ONLINE SIMULATION OF CLASSICAL INORGANIC ANALYSIS - INTERACTIVE, SELF-INSTRUCTING SIMULATIONS GIVE MORE LAB-TIME.*

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Laboratory exercises, investigations, and experiments are invariably included in university chemistry teaching. The learning of empirical facts, chemical procedures and methods in chemistry depends heavily on the experience, which may be obtained from such teaching activities [1]. Experimental work in teaching is, however, both expensive and time consuming, and should therefor effectively benefit from the allotted student time, money, and staff time. If the instructions are too ambitious regarding what the students can manage to do and are overloaded with information [2,3] it may result in the students simply following a recipe, which is probably not effective relative to the efforts. The use of pre labs and post labs may be a way to enhance the effectiveness of the work in the laboratory [4,5]. If the purpose is not that the students become perfectly trained on the manipulative side of the procedure (and in university programmes it often isn't), but rather to give them experience with chemicals and methods, a computer-based laboratory simulation may function as a cheap and fast extension of student lab time. Virtual investigations seem to be a promising kind of tool [6,7,8] for several reasons and this has lead to the development of self-instructing, interactive PC-based learning resources closely related to an actual, running course in introductory inorganic chemistry [8]. Such a development is rather time consuming, but since the first experience was positive [8] it was considered worthwhile to develop the idea further for that course. This development of further resources to simulate a laboratory investigation will be described.

Why use Classical inorganic analysis in laboratory assignments?

Classical qualitative and quantitative analysis of relatively simple soluble salts or co-ordination compounds with inorganic ligands only, has for many years been part of introductory inorganic chemistry in spite of the fact that professional chemical analysis currently is far more advanced than chemical separation and identification reactions in test tubes and volumetric analysis. The reason to keep and use such an kind of old fashioned element in an introductory inorganic chemistry course is first of all that this type of simple and classical procedures has a great learning potential; it offers a practical setting which can give a lot of experience with chemical reactions.

> **Box**: **Example of a written problem:**
> A greenish mineral (**Atakamite**) dissolves in 0.4 M hydrochloric acid with a green colour (A), in conc. hydrochloric acid with a yellow colour and in nitric acid it turns blue (C).
> Solution A treated hot with thioacetamide gave a black precipitate,which treated with nitric acid gave a yellow precipitate (D) and a blue solution (E). E gives with conc. ammonia a more intense blue solution, which decolourise with potassium cyanide. This colourless solution doesn't precipitate with thioacetamide.
> When excess of silver nitrate is added to solution C a white precipitate is formed, which is soluble in ammonium carbonate (1 M). The subsequent addition of potassium bromide gives an off-white precipitate.
> 128.2 mg of the mineral in 50.0ml 0.100 M nitric acid was titrated (Ag-electrode, 12.0 ml 0.050 M silver nitrate). After the precipitate had been removed, the filtrate was titrated (glass-electrode instead, 10.00 ml 0.200 M sodium hydroxide).
> 138.8 mg of the mineral in 0.4 M hydrochloric acid was neutralised and the addition of excess potassium iodide resulted in the formation of a brown slurry. It was titrated with 13.0 ml 0.100 M thiosulfate (starch as indicator: bluish to white slurry). Determine a formula of the mineral.

Our introductory inorganic chemistry course, mainly for biology students, include a 20 hours laboratory assignment where simple soluble solid inorganic compounds and minerals, containing common s-, d- and p-block metal ions together with simple p-block anions and/or ammonium/ammonia are identified within a classical analysis scheme. The quantification of the compounds is not part of this limited laboratory investigation, but certainly of the "dry" part of the course. The students seem to accept this setting and some even enjoy the "game" of finding the identity of "unknowns".

To optimise the outcome of the laboratory assignments it should be supported by other activities. Using written problems about the identification of fairly simple, stoichiometric compounds (see Box for an example) is one way of serving the purpose. The problems use the same language as in the laboratory manual, where observations and procedures are described, not explained, thus being a tool for practicing the interpretation of observations and fir reminding the students of what happens in the laboratory. These two types of resources - the laboratory assignment and the written problems reinforce each other. The third type of teaching and learning resource is the simulation of laboratory assignments.

