerned with the application of the group SO(4,2)⊗SU(2) to the periodic table of chemical elements. It is shown how the Madelung rule of the atomic shell model can be used for setting up a periodic table that can be further rationalized via the group SO(4,2)⊗SU(2) and some of its subgroups. Qualitative results are obtained from the table and the general lines of a programme for a quantitative approach to the properties of chemical elements are developed on the basis of the group SO(4,2)⊗SU(2).

PACS: 03.65.Fd, 31.15.Hz

Key words: hydrogen-like atom, harmonic oscillator, invariance and non-invariance groups, Lie algebra under constraints, Madelung rule, periodic table

1 Introduction

Most of the modern presentations of the periodic table of chemical elements are based on a quantum-mechanical treatment of the atom. In this respect, the simplest atom, namely the hydrogen atom, often constitutes a starting point for studying many-electron atoms. Naively, we may expect to construct an atom with atomic number \(Z\) by distributing \(Z\) electrons on the one-electron energy levels of a hydrogen-like atom. This building-up principle can be rationalized and refined from a group-theoretical point of view. As a matter of fact, we know that the dynamical noninvariance group of a hydrogen-like atom is the special real pseudo-orthogonal group in 4+2 dimensions (or conformal group) SO(4,2) or SO(4,2)⊗SU(2) if we introduce the group SU(2) that labels the spin [1-3]. This result can be derived in several ways. We briefly review two of them.

The first way is quite well-known and corresponds to a symmetry ascent process starting from the geometrical symmetry group SO(3) of a hydrogen-like atom. Then, we go from SO(3) to the dynamical invariance group SO(4) for the discrete spectrum or SO(3,1) for the continuous spectrum. The relevant quantum numbers for the discrete spectrum are \(n\), \(\ell\) and \(m_\ell\) (with \(n = 1, 2, 3, \cdots\); for fixed \(n\): \(\ell = 0, 1, \cdots, n - 1\); for fixed \(\ell\): \(m_\ell = -\ell, -\ell + 1, \cdots, \ell\)). The corresponding state vectors \(\Psi_{ntm_\ell}\) can be organized to span multiplets of SO(3) and SO(4). The set \(\{\Psi_{ntm_\ell} : n \text{ fixed; } m_\ell \text{ ranging}\}\) generates an irreducible representation class (IRC), noted \(\ell\), while the set \(\{\Psi_{ntm_\ell} : n \text{ fixed; } \ell \text{ and } m_\ell \text{ ranging}\}\) generates an IRC of SO(4). The direct sum

\[
h = \bigoplus_{n=1}^{\infty} \bigoplus_{\ell=0}^{n-1} (\ell)
\]
spanned by all the possible state vectors $\Psi_{n\ell m}$ corresponds to an IRC of the de Sitter group SO(4, 1). The IRC $h$ is also an IRC of SO(4, 2). This IRC thus remains irreducible when restricting SO(4, 2) to SO(4, 1) but splits into two IRC’s when restricting SO(4, 2) to SO(3, 2). The groups SO(4, 2), SO(4, 1) and SO(3, 2) are dynamical noninvariance groups in the sense that not all their generators commute with the Hamiltonian of the hydrogen-like atom.

The second way to derive SO(4, 2) corresponds to a symmetry descent process starting from the dynamical noninvariance group Sp(8, $\mathbf{R}$), the real symplectic group in 8 dimensions, for a four-dimensional isotropic harmonic oscillator. We know that there is a connection between the hydrogen-like atom in $\mathbf{R}^3$ and a four-dimensional oscillator in $\mathbf{R}^4$ [3-4]. Such a connection can be established via Lie-like methods (local or infinitesimal approach) or algebraic methods based on the so-called Kustaanheimo-Stiefel transformation (global or partial differential equation approach). Both approaches give rise to a constraint and the introduction of this constraint into the Lie algebra of Sp(8, $\mathbf{R}$) produces a Lie algebra under constraints that turns out to be isomorphic with the Lie algebra of SO(4, 2). From a mathematical point of view, the latter Lie algebra is given by [5]

$$\text{cent}_{\text{sp}(8, \mathbf{R})}/so(2) = su(2, 2) \sim so(4, 2)$$

in terms of Lie algebras.

