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DESIGNING LABORATORY ENVIRONMENT AND EXPERIMENTS FOR SOME DISCIPLINES CORRELATED WITH STRUCTURE, POLLUTANTS TOXICITY AND MOLECULAR INTERACTIONS STUDY (I)

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abstract: In this paper are exposed conceptions considered important for the new design of laboratory environment and experiments for two compulsory disciplines included in the first cycle of the Environmental Chemistry specialization of the Faculty of Chemistry. This action is claimed by recent curricula updates and changes in accord with the Bologna declaration and by some redistribution of space assigned to Physical Chemistry Department.

keywords: design of laboratory environment and experiments, compulsory disciplines, safety requirements, developing students abilities.

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1. Introduction

The Faculty of Chemistry from Bucharest University is now an institution of higher education of indisputable prestige, which operated in the last years more changes in curricula in accord with stipulations of Bologna declaration but the number of students which enters in each year at our faculty is decreasing and the number of the school interruptions is increasing. If the first index can be due to multiple *external causes* (as decreasing interest of young generation for difficult science studies in comparison with the humanistic ones, decreasing importance accorded to chemistry in high school, decreasing demographics reflected in high school population, etc) the second index can be correlated and with faculty's *internal causes*.

The faculty staff should adopt in the exposed above conditions a teaching strategy based essentially on *intuition* and *increasing complexity principles* to direct interest and attitudes of new students to the chemistry and its variety applications in the common life, to convince them that chemistry, in correlation with life sciences, permits a true understanding of the living systems.

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In this direction has became very important the design of laboratory environment and experiments because students in chemistry spend a lot of time in laboratory.

Authors of this paper are implied in the teaching of two disciplines correlated with the structure in the 1st cycle at the section of Environmental chemistry as results from Table 1.

Table 1 Structure correlated disciplines in 1st cycle.

No	Title of course	Position and character of discipline	Hours of course and laboratory/week
1	Molecular Structure	2nd year, 3rd semester, compulsory	2, 3
2	Relationships Structure-Properties-Toxicity of Industrial Pollutants (RSPT)	3rd year, 5th semester, compulsory	2, 1

In the 2nd cycle we are implied in teaching at the *Biomolecules* master course: Advanced techniques for spectral characterization. Also, we are teaching the *Molecular interactions of the pollutants with biological compounds* optional course for the 3rd year students of the same Environmental chemistry section.

For the first and second cycle of university studies at the named disciplines our team published a lot of course-books [1-4], ones in two editions. The elaborated courses for the second cycle [3,4] have a very pronounced practical character because the laboratory works for master students are included in its volume for a better illustration of the corresponding theory, in order to facilitate contact of students with the both essential learning aspects.

In view of recent changes of the curricula, in this paper we resumed conceptions which are considered important in the new design of the laboratory environment and experiments for the named in Table 1 disciplines, included both as compulsory in the first cycle.

Design and Discussion

The Laboratory of Molecular Structure for the Environmental Chemistry section is scheduled in the same space with that of the sister discipline from Chemistry section. Due to redistribution of the space, affected to the Physical Chemistry Department, the laboratory of Molecular Structure was moved from the ground floor to the second floor at the beginning of September 2008 in the room E212.

The schema of the new arrangement, designed and realized in collaboration with lecturer Dr. Sorana Ionescu and lecturer Dr. Alina Jurcă (which teach at the Chemistry section) from beginning of the new scholar year 2008/2009 is done in Fig. 1. Dimensions of the laboratory are: 7.65 m long; 5.04 m wide; 6 m high

Due to minimal space and volume of laboratory in comparison with EU norms laboratory sessions must be scheduled for a subgroup of students

The laboratory works for Molecular Structure are listed in the Table 2.

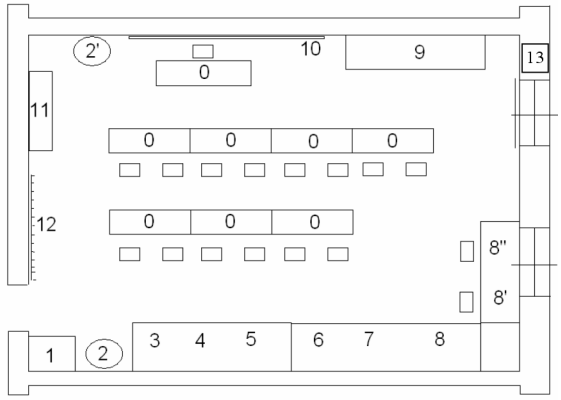

Fig. 1 *Molecular structure laboratory (experiments or apparatus):* 0-desk; 1-parachor; 2,2'-sink; 3-fluorescence; 4-UV-Vis spectrophotometer; 5-refractometer; 6-dielcometer; 7-polarimeter; 8,8''-computers; 9-stiloscope; 10-blackboard; 11-board; 12-peg;13- balance; □-chair

