

## PERIODIC SYSTEM OF ELEMENTS DATABASE AND ITS APPLICATIONS

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**Abstract:** *The paper presents the benefits of SQL phrases used to interrogate a database, which store the periodic system of elements for didactic aim. The article is based on an original developed MySQL database and a PHP application, which can be used to answer at different questions, related to the structure of periodic system of elements. Sets of examples are given.*  
**Keywords:** *Client-server application, e-learning, SQL application, MySQL database server.*

### 1. INTRODUCTION

One of the consequences of the renewed interest in philosophical aspects of chemistry has been the corresponding renewed interest in the periodic system of the elements, which embodies so much chemical knowledge in an implicit form.<sup>1,2</sup> The periodic system reflects the configuration of electrons of the atoms in various shells or quantum states. This is how the system is presently explained in textbooks of chemistry.<sup>3</sup>

The best methods of estimating similarity and of displaying its salient features are methods that would seem most interesting to chemists. Therefore, the results depend critically on the sample of chemical and physical-chemical properties that are chosen.<sup>4</sup>

There are many forms of displaying and structure the chemical elements in the periodic systems. A numerical classification was performed on 69 elements with 54 chemical and physical-chemical properties. The elements fell into clusters in close accord with the electron shell *s*-, *p*- and *d*-blocks. The *f*-block elements were not included for lack of sufficiently complete data. The successive periods of

*s*- and *p*-block elements appeared in an oval configuration, with *d*-block elements lying to one side. More than three axes were required to give good representation of the variation, although the interpretation of the higher axes is difficult. Only 15 properties were scores for the noble gases, but despite the paucity of properties reflecting chemical reactivity, analysis of the 69 elements on these properties still showed the major features seen from the full set. Despite Mendeleev's success in predicting the properties of germanium and gallium, it is still difficult to predict finer details of new artificial elements. Attempts at relating elements quantitatively have mostly been in the form of diagrams, with the elements positioned in two or three dimensions.<sup>4</sup>

Although it is usually found that the numerical classification is not greatly affected by a modest number of missing entries (either not recorded or logically not scored) it was thought best to keep these down as far as possible by omitting elements and properties with many gaps. The proportion of scored entries in the 54×69 table was 74.8 %. Some properties that were likely to be nearly duplicates of others were excluded. The noble gases and lanthanides gave major problems. Only 15 properties could be scored satisfactorily for the former. The data for lanthanides is patchy, and it was thought best to include only lanthanum, which was relatively well documented. Atomic weight and atomic number were excluded in order to see what emerged from an analysis that omitted them. Attempts to explain the periodic system as a manifestation of regularities in the structure of the atoms of the elements are as old as the system itself.<sup>3</sup>

In addition, enormous progress in the evaluation of the chemical properties of the transactinide elements has been made over the past 15 years. While the early studies of chemical properties of *Rf* and *Db* revealed only qualitative features, many of the more recent investigations have yielded quantitative information, i.e., heats of adsorption in the gas-phase chemical studies, and distribution coefficients in the aqueous-phase studies. Relativistic quantum chemical calculations of the molecules, combined with fundamental physical-chemical considerations of their interaction with the chemical environment, have become available, which allow for detailed predictions of the chemical properties of the heaviest elements.<sup>5</sup>

The internationally accepted atomic weights are very important for science and technology. The standard atomic weights of the elements are regularly evaluated, recommended, and published in updated tables by the Commission on Atomic Weights and Isotopic Abundances (CAWIA) of the International Union of Pure and Applied Chemistry (IUPAC). It is known that atomic weights and atomic masses are now scaled to a numerical value of exactly 12 for the mass of the carbon isotope of mass number 12. Technological advances in mass spectrometry and nuclear-reaction energies have enabled atomic masses to be determined with a relative uncertainty of better than  $10^{-7}$ . Isotope abundances for an increasing number of elements can be measured to better than  $10^{-3}$ . The excellent precision of such measurements led to the discovery of many elements, in different specimens, display significant variations in their isotope-abundance ratios, caused by a variety of natural and industrial physical-chemical processes. While such variations increasingly place a constraint on the uncertainties with which some standard atomic weights can be stated, they provide numerous opportunities for investigating a range of important phenomena in physical, chemical, cosmological, biological, and industrial processes. Accurate determinations of the atomic weights of certain elements also influence the values of fundamental constants such as the Avogadro, Faraday, and universal gas constants.<sup>6,7</sup>

