SCIENCO

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

ISSN 0104-5431

AN INTERNATIONAL FORUM FOR THE RAPID PUBLICATION
OF ORIGINAL SCIENTIFIC ARTICLES DEALING WITH CHEMISTRY
AND RELATED INTERDISCIPLINARY AREAS

VOLUME SEVENTEEN NUMBER SEVENTEEN

DECEMBER 2009

EDITOR

LAVINEL G. IONESCU, *SCIENCO*, Consultoria Científica, Viamão, RS, BRASIL

ASSISTANT EDITOR

LUIS ALCIDES BRANDINI DE BONI, Tchequimica LTDA, Porto Alegre, RS. Brasil.

EDITORIAL BOARD

FARUK NOME AGUILERA, Departamento de Química, Universidade Federal de Santa Catarina, Florianópolis, SC, Brasil
D. BALASUBRAMANIAN, Centre for Cellular and Molecular Biology, Hyderabad, INDIA
HECTOR E. BERTORELLO, Departamento de Química Organica, Facultad de Ciencias Químicas, Universidad Nacional de Cordoba, Cordoba, ARGENTINA
AÉCIO P. CHAGAS, Instituto de Química, UNICAMP, Campinas, SP, BRASIL
JUAN JOSÉ COSA, Departamento de Química y Fisica, Facultad de Ciencias Exactas, Universidad Nacional de Rio Cuarto, Rio Cuarto, ARGENTINA
GLENN A. CROSBY, Department of Chemistry, Washington State University, Pullman, WA, USA
VITTORIO DEGIORGIO, Dipartimento di Elettronica, Sezione di Fisica Applicata, Universita di Pavia, Pavia, ITALIA
JOSE C. TEIXEIRA DIAS, Departamento de Química, Universidade de Coimbra, Coimbra, PORTUGAL
OMAR A. EL SEOUD, Instituto de Química, Universidade de São Paulo, São Paulo, SP, BRASIL
FERNANDO GALEMBECK, Instituto de Química, UNICAMP, Campinas, SP, BRASIL
NISSIM GARTI, Casali Institute of Applied Science, Hebrew University of Jerusalem, Jerusalem, ISRAEL
GASPAR GONZALEZ, Centro de Pesquisa, CENPES-PETROBRAS, Ilha do Fundão, Rio de Janeiro, RJ, BRASIL
YOSHITAKA GUSHIKEM, Instituto de Química, UNICAMP, Campinas, SP, BRASIL
WILLIAM RASE, Department of Chemistry, Texas Tech University, Lubbock, Texas, USA
I. B. IVANOV, Laboratory of Thermodynamics and Physico-chemical Hydrodynamics, Faculty of Chemistry, University of Sofia, Sofia, BULGARIA
IVAN IZQUIERDO, Departamento de Bioquímica, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, BRASIL
V.A. KAMINSKY, Karpov Institute of Physical Chemistry, Moscow, RUSSIA
MICHAEL LAING, Department of Chemistry, University of Natal, Durban, SOUTH AFRICA
EDUARDO LISSI, Departamento de Química, Universidad de Santiago de Chile, Santiago, CHILE
WALTER LWOWSKI, 'Department of Chemistry, New Mexico State University, Las Cruces, N.M., USA
CRISTINA MANDRAVEL, Catedra de Chimie Fizica, Facultatea de Chimie Universitatea din Bucuresti, Bucuresti, Romania
C. MANOHAR, Bhabha Atomic Research Centre, Chemistry Division, Bombay, INDIA
AYRTON FIGUEIREDO MARTINS, Departamento de Quimica,Universidade Federal de Santa Maria, Santa Maria, RS, BRASIL
FRED MENGER, Department of Chemistry, Emory University, Atlanta, GA, USA
KASHMIRI LAL MITTAL, Private Consultant, Hopewell Junction, N.Y., USA
ARNO MULLER, Escola de Engenharia, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, BRASIL
JOSE MIGUEL PARERA, Instituto de Investigaciones en Catalisis y Petroquímica, Universidad Nacional del Litoral, Santa Fe, ARGENTINA
LARRY ROMSTED, Department of Chemistry, Rutgers University, Piscataway N.J., USA
GILBERTO FERNANDES DE SA, Departamento de Química Fundamental, Universidade Federal de Pernambuco, Recife, PE, BRASIL
DIMITRIOS SAMIOS, Instituto de Química, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, BRASIL
DIOGENES DOS SANTOS, Department of Molecular Biology, Oxford University, Oxford, ENGLAND.
BEN K. SELINGER, Department of Chemistry, Australian National University, Canberra, AUSTRALIA
KOZO SHINODA, Department of Applied Chemistry, Faculty of Engineering, Yokohama National University, Yokohama, JAPAN
CRISTOFOR I. SIMIONESCU, Academia Romana, Filiala Iasi, Iasi, ROMANIA
BRUNO SZPOGANICZ, Departamento de Química, Universidade Federal de Santa Catarina, Florianopolis, SC, Brasil
UMBERTO TONELLATO, Dipartimento di Chimica Organica, Universita degli Studi di Padova, Padova, ITALIA
DIETER VOLLHARDT, Max Planck Institut fur Kolloid und Grenzflächenforscung, Berlin, GERMANY
RAOUL ZANA, Institut Charles Sadron, CRM-EAHP, Strassbourg, FRANCE

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

ISSN 0104-5431

VOLUME SEVENTEEN, NUMBER SEVENTEEN DECEMBER 2009

CONTENTS / CONTEÚDO

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
SOUTH. BRAZ. J. CHEM., VOL. 17, No. 17, 2009

AN EFFICIENT SYNTHESIS OF β-(3-QUINOLINYL)-α-ALANINE

Stefan Holger Öhlinger

Free University of Berlin, Faculty of Biology, Biochemistry, Chemistry and Pharmacy,
Department of Organic Chemistry, Takustrasse 3, D-14195 Berlin, Germany

---

ABSTRACT:

*A convenient synthesis for β-(3-quinolinyl)-α-alanine (**4**) is presented. Condensation of 2-chloro-3-chloromethylquinoline (**5**) with diethyl acetamidomalonate (**2**) gave high yield of diethyl 2-acetylamino-2-(2-chloro-3-quinolinylmethyl)-propanedionate (**6**), which was dehalogenated in the presence of ammonium formate and palladium/charcoal. Diethyl 2-acetamido-2-(3-quinolinylmethyl)-malonate (**3**) was easily converted to the amino acid. The condensation reaction between **2** and **6** is also useful for the construction of (1H)-2,3-dihydropyrrolo[2,3-b]quinoline-2,2-bis(carboxylic acid) and pyrrolo[2,3-b]quinoline-2-carboxylic acid derivatives.*

KEYWORDS: reductive dehalogenation; unnatural amino acid; β-(3-quinolinyl)-α-alanine; pyrrolo[2,3-b]quinoline-2-carboxylic acid skeleton

RESUMO:

*Uma síntese eficaz para β-(3-quinolinil)-α-alanina (**4**) é apresentada. A condensação de 2-cloro-3-clorometilquinolina (**5**) com dietilacetamido malonato (**2**) levou a um rendimento alto de dietil 2-acetilamino-2-(2-cloro-3-quinolinilmetil)-propanodionato (**6**), que foi sujeito à dehalogenação na presença de Pd/C. O dietil 2-acetamido-2-(3-quinolinilmetil)-malonato (**3**) foi facilmente convertido no amino ácido. A reação de condensação entre **2** e **6** é também útil para a síntese de (1H)-2,3-dihidropirolo[2,3-b]quinolina-2,2-bis(ácido carboxílico) e derivados de pirolo[2,3-b]quinolina-2-ácido carboxílico.*

PALAVRAS CHAVES: dehalogenação redutiva; amino ácido não-natural; β-3-(5-quinolinil)-α-alanina; esqueleto de pirolo[2,3-b]quinolina-2-ácido carboxílico

---

Email: steven@chemie.fu-berlin.de

DOI: 10.48141/SBJCHEM.v17.n17.209.4_2009.pdf

INTRODUCTION

The use of 3-(3-quinolinyl)-alanine (**4**), a rare unnatural amino acid is limited due to difficulties in access. Folkers *et al*. prepared the title compound in the synthesis of highly active peptides as Luteinising Hormone Releasing Hormone (LHRH) antagonists, as drug carriers and also of peptides with activity on central nerve system.[1-4]
In other reports the influence on tryptophan biosynthesis or chorismate mutase has been studied.[5-7] It has also been applied as a replacement of tryptophan in structure-activity studies of brain/gut peptide like Acetyl-cholecystokinin-heptapeptide (Ac-CCK-7) analogues.[8, 9]

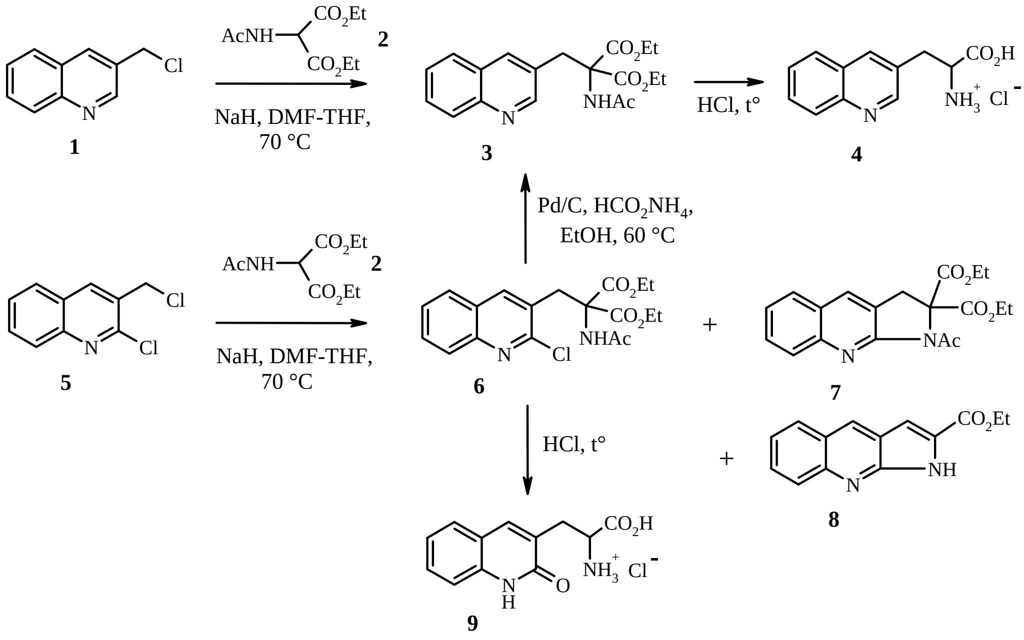
The amino acid was first prepared by Dyer and Yokoyama.[10] Improvements were achieved by using the azlactone approach,[11] which is still useful for preparing enantiopure **4**.[12] Condensation of 3-chloromethylquinoline (**1**) with diethyl acetamidomalonate (**2**) leads to diethyl 2-acetylamino-2-(3-quinolinylmethyl)-propanedionate (**3**).[4, 13] Enantioselective synthesis of **4** or its derivatives was achieved,[8, 9] adapting the Evans oxazolidine auxiliary method. Other enantioselective approaches to derivatives of **4** make use of enzymatic resolution,[11, 13] or asymmetric catalytic hydrogenation of the corresponding enamines.[12, 14] All these approaches suffer from limited availability of 3-substituted quinolinyl derivatives needed as precursors.

In the synthesis of **4** mentioned above,[4, 13] difficulties in separation of **2** and **3** were noticed because of similar polarities. The condensation product **3** on crystallization was always accompanied by unreacted **2**. A high-purity **3** could be produced only by multiple crystallization and careful chromatographic purification.

RESULTS AND DISCUSSION

The synthesis of **4** presented here combines the acetamidomalonate process with reductive dehalogenation of 2-chloro-3-quinoline derivatives. The condensation of **2** and 3-chloromethyl-2-chloroquinoline (**5**) proceeded smoothly in DMF as solvent and sodium hydride as base.[15] Sufficient pure product **6** was isolated after one crystallization; separation of **2** and diethyl 2-acetylamino-2-(2-chloro-3-quinolinylmethyl)-propanedionate (**6**), contained in the mother liquors, is simplified by greater differences in polarity as compared to the original setup.[4, 13] **6** was obtained in reproducible yields greater than 85 %.[16]

Initially, efforts to condense **5** with **2** in the presence of sodium ethylate and ethanol as solvent not only resulted in incomplete reaction and markedly lower yield of the desired product, but also gave side products arising from intramolecular cyclization, such as diethyl N-acetyl-(1*H*)-2,3-dihydropyrrolo[2,3-b]quinoline-2,2-biscarboxylate (**7**) and ethyl pyrrolo[2,3-b]quinoline-2-carboxylate (**8**). Slight modifications of the reaction conditions gave access to **8** in higher yield.