Table 2 Compulsory laboratory works at the discipline Molecular Structure

No	Laboratory works	Notation	Type of the students developed abilities
1	Determination of molecular refraction	RM	Practical
2	Determination of specific rotation	$[\alpha]_D^{20}$	Practical
3	Fluorescence extinction with iodine ions	F.Ex	Practical
4	Determination of dipole moment Method of diluted solutions	M	Practical
5	Determination of molar parachor	Pc	Practical
6	X-Ray spectra	X(Z)	Theoretical
7	Biomolecules RES study	RES	Theoretical
8	Electronic spectra of polyatomic molecules	UV-VIS	Theoretical
9	Isotopic effect in vibration-rotation spectra	Ieff	Theoretical-computational
10	IR spectroscopy. Characteristic frequecies	IR	Correlation capacity/Practical
11	Determination of molecular structure (I)	SM1	Capacity of correlation
12	Determination of molecular structure(II)	SM2	Theoretical Theoretical /Capacity of correlation

As can be noticed the first 5 listed works in the Table 2 develop practical abilities of student which learn the basic modes for measuring of some *macroscopic properties* (refraction index, optical rotation angle, superficial tension, intensity of fluorescence, dielectric constant) of liquid substances and solutions and its inclusion in the simple equations to calculate some *molecular properties*.

Students use very simple non-automated, but relatively new apparatus. This laboratory posses optical instruments as refractometer, polarimeter, fluorimeter or artisanal glass installation (for superficial tension measurement in dynamic regime) and dielcometer.

During execution of these experimental works the student learn to use different nomogramms useful for computation of the molar refraction, or parachor. These nomogramms are attached in the protocol of their scheduled work.

Beginning with the works 6-9 the theoretical abilities of the students are especially solicited because they receive registered diffractogramms, RES, UV-VIS or IR spectra for solid, liquid or gaseous substances. These more elaborated informations are obtained in research laboratories of the Physical Chemistry Department and are registered at more complicated, unique apparatus. The students are directed to make its decipher. Students are counseled by assistant to obtain the issued molecular properties from more complicated equations or graphic plots.

In the most complex works 10, 11, 12 student is solicited to do correlation of minimum 4 type of structural data: those resulted from knowledge of elemental composition, chemical reactivity, IR or UV-VIS spectra and RMN spectra to obtain finally structural formula of the unknown substance. The student dispose in this type of works for a series of data concerning: *infrared absorption-structure correlations*, *values of wavelengths* corresponding to π-π^* and n-π^* transitions *in UV-VIS spectra* for aldehides, ketones and conjugated dienes, *proton chemical shifts* for aromatic, olefins compounds, *proton-proton coupling constants.* These correlation tables are included in their manual [1] realized in conformity with the new curricula. The works with numbers 1, 3, 4, 6-9 in the Table 2 are common with the chemistry section, the works 2, 5, 10, 11, 12 are specifically addressed to students of the Environmental Chemistry section .

From the total of 14 laboratory scheduled sessions two (6 hours) correspond for seminar, one for colloquium (practical exam)

This laboratory posses 3 computers and software for basic quantum mechanics and molecular mechanical modeling notions which are introduced at these seminar sessions

Central part of laboratory is gifted with individual desks (forms) useful for seminar activity, for elaboration of students reports/essays

Results and progress of student is accurately registered by assistant.

The laboratory corresponding to the second analyzed discipline, abbreviated as RSPT, occupy from the autumn of 2007 year a half of space from room E205, situated at second floor in Chemistry building Blv Regina Elisabeta 4-12. The another half space is designated to very performing and costly FTIR spectroscopy and spectro-polarimetry apparatus, related with research concern of our team.

Management of this laboratory claimed additional sanitary (whetstone floor and autonomy temperature room regulatory**)** and safety precautions (a lattice work**).**

General plan of this room (10 m long, 3,3 m wide, 6 m high) is indicated in Fig. 2.

In the space assigned to discipline RSPT for which in new curricula are allocated only 14 hours of applications on semester we proposed the resolving of themes listed in the Table 3.