In the actual form of standardized periodic system, an important roll plays the electronic configuration of every element and in special of extern electrons. It that explain the periodicity of some properties function of atomic number  $Z$  (atomic and ionic ray, ionisation energy of atoms, the size of positive charge of nucleus, the medium distance between electron and nucleus, screening effect of those electrons presented in atom, the type of implied electron). There are also properties, which do not vary continuous, called aperiodic properties (as for example, atomic mass). The aperiodically properties of elements are determined by atomic nucleus while cover of electrons of elements determines the periodic properties.<sup>8</sup>

The periodic system is formed by 110 elements, distributed in groups and periods, but in the last years the elements 111, 112, 114, 116, and 118 were discovered.<sup>9,10</sup>

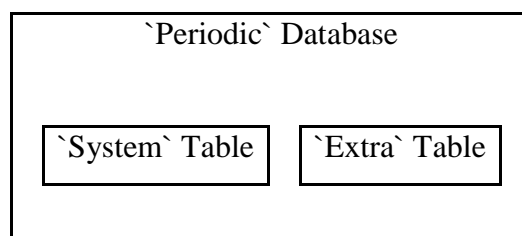
For every element there are presented the information and the values of important properties as general information (discovery, appearance, source, uses, and biological role), physical information (atomic number, relative atomic mass, melting and boiling point, density, ground state electron configuration, electron affinity), information about isotopes (nuclide, atomic mass, natural abundance, and half-life), ionisation energies. Other information (enthalpy of fusion, enthalpy of vaporisation) and oxidation states are also available.

The aim of the presented educational application is to learn the user to make SQL phrases in order to query a pure chemical database (periodic system). The advantages of SQL queries are obvious: fast searching and retrieval of chemical information.<sup>11,12</sup>

### Database Design

A database called `Periodic` with a set of two tables was created (see Figure 1). In order to include great information, the database is design to manage all elements with all properties.

The `System` table contains 23 columns, the `Number` column is the primary key for the table and his value is the Z number of the element. The elements information is stored in rows (the `System` table contains 109 rows), with one row for every element. Every one of the columns contains an element property such as Mass, Melting, Boiling. The `Extra` table contains 23 rows, and every row contains the measurement unit for a property stored in corresponding column from `System` table.



**Figure 1.** `Periodic` database structure.

In order to create a system for periodic system management, a set of programs was created. The web interface was designed for user and administrator use. For special operations on `Periodic` database, the phpMyAdmin program was

enough. A picture of `System` table from phpMyAdmin interface is depicted in Figure 2.

	Field	Type
<input type="checkbox"/>	Discovery	tinytext
<input type="checkbox"/>	Appearance	tinytext
<input type="checkbox"/>	Source	text
<input type="checkbox"/>	Uses	text
<input type="checkbox"/>	Biological	text
<input type="checkbox"/>	General	text
<input type="checkbox"/>	Number	tinyint(3)
<input type="checkbox"/>	Mass	float
<input type="checkbox"/>	Melting	float
<input type="checkbox"/>	Boiling	float
<input type="checkbox"/>	Density	float
<input type="checkbox"/>	Configuration	varchar(65)
<input type="checkbox"/>	Affinity	float
<input type="checkbox"/>	nuclide	varchar(200)
<input type="checkbox"/>	Atomic	varchar(65)
<input type="checkbox"/>	abundance	varchar(90)
<input type="checkbox"/>	life	varchar(100)
<input type="checkbox"/>	Ionisation	text
<input type="checkbox"/>	Fusion	float
<input type="checkbox"/>	Vaporisation	float
<input type="checkbox"/>	main	varchar(200)
<input type="checkbox"/>	others	varchar(165)
<input type="checkbox"/>	Bonds	text
<input type="checkbox"/>	Symbol	char(3)

**Figure 2.** `System` table structure (phpMyAdmin interface).

An user of the periodic system can make queries on `Periodic` database and this task is implemented in our programs using SQL *SELECT* phrases.

