



SQL Application for Periodic System of Elements

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Abstract

The paper presents SQL power of periodic system using for didactic aim. The article is based on a PHP application developed to present a periodic system in a form, which can be used for answer at different questions, which can be asked related at the structure of elements. There are presented all queries that are needed to be use for classification of elements after different properties, the database, and user interface design.

Keywords

Client-server application, e-learning, SQL application

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 [1,2]. 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 [3].

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 [4].

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 [4].

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 [3].

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 [5].

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 [6,7].

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 which explain the periodicity of some properties function of atomic number Z (atomic and ionic ray, ionization 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 [8].

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 [9,10].

In this context, the periodic system that was our main source of documentation can be reached at the address: <http://www.chemsoc.org/viselements/pages/pertable fla.htm>.

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), ionization energies. Other information (enthalpy of fusion, enthalpy of vaporization) and oxidation states are also available. The aim of this study was to use SQL power of periodic system for didactic aim. There are presented all queries that are needed to be use for classification of elements after different properties in order to obtain information about the physical and chemical properties as well as about the capacity to combine the different elements to obtain different compounds.

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

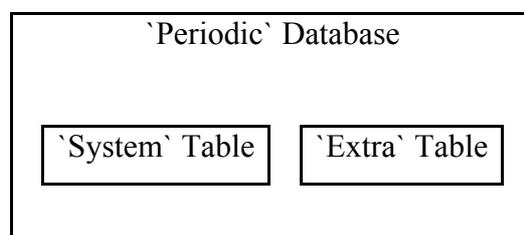


Fig. 1. 'Periodic' database structure

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"/>	<u>Number</u>	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)

Fig. 2. `System` table structure

A 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 used also through a password-protected interface.

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

In fig. 3 are depicted our user interface:

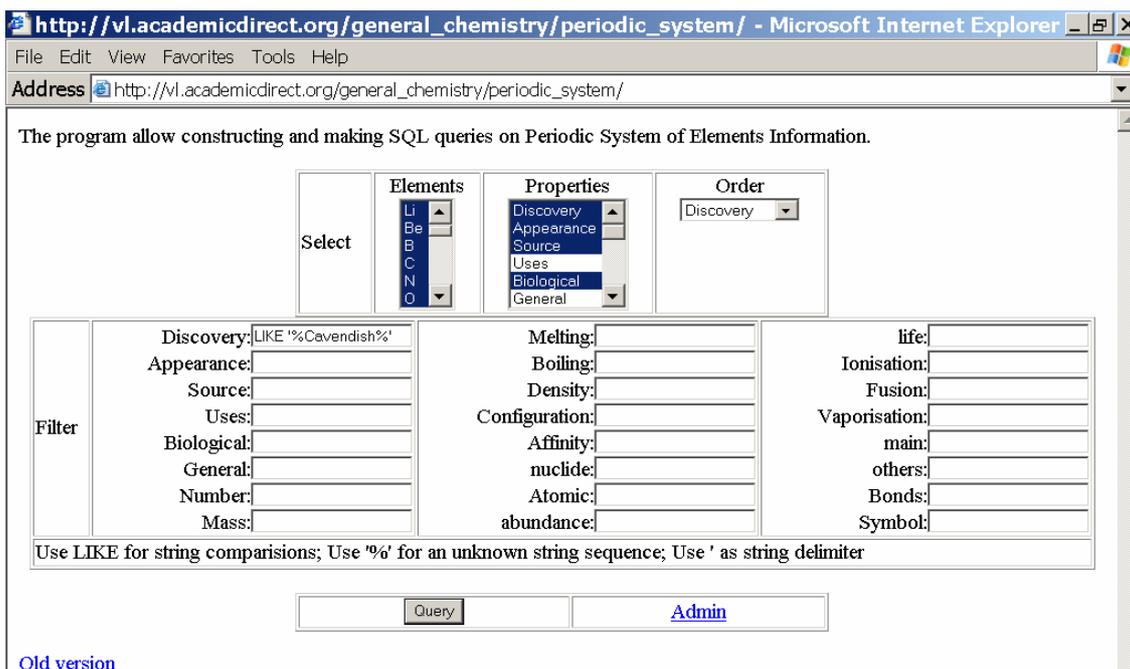


Fig. 3. User interface (define selection and filters and make query)

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 queries are processed by the *view.php* program, are also displayed in front of results page, and is followed by the query results. Independently by the user choice are supplementary selected two columns: `Number` and `Symbol` as can be seen in the previous SELECT phrase.

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 a horizontal line.

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

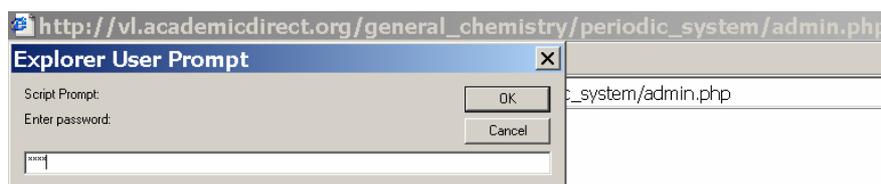


Fig. 4. Entry point in admin interface

A wrong password it produce the appearance again of the explorer user prompt dialog box. The correct password entry produces the appearance of admin interface (fig. 5).