Once we accept that the hydrogen-like atom may serve as a guide for studying the periodic table, the group SO(4, 2) and some of its subgroups play an important role in the construction of this table. This was first realized in by Barut [6] and, independently, by Konopel’chenko [7]. Later, Byakov et al. [8] further developed this group-theoretical approach of the periodic chart of chemical elements by introducing the direct product SO(4, 2)$\otimes$SU(2).

The aim of this paper is to emphasize the importance of a connection between the periodic table à la SO(4, 2)$\otimes$SU(2) and the Madelung rule [9] of atomic spectroscopy. The material is organized as follows. In Section 2, a periodic table is derived from the Madelung rule. In Section 3, this table is rationalized in terms of SO(4, 2)$\otimes$SU(2). Some qualitative and quantitative aspects of the table are described in Sections 4 and 5. This paper constitutes a companion article to four previous papers by the author [10].

2 The periodic table à la Madelung

We first describe the construction of a periodic table based on the so-called Madelung rule [9] which arises from the atomic shell model. This approach to the periodic table uses the quantum numbers occurring in the quantum-mechanical treatment of the hydrogen atom as well as of a many-electron atom.

In the central-field approximation, each of the $Z$ electrons of an atom with atomic number $Z$ is partly characterized by the quantum numbers $n$, $\ell$, and $m_{\ell}$. The numbers $\ell$ and $m_{\ell}$ are the orbital quantum number and the magnetic quantum number, respectively. They are connected to the chain of groups SO(3)$\supset$SO(2): the
quantum number $\ell$ characterizes an IRC, of dimension $2\ell + 1$, of SO(3) and $m_\ell$ a one-dimensional IRC of SO(2). The principal quantum number $n$ is such that $n - \ell - 1$ is the number of nodes of the radial wave function associated with the doublet $(n, \ell)$. In the case of the hydrogen atom or of a hydrogen-like atom, the number $n$ is connected to the group SO(4): the quantum number $n$ characterizes an IRC, of dimension $n^2$, of SO(4). The latter IRC of SO(4) splits into the IRC’s of SO(3) corresponding to $\ell = 0, 1, \ldots, n - 1$ when SO(4) is restricted to SO(3).

A complete characterization of the dynamical state of each electron is provided by the quartet $(n, \ell, j, m)$ or alternatively $(n, j, \ell, m)$. Here, the spin $s = \frac{1}{2}$ of the electron has been introduced and $m_s$ is the $z$-component of the spin. Furthermore, $j = \frac{1}{2}$ for $\ell = 0$ and $j$ can take the values $j = \ell - s$ and $j = \ell + s$ for $\ell \neq 0$. The quantum numbers $j$ and $m$ are connected to the chain of groups SU(2)$\supset$U(1): $j$ characterizes an IRC, of dimension $2j + 1$, of SU(2) and $m$ a one-dimensional IRC of U(1).

Each doublet $(n, \ell)$ defines an atomic shell. The ground state of the atom is obtained by distributing the $Z$ electrons of the atom among the various atomic shells $n\ell, n'\ell', n''\ell'', \cdots$ according to (i) an ordering rule and (ii) the Pauli exclusion principle. A somewhat idealized situation is provided by the Madelung ordering rule: the energy of the shells increases with $n + \ell$ and, for a given value of $n + \ell$, with $n$ [9]. This may be depicted by Fig. 1 where the rows are labelled with $n = 1, 2, 3, \cdots$ and the columns with $\ell = 0, 1, 2, \cdots$ and where the entry in the $n$-th row and $\ell$-th column is $[n + \ell, n]$. We thus have the ordering $[1, 1] < [2, 2] < [3, 2] < [3, 3] < [4, 3] < [4, 4] < [5, 3] < [5, 4] < [5, 5] < [6, 4] < [6, 5] < [6, 6] < \cdots$. This dictionary order corresponds to the following ordering of the $n\ell$ shells

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < \cdots$$

which is verified to a good extent by experimental data. (According to atomic spectroscopy, we use the letters $s$ (for sharp), $p$ (for principal), $d$ (for diffuse), $f$ (for fundamental), \ldots to denote $\ell = 0, 1, 2, 3, \cdots$, respectively.)