An administrator of the periodic system can make updates on `Periodic` database and this task is implemented in our programs using SQL *UPDATE* phrases. The web interface for administration is password protected and our programs check the password before the beginning of the system administration.

In addition, at the creation time of the database, a set of SQL *INSERT* phrases was also used through a password-protected interface.

The *index.php* program (located in *periodic\_system* directory) serves as main entry interface in periodic system querying.

In Figure 3 is depicted our user interface.

The *Query* button constructs the SQL query based on row and column selections, and imposed filters. After the query constructing, the query is displayed together with the retrieved information from MySQL database server querying.

The screenshot shows a web browser window with the address `http://vl.academicdirect.ro/periodic_system/`. The main content area is divided into several sections:

- Select:** A button to initiate a query.
- Elements:** A dropdown menu with options: Li, Be, B, C, N, O.
- Properties:** A dropdown menu with options: Discovery, Appearance, Source, Uses, Biological, General.
- Filter:** A table of input fields for filtering results:
 

Discovery:	LIKE '%Cavendish%'
Appearance:	
Source:	
Uses:	
Biological:	
General:	
Number:	
Mass:	
- Properties Table:** A table of input fields for various chemical properties:
 

Melting:		life:	
Boiling:		Ionisation:	
Density:		Fusion:	
Configuration:		Vaporisation:	
Affinity:		main:	
nuclide:		others:	
Atomic:		Bonds:	
abundance:		Symbol:	

At the bottom, there is a note: "Use LIKE for string comparisons; Use '%' for an unknown string sequence; Use ' as string delimiter". Below the note are two buttons: "Query" and "Admin".

**Figure 3.** User interface (define selections and filters and make query).

The user has at least two opportunities here: to study the construction of SQL SELECT phrase in order to learn the SQL terminology or to refine his selection to rich more specific information and to obtain the desired chemical information.

The query that is produced for the selections from Figure 3 looks like:

```
SELECT `Number`, `Discovery`, `Appearance`, `Source`, `Uses`, `Biological`,
      `Symbol`
FROM `System` WHERE 1 AND (0 OR `Number` = '1' OR `Number` = '2' OR
`Number` = '3' OR `Number` = '4' OR `Number` = '5' OR `Number` = '6' OR
`Number` = '7' OR `Number` = '8') AND (`Discovery` LIKE '%Cavendish%')
```

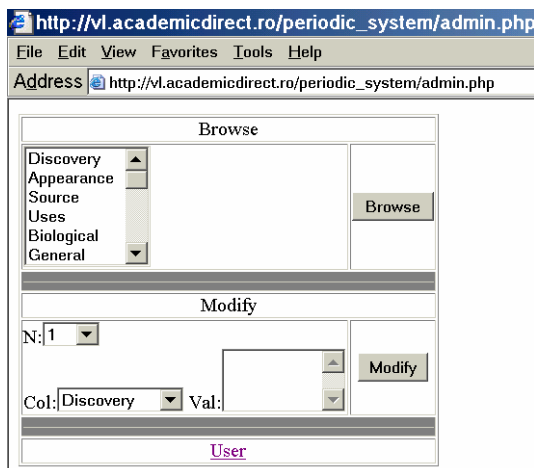
The resulted information is displayed as hypertext with every property (column from `system` table), with line break separator. For better viewing, the elements are separated with an horizontal line.

The management of database is assured through *admin.php* program. As we say previously, the admin interface is password protected (Figure 4).

The screenshot shows a small dialog box titled "Explorer User Prompt" with a close button (X). Inside the dialog, there is a "Script Prompt" label, an "Enter password:" label, and a text input field. At the bottom right, there are "OK" and "Cancel" buttons.

**Figure 4.** Entry point in admin interface.

A wrong password produces a new appearance (in an infinite cycle) of the explorer user prompt dialog box. The correct password entry produces the appearance of admin interface (Figure 5).



**Figure 5.** Admin interface (*admin.php* program).

The admin interface let us to look at a specific property through the `System` table (*Browse* section) and to change a property of an element (*Modify* section).