Scheme: Synthetic pathway to β-(3-quinolinyl)-α-alanine

5 as precursor could easily be obtained by a procedure first developed by Meth-Cohn *et al.*[17–19] or by side-chain chlorination of 2-chloro-3-methylquinoline.[20] Calvin *et al.* have presented a procedure for preparation of **5** from 3-chloro-N-phenylpropanamide.[21]

6 was dehalogenated using ammonium formate and palladium/charcoal in refluxing ethanol to produce **3** in near quantitative yield. Treatment of **3** with refluxing 25 % HCl gave **4**-HCl after removal of excess HCl in vacuum. **4** was liberated by adding ammonium hydroxide solution to a cooled solution of **4**-HCl in water. The N-Boc- and N-Fmoc derivatives of **4** were prepared by standard procedures.

When **6** was subjected to decarbethoxylation in refluxing HCl, complete conversion to 2-amino-3-(2(1*H*)-quinolinone-3-yl)-propanoic acid (**9**) was achieved, which is closely related to the 4-substituted quinolinone anti-ulcer drug “Rebamipide”.[22-24]

EXPERIMENTAL

^{1}H NMR and ^{13}C{^{1}H} NMR spectra were recorded on Bruker AM-400 instrument. Chemical shifts are in ppm relative to tetramethylsilane as internal standard at 0.0 ppm (^{1}H NMR) or relative to shifts of deuterated solvents (^{13}C NMR) according to literature values (CDCl$_3$ middle resonance at 77.0 ppm). Melting points of organic compounds were determined on Büchi B-540 apparatus.

Compound 3: mp. 124-125 °C (from EtOAc-hexanes). ^{1}H NMR (400 MHz, CDCl$_3$, δ): 8.60 (1H, d), 8.03 (1H, dd), 7.83 (1H, d), 7.65-7.75 (2H, m), 7.55 (1H, m), 6.60 (1H, s, NH), 4.35 (4H, q, J = 7.5 Hz), 3.89 (2H, s), 2.10 (3H, s), 1.35 (6H, t, J = 7.5 Hz). ^{13}C NMR (100 MHz, CDCl$_3$, δ): 169.7, 167.4, 152.1, 147.6, 136.8, 129.6, 129.5, 128.5, 128.0, 127.6, 127.1, 67.4, 63.2, 35.5, 23.3, 14.3.

Compound 6: mp. 152-153 °C (from EtOAc-hexanes). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.00 (1H, d), 7.90 (1H, s), 7.75 (2H, dd), 7.55 (1H, dd), 6.62 (1H, s, NH), 4.45-4.25 (4H, m), 4.00 (2H, s), 2.05, (3H, s), 1.30 (6H, t). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 169.8, 167.5, 151.4, 147.0, 140.8, 130.7, 128.3, 127.8, 127.4, 127.3, 127.2, 66.4, 63.0, 35.2, 23.1, 14.1.

Compound 7: yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$, δ): 7.90 (1H, d), 7.83 (1H, s), 7.68 (1H, d), 7.60 (1H, dd), 7.40 (1H, dd), 4.25 (4H, q), 3.70 (2H, s), 2.98, (3H, s), 1.30 (6H, t). ^{13}C-NMR (100 MHz, $CDCl_3$, δ): 170.8, 168.2, 154.2, 146.8, 132.5, 129.6, 128.3, 127.6, 125.7, 125.4, 122.7, 72.2, 62.7, 36.1, 25.8, 14.2.

Compound 8: mp. 173-174 °C (from EtOAc). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 10.63 (1H, s, NH), 8.55 (1H, s), 8.20 (1H, m), 7.95 (1H, m), 7.70 (1H, m), 7.45 (1H, m), 7.35 (1H, s), 4.45 (2H, q), 1.35 (3H, t). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 161.6, 150.4, 147.3, 132.1, 131.1, 129.2, 128.8, 128.2, 125.2, 123.6, 121.6, 106.9, 61.7, 14.4.

Compound 9-hydrochloride: 270-272 °C decomp. ^{1}H NMR (400 MHz, dmso-d6, δ): 11.95 (1H, s), 8.50 (3H, br. s, NH), 7.85 (1H, s), 7.60 (1H, m), 5.50 (1H, m), 7.40 (1H, m), 7.15 (1H, m), 4.25 (1H, m), 3.0 - 3.1 (2H, m). ^{13}C NMR (100 MHz, dmso-d6, δ): 170.8, 163.0, 140.3, 139.0, 130.6, 128.2, 127.8, 122.6, 119.9, 115.5, 51.6, 32.7.

The results of elemental analysis of the new synthesized compounds **3**, **6**, **8** were in agreement with calculated values.

REFERENCES

1. J.-X. Cheng, C. Y. Bowers and K. Folkers, US Pat. 4642332; *Chem. Abstr.*, 106, 214397r (1987).
2. a) K. Folkers, C. Y. Bowers, T. Kubiak and J. Stepinski, *Z. Naturforsch.*, 38B, 1253-1256 (1988); b) A. Ljungqvist, D.-M. Feng, C. Y. Bowers, W. A. Hook and K. Folkers, *Z. Naturforsch.*, 46B, 1231-1236 (1991); c) A. Ljungqvist, D.-M. Feng, W. Hook, Z.-X. Shen, C. Y. Bowers and K. Folkers, *Proc. Natl. Acad. Sci. USA*, 85, 8236-8240 (1988); d) A. Janecka, A. Ljungqvist, C. Y. Bowers and K. Folkers, *Biochem. Biophys. Res. Commun.*, 180, 374-379 (1991).
3. A. Ljungqvist, D.-M. Feng, C. Y. Bowers, K. Folkers and A. Janecka, US Pat. 5480969; *Chem. Abstr.*, 124, 261749p (1996).
4. N. S. Bodor, US Pat. 4888427; Eur. Pat. EP 0293071, German Pat. DE 3883600; *Chem. Abstr.*, 110, P232096d (1989).
5. F. Lingens, H. Kraus and S. Lingens, *Hoppe-Seyler's Z. Physiol. Chem.*, 339, 1-8 (1964).
6. B. Sprössler and F. Lingens, *Hoppe-Seyler's Z. Physiol. Chem.*, 351, 967-974 (1970); *Chem. Abstr.*, 73, 94863r (1970).
7. F. Zymalkowski and U. Jacoby, *Arch. Pharm.*, 304, 271-277 (1971); *Chem. Abstr.*, 75, 48862h (1971).

8. W. Danho, J. W. Tilley, S.-J. Shiuey, I. Kulesha, J. Swistok, R. Makofske, J. Michalewsky, R. Wagner, J. Triscari, D. Nelson, F. Y. Chiruzzo and S. Weatherford, *Int. J. Peptide Protein Res*., 39, 337-347 (1992); *Chem. Abstr*., 117, 143640d (1992).
9. W. Danho, D. J. Nelson, G. L. Olson, S.-J. Shiuey, J. W. Tilley and R. Wagner, US Pat. 518448; *Chem. Abstr*., 118, 213545y (1993).
10. E. Dyer and W. Yokoyama, *J. Org. Chem*., 26, 2124-2125 (1961).
11. Y. Zhang and Z. Shen, *Chem. Res. Chin. Univ*., 7, 261-265 (1991); *Chem. Abstr*., 117, 171995s (1992).
12. C. Cativiela, J. A. Mayoral and E. Meléndez, *J. Org. Chem*., 49, 2502-2504 (1984).
13. C. K. Acosta, M.L. Bahr, J. E. Burdett, J. W. Cessac, R. A. Martinz, P. N. Rao and H. K. Kim, *J. Chem. Res.* (S), 110-111 (1991); *Chem. Abstr*., 115, 72165y (1991).
14. J. J. Bozell, C. E. Vogt and J. Gozum, *J. Org. Chem*., 56, 2584-2587 (1991).
15. Although no difficulties were observed, it should be noted that there have been some reports of runaway reactions using these conditions: J. Buckley, R. Lee Webb, *Chem. Eng. News*, 60 (28), 5 (1982) and G. DeWall, *Chem. Eng. News*, 60 (37), 5, 43 (1982). Successful scaleup of this reaction has, however, been carried out in a solvent mixture of THF and DMF.
16. Details of the procedure will be reported elsewhere.
17. O. Meth-Cohn, B. Narine and B. Tarnowski, *J. Chem. Soc. Perkin Trans. 1*, 1520-1530 (1981).
18. O. Meth-Cohn, S. Rhouati, B. Tarnowski and A. Robinson, *J. Chem. Soc. Perkin Trans. 1*, 1537-1543 (1981).
19. O. Meth-Cohn, B. Narine and B. Tarnowski, *Tetrahedron Lett*., 4885-4886 (1979).
20. F. Korodi, *J. Heterocyclic Chem*., 28, 1549-1552 (1991).
21. J. R. Calvin, G. F. Hillstrom, J. Holland, P. E. Krieger, R. Murugan, E. F. V. Scriven and J. Yang, *Arkivoc*, 3 (IV), 257-263 (2002); *Chem. Abstr*., 138, 368731 (2003).
22. M. Uchida, M. Komatsu and K. Nakagawa, Jpn. Tokkyo Koho JP 60/019767; Jpn. Tokkyo Koho JP 1308258; *Chem. Abstr*., 106, 50063a (1987).
23. M. Uchida, M. Komatsu and K. Nakagawa, US Pat. 4578381; German Pat. DE 3324034; *Chem. Abstr*., 101, P 54936g (1984).
24. M. Uchida, F. Tabusa, M. Komatsu, T. Kanabe and K. Nakagawa, *Chem. Pharm. Bull*., 33, 3775-3786 (1985).

The SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY (ISSN: 2674-6891; 0104-5431) is an open-access journal since 1993. Journal DOI: 10.48141/SBJCHEM.
http://www.sbjchem.com.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
SOUTH. BRAZ. J. CHEM., Vol. 17, No. 17, 2009

ENVIRONMENTAL POLLUTION RESULTING FROM OLIVE OIL PRODUCTION IN PALESTINE

Awni Khatib, Fathi Aqra* and Nader Yaghi
Department of Chemistry,
Faculty of Science and Technology,
Hebron University, P.O. Box 40,
Hebron, West Bank, PALESTINE

Sobhi, Basheer and Isam Sabbah
Research and Development Center,
The Galilee Society, P. O. Box 437
Shefa-Amr, 20200 ISRAEL

Basam Al-Hayek and Mohammed Mosa
Royal Scientific Society,
P.O. Box 1438, Al-Jubaiha 11941,
Amman, JORDAN

ABSTRACT

The level of environmental impact of olive oil production in Palestine was evaluated by measuring the parameters: pH, chemical oxygen demand (COD), biochemical oxygen demand (BOD), total suspended solids (TSS), total dissolved solids (TDS), concentration of fat, oil, and grease (FOG), phenols, electric conductivity (EC) total phosphorus (T-P) and total Kjeldahl nitrogen (TKN, and compared with the Jordanian standard values. The results show that the value of these parameters are too high. A local survey has also been conducted by designing a questionnaire that covers oil production yield, water consumptions in olive washing and in oil recovery, wastewater generation relative to olive processed and oil generated, and solid waste product. The data were collected from 92 local olive oil mills, which were analyzed and organized according to the investigated parameters, and categorized according to local selected areas in the West Bank such as Hebron (South), Nablus (Center) and Jenine (North).

---

*Author to whom all correspondence should be directed, e-mail: fathiaqra2009@hotmail.com

DOI: 10.48141/SBJCHEM.v17.n17.209.9_2009.pdf

The results revealed local variations in oil yield and solid waste product due to variations in the type of olive produced. The olives from the South ware found to contain larger solid content than those from the North, resulting in lower oil yield. The overall results indicated that the average oil yield was 23.7%, the solid waste product was 40,0% while the remaining balance was the water content (36.7%) in the olive fruit. A representative value at 1.7 m^3/ton for wastewater generation was found to be high compared to similar values in other places of the world. This requires a criterious review of the technology and operation of olive mills in Palestine. The characteristics of OMW were found to violate the standards for OMW and this requires the attention of authorities.

KEY WORDS: **Olives, Olive oil, Oil yield, Solid waste, Water Consumption, Wastewater, COD, BOD, TDS, TSS, OMW**

RESUMO:

O impacto da produção de óleo de oliveira na Palestina foi avaliado medindo parâmetros tais como pH, demanda química de oxigênio (DQO), demanda bioquímica de oxigênio (DBO, total de sólidos em suspensão (TSS), total de sólidos dissolvidos (TSD), concentração de óleo e gorduras, fenóis, condutividade elétrica, total de fósforo; total de nitrogênio (Kjeldahl) e comparando com valores padrão do Reino da Jordânia. Os dados experimentais foram coletados em 92 locais diferentes nas regiões de Hebron (Sul), Nablus (Centro) e Jenine (Norte). Os resultados experimentais mostraram um rendimento médio de azeite de 23,7% e dejetos sólidos de 40,0%. O conteúdo de água das azeitonas foi de 36,7%. O valor de 1,7m^3 /ton de água residual pode ser considerado alto quando comparado com outros lugares do mundo e sugere uma avaliação da tecnologia usada na produção do azeite de oliva.

