

## FORUM

### CHEMISTRY IN CATALONIA: 1990-1995\*

The present report\*\* has an antecedent in the work in *La recerca científica i tecnològica a Catalunya* (Research in Science and Technology in Catalonia), published in 1990 in a joint edition by the Institut d'Estudis Catalans and the Comissió Interdepartamental de Ciència i Tecnologia (CIRIT), Generalitat de Catalunya. This is why this report starts at this date and extends up to 1995, covering a period of six years.

We must remember that during this period, the European Union scheduled its 3<sup>rd</sup> Framework Programme on Research and Technology (1991-1994). Though Catalan researchers began to receive European funding during this time, they mainly financed their research through Spanish agencies (DGICYT and CICYT), especially by applying for «Promotion of General Knowledge» and «R&D» Programs, and also through the Catalan agency CIRIT. In 1993, the 1<sup>st</sup> Research Plan of the Generalitat de Catalunya was started, ending in 1996, but this was created as a subsidiary to Spanish national plans, since in 1992 the Spanish Constitutional Court ruled that the Generalitat could not administer its own scientific policy.

During these six years, the campuses in Tarragona, Lleida and Girona became independent from their corresponding central universities. Moreover, newer universities were created, namely the Pompeu Fabra University and the Ramon Llull University, both in Barcelona, the latter built around several pre-existing university centres, such as the Institut Químic de Sarrià (founded in 1916), which is of considerable importance in the field dealt with in this publication.

This work is divided into three main sections and a final summary with conclusions. The first section is dedicated to human resources, and basically intends to establish a census of the chemistry research personnel at the universities and public research centres in Catalonia. The next section classifies and quantifies the research expenditure earmarked for research in chemistry, especially that of public origin, and also includes some indirect indicators of the contributions of the private sector in this area. The last of these main sections describes scientific production and evaluates its quality. As in similar studies, this quantification and evalu-

ation is done using bibliographic data generated by the people who are themselves responsible for the research; in other words, from publications by Catalan researchers appearing in journals of recognised prestige, normally peer reviewed. This was done employing chemical information databases in regular use among chemists, namely the *Science Citation Index (SCI)* from the Institute for Scientific Information, and the *Chemical Abstracts (CA)*, from the American Chemical Society.

The three sections mentioned above are brought together in a last part with comments and conclusions, limited by the insufficiencies of the collected data due to lack of availability or accessibility. In addition, some criticism about research in Catalonia (1990-1995) is included in this last part.

First of all, it is necessary to define the scope of this study. Chemistry, which can be conceived as a classical scientific discipline, in fact has blurred limits; this is the case when observing closely related derived specialities such as biochemistry or chemical engineering, but also with different branches of knowledge employing conceptual and methodological tools borrowed from chemistry. The study of chemistry research in Catalonia has, whenever possible, been circumscribed to the classical specialities of this science: analytical chemistry, physical chemistry, inorganic chemistry and organic chemistry. On the other hand, these branches are also the areas of knowledge that make up the study of chemistry in our universities, and are also part of the curriculum for pharmacy, together with other closely related specialities, such as therapeutic chemistry, also considered here. Research carried out at public research centres, such as the CSIC centres located in Catalonia, also corresponds to the four classical specialities or to other very clearly defined disciplines such as environmental chemistry or solid-state chemistry. On the other hand, other specialities closely connected with chemistry, but usually having their own university degrees, have been excluded from the study. This is the case of chemical engineering or biochemistry.

#### Human resources

##### Personnel at the university and public research centres

Research carried out using public funds is done mainly in universities, linked to the higher education studies of chemistry and pharmacy, and especially, although not exclusively, to postgraduate and Ph.D. studies, supervised by University departments. Some research in chemistry is also done in

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Table 1. Names and acronyms of Catalan and Spanish institutions appearing in the text, and their equivalents into English

Centre d'Investigació i Desenvolupament, CID (CSIC)	Centre of Research and Development, CSIC in Barcelona
Comisión Interministerial de Ciencia y Tecnología, CICYT	Inter-ministry Commission for Science and Technology, Spanish funding agency, Madrid
Comissió Interdepartamental de Recerca i Innovació Tecnològica, CIRIT	Interdepartmental Commission on Research and Technological Innovation, Autonomous Government of Catalonia
Comissionat d'Universitats i Recerca, CUR	Universities and Research Commission, Autonomous Government of Catalonia
Consejo Superior de Investigaciones Científicas, CSIC	Spanish National Council for R&D activities, Madrid
Dirección General para la Innovación Científica y Técnica, DGICYT	Directorate for Scientific and Technical Innovation, Spanish funding agency, Madrid
Fundación COTEC	Private foundation dedicated to the promotion of R&D activities in Spain, Madrid
Generalitat de Catalunya	Autonomous Government of Catalonia
Institut d'Estudis Catalans, IEC	Institute for Catalan Studies, Barcelona
Institut de Ciència dels Materials de Barcelona, ICMAB (CSIC)	Institute of Materials Science of Barcelona, CSIC at Bellaterra
Institut Químic de Sarrià, IQS	Chemical Institute of Sarrià, Barcelona
Instituto Nacional de Estadística, INE	Spanish Statistics Institute, Madrid
Ministerio de Educación y Ciencia, MEC	Science and Education Ministry, Madrid
Universitat Autònoma de Barcelona, UAB	Autonomous University of Barcelona, Bellaterra
Universitat de Barcelona, UB	University of Barcelona, Barcelona
Universitat de Girona, UG	University of Girona, Girona
Universitat de Lleida, UL	University of Lleida, Lleida
Universitat Politècnica de Catalunya, UPC	Polytechnic University of Catalonia, Barcelona
Universitat Ramon Llull, URL	Ramon Llull University, Barcelona
Universitat Rovira i Virgili, URV	Rovira i Virgili University, Tarragona

connection with studies of chemical engineering (UPC, UAB, UB, URV). Several centres run by the Spanish administration also play an important role in chemical research. This is the case of the Centre d'Investigació i Desenvolupament (CID), and the Institut de Ciència dels Materials de Barcelona (ICMAB), both integrated within CSIC. Certain centres run by the town and autonomous administrations also carry out some research activities. Finally, the private sector must also be included. Unfortunately, data referring to this sector are difficult to obtain, and the value of the present study would obviously be significantly enhanced by a more complete account of this sector.