From these considerations of an entirely atomic character, we can construct a periodic table of chemical elements. We start from the Madelung array of Fig. 1. Here, the significance of the quantum numbers $n$ and $\ell$ is abandoned. The numbers $n$ and $\ell$ are now simple row and column indexes, respectively. We thus forget about the significance of the quartet $n, \ell, j, m$. The various blocks $[n + \ell, n]$ are filled in the dictionary order, starting from $[1, 1]$, with chemical elements of increasing atomic numbers. More precisely, the block $[n + \ell, n]$ is filled with $2(2\ell + 1)$ elements, the atomic numbers of which increase from left to right. This yields Fig. 2, where each element is denoted by its atomic number $Z$. For instance, the block $[1, 1]$ is filled with $2(2 \times 0 + 1) = 2$ elements corresponding to $Z = 1$ up to $Z = 2$. In a similar way, the blocks $[2, 2]$ and $[3, 2]$ are filled with $2(2 \times 0 + 1) = 2$ elements and $2(2 \times 1 + 1) = 6$ elements corresponding to $Z = 3$ up to $Z = 4$ and to $Z = 5$ up to $Z = 10$, respectively. It is to be noted, that the so obtained periodic table a priori contains an infinite number of elements: the $n$-th row contains $2n^2$ elements and each column (bounded from top) contains an infinite number of elements.
Fig. 1. The \([n + \ell, n]\) Madelung array. The lines are labelled by \(n = 1, 2, 3, \cdots\) and the columns by \(\ell = 0, 1, 2, \cdots\). For fixed \(n\), the label \(\ell\) assumes the values \(\ell = 0, 1, \cdots, n - 1\).

Fig. 2. The periodic table deduced from the Madelung array. The box \([n + \ell, n]\) is filled with \(2(2\ell + 1)\) elements. The filling of the various boxes \([n + \ell, n]\) is done according to the dictionary order implied by Fig. 1.
On the periodic table . . .

3 The periodic table à la SO(4,2)⊗SU(2)

We are now in a position to give a group-theoretical articulation to the periodic table of Fig. 2. For fixed $n$, the $2(2\ell + 1)$ elements in the block $[n + \ell, n]$, that we shall refer to as an $\ell$-block, may be labelled in the following way. For $\ell = 0$, the $s$-block in the $n$-th row contains two elements that we can distinguish by the number $m$ with $m$ ranging from $-\frac{1}{2}$ to $\frac{1}{2}$ when going from left to right in the row. For $\ell \neq 0$, the $\ell$-block in the $n$-th row can be divided into two sub-blocks, one corresponding to $j = \ell - \frac{1}{2}$ (on the left) and the other to $j = \ell + \frac{1}{2}$ (on the right). Each sub-block contains $2j + 1$ elements (with $2j + 1 = 2\ell$ for $j = \ell - \frac{1}{2}$ and $2j + 1 = 2(\ell + 1)$ for $j = \ell + \frac{1}{2}$) that can be distinguished by the number $m$ with $m$ ranging from $-j$ to $j$ by step of one unit when going from left to right in the row. In other words, a chemical element can be located in the table by the quartet $(n, \ell, j, m)$ (where $j = \frac{1}{2}$ for $\ell = 0$).

Following Byakov et al. [8], it is perhaps interesting to use an image with streets, avenues and houses in a city. Let us call Mendeleev city the city whose (west-east) streets are labelled by $n$ and (north-south) avenues by $(\ell, j, m)$. In the $n$-th street there are $n$ blocks of houses. The $n$ blocks are labelled by $\ell = 0, 1, \cdots, n - 1$ so that the address of a block is $(n, \ell)$. Each block contains one sub-block (for $\ell = 0$) or two sub-blocks (for $\ell \neq 0$). An address $(n, \ell, j, m)$ can be given to each house: $n$ indicates the street, $\ell$ the block, $j$ the sub-block and $m$ the location inside the sub-block. The organization of the city appears in Fig. 3.