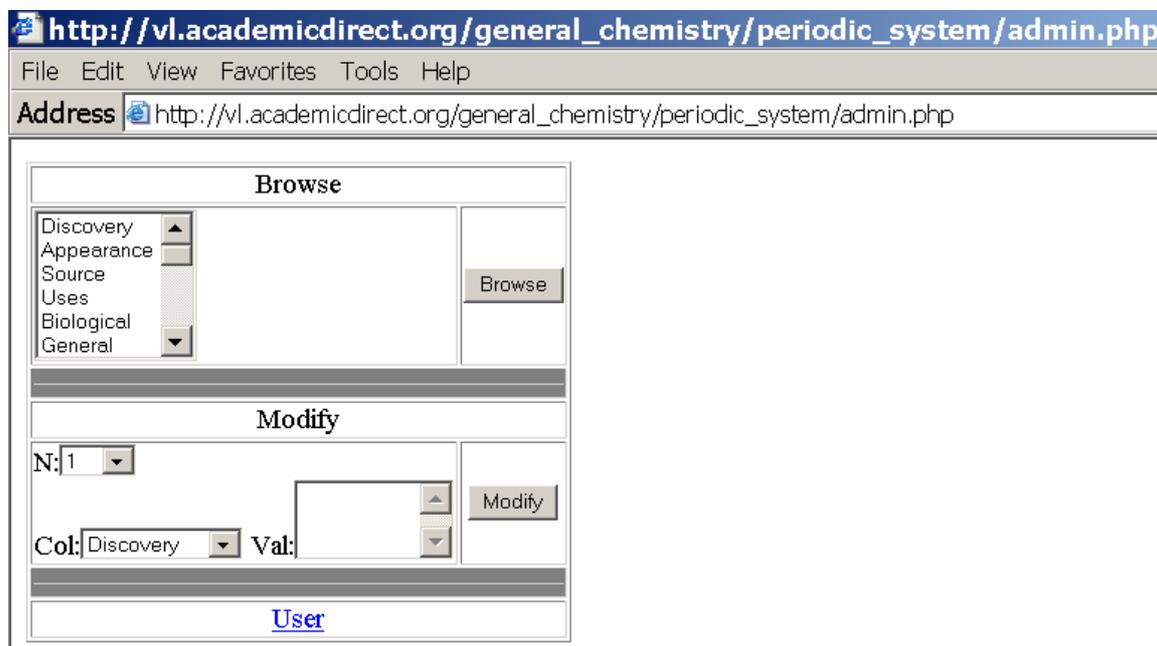


Fig. 5. Admin interface (*admin.php* program)

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).

The program that is responsible for updates are *modify.php* and the program that is responsible for 'System' table browsing is *browse.php*.

Problems and Solutions

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. To do this, a SELECT command is enough:

*SELECT * FROM `System` WHERE 1*

This is obtained from user interface without any element or property express selection.

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):

Fig. 6. Selection making

The following table presents a set of examples of program using:

Table 1. Information about the periodical properties of the elements

Other properties of elements, a list with ionization energies, enthalpy of fusion, enthalpy of vaporization, oxidation states, ordered by element number and by symbol of the element	<i>SELECT `Ionisation`, `Fusion`, `Vaporisation`, `Main`, `Others`, `Bonds`, `Symbol` FROM `System` ORDER BY `Number`, `Symbol`</i>
Select the elements that present the highest ionization energy for the first electron from the atom	<i>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`</i>
Establish the group and the period of Ca, based on its electronic configuration	<i>SELECT `Number`, `Configuration`, `Symbol` FROM `System` WHERE 1 AND (0 OR `Number` = '20') ORDER BY `Configuration`</i>
Arrange the elements from the seventh principal group in the increasing order of electron affinity	<i>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`</i>
Arrange the elements from periodic system in the increasing order of melting point	<i>SELECT `Number`, `Melting`, `Symbol` FROM `System` WHERE 1 ORDER BY `Melting`</i>
In order to find the heaviest element from periodic system, arrange the elements in the increasing order of density	<i>SELECT `Number`, `Density`, `Symbol` FROM `System` WHERE 1 ORDER BY `Density`</i>

Table 1. Information about the periodical properties of the elements

Establish based on the electronic properties the period of Cu	<i>SELECT `Number`, `General`, `Symbol` FROM `System` WHERE 1 AND (0 OR `Number` = '29') ORDER BY `Configuration`</i>
In order to establish the number of principal group for the elements from the first period, it is necessary the electronic configuration. Display configuration	<i>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`</i>
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	<i>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` <i>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` <i>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` <i>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`</i></i></i></i>
Ordering the periodic elements based on the greater ionization energy	<i>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`</i>
The periodic elements based on affinity order by element mass	<i>SELECT `Number`, `Affinity`, `Symbol` FROM `System` WHERE 1 AND (0 OR `Number` = '1' OR ...) ORDER BY `Mass`</i>
The periodic elements based on the bonds order by on others	<i>SELECT `Number`, `Bonds`, `Symbol` FROM `System` WHERE 1 AND (0 OR `Number` = '2' OR `Number` = '3' OR...) ORDER BY `others`</i>

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 students must read the questions, which can be ask and try to answer based on the information presented above.

- Select the elements, which have the highest ionization 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;

Conclusions

The application hit two major points: learning about elements and learning about SQL phrases construction. The information presented in this periodic system are 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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