#### *University research personnel*

Table 2 shows the overall figures for personnel in the more relevant research centres in Catalonia, mainly of public nature. For an easy comparison, the data have been grouped under the concepts: «permanent personnel», P (full professors and associate professors at the universities, or research professor, research fellow or scientific collaborator at CSIC);

«contracted personnel», C (assistant professors, laboratory assistants, and visiting professors at the universities, or specialised personnel, contract research fellows and research assistants at CSIC); and «research students», S (postgraduate and postdoctoral fellowships). No data concerning auxiliary personnel have been included because of their very small number, which is not even included in official reports. In fact, this is an indication of a deficiency, especially at the universities. By comparison, countries such as the United Kingdom, France or Germany usually furnish more than one technician per each permanent professor or research fellow. Table 2 reveals a comparable distribution of permanent (P) and contracted (C) personnel, although it is not maintained for the research students (S); this is due to the varying criteria which the different organisations employ to account for them. It must also be taken into consideration that in certain public and research laboratories there are people known as honorary contributors, personnel without any contractual relationship to the centre, who are there over a more or less prolonged training period. In general, figures for personnel

Table 2. Research personnel at the main Catalan public research centres in chemistry (1990-1995)

Centre	1990			1995		
	P	C	S	P	C	S
Universitat de Barcelona, Faculty of Chemistry	88	46	26 <sup>(1)</sup>	112	31	53 <sup>(1)</sup>
Universitat de Barcelona, Faculty of Pharmacy <sup>(2)</sup>	32	19	11 <sup>(1)</sup>	41	15	21 <sup>(1)</sup>
Universitat Autònoma de Barcelona	52	31	34 <sup>(3)</sup>	47	45	55 <sup>(3)</sup>
Universitat de Girona <sup>(4)</sup>	11	12	4	13	22	7
Universitat Rovira i Virgili	21 <sup>(5)</sup>	15 <sup>(5)</sup>	(10) <sup>(6)</sup>	24	39	(12) <sup>(6)</sup>
Universitat de Lleida	11	3	0	11	3	0
Institut de Ciència dels Materials de Barcelona, ICMAB (CSIC)	8	2	15	7	5	27
Centre d'Investigació i Desenvolupament, CID (CSIC) <sup>(8)</sup>	37 <sup>(7)</sup>	53	47	40	70	49
<i>Totals</i>	260	181	137	295	230	212
		578 <sup>(9)</sup>			737	

(1) These data only include predoctoral fellowships from CIRIT and MEC

(2) These data include the pharmacology area (according to data from the 1997-98 academic year, there were 23 P, 5 C and 30 S only considering organic chemistry and pharmaceutical chemistry).

(3) Number of fellowships from any kind of funding

(4) Prior to 1992, the teaching staff was counted as part of the Chemistry Department of the UAB.

(5) Data taken from the UB reports, considering the campus at Tarragona

(6) Fellowship data are not available, only estimative data are given which are not included in the total count.

(7) There is no separate data previous to 1992

(8) Including the department of ecotechnology.

(9) 1990 or closest year

in training must be considered as low estimates of actual values.

Table 2 also shows in rough the evolution of figures for research personnel, showing overall figures for 1990 and 1995. Research personnel at the beginning and at the end of the period under consideration were 578 and 737 people respectively. These figures represent an annual steady increase index of 4.9%, or, in general, a factor of 1.275 for the six years considered. Distribution for the different classes were 45%, 31%, and 24% for P, C and S in 1990, and 40%, 31% and 29% respectively in 1995.

When observed separately, the growth of each class of personnel show factors of 1.13, 1.27 and 1.54 for P, C and S personnel over the six years considered. These values reveal that the more appreciable growth corresponds to the predoctoral personnel, together with the contracted personnel, both classes which are very close to research activities.

Initially, all research personnel are full-time, but in the case of academics, full-time work is really only done by personnel in training. So, due to teaching and administrative tasks, permanent professors and also contracted personnel account for 50% full-time equivalent personnel in terms of research potential.

It must be mentioned that contracted personnel at the universities correspond mainly to lecturers and laboratory assistants that are simultaneously engaged in their doctoral studies, and this means that they must also be considered as research students. So, if we consider the ratio of the sum of C and S to permanent personnel, P, the obtained figures are 1.22 for 1990, and 1.50 for 1995. The increase of this ratio clearly indicates the growth of research potential in public

centres, as it also represents grosso modo Ph.D. students and Ph.D. supervisors. However, this index is very different for the different research centres.

Attempting to take a more profound look at personnel distribution over the four main areas of knowledge (analytical, physical, inorganic and organic), we get similar figures for each one: around 90 researchers within each area in 1990, or around 120 in 1995 (this is mainly true for different departments at the university or in the ICMAB-CSIC).

#### Organisation of research personnel

In research institutions, the R&D personnel are organised in departments or units, while organisation in academic institutions is of a more administrative nature, or is done in terms of research groups and research projects that show a more functional and temporary character.

*University departments and research centres.* In table 3 we summarise the list of university departments and research centres working in chemistry on a regular basis. Almost all these departments and centres carry on their research activities within the scope under consideration. It must be remembered that the universities of Girona, Lleida and Rovira i Virgili were separated from the UAB or UB in 1992. Obviously, other institutions also carry on some research in chemistry, although not so exclusively. This is the case of different university departments in the fields of biochemistry (UB, UAB and URV), and chemical engineering (UB, UAB, UPC and URV), together with some CSIC centres or others not directly considered here.

*Research groups.* The public research nuclei in Catalonia, once they reach a certain critical mass, can be declared con-

Table 3. University departments and research centres working regularly in chemistry (1995)

Universitat de Barcelona	Faculty of Chemistry	Department of Analytical Chemistry Department of Physical Chemistry Department of Inorganic Chemistry Department of Organic Chemistry
	Faculty of Pharmacy	Department of Pharmacology and Therapeutical Chemistry Unit of Pharmaceutical Chemistry Unit of Organic Chemistry
Universitat Autònoma de Barcelona	Department of Chemistry	Unit of Analytical Chemistry Unit of Physical Chemistry Unit of Inorganic Chemistry Unit of Organic Chemistry
Universitat de Girona	Department of Chemistry	Unit of Analytical Chemistry Unit of Physical Chemistry Unit of Inorganic Chemistry Unit of Organic Chemistry
Universitat de Lleida	Department of Chemistry	
Universitat Rovira i Virgili	Faculty of Chemistry	Department of Chemistry
Universitat Ramon Llull	Institut Químic de Sarrià	Department of Analytical Chemistry Department of Physical Chemistry Department of Organic Chemistry Department of Chemometrics
Consell Superior d'Investigacions Científiques	Centre d'Investigació i Desenvolupament (CID)	Department of Peptides and Proteins Department of Environmental Chemistry Department of Biological Organic Chemistry Department of Surfactant Technology
	Institut de Ciència dels Materials (ICMAB)	Laboratory of Organic Materials Laboratory of Solid-State Chemistry Laboratory of Inorganic Chemistry

solidated chemistry research groups by the Comissionat per a Universitats i Recerca (CUR), of the Generalitat de Catalunya.\*

From this census, some general information can be taken: the number of consolidated groups in chemistry is 52, and the total staff 851 people, noticeably larger than the figures referred to in table 2 (737 in 1995) which were obtained from the annual reports published by the research centres. This discrepancy is reasonable, since, as previously stated, the data in table 2 are low estimates of personnel. This is the case especially for the predoctoral personnel, which is very difficult to quantify, considering all its varying types. An interesting observation can be made when comparing the data from both mentioned sources: all public research personnel in chemistry can be considered as active. From the 52 research groups considered, 24 correspond to UB, 12 to UAB, 1 to UG, 6 to URV, 1 to UL, 2 to URL and 6 to CSIC. The fine distribution associates 11 of these groups with analytical chemistry, 13 with physical chemistry, 9 with inorganic chemistry and 19 with organic chemistry.