At this stage, it is worthwhile to re-give to the quartet $(n, \ell, j, m)$ its group-theoretical significance. Then, Mendeleev city is clearly associated to the IRC class $h \otimes [2]$ of SO(4,2)⊗SU(2) where $[2]$ stands for the fundamental representation of SU(2). The whole city corresponds to the IRC $\bigoplus_{n=1}^{\infty} \bigoplus_{\ell=0}^{n-1} \bigoplus_{j=|\ell-\frac{1}{2}|}^{\ell+\frac{1}{2}} (j) = \left( \bigoplus_{n=1}^{\infty} \bigoplus_{\ell=0}^{n-1} (\ell) \right) \otimes [2]$ of SO(4,2)⊗SU(2) in the sense that all the possible quartets $(n, \ell, j, m)$, or alternatively $(n, \ell, m_\ell, m_s)$, can be associated to state vectors spanning this IRC. (In the latter equation, $(\ell)$ and $(j)$ stand for the IRC’s of SO(3) and SU(2) associated with the quantum numbers $\ell$ and $j$, respectively.)

We can ask the question: how to move in Mendeleev city? Indeed, there are several bus lines to go from one house to another one? The SO(3) bus lines (also called SO(3)⊗SU(2) ladder operators) make it possible to go from one house in a given $\ell$-block to another house in the same $\ell$-block (see Fig. 4). The SO(4) bus lines (also called SO(4)⊗SU(2) ladder operators) and the SO(2,1) bus lines (also called SO(2,1) ladder operators) allow to move in a given street (see Fig. 5) and in a given avenue (see Fig. 6), respectively. Finally, it should be noted that there are taxis (also called SO(4,2)⊗SU(2) ladder operators) to go from a given house to an arbitrary house.

Another question concerns the inhabitants (also called chemical elements) of Mendeleev city. In fact, they are distinguished by a number $Z$ (also called the
atomic number). The inhabitant living at the address \((n, \ell, j, m)\) has the number

\[
Z(n\ell jm) = \frac{1}{6}(n + \ell)(n + \ell + 1)^2 - \frac{1}{2}(n + \ell + 1)^2 \\
-\frac{1}{4}[1 + (-1)^{n+\ell}](n + \ell + 1) - 4\ell(\ell + 1) + \ell + j(2\ell + 1) + m - 1
\]

Each inhabitant may also have a nickname. All the inhabitants up to \(Z = 110\) have a nickname. For example, we have Ds, or darmstadtium in full, for \(Z = 110\). Not all the houses in Mendeleev city are inhabited. The inhabited houses go from \(Z = 1\) to \(Z = 116\) (the houses \(Z = 113\) and \(Z = 115\) are occupied since the beginning of 2004 [11]). The houses corresponding to \(Z \geq 117\) are not presently inhabited. (When a house is not inhabited, we also say that the corresponding element has not been observed yet.) The houses from \(Z = 111\) to \(Z = 116\) are inhabited but have not received a nickname yet. The various inhabitants known at the present time are indicated on Fig. 7.

It is not forbidden to get married in Mendeleev city. Each inhabitant may get married with one or several inhabitants (including one or several clones). For example, we know \(\text{H}_2\) (including \(\text{H}\) and its clone), \(\text{HCl}\) (including \(\text{H}\) and \(\text{Cl}\)), and \(\text{H}_2\text{O}\) (including \(\text{O}\), \(\text{H}\) and its clone). However, there is a strict rule in the city: the assemblages or married inhabitants have to leave the city. They must live in another city and go to a city sometimes referred to as a molecular city. (Only the clones can stay in Mendeleev city.)