PALAVRAS-CHAVE: Azeitonas, Azeite de oliveira, Rendimento de azeite, Dejetos sólidos, Consumo de água, DQO, DBO, TSS, TSD.

INTRODUCTION

Olive oil extraction is one of the most traditional food industries in the Mediterranean region. In addition to olive oil, this industry produces by-products, in particular olive mill wastewaters (OMWs) and olive husks, which represent a serious environmental problem. Olive mill effluents constitute a serious environmental problem in the Mediterranean sea region due to the unique features associated with this type of agro-waste (i.e. seasonal and localized production, high and diverse organic load, low flow rates). Therefore, it is not surprising that research efforts have been directed towards the development of efficient treatment technologies including various physico-chemical and biological processes. Annually, approximately 1.8x10^6 tons of olive oil is produced worldwide, with a majority being produced in the Mediterranean basin (1-3). Treatability of olive mill wastewater has been investigated using respirometric method (4) and other methods (5-11). Olive oil industries were considered responsible for a great amount of pollution and there has been a strong need for optimization of olive oil waste treatment systems. Study of the inhibitory activity of phenolic compounds found in olive products has been investigated (12). Olive mill sludge (OMS), a by-product resulting from natural evaporation of olive oil processing effluent, poses a major environmental threat (13). In Palestine, olive and olive oil production is an important source of income for a considerable sector of farmers. From an agricultural prospective, olives and their oil have a major contribution in the Palestinian economy. Olive farms cover almost half of the cultivated area in The West Bank, and oil production contributes about 28.7% of the agriculture domestic income. There are about 246 olive mills in the West Bank (14). The operations of these mills are split between modern and traditional models. Naturally, olive mills are generally situated close to olive orchards. The Palestinian Nation Information Center published the overall statistical information about the number of mills, and total amounts of olive and olive oil produced in The West Bank and Gaza between the years 1998 to 2002. There is a slight change in the overall percentage oil yield from year to year. Generally extraction of oil is carried out either by continuous or discontinuous processes, and both methods generate wastewater, which consists of the water contained in olive fruit, the added water required for washing the fruit, and for the centrifugation process. With the continuous process, the average amount of olive mill wastewater (OMW) is 1.2-1.8 m^3/ton of olives, while with the discontinuous process; it is only 0.4 - 0.5 m^3/ton of olives (15).

The color of the wastewater produced by both methods is usually black or reddish black due to the presence of phenolic compounds. The typical composition of OMW includes water (83%), organic compounds (15%), and inorganic chemicals (about 2%). The organic load in OMW is considered one of the highest of all concentrated effluents, being 100-150 times higher than the organic load of domestic wastewater. In general, OMW produced in discontinuous mills contains higher organic load than those generated in continuous mills. OMW is acidic, and contains a high concentration of total dissolved solids (TDS), total suspended solids (TSS), phenols, and other organic matter. The organic content is characterized by high levels of chemical oxygen demand (COD), biochemical oxygen demand (BOD), and very high concentration of fat, oil, and grease (FOG) (Jordanian Ministry of Agriculture 1998). No standard for OMW discharge disposal is currently imposed in Palestine, but the Jordanian standards are adopted (Table 1) (16-18). The BOD and COD maximum concentrations in OMW reach 100,000 and 220,000 mg/L, respectively. The OMW consist of toxic and non-toxic organic materials such as sugars, tannins, polyphenols, polyalcohols, pectins, proteins, and lipids. Ecological stabilization and detoxification of their effects are expensive and ineffective (19-20).

Currently, there is no appropriate method applied for treating OMW in Palestine; it is usually disposed of in sewage systems and/or cesspools in addition to being discharged into water streams and valleys of the region. Due to the presence of a high load of toxic organic compounds, the improper discharge of OMW causes the disruption of biological activities in domestic wastewater ponds. This creates a strong and unpleasant odor due to aerobic digestion in open air systems, and poses a threat to surface and groundwater (21). The disposal of OMW causes serious environmental problems during the olive harvest season. Also, a large amount of solid waste is generated with wastewater.

Table 1. Characteristics of OMW in Jordan and comparison with Jordanian standards and regulations for OMW.

Parameter	Unit	OMW Characteristics Min.-Max.	Maximum Allowable Limit- Jordanian Standards		
			Disposal to wadis and rivers	Reuse for irrigation	Discharge to sanitary systems
pH	SU	5.48-5.91	6.8-9.0	6.5-8.4	5.5-9.5
COD	mg/L	78536-160096	150	undetermined	2100
BOD_5	mg/L	23248-63271	50	undetermined	800
TSS	mg/L	14207-46188	50	100	1100
TDS	mg/L	16984-80355	3000	2000	
FOG	mg/L	2008-13118	5	5	50
Phenol	mg/L	1739-4432	0.002	0.002	10

This emphasizes the environmental pollution associated with olive oil production and highlights the need for this study. In continuation to our earlier studies (22-23), this article describes the water consumption and water extracted during olive oil extraction processes, as well as the physical-chemical analysis of the wastewater from this agribusiness industry. It evaluates the level of environmental impact of olive oil production in Palestine through two routes; first by measuring the parameters PH, COD, BOD, TDS, TSS and TKN of 61 samples from different areas and secondly by conducting a survey covering 92 olive mills in the West Bank.

EXPERIMENTAL

Ninety two olive mills through out The West Bank could be reached and included in the survey. A questionnaire was prepared and the obtained data were analyzed and organized according to the oil yield and solid waste product, and then categorized with respect to local areas in the West Bank; Hebron (south), Nablus (middle) and Jenine (North). Experimental work was performed for determining typical characteristics of OMW in Palestine, by analyzing samples from 61 olive mills from North, Middle and South Palestine during three intervals of the harvest season (beginning, middle and end of season). The methods used to obtained the physical chemical data of the wastewater and the major characteristic methods and analysis of the parameters pH, COD, BOD, TSS, TDS, FOG, TKN, phenols, electric conductivity (EC) and total Phosphorus (T-P) of the wastewater were determined using the standard tests (24).

RESULTS AND DISCUSSION

Analysis of the overall data published by the Palestinian National Information Center (PNIC) [14] provides (Fig 1) oil yield (defined as percentage of amount of oil produced per amount of olive processed), which compares the amount of olives and olive oil produced in various parts of the West Bank and the overall yield in 2002. The largest amounts of olives and olive oil were produced in Jenine. There are some variations in the overall yield between the locations. The estimated average overall yield was 22.3%. Obviously, olives and olive oil production is more popular in the North areas, and the oil yield is higher than that in the South. The obtained fitting R^2 values are above 0.99. The oil yield (%Oil/Olive) has an average value of 23.7%, which is in accordance with the previous reports [5-7], with a difference of 1.4%. Both the linearity of the data and the closeness of the obtained yield to that estimated previously confirm the validity of the survey conducted. This emphasizes the fact that the oil yield in Hebron (South) is lower than that in the Middle or North (Jenine and Nablus). Similar to oil yield data, the obtained fitting R^2 values are high (almost above 0.99) confirming linearity. The fraction of solid waste (quantity of solid waste produced per quantity of processed olives) has an average value of 40,0%. Relatively, olive mills in Hebron area produced a larger fraction of solid waste compared to those in the North areas.

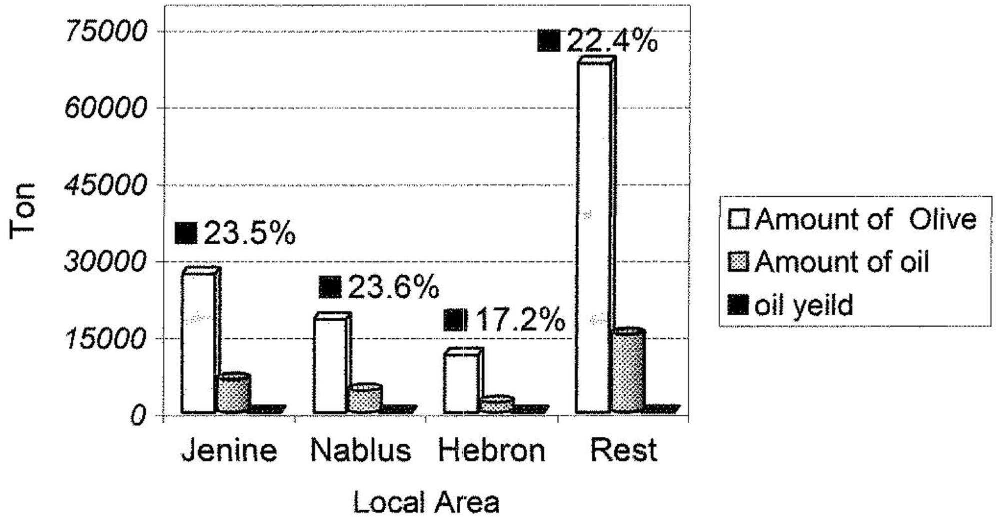


Figure 1.Comparison of the amount of olives and olive oil produced in various parts of The West Bank and Gaza and the overall oil yield in the year 2002

In olive mills, wastewater is generated from various sources including water coming from olives and water used for processing (water consumption). The latest source comes from two different steps; washing of olives and extraction of oil. The designed questionnaire enabled us to gather data for total wastewater, water used for washing and water used in extraction. The summation of water used for washing and extraction provided data for water consumption, while the difference between total wastewater and water consumption provided data for water coming from fruit. The results obtained for the various forms of water are plotted against quantity of processed olives and presented in Figs. 2, 3 and 4. Figure 2 represents the data for water coming from olive fruit versus quantity of processed olives, in Hebron, Nablus and Jenine. Obviously, the general trend is linear, the slope of which provides a representative value of the fraction of water content in the olive fruits. Table 2 provides the results of linear curve fitting for these data. Similar to both oil yield and solid fraction, the obtained fitting R^2 values are all above 0.99. Relatively, olives in Hebron area contain a slightly larger fraction of water than those in the North areas. In general, the fraction of water content in olive (quantity of water from olive fruit per quantity of processed olives) has an average value of nearly 40%.

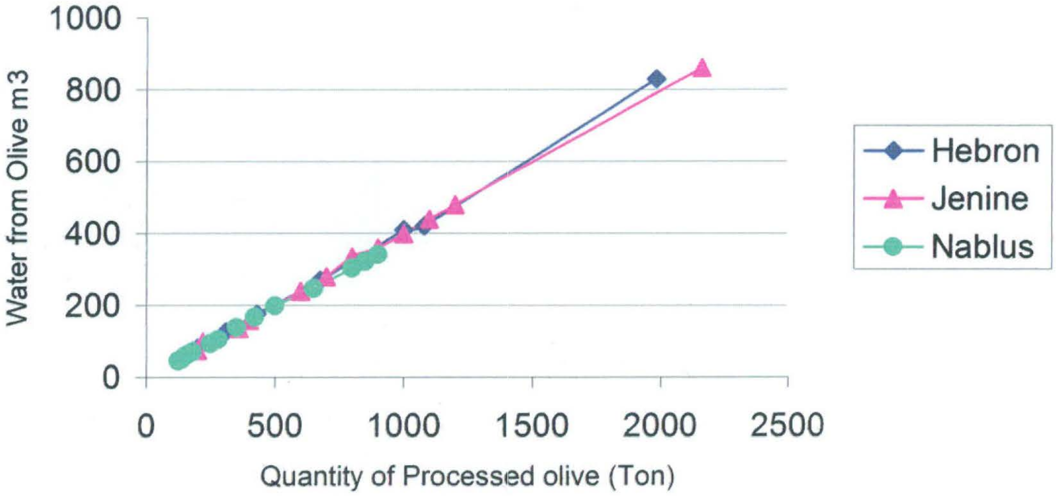


Figure 2.Quantity of water coming from olive fruit versus quantity of processed olives for data from Hebron (triangles), Nablus (circles) and Jenine (diamonds)

Table 2. Results of linear curve fitting for data of water from olive fruit obtained from the conducted survey.

Local Area	Fitting Line	Fitting R^2	Fraction of Water coming from olive fruits
Hebron	Y=0.411 X	0.9983	0.411
Nablus	Y=0.382 X	0.9991	0.382
Jenine	Y=0.401 X	0.9992	0.401
All data as one plot (Average)	Y=0.398 X	0.9988	0.398

Table 3 summarizes the obtained characteristics of olives. From mass balance, the weight of the oil yield, the solid waste and the water content should be equal to the mass of the olive fruit used, that is the ratio must be unity. With the obtained average values, the sum is greater than unity (1.038) with a percentage error of 3.8 %. Thus, these average values provide representative values for olives characteristic in Palestine with reasonable accuracy. Figure 3 represents water consumption (for washing and extraction of oil) versus quantity of processed olive. Similar to other parameters, the tend is linear. Using linear curve fitting for these data provides fitting values (R^2) all above 0.99 as listed in Table 4. The slope represents the average value of water consumption per ton of processed olives. The average value is 1.193 m^3/ton. This value is relatively high, and it is of special concern in Palestine where water resources are very limited. Water consumption shall be minimized not only to reduce the generated wastewater, but also to reduce fresh water demand. This would require a technical review for operation of olive mills.