### Periodic System Database SQL SELECT Examples

The problems which appear in the use of periodic system for didactic aim are the complexity of properties, which characterize every element and the great number of elements (109).

For this, for all elements, the control key is represented by the specific properties. At the beginning of the periodic system study, it must display a list with all elements and their properties stored into the database. To do this, is enough:

*SELECT \* FROM `System` WHERE 1*

This SELECT phrase is obtained from user interface without any element or property express selection (only pressing of Query button from user interface).

An easy task is to select the `General` property from the `System` table, selecting the General option from the Select/Properties list (see Figure 2):

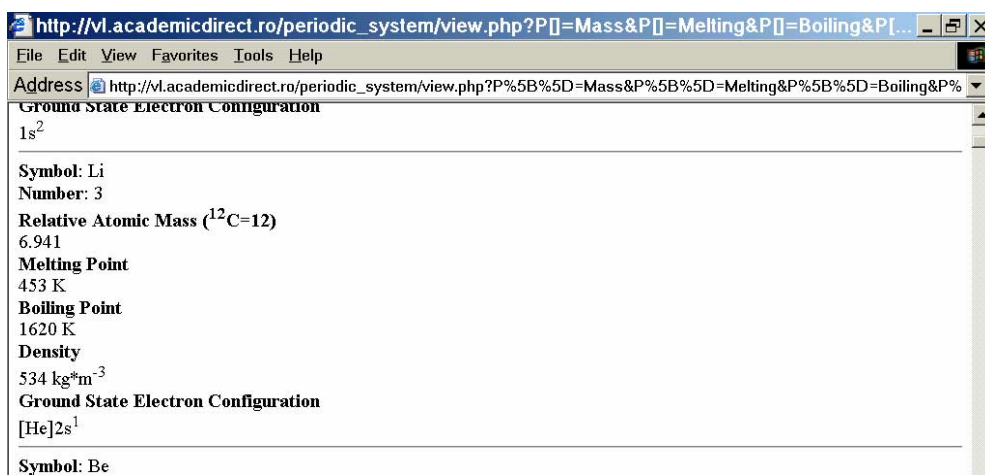
*SELECT `Number`, `General`, `Symbol` FROM `System` WHERE 1*

This SELECT phrase shows the general properties for all chemical elements.

A selection like:

```
SELECT `Number`, `Mass`, `Melting`, `Boiling`, `Density`, `Configuration`,
      `Symbol`
FROM `System` WHERE 1 AND (0 OR `Number` = '1' OR `Number` = '2' OR
`Number` = '3' OR `Number` = '4' OR `Number` = '5' OR `Number` = '6' OR
`Number` = '7' OR `Number` = '8')
```

produces a result such as we depicted in Figure 6.



**Figure 6.** Selection of properties from `System` table.

These SQL SELECT phrases allow us to access the melting and boiling point of selected elements (H, He, Li, Be, B, C, N, O).

Note that the elements and the properties are not necessary to be selected consecutively (see elements list from Figure 7).

Before the beginning the presentation of key isotopes, a list with nuclide, atomic mass, abundance, and half-life, ordered by element number and by name of the element must be generated. The selection is:

```
SELECT `nuclide`, `Atomic`, `abundance`, `life`, `Symbol` FROM `System`
```

and it will produce the expected result. Deselecting all elements makes the including of all elements.



	Select	Elements Be B C N O F	Properties Affinity nuclide Atomic abundance life Ionisation	Order Number	
Filter	Discovery:		Melting:		life:
	Appearance:		Boiling:		Ionisation:
	Source:		Density:		Fusion:
	Uses:		Configuration:		Vaporisation:
	Biological:		Affinity:		main:
General:		nuclide:		others:	
Number:		Atomic:		Bonds:	
Mass:		abundance:		Symbol:	
Use LIKE for string comparisons; Use '%' for an unknown string sequence; Use ' as string delimiter					
		Query	<a href="#">Admin</a>		

**Figure 7.** Selection of isotopes from periodic system MySQL database.

A lot of specific structured information is now accessible and we present a set of SQL examples:

- Other properties of elements, a list with ionisation energies, enthalpy of fusion, enthalpy of vaporisation, oxidation states, ordered by element number and by symbol of the element:

```
SELECT `Ionisation`, `Fusion`, `Vaporisation`, `Main`, `Others`, `Bonds`,
      `Symbol` FROM `System` ORDER BY `Number`, `Symbol`
```

- Select the elements that present the highest ionisation energy for the first electron from the atom:

```
SELECT `Number`, `Ionisation`, `Symbol` FROM `System` WHERE 1 AND (0 OR
  `Number` = '10' OR `Number` = '18' OR `Number` = '36' OR `Number` = '54'
  OR `Number` = '86') ORDER BY `Ionisation`
```

- Establish the group and the period of Ca, based on its electronic configuration:
- ```
SELECT `Number`, `Configuration`, `Symbol` FROM `System` WHERE 1 AND (0
  OR `Number` = '20') ORDER BY `Configuration`
```

- Arrange the elements from the seventh principal group in the increasing order of electron affinity:

```
SELECT `Number`, `Affinity`, `Symbol` FROM `System` WHERE 1 AND (0 OR
  `Number` = '9' OR `Number` = '17' OR `Number` = '35' OR `Number` = '53')
  ORDER BY `Affinity`
```

- Arrange the elements from periodic system in the increasing order of melting point:

*SELECT `Number`, `Melting`, `Symbol` FROM `System` WHERE 1 ORDER BY  
`Melting`*

- In order to find the heaviest element from periodic system, arrange the elements in the increasing order of density:

*SELECT `Number`, `Density`, `Symbol` FROM `System` WHERE 1 ORDER BY  
`Density`*

- Establish the electronic configuration of elements from the fourth period:

*SELECT `Number`, `Configuration`, `Symbol` FROM `System` WHERE 1 AND  
(`Configuration` LIKE '[Ar]%)' ORDER BY `Number`*

- In order to establish the number of principal group for the elements from the first period, it is necessary the electronic configuration. Display configuration:

*SELECT `Number`, `Configuration`, `Symbol` FROM `System` WHERE 1 AND (0  
OR `Number` = '3' OR `Number` = '4' OR `Number` = '5' OR `Number` = '6'  
OR `Number` = '7' OR `Number` = '8' OR `Number` = '9' OR `Number` = '10')  
ORDER BY `Configuration`*

- In order to have information about isotopes, it is necessary to know the nuclide and the values of atomic mass, natural abundance and half-life of isotopes. Retrieve this information separately for four elements:

*SELECT `Number`, `nuclide`, `Symbol` FROM `System` WHERE 1 AND (0 OR  
`Number` = '7' OR `Number` = '15' OR `Number` = '33' OR `Number` = '51'  
OR `Number` = '83') ORDER BY `nuclide`*

*SELECT `Number`, `Atomic`, `Symbol` FROM `System` WHERE 1 AND (0 OR  
`Number` = '7' OR `Number` = '15' OR `Number` = '33' OR `Number` = '51'  
OR `Number` = '83') ORDER BY `Atomic`*

*SELECT `Number`, `abundance`, `Symbol` FROM `System` WHERE 1 AND (0  
OR `Number` = '7' OR `Number` = '15' OR `Number` = '33' OR `Number` =  
'51' OR `Number` = '83') ORDER BY `abundance`*

*SELECT `Number`, `life`, `Symbol` FROM `System` WHERE 1 AND (0 OR  
`Number` = '7' OR `Number` = '15' OR `Number` = '33' OR `Number` = '51'  
OR `Number` = '83') ORDER BY `life`*

- Order and display the first four elements from periodic system, by values of ionisation energy:

```
SELECT `Number`, `Ionisation`, `Symbol` FROM `System` WHERE 1 AND (0 OR  
`Number` = '1' OR `Number` = '2' OR `Number` = '3' OR `Number` = '4')  
ORDER BY `Ionisation`
```

- List the elements from the fourth period based on electron affinity order:

```
SELECT `Number`, `Affinity`, `Symbol` FROM `System` WHERE 1 AND  
(`Configuration` LIKE '[Ar]%)' ORDER BY `Affinity`
```

- Order the periodic elements with two electrons in the last `s` substrate based on the enthalpy of vaporisation:

```
SELECT `Number`, `Configuration`, `Affinity`, `Vaporisation`, `others`, `Symbol`  
FROM `System` WHERE 1 AND (`Configuration` LIKE '%s<sup>2</sup>')  
ORDER BY `Vaporisation`
```

## 2. RESULTS AND DISCUSSION

In order to obtain the required lists, all that we have to do is to submit queries to the SQL server (in our case MySQL) and to fetch the results. One solution is to create a drop down list with all SQL phrases for selection and more, for classification based on property element to create three input boxes for start value.