4 Qualitative aspects of the periodic table

Going back to Physics and Chemistry, we now describe Mendeleev city as a periodic table for chemical elements. We have obtained a table with rows and columns for which the \(n\)-th row contains \(2n^2\) elements and the \((\ell, j, m)\)-th column contains an infinite number of elements. A given column corresponds to a family of chemical analogs in the standard periodic table and a given row may contain several periods of the standard periodic table.

The chemical elements in their ground state are considered as different states of atomic matter: each atom in the table appears as a particular partner for the (infinite-dimensional) unitary irreducible representation \(h \otimes [2]\) of the group \(\text{SO}(4, 2) \otimes \text{SU}(2)\), where \(\text{SO}(4, 2)\) is reminiscent of the hydrogen atom and \(\text{SU}(2)\) is introduced for a doubling purpose. In fact, it is possible to connect two partners of the representation \(h \otimes [2]\) by making use of shift operators of the Lie algebra of \(\text{SO}(4, 2) \otimes \text{SU}(2)\). In other words, it is possible to pass from one atom to another one by means of raising or lowering operators. The internal dynamics of each element is ignored. In other words, each neutral atom is assumed to be a noncomposite physical system. By way of illustration, we give a brief description of some particular columns and rows of the table.

The alkali-metal atoms (see Fig. 8) are in the first column (with \(\ell = 0, j = \frac{1}{2}\), and \(m = -\frac{1}{2}\)); in the atomic shell model, they correspond to an external shell of type \(1s, 2s, 3s, \cdots\); we note that hydrogen (H) belongs to the alkali-metal atoms.
On the periodic table . . .

The second column (with $\ell = 0$, $j = \frac{1}{2}$, and $m = \frac{1}{2}$) concerns the alkaline earth metals (see Fig. 9) with an external atomic shell of type $1s^2, 2s^2, 3s^2, \ldots$; we note that helium (He) belongs to the alkaline earth metals. The sixth column corresponds to chalcogens (see Fig. 10) and the seventh column to halogens (see Fig. 11); it is to be observed that hydrogen does not belong to halogens as it is often the case in usual periodic tables. The eighth column (with $\ell = 1$, $j = \frac{3}{2}$, and $m = \frac{3}{2}$) gives the noble gases (see Fig. 12) with an external atomic shell of type $2p^6, 3p^6, 4p^6, \ldots$; helium (with the atomic configuration $1s^22s^2$) does not belong to the noble gases in contrast with usual periodic tables.

The $d$-blocks with $n = 3, 4$ and 5 yield the three familiar transition series (see Fig. 13): the iron group goes from Sc(21) to Zn(30), the palladium group from Y(39) to Cd(48) and the platinum group from Lu(71) to Hg(80). A fourth transition series goes from Lr(103) to $Z = 112$ (observed but not named yet). In the shell model, the four transition series correspond to the filling of the $nd$ shell while the $(n + 1)s$ shell is fully occupied, with $n = 3$ (iron group series), $n = 4$ (palladium group series), $n = 5$ (platinum group series) and $n = 6$ (fourth series). The two familiar inner transition series are the $f$-blocks with $n = 4$ and $n = 5$ (see Fig. 14): the lanthanide series goes from La(57) to Yb(70) and the actinide series from Ac(89) to No(102). Observe that lanthanides start with La(57) not Ce(58) and actinides start with Ac(89) not Th(90). We note that lanthanides and actinides occupy a natural place in the table and are not reduced to appendages as it is generally the case in usual periodic tables in 18 columns. A superactinide series is predicted to go from $Z = 139$ to $Z = 152$ (and not from $Z = 122$ to $Z = 153$ as predicted by Seaborg [12]). In a shell model approach, the inner transition series correspond to the filling of the $nf$ shell while the $(n + 2)s$ shell is fully occupied, with $n = 4$ (lanthanides), $n = 5$ (actinides) and $n = 6$ (superactinides). The table in Fig. 7 shows that the elements from $Z = 121$ to $Z = 138$ form a new period having no homologue among the known elements.