Among the 851 researchers counted, 30% (255) correspond to analytical chemistry, 20% (174) to physical chem-

istry, 15% (129) to inorganic chemistry and 35% (293) to organic chemistry. A deeper look at the census of consolidated research groups permits us to outline a mean description of their personnel. The size of the typical group is 16 people: 7 of which have reached the doctoral level (D), and 9 doing predoctoral graduate activities (G). The corresponding G/D ratio is then 1.27, which compares well with the value 1.55, which corresponds to the ratio between the sum of contracted plus in training personnel and personnel in permanent positions, mentioned at the beginning of this part, and considered as a measure of the research potentiality. Slightly different values are observed in the G/D ratios in the different research areas. The highest value is noticed among the analytical chemistry groups (1.57), while inorganic chemistry has the lower value (0.87). The organic chemistry (1.34) and physical chemistry (1.15) groups present values close to the mean.

Finally, from the denomination of these research groups, some interesting information can be derived regarding the main themes in their research activity. Key topics in the category of analytical chemistry are studies of equilibrium, speciation, chromatographic techniques, chemical sensors and biosensors, chemometrics and environmental analysis. In the physical chemistry field, outstanding topics are quantum chemistry (several groups), the study of reactivity or reaction

\* The last published census appeared in 1997, in the work *Recerca a Catalunya* (Research in Catalonia).

dynamics, electrochemistry, physics of materials, solid-state chemistry and environmental applications. In relation to inorganic chemistry, some fields of the research groups are organometallics, catalysis (various groups), magnetism, electronic structure, macromolecular chemistry, host-guest chemistry, macrocycles and bioinorganics. Organic chemistry, the largest class, includes groups working on synthesis relative to antibiotics, biomolecules, peptides and proteins, or focused on stereoselective or asymmetric synthesis. Other research lines are concerned with macromolecular chemistry, theoretical computation, electrochemical applications, polymers, materials or biological organic chemistry. It must also be mentioned that in our country the themes related to the use of nuclear magnetic resonance, with different groups, are normally ascribed to this speciality. Due to the affinity of the working issues, it is normal to add to the latter class of organic chemistry several groups who carry on activity connected with pharmacy studies such as those who work on the synthesis of alkaloids, polycycles or are focused on pharmaceutical chemistry.

Two final observations must be made concerning these consolidated research groups. First, as is to be expected in the academic world, the research topics are closer to pure than to applied chemistry, perhaps in a unbalanced way. Apart from that, it must be stated that many of the consolidated research groups may be associations of smaller research sub-units, related to a greater or lesser extent. So, the name identifying the group is sometimes not clear enough or is too generic to be adequately understood.

#### Research personnel in the private sector

It has not been possible to obtain reliable data concerning research people in chemistry in the private sector. A reference value is given by the COTEC foundation in Madrid. It gives, for the considered period, an estimate of 2 214 people dedicated to R&D tasks in the chemical industry sector in the whole of Spain. Assuming that around 50-75% of this sector is located in Catalonia (see next part of the manuscript), an estimate of 1 100 to 1 500 people would be dedicated to R&D activities. This is again a low estimate, considering that additional people from the sectors of pharmaceutical products, petroleum and food should be also considered.

In addition, if we consider the macroscopic indicator of 2.0 researchers per 1000 inhabitants in Catalonia (data from the sources), then, the number of Catalan researchers dedicated to chemistry in the private sector represents the 9.2-12.5% of the total number of personnel dedicated to R&D activities in Catalonia. If, additionally, we include the staff in the public sector (Table 2), this results in a very significant number of people, as might be expected given the importance of the chemical industry at Catalonia.

#### Research expenditure

Data for R&D funding are fully available for Catalan universities and other public research organisms (mainly CSIC), and

can be obtained with reasonable accuracy from the annual reports of these public institutions and the funding agencies. The structure of these reports, usually organised according to teaching criteria (faculties or departments), prevents the precise attribution of funds to individual research groups or lines. Accordingly, the present report shows the funding of these institutions classified by origin, by destination (research projects, research equipment, personnel, etc.) and by the general area of chemistry (analytical, inorganic, etc.) receiving the funds.

In sharp contrast with the abundance and accuracy of data relative to these public institutions, R&D expenditure in the private chemical sector could not be obtained from direct sources. Instead use was made of indirect statistical data, namely the yearly reports entitled *Informe anual de l'empresa catalana* (Annual report on Catalan industries), published by the Generalitat, the Catalan Autonomous Government. These yearly reports separately list figures relative to chemical firms and to pharmaceutical firms. However, the R&D figures are given only as a percentage of the added value. Thus, the figures shown in the present report for the private sector can only be taken as minimum estimates, since they do not include expenditures for chemical research in the pharmaceutical and other chemistry-related industries.

#### Public expenditure and research funding

Table 4 shows all public expenditure for chemistry in Catalonia, 1990-1995. This table includes the research funds allocated by individual agencies (European, Spanish and Catalan) not only to universities and CSIC, but also to firms and organisms engaged in chemical research activities. The table also includes data for research contracts, funded by public or private companies and organisms, received by the universities.

The low figure for the European funds in Table 4 reflects the marginal budget for chemistry (except in materials science) in the Framework Programs of the EU. On the other hand, the relatively high figure for the funds from the Catalan Government is due to the sizeable contribution in those years from the Fine Chemicals research program, now discontinued, which was managed by the Generalitat. Undoubtedly, future reports will show a sharp decrease in overall funding from the Catalan agencies. Table 5 shows the funding for all Universities and for CSIC according to the destination of the funds.

Comparison between the gross totals of Tables 4 (64.78 M€) and 5 (50.51 M€) shows that in the period 1990-95 the public funding of chemistry R&D at universities and CSIC amounts to about 80% of the total public expenditure, while the remaining 20% of public funding was allocated to other organisms and firms.

The comparison between the total figures for individual organisms in Table 5 reflects the relative sizes of chemistry-related research in these universities. In this context, it is worth mentioning here that the biggest chemistry departments in Catalonia belong to UB (which is also the largest

Table 4. Global R&amp;D expenditure in Chemistry by funding sources, 1990-95, in thousand €. (Includes all public funding to Universities and CSIC, as well as firms and other organisms)

Source	1990	1991	1992	1993	1994	1995	Total	%
EU	0	1,052	1,022	2,434	228	1,142	5,878	9.1
MEC	2,476	4,838	3,215	4,796	4,249	4,435	24,010	37.1
Generalitat	619	3,937	3,396	5,018	4,003	6,581	23,554	36.3
Contracts/Other	1,430	1,382	1,797	2,434	2,422	1,875	11,341	17.5
Total	4,526	11,209	9,430	14,683	10,902	14,034	64,783	100

Table 5. Overall R&amp;D chemistry funding (1990-95) for Catalan universities and CSIC (in thousand €) according to destination of the funds

Organism	Projects	Contracts	Equipment	Personnel	Other	Total	%
UB	5,860	5,427	6,112	3,402	805	21,606	42.8
CSIC	7,362	*	2,188	2,350	294	12,195	24.1
UAB	3,732	3,059	859	2,711	793	11,149	22.1
URV	998	1,298	331	258	258	3,137	6.2
UG	385		463	397	114	1,364	2.7
URL	301	*	288	282	12	877	1.7
UL	144			30	6	180	0.4
Total	18,788	9,778	10,247	9,424	2,278	50,509	100
%	37.2	19.3	20.2	18.7	4.6	100	

(\*) Data not available

Catalan university), and that the only Faculty of Pharmacy in Catalonia with considerable chemistry research also belongs to UB. On the other hand, the smaller universities (URV, UG, URL and UL) were created during the period under study, and their data in Table 5 reflect both their (small) size and their youth. One outstanding feature of the young but very active URV is its location in Tarragona, quite close to an important concentration of major petrochemical industries, which explains its success in obtaining research contracts.