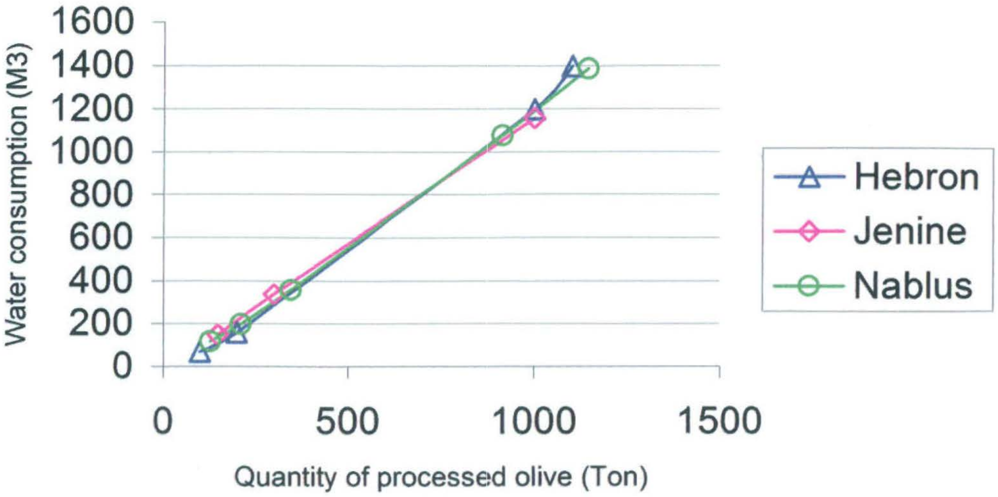


Figure 3.Quantity of consumption water versus quantity of processed olives for data from Hebron (triangles), Nablus (circles) and Jenine (diamonds)

Table 3. Summary of typical olive characteristics in Palestine.

Local area	Fraction of oil*	Fraction of solid*	Fraction of water*	Total*
Hebron	0.219	0.429	0.414	1.062
Nablus	0.248	0.399	0.382	1.029
Jenine	0.243	0.379	0.401	1.023
Average	0.237	0.403	0.398	1.038

* *1Kg*

Table 4. Results of linear curve fitting for water consumption data.

Local Area	Fitting Line	Fitting R^2	Fraction of consumption water
Hebron	Y=1.230X	0.9907	1.230
Nablus	Y=1.188X	0.9945	1.188
Jenine	Y=1.155X	0.999	1.155
All data as one plot (Average)	Y=1.191X	0.9947	1.191

The average value is nearly 1.7 m^3 wastewater/ton olives. This value is within the range of 1.2- 1.8 m^3/ton published in the literature as the range of OMW for continuous processes. For discontinuous processes, the range is 0.4 -0.5 m^3/ton. In Palestine, the operations are split between continuous and discontinuous processes. However, the average value of the volume of OMW in Palestine fits within the range for continuous processes (which generates almost three time more wastewater than discontinuous processes). It is also more close to the maximum limit of that range. Consequently, it is important to perform a technical review for the implemented technology and procedures followed in Palestinian olive mill to reduce the rate of wastewater generation. Table 5 summarizes the results for water consumption and wastewater. In Hebron area, although the levels of production of olives and olive oil are lower than those in the north, both water consumption levels and the total wastewater levels are higher. This indicates that the environmental concerns in Hebron are still considerable. Figure 4 indicates that washing water in Hebron is comparable to that in north area. Thus, the rise in the total wastewater in Hebron comes from the high relative water content and high level of water used for extraction. Figure 5 presents plots of the total wastewater versus quantity of produced oil. Obviously, the curve for Hebron is above the other two curves for Jenine and Nablus. In addition to the previous reasoning regarding wastewater, the oil yield is lower, which contributes in raising this curve above the others.

Table 5. Summary of results of wastewater from olive mills.

Local Area	Water Consumption (*)	Water coming from olive(*)	Total wastewater (*)
Hebron	1.230	0.411	1.641
Nablus	1.188	0.382	1.570
Jenine	1.155	0.401	1.556
All data as one plot (Average)	1.191	0.398	1.589
(*) **m^3 water / ton olives**			

The results of the experimental work for the obtained typical characteristics of olive mills wastewater are illustrated in Table 6. The values obtained at three intervals (beginning, middle and end of the harvest season) are listed and compared to the Jordanian standards for OMW for discharge to sanitary systems. The results indicate that there are some variations from time to time during the season However; the investigation of these variations requires a more extensive analysis and larger amount of data. The average values for the investigated characteristic parameters such as COD, TDS, TSS, BOD, FOG, TKN and phenols are too high and are all above the permitted values and thus the discharge of such OMW violates these standards and should receive sufficient attention from authorities to encounter the environmental problem. Comparison of the data obtained (Table 6) for the investigated parameters of pollution with previously reported data (Table 1) indicates that the chosen olive mills generate wastewater with characteristics within the range of the OMW in Jordan.

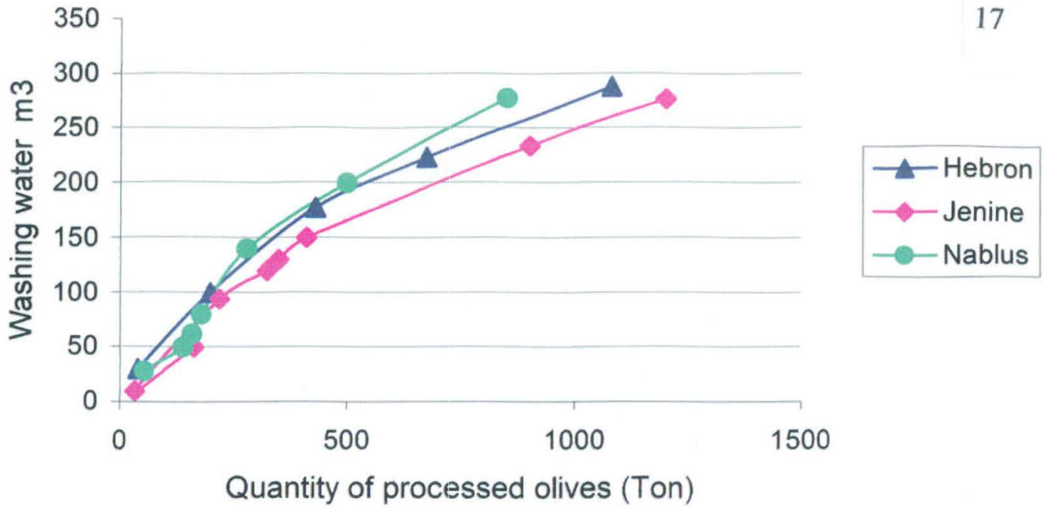


Figure 4.Quantity of washing water versus quantity of processed olive for data from Hebron (triangles), Nablus (circles) and Jenine (diamonds)

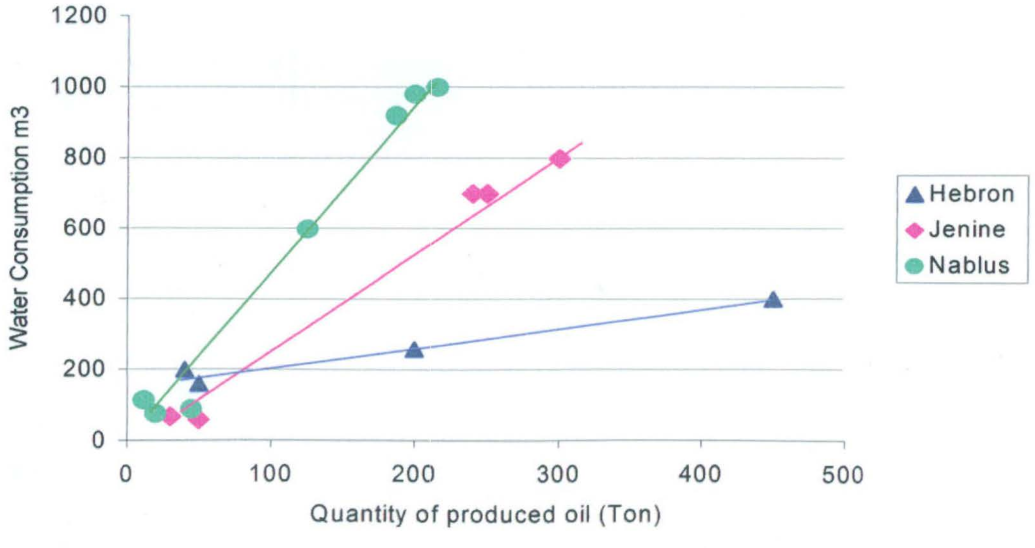


Figure 5.Quantity of total wastewater versus quantity of produced oil for data from Hebron (triangles), Nablus (circles) and Jenine (diamonds)

Table 6. Experimental results of OMW characteristics for sample obtained at the beginning, middle and end of harvest season.

Parameter	Unit	Value				Maximum Allowable Limit- Jordanian Standards(Discharge to sanitary systems)
		Beginning	Middle	End	Average	
pH	SU	4.8	5.08	5.1	4.99	5.5-9.5
COD	mg/L	7121	6190	6815	6708.7	2100
BOD_5	mg/L	88535	98882	109582	98999.7	800
TSS	mg/L	42667	45680	48527	45624.7	1100
TDS	mg/L	11271	17335	22285	16963.7	-
FOG	mg/L	39063	27437	39138	35212.7	50
Phenol	mg/L	3361	3363	4466	3730	10
EC	µs/cm	287	198	228	237.7	-
T-P	mg/L	648	348	587	527.7	-
TKN	mg/L	3057	3087	3304	3149.3	-

CONCLUSION

The ongoing stricter policy rules on environmental issues, recent changes in consumer towards the environmental effects of food production, and even stricter regulations voted by the European Union towards reduction of the use of natural resources initiated a great amount of research towards improving the thermal waste treatment methodology. The olive oil industry continues to be one of the most heavily polluting ones among the food industries. Food industry will have to focus on waste avoidance as well as utilization of the process waste. Application of clean technologies greatly enhances the safety and quality of the product as well as reducing the energy requirements and environmental impact of the food industry. The main environmental impacts of the food sector are aquatic, atmospheric and solid waste emissions. Nowadays, the main treatment method of solid wastes is composting, while recovery and reuse of by-products and wastes as raw materials stand for another effective option. Olive-mill wastes are produced by the industry of olive oil production, which is very important economic activity, particularly, for Mediterranean basin countries, leading to a large environmental problem of current concern in this region. This paper presents a current and interesting theme and highlights the environmental concerns associated with olive oil production in Palestine. Although there is no novelty in this field, the results show some interest. The novelty, contribution to the field, technical quality and depth of research are good. The survey conducted reveals that there are local variations in the parameters investigated due to variations in the types of olives. Oil and water content in olives are dependent on location. The olives from the South are found to contain larger solid content than those from either Middle (Center) or North, resulting in lower oil yield and higher solid generation per ton of olive produced. A representative value at 1.7 m^3/ton for wastewater generation is found to be high compared to those values in other places of the world. This requires a technical review of the technology and operation of olive mills in Palestine. The characteristics of OMW are found to violate the standards for OMW and this requires the attention of authorities. This work presents a warning about the impact of OMW in the environment in Palestine.