Because the program was created and completed without applying the real situation at student course, before the designed interface is adaptive one that allow user to construct SQL phrases. Note that is not a perfect one, because do not consider the classification of elements based on the chemical character (metals and nemetals and the metals can be classified in different types).

First list is field list a header message follow, then filter list, then ordering criterions, a footer message, a drop down list to draw supplementary columns in resulted table for information, which is not available for all elements, like discovery, biological role, and other information. Both filter and order drop down lists contain all fields from 'elements' table and was retrieved using another SQL phrase:

***SHOW COLUMNS FROM 'elements' and SHOW TABLES FROM 'System'***

**Final reports**

The application was tested with students from Departments of Materials Science, and Automation and Computer Science from Technical University of Cluj-Napoca.

On the labs, the students must read the following questions, and to answer based on the information presented above:

- Select the elements, which have the highest ionisation energies;
- Establish the group and the period of one element, based on its electronic configuration;
- Establish the valence towards hydrogen for the elements from second principal group;
- Arrange the elements in the increased order of electron affinity;
- Establish the chemical character of elements in accordance with the electronic configuration and the position in the periodic system;
- Select the elements with valence  $-1$  and  $+2$  and form the corresponding compounds;
- Arrange the elements from the first principal group in the increasing order of the base character of metallic hydroxides;
- Arrange the elements from the second period in the increasing order of the acidity character of binary combinations of hydrogen with the corresponding elements.

The application use demonstrates that both categories of students perform successfully the desired queries.

All queries are performed by 68 from 130 for the students from Department of Materials Science, which demonstrate full assimilation of SQL SELECT phrase constructing and it's chemical applications for 52%. The students

from Department of Automation and Computer Science based on his database knowledge perform in a percent of 63% all desired queries (55 from 88).

Anyway, the program testing demonstrates that the SQL SELECT concept can be assimilated and successfully used by users, which haven't strong computer science knowledge in a percent approximately equal with the users which posses this type of knowledge.

In order to compare statistically these results, we can use the t Test:

$$t_{exp} = \frac{m_1 - m_2}{\sqrt{\frac{s_1^2}{n_1} - \frac{s_2^2}{n_2}}} \quad (1)$$

Supposing that the number of students which answer correctly at all questions is a binomial distribution, the t Test parameters are calculated as below:

$m_1 = 68/130$  (mean value from first population);

$m_2 = 55/88$  (mean value from second population);

$n_1 = 130$  (size of first population);

$n_2 = 88$  (size of second population);

$s_1^2 = n_1 \cdot m_1 \cdot (1 - m_1)$  (variance for first population);

$s_2^2 = n_2 \cdot m_2 \cdot (1 - m_2)$  (variance for second population).

The  $t_{exp}$  value is 0.83. The number of degrees of freedom is  $n = n_1 + n_2 - 2 = 216$ .

The theoretical value of t, for a 95% probability and n degrees of freedom is  $t_{the} = 1.97$ .

Because  $t_{exp} = 0.83 < 1.97$  for 95% probability, we can say that the percent of students from first population which got all answers correctly is not significantly different from the percent of students from second population which got all answers correctly with a probability of 95%.

### 3. CONCLUSIONS

The application hit two major points: learning about elements and learning about SQL phrases construction. The information presented in this periodic system is complex and can be used to answer at different questions related to the structure, chemical character and the possibility to combine different elements.

The presented application for periodic system used hardly the performances of SQL kernel from MySQL database server for multiple filters, multiple sorting, and specific fetching of the records. The PHP implementation of the program shortens the implementation time and makes as easy to run and update applications.

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