Table 6 shows the global funding of UB, CSIC, UAB and URV, along with the distribution over several chemistry areas. The reason for selecting only these four institutions is that their combined funding (48.1 M€) amounts to 95% of the

total reflected in Table 5, while the distribution among the selected fields of chemistry still yields significant figures.

Examination of data in Table 6 shows that almost 22% of the funding could not be assigned to any individual field of chemistry. There are several reasons for this, such as funding allocated to the whole Faculty of Chemistry, or in some cases to the Department of Chemistry. Out of the allocated budget, two large fields receive most of the funding. Thus, Organic Chemistry receives 34% of the total funding available, while Analytical Chemistry gets almost 20% of it. On the other hand, Inorganic Chemistry (9%) and Physical Chemistry (10%) receive almost equal amounts, while other areas (such as Pharmaceutical or Therapeutic Chemistry) have smaller shares.

Table 6. Distribution of R&amp;D chemistry funding (in thousand €) for UB, CSIC, UAB and URV, 1990-95

	UB	UAB	URV	CSIC	Total
Analytical Chem.	3,294	2,759	992	2,404 <sup>(1)</sup>	9,442
Physical Chem.	1,653	655	234	2,338 <sup>(2)</sup>	4,874
Inorganic Chem.	2,482	1,424	174	433	4,520
Organic Chem.	9,748	3,684	974	2,055 <sup>(3)</sup>	16,462
Pharmaceutical/Therap. Chem.	2,073	–	–	–	2,073
Other / Unspecified	2,356	2,632	763	4,964	10,710
Total	21,606	11,149	3,137	12,195	48,087

1. Includes Environmental Chemistry

2. Includes Materials Science and Solid State

3. Includes Biological Organic Chemistry

Table 7. Number of Chemistry projects allocated by Spanish funding agencies CICYT and DGICYT, 1992-95

UNESCO code	CICYT projects		DGICYT projects	
	Rest of Spain	Catalonia	Rest of Spain	Catalonia
2210	26	3	113	20
2301	26	4	71	15
2303	6	8	102	23
2304	18	4	26	7
2305	0	2	-	-
2306	23	17	135	37
2307	7	1	62	6
2390	13	3	2	0
2391	8	9	-	-
Total	127	51	511	108

UNESCO codes: 2210: Physical Chemistry; 2301: Analytical Chemistry; 2303: Inorganic Chemistry; 2304: Macromolecular Chemistry; 2305: Nuclear Chemistry; 2306: Organic Chemistry; 2307: Physical Chemistry; 2390: Pharmaceutical Chemistry; 2391: Environmental Chemistry.

Table 7 compares the success of funding by the Spanish agencies CICYT and DGICYT of chemistry research projects in Catalonia and in the rest of Spain. With about 15.1% of the total Spanish population, Catalonia obtained 29% of the projects allocated by CICYT for research in chemistry, as well as 17.4% of the projects from DGICYT.

#### Research expenditure in the private sector

As stated above, data for the R&D expenditure in the private sector of chemistry are much more difficult to gather than for the public research institutions, and in addition, the two series of data are not strictly comparable. Indeed, industrial firms rightly consider the wages of all kinds of personnel involved in research activities as research expenses, while for public institutions the salaries of permanent staff are not usually taken into account. The same is sometimes also true for the costs of facilities, services, equipment and administration, to mention just a few traditional differences between the accounting systems of the two sectors.

With these differences in mind, in the present report fig-

ures are tentatively given for the R&D expenditure of the chemical industry in Catalonia for the period 1990-95 (see Table 8), using the statistical data shown in the yearly reports entitled *Informe anual de l'empresa catalana* (Annual Report of the Catalan Industries), published by the Catalan Government.

From Table 8, excluding year 1990, it can be seen that the ratio between total public funding for chemical research and total chemistry R&D expenditure in Catalonia oscillates around 20%, with a maximum of 22.5% in 1993 and a minimum of 18.5% in 1992. Another significant aspect is that R&D payments to foreign firms and organisms (collected in Table 8 as «Royalties») amount to about 15% of the total expenditure (including both private and public funding). This figure should be compared with the total public funding of chemistry R&D, which is only slightly higher (20%). On the other hand, for the year 1995 the total figure for research contracts in Catalan universities and CSIC amounts to only 2.6% of the total expenditure (including both private and public funding). This is only about one sixth of the technolo-

Table 8. R&amp;D expenditure of Catalan chemical firms and global funding from agencies financing public research in Catalonia, 1990-1995 (absolute values in M€)

YEAR	1990		1991		1992		1993		1994		1995	
	%	M€	%	M€	%	M€	%	M€	%	M€	%	M€
<i>Chemical firms<sup>(1)</sup></i>												
Value added .	<b>892.74</b>		<b>965.96</b>		<b>1,025.69</b>		<b>1,038.64</b>		<b>1,271.98</b>		<b>1,416.10</b>	
R&D	<b>2.9</b>	25.89	<b>3.87</b>	37.38	<b>3.6</b>	37.13	<b>3.94</b>	40.92	<b>3.12</b>	39.68	<b>3.32</b>	47.02
Royalties	<b>0.56</b>	5.00	<b>0.68</b>	6.57	<b>0.42</b>	4.31	<b>0.92</b>	9.56	<b>0.63</b>	8.01	<b>0.78</b>	11.05
<i>Total public funding (Table 4)</i>												
R&D		4.52		11.21		9.43		14.68		10.90		14.03
(Contracts)		(1.43)		(1.38)		(1.80)		(2.43)		(2.42)		(1.88)
Private R&D + Royalties + Public R&D		35.42		55.16		50.87		65.16		58.60		72.10

(1) Primary data, given in boldface, are taken from the series *Informe anual de l'empresa catalana* (Annual Report on Catalan Firms), published by Departament d'Economia i Finances. Generalitat de Catalunya, (Ministry of Economy of the Catalan Government), in the chapters on «Indústria Química» (Chemical Industry) for the corresponding years. The series also contains separate chapters on the pharmaceutical industry, which is therefore not covered in this table.

gy payments made abroad in the same year. The reader is invited to draw his/her own conclusions from this fact.

## Scientific productivity

In order to evaluate the productivity and the quality of the Catalan chemistry research we have selected three indicators. (i) Number of Bachelors degrees (*Llicenciat*) and number of Ph.D. degrees in Chemistry, (ii) number of papers published, and (iii) number of Patents reported.