REFERENCES

1. C. Paredson, J. Cegarra, A. Roig, M. Sanchez-Monedero and S. Bernal, *Bioresource Technology, 67* , 111(1999)
2. V. Tamburino, S. Zimbone and P. Quattrone, *OLIVAE, 76*, 36(1999)
3. S. Hanifi and I Hadrami, *J. Agronomy*, 7, 63 (2008)
4. B. Kiril, K. Kestioglu and M. Yalili, *Ekoloji 17*, 39(2008)
5. I.S. Arvanitoyannis, A. Kassaveti and S. Stefanatos, *Critical Reviews in Food Science and Nutrition, 47*, 187 (2007)
6. I.S. Arvanitoyannis, A. Kassaveti and S. Stefanatos, *International J. Food Science and Tech., 42*, 852 (2007)
7. I.S. Arvanitoyannis and A. Kassaveti, *International J. Food Science and Tech.., 42,* 281 (2007)
8. E. Bettazzi, M. Morelli, S. Caffaz, C. Caretti, E. Azzari and C. Lubello, *Water Science Tech., 54*, 17 (2006)

9. S. Caffaz, C. Caretti, M. Morelli, C. Lubello and E. Azzari, *Water Science and Tech.*, *55*, 89 (2007)
10. D. Mantzavinos and N. Kalogerakis, *Environ. Int.*, 31, 289(2005)
11. M. Ugurlu and I. Kula, *Environ. Sci. Pollut. Res. Int.*, *14*, 319(2007)
12. J.M. Landete, J.A. Curiel, H. Rodriguez, B. Rivas and R. Munaz, *Food Chemistry*, *107*, 320(2008)
13. S. Hachicha, F. Sellami, J. Cegarra, R. Hachicha, N. Drira, K. Medhioub and E. Ammar, *J. Hazard. Mat.*, *162*, 402(2009)
14. Palestinian National Information Center, 2005 (www.pnic.gov.ps)
15. U. Tomati, E. Galli, F. Fiorelli and L. Pasetti, *International Biodeterioration and Biodegradation*, *38*, 155 (1996)
16. Jordanian Ministry of Agriculture. Annual Report, 1998
17. Jordanian Standards No.202 "Industrial Wastewater" (1991) Ministry of Trade and Industry, Department of Specification and Standards
18. Water Authority Law No.18 (1988) Disposal of Industrial and Commercial Wastewater to the Sewer Network, Jordan
19. R. Borja, A. Martin, R. Maestro, J. Alba and J. Fiestas, *Process Biochem.*, *27*, 231 (1992)
20. V. Martin, R. Borja, V. Alonso, I. Garcia and C. Banks, *Water Research*, *28*, 489 (1995)
21. M. Hamdi, *Applied Biochem. Biotechnol.*, *37*, 155(1992)
22. A. Khatib, F. Aqra, N. Yaghi, Y. Subuh, B. Hayeek, M. Musa, S. Basheer and I. Sabbah, *Am. J. Environ. Sci.*, *5*, 1 (2009)
23. J.A. Morillo, B. Antizar-Ladislao, M. Sánchez, R. Cormenzana and N.J. Russell, *Applied Microbiology and Biotechnology*, *82*, 25(2009)
24. Standard Methods for the Examination of Water and Wastewater, American Public Health Association, Edit. 14, 1981

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
SOUTH. BRAZ. J. CHEM., Vol 17, N° 17, 2009

PHYSICAL CHEMICAL STUDIES OF THE SURFACTANT DILAURYLDIMETHYLAMMONIUM BROMIDE (DLDMAB): AGGREGATION AND CATALYTIC PROPERTIES

Elizabeth Fátima de Souza[a], Sílvia Dani[b] and Lavinel G. Ionescu[c,d]

[a] Faculdade de Química, CEATEC, Pontifícia Universidade Católica de Campinas - PUC-CAMPINAS, Campinas, SP, Brazil
[b] Departamento de Química, Centro de Ciências Naturais e Exatas, Universidade Luterana do Brasil, ULBRA, Canoas, RS, Brazil
[c] Scienco Scientific Consulting Services Viamão, RS, Brazil
[d] Sarmisegetusa Research Group, Santa Fe, New Mexico, USA

ABSTRACT

The micellization of dilauryldimethylammonium bromide (DLDMAB) in water was studied by using surface tension measurements. The critical micellar concentration (CMC) was determined at 25°, 32° and 40 °C and thermodynamic parameters such as the free energy of micellization (ΔG^{o}_{mic})*, enthalpy* (ΔH^{o}_{mic}) *and entropy* (ΔS^{o}_{mic}) *of micellization were measured. The CMC at 25 °C was 4.93 ×* 10^{-5} *M and the corresponding values of the thermodynamic parameters were:* $\Delta G^{o}_{mic} = -5.87$ *kcal/mol;* $\Delta H^{o}_{mic} = -1.12$ *kcal/mol and* $\Delta S^{o}_{mic} = +16.00$ *e.u. Micelles of the surfactant DLDMAB act as catalysts for the alkaline hydrolysis of p-nitrophenyl diphenyl phosphate (NPDPP) with a maximum catalytic factor of approximately 120 compared to 80 for CTAB. Typical activation parameters measured for 1.00 ×* 10^{-3} *M surfactant and 0.005 M NaOH were:* $E_a = 9.7$ *kcal/mol;* $\Delta H^{o\neq} = 9.1$ *kcal/mol;* $\Delta G^{o\neq} = 19.6$ *kcal/mol and* $\Delta S^{o\neq} = -33.9$ *e.u. The kinetic results were also analyzed in terms of the pseudo-phase ion exchange models (PPIE) and showed that the model is applicable to describe the experimental results.*

KEYWORDS: dilauryldimethylammonium bromide; micellization; micellar catalysis; phosphate esters

RESUMO:

A micelização do brometo de dilaurildimetilamônio (DLDMAB) em água foi estudada por medidas de tensão superficial. A concentração micelar crítica (CMC) foi determinada a 25°, 32° e 40 °C e propriedades termodinâmicas tais como a energia livre (ΔG^{o}_{mic}) *de micelização, a entalpia* (ΔH^{o}_{mic}) *e a entropia* (ΔS^{o}_{mic}) *de micelização foram medidas. A 25 °C CMC foi de 4,93 ×* 10^{-5} *M e os valores correspondentes para os parâmetros termodinâmicos foram os seguintes:* $\Delta G^{o}_{mic} = -5{,}87$ *kcal/mol;* $\Delta H^{o}_{mic} = -1{,}12$ *kcal/mol e* $\Delta S^{o}_{mic} = +16{,}00$ *e.u. Micelas do surfactante DLDMAB atuam como catalisadoras para a hidrólise alcalina do p-nitrofenil difenil fosfato (NPDPP), com um fator catalítico máximo de aproximadamente 120, comparável ao de 80 do CTAB. Parâmetros de ativação representativos medidos experimentalmente para DLDMAB 1,00 ×* 10^{-3} *M e NaOH 0,005 M foram:* $E_a = 9{,}7$ *kcal/mol;* $\Delta H^{o\neq} = 9{,}1$ *kcal/mol;* $\Delta G^{o\neq} = 19{,}2$ *kcal/mol e* $\Delta S^{o\neq} = -33{,}9$ *e.u. Os resultados cinéticos foram analisados em termos do modelo de pseudofase de troca iônica (PPIE) e mostraram que o modelo é aplicável para a descrição dos resultados experimentais.*

PALAVRAS CHAVE: brometo de dilaurildimetilamônio, micelização, catálise micelar, ésteres de fosfato

DOI: 10.48141/SBJCHEM.v17.n17.2009.23_2009.pdf

INTRODUCTION

This article reports the results obtained for the study of the micellization of dilauryldimethylammonium bromide (DLDMAB) and its application in the micellar catalyzed hydrolysis of p-nitrophenyl diphenyl phosphate.

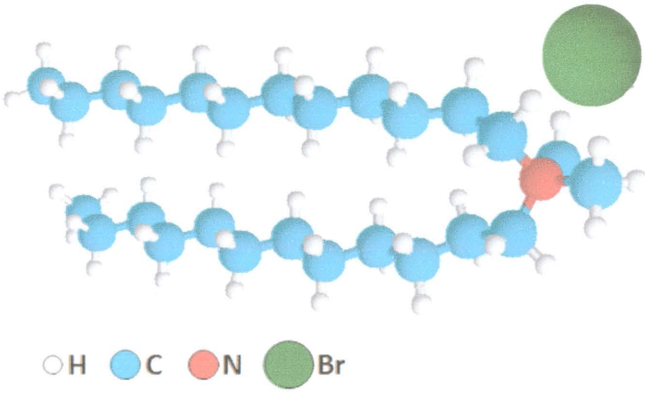


Figure 1. Structural formula of the dilauryldimethylammonium bromide (DLDMAB). **Software ACD/ChemSketch.**

As a part of a systematic study of the micellization process we have studied a variety of surfactants in water, non-aqueous solvents and water solutions containing co-solvents or additives using experimental methods such as surface tensiometry, nuclear magnetic resonance (NMR) and quasi-elastic light scattering (QELS) [1-14]. The study of the surfactant under consideration, DLDMAB, was motivated by its similarity to cetyltrimethylammonium bromide, CTAB, the main difference being the presence of two shorter, C12, carbon tails.

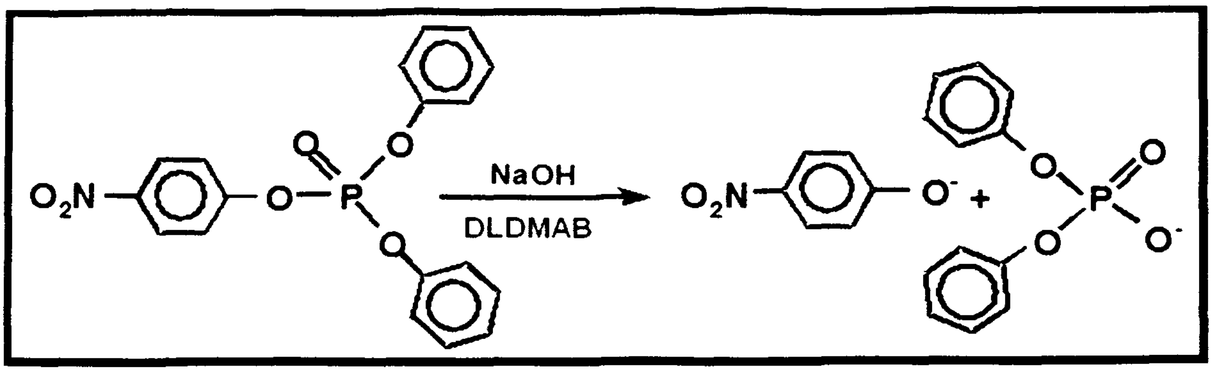
Organic phosphorus compounds, and in particular phosphate esters, are of paramount biological and pharmacological importance and have been widely used as drugs, nerve gases and pesticides [15-17].

In studies described in the literature we have reported the hydrolysis of di- and tri-substituted phosphate esters in the presence of micelles of a variety of surfactants, including some that form functional micelles [18-21].

The micellar catalyzed oxidative cleavage of a carbon-carbon bond in Dicofol(TM) [22] and the micellar catalyzed dehydrochlorination of 1,1,1-trichloro-2,2-bis(*p*-chlorophenyl)ethane (DDT) and some of its derivatives have also been subject of our investigations [23,24].

We have also reported results obtained for the hydrolysis of p-nitrophenyl diphenyl phosphate in aqueous solutions in the presence of micelles of diethyl heptadecyl imidazolinium ethyl sulfate (DEHIES) and CTAB, sodium hydroxide and dimethylsulfoxide (DMSO) and analyzed the effect of internal pressure of the medium, dielectric constant, donor number and polarity of the solvent and the effect of DMSO on micellization [25-29]. In a more recent article we have described the physical chemical studies of the aggregation and catalytic properties of the surfactant cetyldimethylethylammonium bromide (CDEAB) [30].

The present article deals with the study of the hydrolysis of p-nitrophenyl diphenyl phosphate (NPDPP) in the presence of micelles of dilauryldimethylammonium bromide (DLDMAB) in aqueous solutions containing NaOH, as illustrated by the Scheme 1.



Scheme 1. Hydrolysis of p-nitrophenyl diphenyl phosphate (NPDPP) in the presence of micelles of dilauryldimethylammonium bromide (DLDMAB) within aqueous solutions containing sodium hydroxide (NaOH).

EXPERIMENTAL PROCEDURE

Materials. The p-nitrophenyl diphenyl phosphate (NPDPP) was prepared using standard methods [31,32]. A sample was also obtained from Prof. Fred Menger, Emory University, Atlanta, Georgia, USA. The surfactant dilauryldimethylammonium bromide (DLDMAB) was purchased from Chem. Service, West Chester, Pa., USA. The sodium hydroxide was analytical reagent grade and was purchased from Merck Co.

Surface Tension Measurements. All solutions were prepared volumetrically with deionized double distilled water and contained a series of at least fifteen different concentrations of DLDMAB. The surface tension of the DLDMAB-H_2O solutions was measured at 25°, 32° and 40 °C by means of a Fisher Model 21, Semi-Automatic Tensiometer. Ten milliliters aliquots of the solutions were placed in a Petri dish with a diameter of 6 cm. The temperature of the solutions was brought to the chosen temperature using a water bath and the Petri dish was kept at the desired temperature by placing it in a container through which water was circulated from the constant temperature bath. The tensiometer was set a constant height. The final surface tension of any solution was the average of at least three independent measurements.

The critical micellar concentrations (CMC's) were determined from plots of the surface tension of the solutions versus the concentration or log concentration of DLDMAB. The marked change in the plots was taken as an indication of micelle formation and the inflection point was considered to correspond to the CMC [33].

The thermodynamic parameters ΔG^o_{mic}, ΔH^o_{mic} and ΔS^o_{mic} were determined using standard equations [34,35] derived on the basis of the assumption that the process of micellization involves the formation of a distinct micellar phase at the CMC and that the concentration of monomers in solution is constant, once micelles are formed. The experimental accuracy in the values determined for ΔG^o_{mic} is about ± 100 cal/mole. On the other hand, ΔH^o_{mic} and ΔS^o_{mic} are more approximate since they were calculated on the basis of measurements at three temperatures only.