In Section 3, we have noted that each $\ell$-block with $\ell \neq 0$ gives rise to two sub-blocks. As an example, the $f$-block for the lanthanides is composed of a sub-block (corresponding to $j = \frac{1}{2}$) from La(57) to Sm(62) and another one (corresponding to $j = \frac{5}{2}$) from Eu(63) to Yb(70) (see Fig. 15). This division corresponds to the classification in light or ceric rare earths and heavy or yttric rare earths. It has received justifications both from the experimental and the theoretical sides.

5 Quantitative aspects of the periodic table

To date, the use of $SO(4,2)$ or $SO(4,2)\otimes SU(2)$ in connection with periodic charts has been limited to qualitative aspects only, viz., classification of neutral atoms and ions as well. We would like to give here the main lines of a programme under development (inherited from nuclear physics and particle physics) for dealing with quantitative aspects.

The first step concerns the mathematics of the programme. The direct product group $SO(4,2)\otimes SU(2)$ is a Lie group of order eighteen. Let us first consider the
Fig. 3. Mendeleev city. The streets are labelled by \( n \in \mathbb{N}^* \) and the avenues by \((\ell, j, m)\) \([\ell = 0, 1, \ldots, n - 1; j = \frac{1}{2} for \ell = 0, j = \ell - \frac{1}{2} or j = \ell + \frac{1}{2} for \ell \neq 0; m = -j, -j + 1, \ldots, j]\).
Fig. 4. How to move in Mendeleev city? To move inside a block, take an SO(3)⊗SU(2) bus line! The shaded bus line corresponds to \( l = 3 \) and \( n = 6 \).
Fig. 5. How to move in Mendeleev city? To move inside a west-east street, take an $SO(4) \otimes SU(2)$ bus line! The shaded bus line corresponds to $n = 4$. 

\begin{tabular}{cccccccccccccccccccccccc}
\hline
\hline
\end{tabular}
Fig. 6. How to move in Mendeleev city? To move inside a north-south avenue, take an \(SO(2,1)\) bus line! The shaded bus line corresponds to \(\ell = 0\), \(j = \frac{1}{2}\), and \(m = -\frac{1}{2}\).
Fig. 7. The inhabitants of Mendeleev city. The houses up to number $Z = 116$ are inhabited. 'X?' means inhabited (or observed) but not named, 'no' means not inhabited (or not observed).
Fig. 8. The inhabitants of Mendeleev city. The family of alkali metals (with an infinite number of elements) corresponds to \((\frac{\ell}{2} = \frac{j}{2} = \frac{m}{2} = \ell = j = m = 0, n \in \mathbb{N})\).
Fig. 9. The inhabitants of Mendeleev city. The family of alkaline earth metals corresponds to \((\ell = 0, j = 1, m = \frac{1}{2}, n \in \mathbb{N})\).
Fig. 10. The inhabitants of Mendeleev city. The family of chalcogens (with an infinite number of elements) corresponds to \((\ell = 1, j = \frac{3}{2}, m = -\frac{1}{2}, n = 2, 3, 4, \ldots)\).
The inhabitants of Mendeleev city. The family of halogens (with an infinite number of elements) corresponds to \( (\ell = 1, j = \frac{3}{2}, m = \frac{1}{2}) \) and \( n = 2, 3, 4, \ldots \).
Fig. 12. The inhabitants of Mendeleev city. The family of noble gases (with an infinite number of elements) corresponds to \( \ell = 1, j = \frac{3}{2}, m = \pm \frac{3}{2}, \ldots \).
Fig. 13. The inhabitants of Mendeleev city. The three transition series: the iron group series [from Sc(21) to Zn(30)], the palladium group series [from Y(39) to Cd(48)], and the platinum group series [from Lu(71) to Hg(80)].
Fig. 14. The inhabitants of Mendeleev city. The three inner transition series: the lanthanide series [from La(57) to Yb(70)], the actinide series [from Ac(89) to No(102)], and the superactinides series [from (139) to (152)].
Fig. 15. The inhabitants of Mendeleev city. The lanthanides or rare earths can be divided into two sub-blocks. The lighter (or ceric) rare earths [from La(57) to Sm(62)] correspond to $\frac{1}{2} \leq \ell = \ell'$ and the heavier (or yttric) rare earths [from Eu(63) to Yb(70)] to $\ell = \ell'$. The lanthanides or rare earths can be divided...
SO(4, 2) part which is a semi-simple Lie group of order \( r = 15 \) and of rank \( \ell = 3 \). It has thus fifteen generators involving three Cartan generators (i.e., generators commuting between themselves). Furthermore, it has three invariant operators or Casimir operators (i.e., independent polynomials, in the enveloping algebra of the Lie algebra of SO(4, 2), that commute with all generators of the group SO(4, 2)). Therefore, we have a set of six \((3 + 3)\) operators that commute between themselves: the three Cartan generators and the three Casimir operators. Indeed, this set is not complete from the mathematical point of view. In other words, the eigenvalues of the six above-mentioned operators are not sufficient for labelling the state vectors in the representation space of SO(4, 2). According to a (not very well-known) result popularised by Racah, we need to find \( \frac{1}{2}(r - 3\ell) = 3 \) additional operators in order to complete the set of the six preceding operators. This yields a complete set of nine \((6 + 3)\) commuting operators and this solves the state labelling problem for the group SO(4, 2). The consideration of the group SU(2) is trivial: SU(2) is a semi-simple Lie group of order \( r = 3 \) and of rank \( \ell = 1 \) so that \( \frac{1}{2}(r - 3\ell) = 0 \) in that case. As a result, we end up with a complete set of eleven \((9 + 2)\) commuting operators. It is to be stressed that this result constitutes the key and original starting point of the programme.