### Bachelors degrees and Ph.Ds. in Chemistry

In the period 1990-1995, 2 850 students obtained their Bachelors' degrees in chemistry from the five Catalan Universities (UB, UAB, URV, UG, and IQS), on an average of 475 per year. In Catalonia as well as in the rest of Spain the Bachelor's degree is a five year course. A recent official change has reduced its duration to four years for purposes of unification of criteria. From the first year of the period studied, 1990, the number of degrees increased 11% every year. However, it is now going down, due to different factors, the demographic decrease being one of the most important. In the same period the number of Ph.D. degrees granted was 357 per year, 12% of graduate students. In the whole of Spain the number of Bachelors and Ph.D. degrees awarded in the same period was 13 995 (2 332 per year) and 1 775 (296 per year), respectively. These figures show that the Catalan universities awarded 20% of the Spanish Bachelors' and Ph.D. degrees, although Catalonia represents 15% of the Spanish population. While the number of bachelors degrees is high, on the other hand, the number of Ph.Ds. is low when compared with other industrially developed countries. By comparison, the number of American Chemical Society-certified Bachelors and Ph.D. degrees awarded in the USA in the year 1996 was 4 309 and 2 127, respectively.

### Publications

In order to analyse the Catalan chemical productivity in research during the period studied (1990-1995), Chemical

Abstracts (CA) and Science Citation Index (SCI) databases have been used. The following eleven categories of the SCI were selected: *Chemistry, Analytical Chemistry, Applied Chemistry, Inorganic & Nuclear Chemistry, Medicinal Chemistry, Organic Chemistry, Physical Chemistry, Electrochemistry, Physics (Atomic, Molecular & Chemical), Polymer Science* and *Spectroscopy*. Thus, categories that contains other aspects of chemistry, such as Biochemistry, Chemical Engineering, Materials Science, Environmental Chemistry, etc. have not been considered in the present report.

### Focus of the production

In the eleven research categories previously chosen from the SCI data base, a total number of 3281 scientific papers published during the period under study have been found in which at least one of the authors is associated with a Catalan institution. In Table 9 a comparison of the papers produced in Catalonia and Spain with worldwide production is given as well as comparisons with selected Western countries. Ireland and Italy have been considered since their percentage of the GNP invested in R&D is similar to Catalonia, while Sweden, with a well consolidated research infrastructure, shows a much larger investment in R&D. Figure 1 graphically presents the percentile distribution of the papers found among the eleven categories for the countries examined. Table 10 shows the relative production (in %) with respect to the world-wide production for each category as well as (in brackets) the relative values in relation to the overall average production for each country.

A particular comparison between Catalonia and Spain of the distribution of the collected publications over the different categories is shown in Figure 2, where a close similarity is evident.

From the analysis of Tables 9 and 10, and in order to assess the yield for each one of the research categories in Catalonia by comparison with world-wide productivity, the following trends can be discerned:

Table 9. Number of publications in the eleven categories studied in the countries under consideration

Category	World	Catalonia	Spain	Ireland	Italy	Sweden
Chemistry	181,076	601	2,969	313	3,526	1,438
Analytical Chemistry	63,947	605	3,453	331	2,361	1,135
Applied Chemistry	18,926	117	761	61	395	180
Inorganic Chemistry	50,301	392	1,890	216	2,581	287
Medicinal Chemistry	9,478	88	214	60	520	141
Organic Chemistry	78,248	604	3,069	294	3,770	770
Physical Chemistry	91,800	402	3,477	349	3,540	1,763
Electrochemistry	15,877	77	432	75	422	178
Phys., At. Mol. & Chemical	48,407	212	1,139	442	1,894	1,014
Polymer Science	48,748	121	992	95	1,503	558
Spectroscopy	28,086	62	611	37	1,844	468
TOTAL	634,894	3,281	19,007	2,273	22,356	7,932



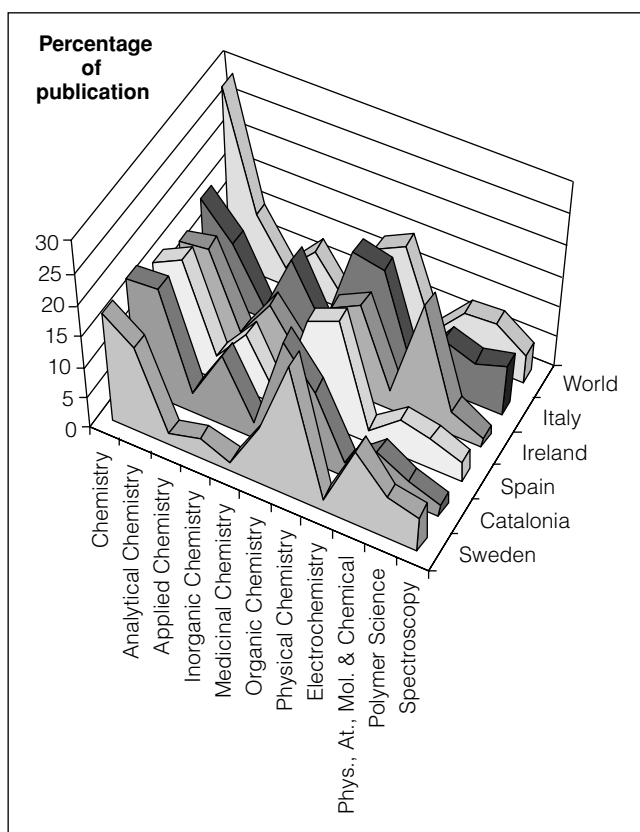


Figure 1. Relative distribution of the overall scientific production among the eleven categories for the countries considered.

- A larger production in relation to the world-wide average in analytical chemistry and medicinal chemistry.
- A slightly larger production focused on organic chemistry and inorganic chemistry.
- A slightly lower concentration than the world-wide average in physical chemistry, atomic and molecular physics and electrochemistry.
- A significantly lower production in chemistry and particularly in polymer science, and spectroscopy.

By comparison with the other countries considered (Table 10) the following trends have been observed:

- Outstanding production in analytical chemistry which is moreover quite similar to the Spanish figure but clearly more extensive than the Italian.
- Organic chemistry and inorganic chemistry also show a larger concentration especially in relation to Sweden, which produces 1.25% of the world-wide production in all categories but with a comparatively lower rate of contribution in this areas.
- Coming back to physical chemistry production, this category appears to be lower in comparison with the other countries, particularly with Sweden, which has recognised prestige and relevance in this field. Even when we include in this category papers coming from other fields like electrochemistry, atomic, molecular and chemical physics, the relative productivity remains essentially unchanged, though the number of scientific papers in this more general area rises significantly.
- In medicinal chemistry, Catalonia presents a very high rate of production, with a percentage close to the Irish, somewhat larger than the Italian and Swedish ones and twice the Spanish production in this category. The outstanding productivity as compared to Spain is probably due to the concentration of the pharmaceutical industry in Catalonia.
- As to polymer science and spectroscopy, tables clearly show the lowest concentration among all categories in Catalonia as well as one of the lowest with respect to the other countries considered.