Kinetic Measurements. The hydrolysis of p-nitrophenyl diphenyl phosphate was studied spectrophotometrically by measuring the rate of appearance of the p-nitrophenoxide anion at 4030 Å with a Varian DMS-80 spectrophotometer equipped with a temperature controlled cell compartment. The reaction was studied at 15°, 25° and 35°C at various concentrations of NaOH and MDBTACL. The pseudo-first order rate constant (k_ψ), in s^{-1}, was determined from linear plots of logarithm of absorbance versus time and the second order rate constants (k_{2m}) in the micellar phase and (k_2^0) in the aqueous phase, in $s^{-1}M^{-1}$, were calculated from k_ψ and the hydroxide ion concentration. Activation parameters such as the activation energy (E_a), the activation enthalpy ($\Delta H^{o\neq}$) and the activation entropy ($\Delta S^{o\neq}$) were determined from experimental k_ψ values measured at three different temperatures using the following equations.

$$\ln k_\psi = \ln A - (E_a/R)(1/T) \quad (1)$$

$$\Delta H^{o\neq} = E_a - RT \quad (2)$$

$$\Delta S^{o\neq} = 4.576 (\log k_\psi - 10.753 - \log T + E_a/4.576T) \quad (3)$$

$$\Delta G^{o\neq} = \Delta H^{o\neq} + \Delta S^{o\neq} \quad (4)$$

where, R corresponds to the gas constant and T to the absolute temperature.

RESULTS AND DISCUSSION

Representative results obtained for the surface tension of DLDMAB in water solutions at 25°, 32° and 40°C are illustrated in Figure 2.

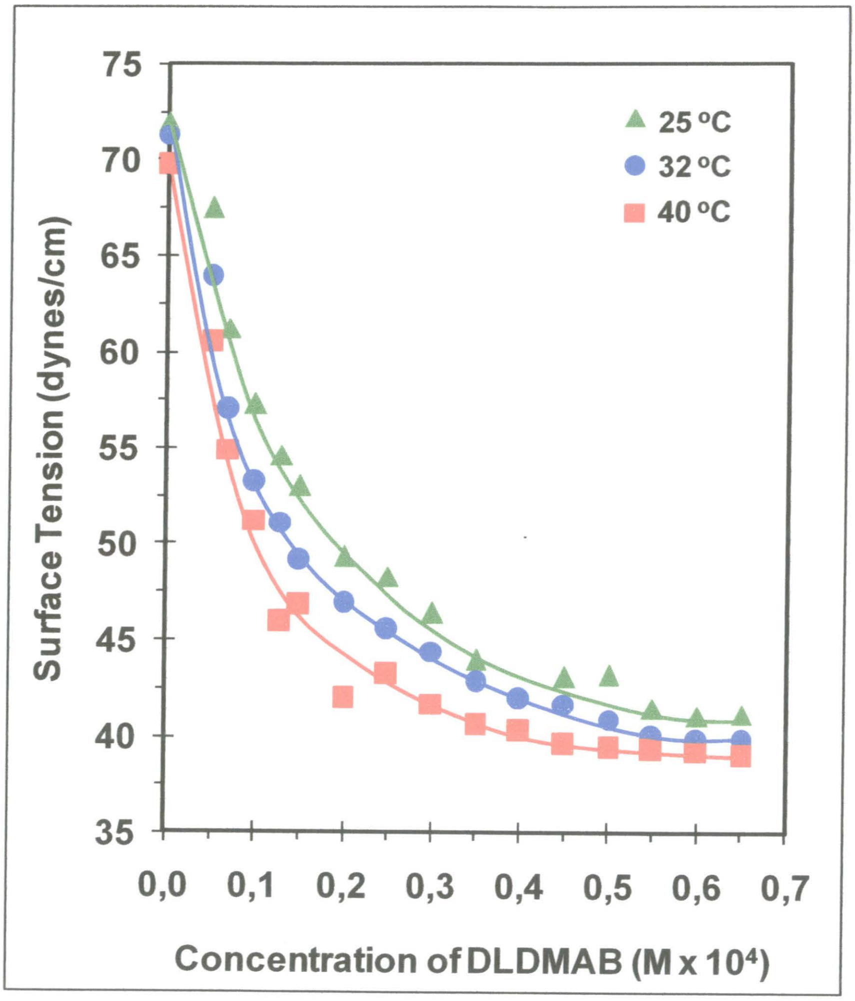


Figure 2. Plot of Surface Tension versus Concentration of Dilauryldimethylammonium Bromide (DLDMAB) in Water at 25°, 32° and 40°C.

All plots of surface tension versus the concentration of DLDMAB exhibited initial marked drops and subsequent leveled off. The inflection point in the given curve was taken as the CMC. At times, plots of surface tension versus the logarithm of the concentration of surfactant gave a better determination for the CMC. Such results are shown in Figure 3 for the same temperatures.

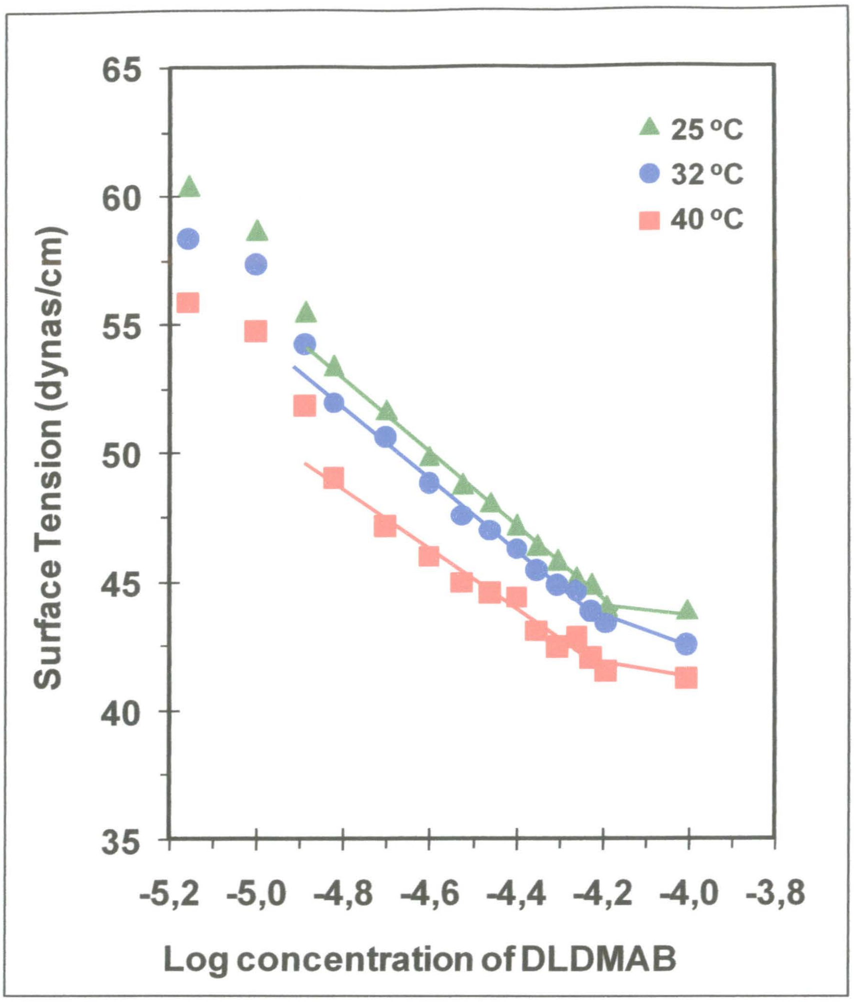


Figure 3. Plot of Surface Tension versus Logarithm of the Concentration of Dilauryldimethylammonium bromide (DLDMAB) in Water at 25° and 32° and 40°C.

The experimental results obtained for the critical micellar concentration (CMC) are shown in Table I and compared to cetyltrimethylammonium bromide (CTAB). Table II shows the experimental values obtained for the thermodynamic functions, i.e., the standard free energy of micellization, ΔG^o_{mic}, the enthalpy, ΔH^o_{mic}, and the standard entropy of micellization ΔS^o_{mic} at 25°C, again compared to CTAB [7,11,14]. As expected, the difference between the experimental values obtained for the CMC and the thermodynamic properties for the two surfactants is small, the difference being mainly due to the nature of the tails.

Table I. Critical Micellar Concentration (CMC) of Dilauryldimethylammonium Bromide (DLDMAB) in Aqueous Solutions Compared to CTAB [14,29]

Surfactant	**Temperature (°C)**		
	25	**32**	**40**
DLDMAB	4.93×10^{-5} M	5.24×10^{-5} M	5.40×10^{-5} M
CTAB	9.00×10^{-4} M	--	10.00×10^{-4} M

Table II. Some Thermodynamic Properties for the Formation of Micelles of Dilauryldimethylammonium Bromide (DLDMAB) in Water at 25 °C Compared to CTAB [14,29]

Surfactant	**Free Energy of Micellization at 25 °C ΔG^0_{mic} (kcal/mole)**	**Enthalpy of Micellization ΔH^0_{mic} (kcal/mole)**	**Entropy of Micellization at 25 °C ΔS^0_{mic} (e.u.)**
DLDMAB	-5.87	-1.12	+16.00
CTAB	-4.14	-1.03	+10.43

Typical profiles for the pseudo-first order rate constant, k_ψ, as a function of the concentration of DLDMAB for the hydrolysis of p-nitrophenyl diphenyl phosphate (NPDPP) at 25°C in aqueous solutions containing NaOH between 0.002 M to 0.005 M are shown in Figure 4 and between 0.0005 and 0.005 M in Figure 5.

The experimental rate profiles obtained in the presence of DLDMAB are characteristic of micellar catalyzed reaction in aqueous solutions with a maximum at 1.0×10^{-3}M. The addition of DLDMAB to the reaction medium causes an increase in the rate of hydrolysis up to a point (the maximum in rate) where there is total incorporation of the substrate in the micellar phase. Subsequent addition of the surfactant causes a decrease in the reaction rate, probably due to the dilution of the reactive counter-ions in the Stern layer of a higher number of micelles. The catalytic factor measured is approximately 120 compared to 80 for CTAB and CDEAB [29]. The higher catalytic factor (k_ψ/k_W) can probably be explained by the presence of the two hydrophobic tails of the surfactant DLDMAB.

Representative activation parameters determined for the reaction with DLDMAB are shown in Table III and compared to CTAB and CDEAB [30]. As can be seen from the analysis of the results the activation parameters for the three surfactants are comparable and similar and to others measured for micellar catalyzed reactions [30,31].

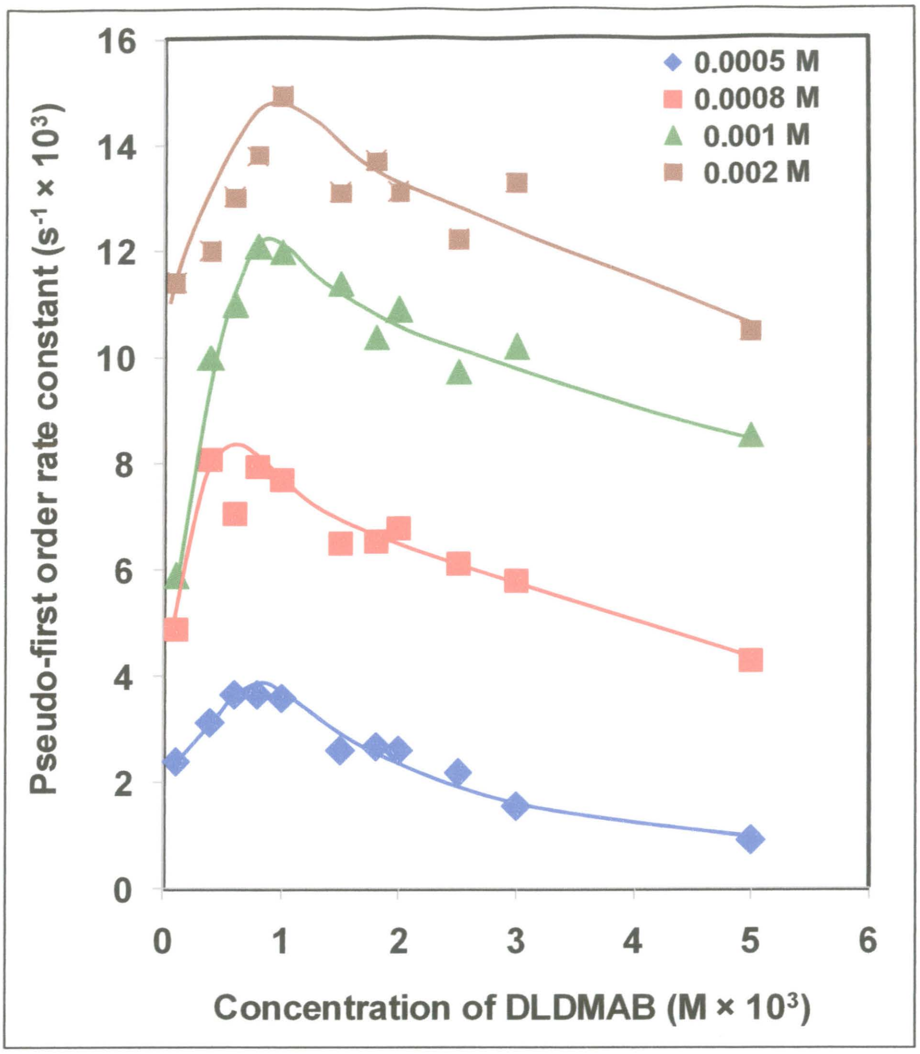


Figure 4. Rate Profiles for the Hydrolysis of p-Nitrophenyl Diphenyl Phosphate in Aqueous Solutions of NaOH (0.0005 – 0.002 M) and Various Concentrations of MDBTACL at 25°C

Table III. Activation Parameters for the Hydrolysis of p-Nitrophenyl Diphenyl Phosphate in Aqueous Solutions of 0.005 M NaOH in the Presence of DLDMAB, CDEAB and CTAB [28-30] at 25 °C.