Simulations are supporting tools for giving more chemical experience.
A new interactive laboratory simulation for that purpose was developed, and the procedures in this electronic simulation follow the laboratory manual, which should be in mind (and/or at hand) when working with the simulation. The students are thus offered three different, but closely related learning resources to reinforce each other: the laboratory assignment, the computer simulation of it, and written problems involving the same macroscopic description of the chemistry to be solved by the paper-and-pencil method. The laboratory simulation programme was designed for use on a standard web-browser platform. Fig.1 illustrates its simple appearance, and the lay-out was deliberately chosen to be very close to the previously described simulation programme [8] for another of the assignments of the same course.
Fig. 1 may also illustrate the type of interactivity. After the computer have loaded a randomly chosen specific "unknown" (activate *Get an "unknown"* in the blue left-side menu), which in this case is presented as a pile of blue crystals on a watch glass, different introductory investigations may be done in some order. The flame colour of the solid (activate: *Heating the sample*) may give an indication of the presence of a metal ion, which changes the colour of a gas flame. Among the "Tables", one deals with such metals and their respective flame colours. Next the solubility properties of the sample are tested. In fig. 1 it is seen, that if you try to dissolve the

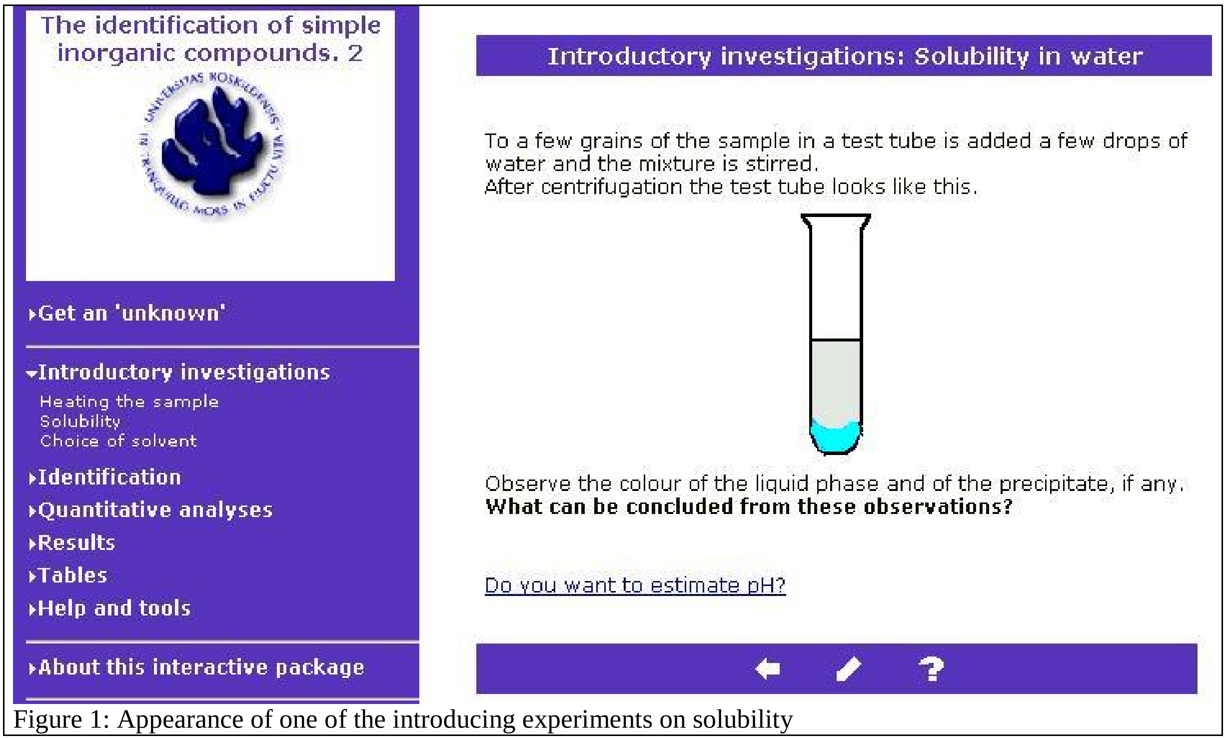

Figure 1: Appearance of one of the introducing experiments on solubility

blue crystals in water the result is a precipitate which is **light** blue (a colour change occurs!). The programme asks the user to think of what could be concluded (that the composition of the "unknown" is probably different from the precipitate obtained).