It must be remarked that the industries in Spain do not produce any scientific publications, while the opposite is true for other countries. This fact means that only researchers in public institutions in Catalonia have progressively increased their research in chemistry in the last years

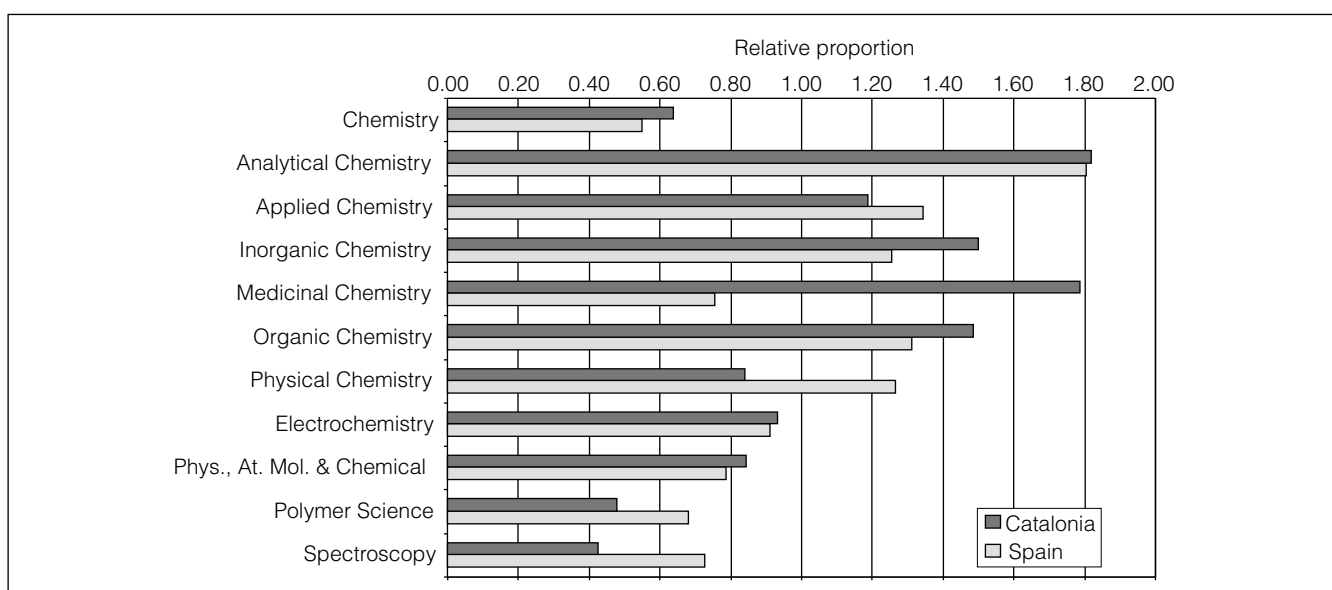


Figure 2. Normalized Catalan and Spanish production relative to the world average production (=1.0) for each category.

Table 10. Focus of the publications in each category for the considered countries in relation to the world-wide productivity. Relative values to the average world-wide production are given in brackets

Category	Catalonia		Spain		Ireland		Italy		Sweden	
Chemistry	0.33	(0.64)	1.64	(0.55)	0.17	(0.48)	1.95	(0.55)	0.79	(0.64)
Analytical Chemistry	0.95	(1.82)	5.40	(1.81)	0.52	(1.44)	3.69	(1.05)	1.77	(1.42)
Applied Chemistry	0.62	(1.19)	4.02	(1.34)	0.32	(0.90)	2.09	(0.59)	0.95	(0.76)
Inorganic Chemistry	0.78	(1.50)	3.76	(1.26)	0.43	(1.19)	5.13	(1.46)	0.57	(0.46)
Medicinal Chemistry	0.93	(1.79)	2.26	(0.76)	0.63	(1.76)	5.49	(1.56)	1.49	(1.19)
Organic Chemistry	0.77	(1.48)	3.92	(1.31)	0.38	(1.04)	4.82	(1.37)	0.98	(0.79)
Physical Chemistry	0.44	(0.84)	3.79	(1.27)	0.38	(1.06)	3.86	(1.10)	1.92	(1.54)
Electrochemistry	0.48	(0.93)	2.72	(0.91)	0.47	(1.31)	2.66	(0.76)	1.12	(0.90)
Phys., At. Mol. & Chemical	0.44	(0.84)	2.35	(0.79)	0.91	(2.54)	3.91	(1.11)	2.09	(1.68)
Polymer Science	0.25	(0.48)	2.03	(0.68)	0.19	(0.54)	3.08	(0.88)	1.14	(0.92)
Spectroscopy	0.22	(0.42)	2.18	(0.73)	0.13	(0.37)	6.57	(1.87)	1.67	(1.33)
Total Average (Country/World)	0.52	(1.00)	2.99	(1.00)	0.36	(1.00)	3.52	(1.00)	1.25	(1.00)

As to the evolution in productivity for each of the categories considered and particularly for Catalonia, the general trend is a continuous increase during the period 1990/1995 as shown in Figure 3. In any case, graphics seem to point out that the production in the different categories shows some tendency to stabilise. Any conclusion on such behaviour can only be corroborated by a proper analysis of the productivity in a period of time following this report.

Another aspect which has been considered in this report is the correlation between scientific production, investment effort in R&D (in terms of the percentage of the GNP), the personal effort (given by the percentage of the total population engaged in research) and the combined effort (given by the geometrical average of the investment and personal effort)

considering different countries around the world, and including in this case the most relevant countries in research and industry (USA and Japan). All mentioned quantities are given in Table 11, taking the Catalonia values as reference. The last column in that table gives the productivity / combined effort ratio which can be taken as a measure of the efficiency in R&D on the assumption that different countries invest the same percentage of their overall R&D budget in chemistry.

According to values reported in Table 11 we can see a similar rate of efficiency for Catalonia and Spain, slightly higher for the latter. Lower efficiency is found for those countries with a similar economy like Italy and Ireland or for those countries with a longer scientific tradition like Sweden. This consideration seems to indicate that countries with consoli-