Surfactant	**Concentration (M)**	**E_a (kcal/mole)**	**$\Delta H^{0\neq}$ (kcal/mole)**	**$\Delta G^{0\neq}$ (kcal/mole)**	**$\Delta S^{0\neq}$ (e.u.)**
No surfactant	--	+ 15.2	+14.6	+21.3	-22.2
DLDMAB	1,0 x 10^{-3}	+ 9.7	+ 9.1	+19.2	-33.9
CDEAB	18 x 10^{-4}	+ 9.0	+ 8.4	+19.2	-36.3
CTAB	15 x 10^{-4}	+ 11.4	+10.8	+18.7	-26.6
CTAB	20 x 10^{-4}	+ 10.5	+ 9.9	+18.8	-29.9

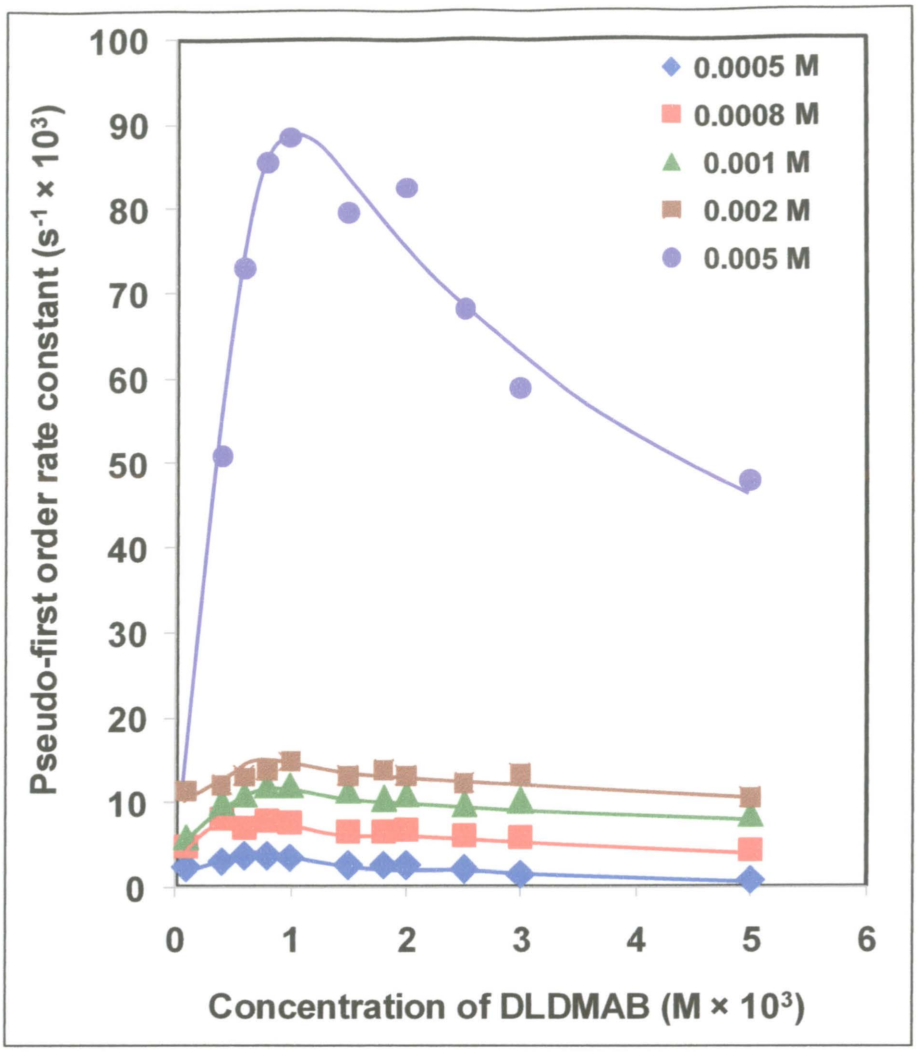


Figure 5. Rate Profiles for the Hydrolysis of p-Nitrophenyl Diphenyl Phosphate in Aqueous Solutions of NaOH (0.0005 – 0.005 M) and Various Concentrations of MDBTACL at 25°C

Most of the models proposed for micellar catalysis [34-55] consider the partition coefficient for the substrate between the micellar and aqueous phase and the distribution of the reagents between the two phases. The hydrolysis of NPDPP with hydroxide ion in the presence of DLDMAB may be considered a bimolecular reaction of OH^- ion and the substrate. Since the concentration of OH^- in the micellar phase is dependent on the concentration of both bromide ions and surfactant, a quantitative treatment of the reaction rate must consider ion exchange on or near the micellar surface. For the reaction under consideration, the model proposed by Quina and Chaimovich [41] reduces to Equation 5, which gives the theoretical dependence of the pseudo-first order constant, k_ψ, as a function of the total hydroxide ion concentration:

$$k_\psi = \frac{\{(k_{2m}/V)K_s K_{OH/Br}[(Br)_m/(Br)_w] + k_2^0\}(OH)_T}{(1+K_s C_D)[1+K_{OH/Br}(Br)_m(Br)_w]} \qquad (5)$$

where, C_D is the concentration of micellized surfactant, V is the molar volume of the reactive region at the micellar surface, k_ψ is the pseudo-first order rate constant, k_{2m} is the second order rate constant in the micellar phase, k_2^0 is the second order constant in the aqueous phase, $K_{OH/Br}$ is the ion exchange constant, K_s is the binding constant for the substrate, $(Br)_m$ is the concentration of Br^- in micellar phase, $(Br)_w$ is the concentration of Br^- in aqueous phase, $(OH)_T$ is the total concentration of hydroxide ions and V is the molar volume of surfactant.

With substrates such as p-nitrophenyl diphenyl phosphate that are very insoluble in water and are solubilized by DLDMAB the expression for k_ψ can be reduced to a simpler form given by Equation (6):

$$k_\psi = \frac{k_{2m}}{C_D V}(OH)_T \frac{K_{OH/Br}[(Br)_m/(Br)_w]}{[1 + K_{OH/Br}(Br)_m(Br)_w]} \qquad (6)$$

The concentration of Br^- in the micellar and aqueous phases can be obtained using the following equations [38-42]:

$$A_1 = C_D + CMC + K_{OH/Br}\,(OH)_T + (1 - \alpha)\, C_D\, K_{OH/Br} \qquad (7)$$

$$(OH)_m = \frac{(-A_1) + \left[(A_1)^2 + 4(1 - K_{OH/Br})(OH)_T K_{OH/Br}(1 - \alpha)c\right]^{0.5}}{2(1 - K_{OH/Br})} \qquad (8)$$

$$(Br)_m = (1 - \alpha)\, C_D - (OH)_m \qquad (9)$$

$$(Br)_w = \alpha\, C_D + CMC + (OH)_m \qquad (10)$$

where CMC is the critical micellar concentration, α is the degree of ionization of the micelle and $(OH)_m$ is the concentration of OH^- in the micellar phase. For systems exhibiting saturation behavior, further analysis of the results using the PPIE treatment as modified to account for HO^-/Br^- exchange allows the evaluation of substrate binding constants, K_S, and micellar rate constants, k_{2m}.[49]

We have calculated the theoretical values of k_ψ for the reaction discussed above using $\overline{V} = 0.37$ L/mol [44]; $K_{OH/Br} = 0.08$ [45]; $\alpha = 0.20$ [46,47] and various concentrations of DLDMAB and NaOH.

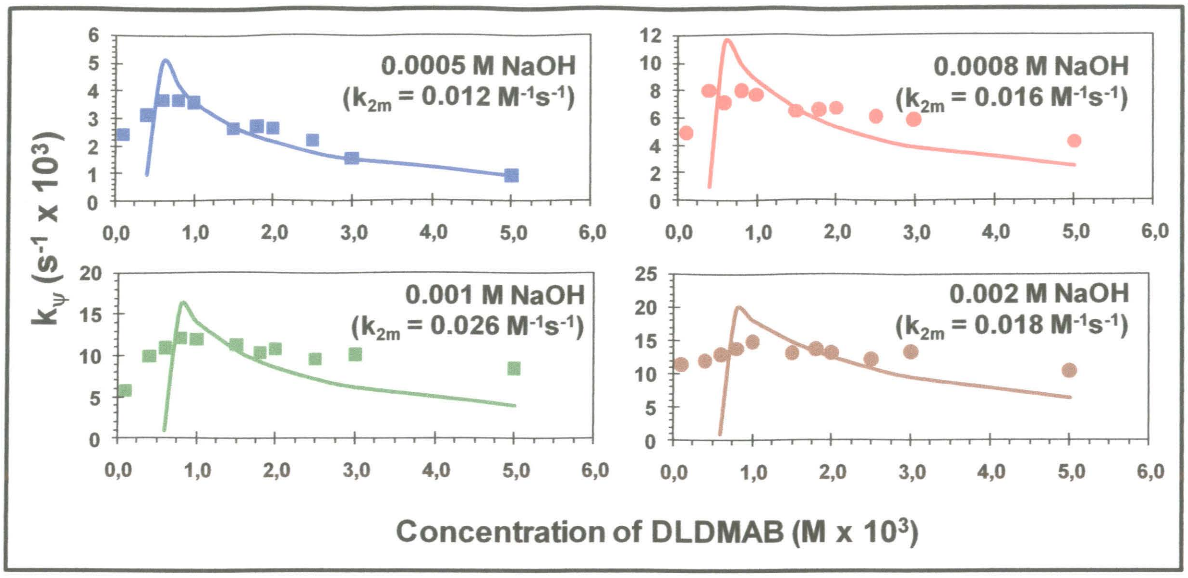


Figure 6. Experimental and Theoretical (—) k_ψ Values for the Hydrolysis of p-Nitrophenyl Diphenyl Phosphate in Aqueous Solutions of NaOH and Various Concentrations of DLDMAB at 25°C.

The values for k_ψ were calculated using different values for k_{2m} ranging from 0.012 $M^{-1}s^{-1}$ and 0.026 $M^{-1}s^{-1}$ and are illustrated in Figure 6. As can be seen, the pseudo-phase ion exchange model gives a reasonable agreement for this micellar catalyzed reaction. At low concentrations of DLDMAB (bellow the CMC), the presence of the highly hydrophobic solute probably induces the formation of kinetically active premicelles.

ACKNOWLEDGMENTS

Support received from Sarmisegetusa Research Group, Las Cruces and Santa Fe, New Mexico, USA is gratefully acknowledged. EFS also acknowledges the financial support from CNPq - National Research Council of Brazil (310347/2006-8).

REFERENCES

1. L. G. Ionescu and J. K. Tsang, *Rev. Roum. Biochim., 15*, 211 (1978).
2. L. G. Ionescu, T. Tokuhiro, B. J. Czerniawski and E. S. Smith, in "*Solution Chemistry of Surfactants*", K. L. Mittal, Ed., Plenum Press, New York, Vol. 1, p. 487, 1979.
3. T. Tokuhiro and L. G. Ionescu, in "*Solution Chemistry of Surfactants*", K. L. Mittal, Ed., Plenum Press, New York, Vol. 1, p. 507, 1979.
4. L. G. Ionescu, T. Tokuhiro and B. J. Czerniawski , *Bull. Chem. Soc. Jpn., 52*, 922 (1979).
5. T. Tokuhiro, D. S. Fung and L. G. Ionescu,. *J. Chem. Soc. Faraday Trans. II, 75*, 975 (1979).
6. L. G. Ionescu and B. J. Czerniawski, *Rev. Roum. Biochim., 18*, 103 (1981).
7. L. G. Ionescu, and V. T. De Fávere in "*Solution Behavior of Surfactants: Theoretical and Applied Aspects*", K. L. Mittal and E. J. Fendler, Eds., Plenum Press, New York, Vol. 1, p. 407, 1982.
8. L. G. Ionescu, *Arch. Biol. Med. Exp., 12(2)*, 272 (1979).
9. L. G. Ionescu and D. S. Fung, *Bull. Chem. Soc. Jpn., 54*, 2503 (1981).