The second step establishes contact with chemical physics. Each of the eleven operators can be taken to be self-adjoint and thus, from the quantum-mechanical point of view, can describe an observable. Indeed, four of the eleven operators, namely, the three Casimir operators of SO(4, 2) and the Casimir operator of SU(2), serve for labelling the representation \( h \otimes [2] \) of SO(4, 2) \( \otimes \) SU(2) for which the various chemical elements are partners. The seven remaining operators can thus be used for describing chemical and physical properties of the elements like: ionization energy; oxidation degree; electron affinity; electronegativity; melting and boiling points; specific heat; atomic radius; atomic volume; density; magnetic susceptibility; solubility; etc. In most cases, this can be done by expressing a chemical observable associated with a given property in terms of the seven operators which serve as an integrity basis for the various observables. Each observable can be developed as a linear combination of operators constructed from the integrity basis. This is reminiscent of group-theoretical techniques used in nuclear and atomic spectroscopy (cf. the Interacting Boson Model) or in hadronic spectroscopy (cf. the Gell-Mann/Okubo mass formulas for baryons and mesons).

The last step is to proceed to a diagonalisation process and then to fit the various linear combinations to experimental data. This can be achieved through fitting procedures concerning either a period of elements (taken along a same line of the periodic table) or a family of elements (taken along a same column of the periodic table). For each property this will lead to a formula or phenomenological law that can be used in turn for making predictions concerning the chemical elements for which no data are available. In addition, it is hoped that this will shed light on regularities and well-known (as well as recently discovered) patterns of the periodic table. This programme, referred to as the KGR programme, was briefly presented at the 2003 Harry Wiener International Conference. It is presently under progress.
6 Closing remarks

We close this paper with two remarks. Possible extensions of this work concern isotopes and molecules. The consideration of isotopes needs the introduction of the number of nucleons in the atomic nucleus. With such an introduction we have to consider other dimensions for Mendeleev city: the city is not anymore restricted to spread in Flatland. Group-theoretical analyses of periodic systems of molecules can be achieved by considering direct products involving several copies of $\text{SO}(4,2) \otimes \text{SU}(2)$. Several works have been already devoted to this subject [13].

Acknowledgments. The author is indebted to M.S. Antony for comments concerning the elements $Z = 110, 113$ and 115 and to Yu.Ts. Oganessian for providing him with Ref. [11]. He would like also to thank I. Berkes, M. Cox, R.A. Hefferlin and M. Laing for interesting discussions and correspondence.

References