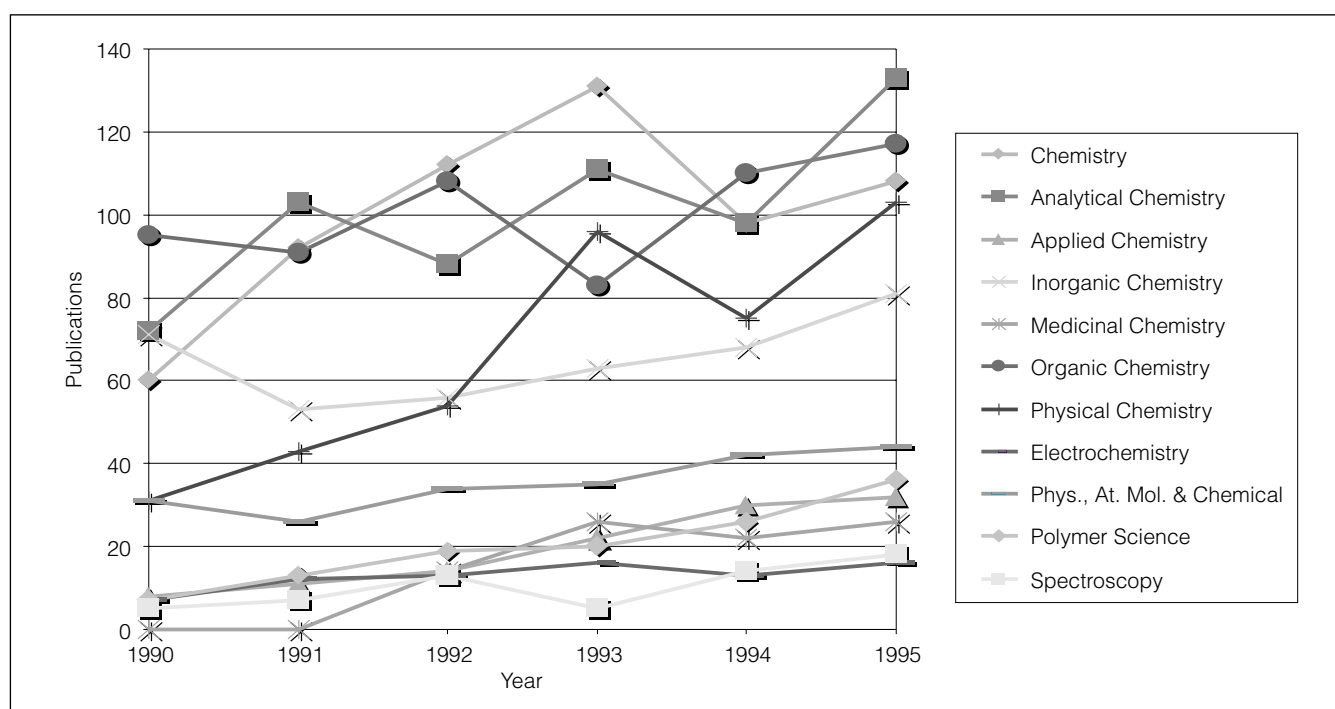


Figure 3. Evolution of the number of chemistry articles by Catalan authors appearing in CA for each of the eleven considered categories.

Table 11. Productivity, Personal effort, Investment effort, Combined effort and Productivity/Combined effort Ratio for the countries considered, in relation to values for Catalonia

Country	Productivity	Personal effort	Investment effort	Combined effort	Productivity / Combined effort
Catalonia	1	1	1	1	1
Spain	5.78	5.28	4.87	5.07	1.14
Ireland	0.69	0.74	1.11	0.90	0.77
Italy	6.80	10.05	13.51	11.65	0.58
Sweden	2.42	5.16	8.53	6.63	0.36
Germany	11.60	29.42	49.99	38.35	0.30
Austria	1.08	1.62	3.32	2.32	0.47
Belgium	1.78	3.37	4.08	3.71	0.48
Denmark	0.99	2.30	3.42	2.80	0.35
France	10.27	26.33	34.15	29.98	0.34
Greece	0.78	0.97	0.48	0.68	1.15
Portugal	0.45	1.16	0.67	0.88	0.51
UK	10.26	16.58	27.50	21.35	0.48
Japan	18.20	74.55	130.11	98.49	0.18
USA	54.99	81.54	207.81	130.17	0.42

dated R&D activity show lower efficiency ratios and comparatively, those countries with an emergent research activity show higher productivity.

### Quality

In order to evaluate the quality of the Catalan chemical publications, we have done a quartile analysis of the impact factor of the 450 journals contained in the eleven categories studied. According to Table 12, the impact factor of the journals in the first quartile is between 18.286 and 1.716.

In the period studied, Chemical Abstracts (CA) contains 4 028 papers whose first author works in a Catalan laboratory. These papers are found in practically all of the 80 sections of CA, showing that all aspects of Chemistry are studied. 80% of these papers were published in some of the Chemical categories of Science Citation Index (SCI) and the remaining 20% correspond to scientific fields closer to Physics, Geology, etc. than to Chemistry. From the total amount, 1 968 papers belong to the eleven chemical categories of SCI chosen for the present report.

In the table, we also present the distribution, according to their impact factor, of the 1 968 papers in the quartiles of the 450 different journals they appeared in, which represented the eleven categories studied. It shows that more than half, 52% of the Catalan papers, have been published in journals of the first quartile. A similar study of the Spanish papers

shows analogous results; in this case, 49% of the papers were published in journals of the first quartile. Figure 4 shows the distribution of the papers of Catalan authors appearing in journals of the first quartile among the categories studied.

Some additional information can be gathered from studies done by bibliometric organisations. In 1999, the Institute for Scientific Information (ISI) published a report on Science in Spain for the period 1994-1998, comprising science and social science fields. ISI indexed 83 757 papers that listed at least one author's address in Spain. The percentage of such papers in all the fields was 2.50%, but the percentage for chemistry papers was higher, 3.71%. As far as the relative-impact figures are concerned, the citations-per-paper averages in Chemistry are close to the world average, -1. Here -1 means that the impact of the Spanish Chemistry papers was 1% lower than the average world impact.

### Patents

The last concept correlated with the productivity considered in this report is the number of patents produced, which can provide in some way information about the applicability of the research developed, as a consequence of their intrinsic character of completeness, including methods and procedures. Information about the number of patents in the period considered was obtained from the Centre de Documentació de Patents of the UB-FBG and the CIDEM.

Table 12. Quartile distribution of the chemistry journals reported in the SCI according to their impact factor, and distribution of the papers from Catalan authors

Quartile	Journals	Impact factor	Papers in the quartile	Corresponding Journals	% Papers
1st	1-113	18.226 - 1.716	1,026	57	52.13
2nd	114-225	1.708 - 0.984	469	64	23.83
3rd	226-338	0.983 - 0.513	281	53	14.28
4th	339-450	0.504 - 0.009	192	26	9.76

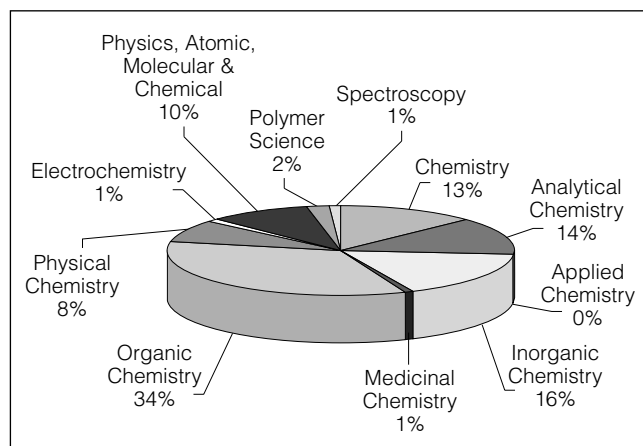


Figure 4. Distribution of the papers by Catalan authors in journals of the first quartile among the categories studied.

It should be said that when using patents as a measure it is the number of active ones that ought to be considered rather than the total, but unfortunately that information is not available.

Patents registered in the 1990/95 period were 1423 in Spain, and of these 449 came from Catalonia (31.5 % of the total). The average number of patents per year in Catalonia was about 75 while 237 was the average for the whole of Spain including Catalonia. By comparing this number with the percentage of population (15.1%) and of GNP (19.9%) for Catalonia, the Catalan patent productivity is quite outstanding. In spite of this favourable result, which corresponds to the large number of chemical industries located in Catalonia, and considering the importance of this industrial sector, the absolute number of patents is very low.

The majority of patents in Spain and also in Catalonia come from the private sector and are of industrial character, while the contribution from public institutions is insignificant (a total of ten patents in Catalonia for the period considered). The COTEC database estimates the number of patents in chemistry for Spain at 60% of the whole.