Further the test of pH may give some information and a click on the hypertext Do you want to estimate pH? in fig. 1 leads you to a new window with a bluish green strip of pH-paper and the usual scale of universal indicator paper; further you are asked to submit how you interpret the colour of the strip (that pH is around 9) and the response will support your conclusion and urge you to consider what that could indicate about the "unknown"; furthermore hypertexts to tables of acidity properties of some components are given. Other solvents offered are dilute hydrochloric acid, dilute nitric acid, aqua regia and sodium hydroxide. With this sample the solution turns light blue in nitric acid and green in dilute hydrochloric acid. In 0.1 M sodium hydroxide a light blue precipitate appears. These observations may give you some clues to what the colours reflect. (cf. also Box above dealing with the mineral Atakamite).
There is a blue bar at the bottom of the window. The back-arrow icon on the left takes you back to the preceding window, and the question mark icon on the right gives you some relevant information which may refer to a table or to "Help and tools" or give other specific information in a separate window. The comment icon in the middle of the blue bar gives you an opportunity to store a conclusion or a suggestion of yours under

"Results". If you click the comment icon, the browser's dialogue box appears as in fig. 2 and you may write and store a comment.
Fig. 2 shows the window which presents the result of trying to dissolve the "unknown" in concentrated hydrochloric acid. The many blue or bluish colours of solids and solutions and the yellow colour in concentrated hydrochloric acid seen so far may lead to a possible interpretation (is it the yellow tetrachlorocuprate in solution?). This suggestion could be entered into the browser's dialogue box, showing up after a click on the comment icon. In fig. 2 it is also seen how the dialogue box looks like, when a comment have been filled in. Activation of the OK button stores the comment and removes the dialogue box.

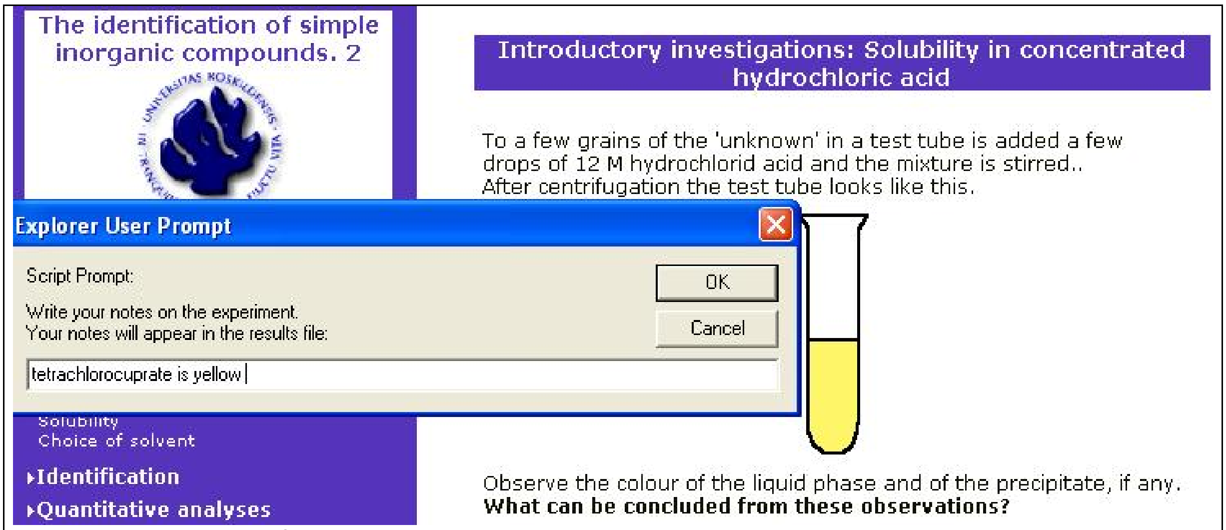

Figure 2: The response of trying to dissolve the "unknown" in concentrated hydrochloric acid.

If you skip some of the introductory investigations and proceed to some other available test the programme rejects to let you perform the test before having completed the introductory investigations. Having done so, you are prompted to go to the "Identification" in the menu.

The identification follows the systematic procedure in the lab manual. Now it is obvious that when the sample is soluble in hydrochloric acid, there is no need to test for insoluble chlorides. With this "unknown" a black sulphide precipitates in 0.4 M hydrochloric acid and this sulphide doesn't dissolve with an excess of sulphide/disulphide. With the present procedure and limited number of possible metal ions in the "unknown" this means copper, which is confirmed by the results of the next steps of the systematic procedure. If we look for barium and strontium the result of the test in fig. 3 suggests that these ions are absent. The next step in the classical qualitative analysis procedure is the "Alkaline oxidation", and if you choose that by entering a dot in the appropriate circle the message "Yes, this is where you are in the systematic procedure. Please proceed." appears. Clicking "Alkaline oxidation" in the left blue menu, a new window shows no precipitate as a result of heating the solution of fig. 3 with an excess of sodium carbonate, a little sodium hydroxide, and sodium peroxide (these details also appear in the window). The following systematic procedure does not identify any other component. Since copper is the only metal ion identified in this "unknown" some other components (ligands and anions) should be identified also (in this case ammonia/ammonium and chloride) and you go on to the "Quantitative analyses".