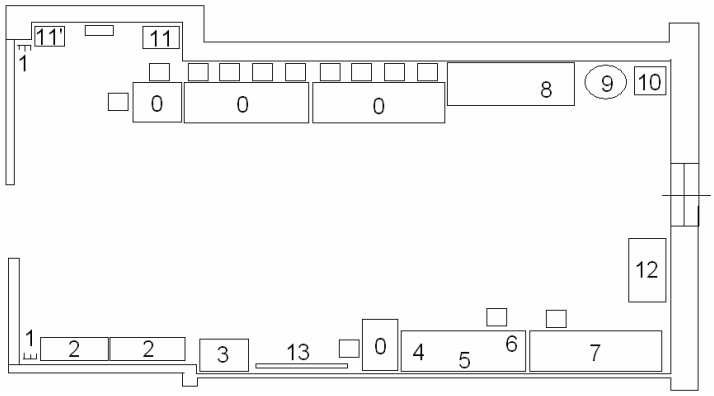

Fig. 2 *RSTP laboratory (equipments)* 0-desk; 1-peg; 2-board; 3-work table; 4-oxigenometer; 5-printer; 6-computer; 7 FTIR spectrophotometer; 8-spectropolarimer; 9-sink; 10-refrigerator; 11-bookcase; 12-IR variable temperature accessories; 13-blackboard; □-chair.

Table 3 Themes selected for discipline RSPT

No	Theme	Number of hours	Developed student abilities
1	Computation of toxic risk and monophasic toxicity from physical - chemical data	1	computational
2	Determination of respiratory capacity with Air-life spirometer	2	practical
3	Determination of concentration, partial pressure and saturation grade of O_2 in rivers waters with oxygenometer Inolab Oxylevel-2	2	practical
4	Applications of Hammett equation	2	Theoretical
5	Hansch analysis	3	Theoretical
6	Calculation of pollutants maximum admitted concentrations from physical-chemical data	2	Computational
7	Calculation of biological response from physical-chemical data	2	Computational and Theoretical

It is obvious from analysis of the Table 2 data (s. themes 4-7) that at this second analyzed discipline, placed in the third year of study, in respect of the *increasing complexity principle*, the ponder of theoretical and computational applications is significant increased (in consequence are developed these student abilities). For this reason the most space with didactic destination is occupied by a big common desk useful for students preparing their reports, or participating to different discussions, or open lessons, axed on environmental problems [6-9]. To facilitate this type of activities RSPT laboratory dispose also from a classical projector.

The practical abilities developed by the resolving of themes 2, 3, listed in the Table 3, are very special for future occupational environmentalist (which must learn to use this type of data in evaluation of the occupational toxic risk) [5,8].

Students hearing compulsory course RSPT and those preparing bachelor and master dissertations under our coordination dispose in this laboratory from a specialized books library space, where they have a free access in conditions of comfort.

On the walls of this laboratory are exposed a lot of selected posters (some purchased, some realized by us in collaboration with our students) which may be related with the both named

destinations of this space, as results from Table 4. We give titles of these posters and some specifications concerning its type and destination in the Table 4.

Table 4 Posters titles in laboratory E205 with double destination.

No	Title of poster	Type (purchased or realized)	Destination
1	Algorithm for determination of symmetry group	realized	Didactic (for 2nd cycle)
2	Classification of structural analysis methods	realized	Didactic (for 1st cycle)
3	IR spectroscopy and sampling techniques	realized	Didactic (2nd cycle)+Research
4	FTIR and Raman spectroscopy	purchased	Research
5	Fluorescence	realized	Didactic (1st cycle)
6	Sensors used in environmental research	purchased	Didactic (1st and 2nd cycle)
7	Safety instructions in laboratory work	realized	Didactic +Research
8	Molecular machinery: A Tour of the Protein Data Bank	purchased	Didactic +Research
9	Pollutants interactions with biomolecules	realized	Didactic (1st cycle)

We consider that this new designed environment of the laboratory is more attractive for our students, future specialists in environmental chemistry.

Finally, we can mention provenience of the funds for design realization of this double destination laboratory:

- costs for extension, consolidation of this room (space finished in 2003) and of the needed safety precautions (a lattice work manufactured in 2007) – was supported from University budget.
- the Vertex70 FTIR spectrometer, computer interfaced, doted with OPUS-software (Bruker-Germany)-with very high performance in research profile and the oxygenometer Inolab-Oxylevel-2 for RSPT laboratory were obtained with the funds from the grants gained by our team in announced by CNCSIS (NARHE) competitions in the period 2003-2008.
- many small apparatus, a lot of laboratory accessories and books were obtained by donation from the part of professor Cristina Mandravel friends-chemists, practitioners world wide.

Surely, our work and our technicians' staff help in realization of this new design of laboratory environment and experiments for the mentioned disciplines cannot be *in money* evaluated!

Conclusions

In this paper are exposed basic conceptions and results in design of laboratory environment and experiments in accord with new curricula for compulsory disciplines: **Molecular**

structure and **Relationships Structure-Properties-Toxicity of industrial pollutants (RSPT)**, both from Environmental chemistry section.

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