Comparing the number of scientific papers and the number of patents produced we obtain a ratio of seven scientific papers per patent in Catalonia while the same ratio is about thirteen for all of Spain. While another source\* raises this ratio to about thirty when all scientific areas are considered; ratios must be improved (get smaller) if we want a more favourable comparison with those countries with consolidated R&D activity.

## Conclusions

### Public sector

In human resources a steady increase has been shown in research personnel, from 578 to 737 people from 1990 to 1995. This represents a cumulative continuous increase of 4.9% per year, always as a low estimate. The total of research personnel in the chemistry field (737) forms approximately 6.1% of the total amount of research personnel in

Catalonia, if we consider the mean value of 2.0 researchers per 1000 inhabitants. This represents a very significant figure of researchers, as could be expected.

The evolution of the ratio of research students to permanent staff during the period studied is from 1.22 to 1.50. This results in an increase of overall training capacity, which also represents an increase in research potential. This trend also expresses a clear benefit for university research, in direct relationship with the training of researchers. However, we should not forget that this is a low value if compared with countries having more consolidated research systems.

If we compare the data for personnel pertaining to the public research centres carrying out chemistry research with the census of consolidated research groups in chemistry, an interesting fact is observed. Almost all the personnel at the public research centres are active researchers in the consolidated groups. In other words, there are no islands of inactive personnel in research. A mean profile of such a consolidated group is seven doctorate personnel and nine research students. This specific accreditation of the consolidated research groups, started during the period under consideration, should be monitored with attention in the future. It has represented an important stimulus for bringing people together, but if research with its own particular profile is sought, more significant funding should be provided for.

Concerning economic resources, almost equal shares were obtained from the Catalan government (36%) and from the Spanish ministry (37%). This was due to the regional management of the specific research plan for fine chemistry, with a significant involvement of Catalan centres. Once it disappears, a different distribution of funding is to be expected.

We can make a special observation concerning the distribution of funding. Spanish national funds normally correspond to carrying out research projects, while the regional funds are dedicated to other concepts, such as scientific infrastructure or mobility of researchers, also covered by the Spanish ministry. This distribution reveals that a truly Catalan scientific policy does not exist, although Catalan researchers have great success in national fund applications. On the other hand, European funding is of little significance (9%), but it is known that the different framework programmes of the EU almost forgot to include chemistry among their top priorities. Other international contributions lack funding significance.

From the above observations, a main conclusion is that it is absolutely necessary to establish a policy of continuous growth of resources for innovation and for personnel devoted to R&D tasks, as well as in project funding, in order to get closer to the level of neighbouring countries.

In terms of production aspects, progressive and effective training of chemistry graduates and doctorates is clearly established, with a certain imbalance in favour of the former. In comparison with graduates, few Ph.Ds. are trained, undoubtedly due to a lack of professional recognition by industry.

\* See A. Pestaña's articles.

The research topics getting prime attention in Catalonia are distributed among the different fields of the speciality, without leaving any unattended. In a very significant way, the distribution of research topics is almost identical to the situation in Spain, except for the case of Medicinal Chemistry. This topic is much more significant in Catalonia, surely due to the existence of specific research groups in the public research centres and also to the importance of the pharmaceutical industry. Unfortunately, these facts only reveal the lack of a specific national scientific policy.

In quantitative terms, there is a clear trend towards increase of scientific productivity, in terms of research articles, although a certain stabilisation could be anticipated at the end of the studied period, which should be monitored. Production is especially significant for the four main academic fields (Analytical, Physical, Inorganic and Organic Chemistries). A small number of contributions in the fields of polymers or spectroscopy is also detected.

In relation to the quality of research, one of the indicators observed is clear: half of the scientific articles appear in journals with a maximum impact factor (first quartile). In this way, research is not only a mere communication to others, but is of high quality and is on a level comparable to that of other countries with a longer scientific tradition.

Figures for elaboration of patents, from either the public or private sector, are only estimates. In any case, the lack of patents in the different fields is a fact already pointed out in general studies of our science system.

Regarding the quantitative aspects of production, it should be pointed out that the chemistry research in Catalonia has considerable «visibility», basically due to researchers from the public sector (0.52% of the world production). In contrast, the private sector hardly contributes at all to this «visibility». Of all the personnel dedicated to R&D activities in Catalonia, the public sector in the chemistry field represents 6.1%. This group (737 researchers) produces approximately 17% of all Spanish publications in the field of chemistry (coincident data from our bibliometric data and from the COTEC reports). In addition, this extensive productivity is accomplished without a large funding effort, unlike other fields which receive special treatment from the Spanish ministry through its national R&D plans. Finally, we should point to the high productivity of the chemistry sector of our R&D system, in qualitative and quantitative aspects. If this level is to be sustained, its activity and the carrying out of research projects must continue and be promoted.

#### Private sector

Difficulties in accessing data for the private R&D sector oblige us to treat it separately. Almost all the working data have been extrapolated from macroscopic indicators obtained from INE, COTEC or the Generalitat de Catalunya.

First, a direct survey is needed for R&D personnel in the private sector, because information is unavailable. A reference value is given by the COTEC foundation. The proportional extrapolation for Catalonia (75% of chemistry activity) shows around 1 500 people dedicated to R&D tasks in the

private sector (twice the value of research people in the public sector), but this value is again a low estimate, as a significant number of people from related sectors must be added.

Next, the public research carried out with private funding, that is, research contracts established with industry, is undoubtedly more extensive than the 17.5% share obtained, but much lower than the value to be expected given the importance of the chemical industry in Catalonia. This indicates that public centres are not aware to cooperate with industry, or perhaps points to a passive role on the part of our industry, more dedicated to reproduction of knowledge or products than generation or development of newer ones. It is worth noting that the amount paid for royalties abroad by the Catalan chemical industry is equivalent to the funding for all the public research in chemistry in Catalonia. A second observation is related to the insufficient use of research personnel trained at public centres, especially Ph.Ds., who once they are working in industry seldom carry out tasks connected with R&D.

A startling fact is the low level of private sector activity in the publication of their research activities, while this sector represents a large share of the total R&D expense (65%). An indirect estimation (COTEC Foundation) gives a share of 1.8% of the publications in the chemistry field. On the other hand, the private sector is very significant in the aspect of patents, as is to be expected, though the absolute value of the number of patents is still very low. This suggests that the main result of private R&D is related to the internal improvement of products and processes. In addition, the private sector undoubtedly includes wages in its expenses (estimated as a share of 33%), a concept that is not taken into account in the public sector figures.

#### Final Remarks

The final conclusion, after the collection of data on the persons involved in and the subjects of research in Catalonia, the funding expended and the output of their activity, mainly in the form of the publication of results, during the period 1990-95, is that the public sector shows a consolidated R&D system, with a level comparable to our neighbour countries. On the other hand, the chemical industry is also a consolidated traditional sector, with growing expenditures for innovation, in order to maintain its competitiveness. In other words the two sectors, when considered separately, receive favourable recognition. However, if considered together, there is no doubt that there is a lack of co-operation between the two. An increase in co-operative activities is an objective, among others, that R&D policies in Catalonia should particularly stress in the future.

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