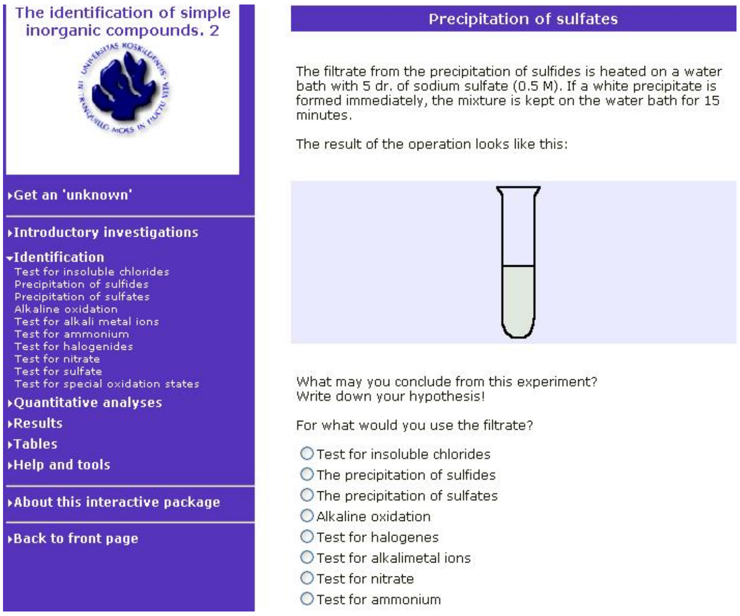

Figure 3: One of the first steps in the systematic procedure of a classical qualitative analysis scheme

Available methods are Atomic Absorption Spectrometry (metals), Flame Photometry (s-block-metals), Kjeldahl analysis (ammonia/ammonium, nitrate), potentiometric determination of halogenides, and gravimetric determination of sulphate.
The simulation programme asks you to select a method - and when you have - to calculate the amount of the sample to be weighed out in order to get a reliable result relative to the performance of the actual method; and as a part of the interactivity the entered results of the calculation is further rejected or accepted. When a calculated amount of "unknown" is accepted, the computer calculates and gives you raw data which would have been obtained from a correctly performed quantitative procedure. You are then asked to calculate a relative molar mass with respect to the analysed component. Your result is again "controlled". When this procedure has been performed (and the results are accepted) for all the components, the computer asks you to forward a formula for the "unknown" which fits the results. Here again a correct result is accepted while an error results in a (helpful) response.

Are such interactive simulation programmes useful?

The students actually like to work with the simulation programme. When they enter the programme for the first time they use more than one hour to complete an identification of an "unknown", while the real thing would have taken up to 10 hours in the lab. It is an important point that they work in pairs because it gives the students the opportunity to formulate in their own words their hypotheses and perhaps some immature views and to discuss it over, while approaching the solution. We think it is worthwhile asking the students to spend their time in this way in relation to the laboratory assignments. It is a third resource to get through the procedures in the laboratory manuals, which are very often overloaded relative to the time spent on them. Our lab manual on this very assignment is a mixture of textbook-notes with systematic descriptions of simple chemistry and recipes of identification and quantification procedures; it is more than 50 pages. It appears that this type of post-lab [4,5] (or rather "in-between-lab" [8]) is a way to get the students read and try to memorise (and as a result: remember) some chemistry and procedures from the laboratory manual. The programme thus provides the students with the opportunity to do (virtual) experiments (to use different laboratory procedures and investigate different substances) outside the laboratory at the time, speed, and place chosen by the students themselves. The point is that if a certain amount of knowledge-by heart of empirical facts and procedures is present in the students' minds the understanding of underlying chemical principles and models could easier be taken in (internalised). This facilitates the translation between observation and its interpretation which again makes it possible to use the chemistry as a tool and to think as a chemist to a certain extent.
In conclusion it is suggested that this type of resource is a valuable supplement to laboratory manuals and written "problems" so that students get more learning and experience out of the laboratory assignments, which are expensive with respect to time and other resources. With present days learning style of many freshman students who want to get to their immediate interest right away - it is essential to offer a variety of entrances into the learning of chemistry. This type of teaching and learning resource apparently does.

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