10. L. G. Ionescu, and D. S. Fung, *J. Chem. Soc. Faraday Trans. I, 77,* 2907 (1981).
11. L. G. Ionescu, L. S. Romanesco and F. Nome in "*Surfactants in Solution*", K. L. Mittal and B. Lindman, Eds., Plenum Press, New York, Vol. 2, p. 789, 1984.
12. L. G. Ionescu and P. E. De Brito Moreira, *Atual. Fís. Quim. Org., 2,* 79 (1984).
13. L. G. Ionescu, *Química Nova, 8(3),* 191 (1985).
14. L. G. Ionescu, S. M. H. Probst, E. F. de Souza, *South. Braz. J. Chem., 6(7),* 67-76 (1998).
15. M. C. Newman, M. A. Unger "*Fundamentals of Ecotoxicology*", 2 ed. CRC Press, Boca Raton, 2003. 458 p.
16. C. Baird, "Química Ambiental"; M. A. L. Recio, L. C. M. Carrera, M. T. Grassi, Trad., 2 ed. Bookman, Porto Alegre, 2002. 622 p.
17. T. Katagi in "Reviews of Environmental Contamination and Toxicology", D. M. Whitacre, Ed., Springer, New York, p. 99-102, 2008.
18. C. A. Bunton, L. G. Ionescu, *J. Am. Chem. Soc., 95,* 2912 (1973).
19. L. G. Ionescu, D. A. Martinez, *J. Colo. Wyo. Acad. Sci., 7,* 13 (1974).
20. L. G. Ionescu, *Bull. N. Mex. Acad. Sci., 14,* 65 (1973).
21. C. A. Bunton, S. Diaz, J.M. Hellyer, I. Ihara, L. G. Ionescu, *J. Org. Chem., 40,* 2313 (1975).
22. F. Nome, E. W. Schwingel, L. G. Ionescu, *J. Org. Chem., 45,* 705 (1980).
23. F. Nome, A. Rubira, L. G. Ionescu, *J. Phys. Chem., 86,* 1181 (1982).
24. L. G. Ionescu, F. Nome, In *Surfactants in Solution*; K. L. Mittal, B. Lindman, Eds.; Plenum Press: New York, Vol. 2, p. 1107, 1984.
25. L. G. Ionescu, E. F. Souza, *South. Braz. J. Chem., 1,* 75 (1993).
26. L. G. Ionescu, E. F. Souza, in "*Surfactants in Solution*"; A. K. Chattopadhyay, K. L. Mittal, Eds.; Marcel Dekker: New York, Vol. 64, p. 123, 1996.
27. L. G. Ionescu, E. F. Souza, *South. Braz. J. Chem., 3,* 63 (1995).
28. L. G. Ionescu, D. A. R. Rubio, E. F. Souza, *South. Braz. J. Chem., 4,* 59 (1996).
29. E. F. Souza, L. G. Ionescu, *Coll. and Surfaces A, 149,* 609 (1999).
20. L.G. Ionescu, S. Dani and E.F. Souza, *South. Braz. J. Chem., 7(8),* 105 (1999).
31. L.G. Ionescu, V.L. Trindade and E.F. Souza, *Langmuir, 16(3),* 988 (2000).
32. A. M. Ross, J. Toet, *Rec. Trav. Chim., 77,* 1946 (1958).
33. A. S. Kirby, J. Jounas, *J. Chem. Soc. B* , 1165 (1970).
34. N. Muller in "*Reaction Kynetics in Micelles*", E. H. Cordes, Ed., Plenum Press, New York, p.1-23, 1973.
35. D. G. Hall, *Trans. Faraday Soc., 66,* 1351, 1359 (1970).
36. S. Dani, Master's Thesis, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazsil, 1991, 169 pp.
37. J. H. Fendler, E. J. Fendler, "*Catalysis in Micellar and Macromolecular Systems,*" Academic Press, New York, 1975.
38. I. V. Berezin, K. Martinek, A. K. Yatsimirskii, *Russ. Chem. Rev., 42,* 787 (1973).
39. K. Martinek, A. K. Yatsimirskii, A. V. Levasov, I. V. Berezin, in "*Solubilization and Microemulsion"s*; K. L. Mittal, Plenum Press, New York, Vol. 2, p. 489, 1977.
40. L. S. Romsted, in "*Solubilization and Microemulsions*"; K. L. Mittal, Ed., Plenum Press, New York, Vol. 2, p. 509, 1977.
41. F. Quina, H. Chaimovich, *J. Phys. Chem., 83,* 1844 (1979).
42. N. Funasaki, *J. Phys. Chem., 83,* 1998 (1979).
43. C. Otero, E. Rodenas, *Can. J. Chem., 63,* 2892 (1984).
44. R.F. Bakeeva, L.A. Kudryavtseva, V.E. Bel'skii, S.B. Fedorov, B.E. Inanov, *Russ. Chem. Bull, 45(8),* 1900 (1996).

45. L.Ya. Zakharova, L.A. Kudryavtseva, A. I. Konovalov, *Russ. Chem. Bull, 47(10)*, 1868 (1998).
46. O. El Seoud, A. Blasko, C.A. Bunton, *Langmuir, 10*, 653 (1994).
47. T. A. S. Brandão, E. S. Orth, W. R. Rocha, A. J. Bortoluzzi, C. A. Bunton, F. Nome, *J. Org. Chem, 207*, 3800 (2007).
48. R. C. Beber, C. A. Bunton, G. Savelli, F. Nome, *Prog. Polymer Sci, 128*, 249 (2004).
49. X. Han, V. K. Balakrishnan, E. Buncel, *Langmuir*, *23* (12), 6519 (2007).
50. E. A. Karpichev , T. M. Prokop'eva, M. K. Turovskaya, V. A. Mikhailov, I. V. Kapitanov, V. A. Savelova, A. F. Popov, *Theor. Exp. Chem.*, *43* (4), 241 (2007).
51. M. Ferrit, C. Del Valle, F. Martinez, *J. Molec. Liquids*, *142* (1-3), 64 (2008).
52. M. Li, X.-G. Meng, J. Du, P. Zhang, W.-P. Zeng, Y. Liu, X.-C. Zeng, *J. Dispersion Sci. Technol.*, *30* (8), 1181 (2009).
53. M. N. Khan, E. Ismail, *J. Phys. Chem. A*, *113* (23), 6484 (2009).
54. Y. Zhu, W. T. Ford, *Langmuir*, *25* (6), 3435, (2009).
55. E. Fernández, L. García-Río, M. Méndez-Pérez, P. Rodríguez-Dafonte, *J. Phys. Chem. B*, *113* (26), 8828 (2009).

The SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY (ISSN: 2674-6891; 0104-5431) is an open-access journal since 1993. Journal DOI: 10.48141/SBJCHEM.
http://www.sbjchem.com.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
SOUTH. BRAZ. J. CHEM., Vol. 17, No. 17, 2009

CONDUCTOMETRIC EVALUATION OF ASSOCIATION CONSTANTS FOR AQUEOUS SOLUTIONS OF $CoCl_2$ IN THE ABSENCE AND PRESENCE OF A MAGNETIC FIELD

Maany A. Hamada*, Nagah El-Shishtawi ** and Esam A.Gomaa *
Department of Chemistry* and Department of Physics **
Faculty of Science, Mansoura University,
35516-Mansoura, EGYPT

ABSTRACT

The association constants K_A for $CoCl_2$ aqueous solutions were calculated using the experimental conductivity values at different salt concentrations. The molar conductivities were measured in the absence and presence of a magnetic field with an average power of 0.677 KGauss.

A new equation for asymmetric 1:2 salts was suggested and used .This equation was derived from Ostwald, Arrhenius and Fuoss-Shedlovsky theories. The results obtained were discussed and the effect of the magnetic field on the association constants was explained.

RESUMO

As constantes de associação, K_A, para soluções aquosas de $CoCl_2$ foram calculadas a partir de valores experimentais da condutividade para várias concentrações do sal. As condutividades molares foram medidas na ausência e na presença de um campo magnético médio de 0.677 KGauss.

Uma nova equação foi sugerida para sais assimétricos 1:2 e foi usada. Esta equação foi derivada a partir das teorias de Ostwald, Arrhenius e Fuoss-Shedlovsky. Os resultados obtidos foram discutidos e o efeito do campo magnético sobre as constantes de associação foi explicado.

DOI: 10.48141/SBJCHEM.v17.n17.2009.35_2009.pdf

INTRODUCTION

Association of salt solutions were studied by Barthel (1) and Deepa (2). The ion-solvent interactions was explained in different electrolytes and polymers using conductivity, relaxation and FTIR measurements(1). Schori *et al.*, (3.4) used conductivity as an electrical method for studying the complexation of Na^+ with some crown ethers in DMF and in dimethoxyethane solutions.

Different Fuoss theories - Fuoss-Shedlovsky, Fuoss-Kraus, Fuoss-Edelson and Fuoss-Debye theories (5, 6) were used for the estimation of the association constants (K_A) for symmetric electrolytes (1:1 electrolytes).

On applying these theories for the association of asymmetric electrolytes, low values of the association constants are obtained .These values lie in the same range of symmetric electrolytes which is not accepted due to the presence of increased number of ions. Therefore, a new equation was required for 1:2 asymmetric electrolytes which facilitates the calculation of K_A easily and accurately.

This paper deals with the application of a new equation for the asymmetric 1:2 salts which are ionized in solutions. This equation was derived from Fuoss-Shedlovsky and Ostwald laws (6). Also, the effect of magnetic field on the association of strong electrolytes was studied. This effect has never been reported before in the literature.

EXPERIMENTAL

Cobalt chloride was provided by Merck Co. Different $CoCl_2$ amounts were added to 5 ml portions of doubly distilled water contained in test tubes and dissolved to give different corresponding concentrations. These solutions were thermostated at 298.15 K for two hours by using a thermostat of the type (Polyscience 8105, USA) and used for measurement of densities, conductivities and capacitance . A cell of two solid carbon electrodes with 1cm distance and cell constant = 0.96 was joined with a multimeter of the type [Macom (MX 620)] for the measurement of conductivity and capacitance. The densities were measured by weighing 1 ml of each solution using Mettler Toledo DA analytical balance.

A two pole permanent magnet (power of 1.26 KGauss with an average value of 0.677 Kilo Gauss between the two poles, measured by a Gauss Meter Model GM-54) was used to study the effect of the magnetic field. The tube containing the solution was placed between the two poles of the magnet and the conductivity was then measured.

RESULTS AND DISCUSSION

From the densities of different $CoCl_2$ solutions ranging from 0.084-0.520 mole/l the molar volumes were calculated by dividing the molecular weight by the density (V= M.W/d) and the calculated values are shown in Table 1. From the molar volumes the solvated radii for the solutions used were also calculated by using equation 1(7; 8).

$$r = \sqrt[3]{V.0.239N} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\; (1)$$

where N is Avogadro's number.

The relative capacitances of solutions $\in$ were estimated by dividing the measured capacity values (in micro Farad, μ F) of the electrolytes by that of pure doubly distilled water and their values are listed also in Table 1.

The mean activity coefficients ($\gamma_{\pm}$) were calculated by the use of modified Born equation (8, 9) as given in equation (2).

$$\log \gamma_{\pm} = -\frac{AZ^{+}Z^{-}\sqrt{C}}{1+Br\sqrt{C}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

where Z^+ and Z^- are the charges of the positive and negative ions of the electrolyte used, r the solvated radius and A, B are constants equal:

$$\mathbf{A = 1.823.10^{6}\,(\in.T)^{-3/2} \ldots\ldots\ldots\ldots\ldots (3)}$$

$$\mathbf{B = 50.29\,(\in.T)^{-½} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)}$$

where $\in$ is the measured relative capacitances in micro Farad of the solutions. The calculated mean activity coefficients are presented in Table 1 for different $CoCl_2$ solutions. It was concluded that the activity coefficients increased by increasing the $CoCl_2$ concentrations due to more interactions in concentrated solutions.

Table 1. Molar volumes (V), relative capacitances (ε), solvated radii (r), Born constants A, B and mean activity coefficients ($\gamma_\pm$) of different $CoCl_2$ concentrations at 298.15 K.

Cm $CoCl_2$ conc. Mol/gl	$\sqrt{C_m}$	V Cm^3/mol	∈*	r in (A°)	A	B $\times 10^8$	- Log $\gamma_\pm$
0.084	**0.29**	**130.623**	**32.5**	**3.727**	**1.913**	**0.511**	**0.712**
0.100	**0.32**	**130.491**	**34.5**	**3.726**	**1.749**	**0.496**	**0.699**
0.150	**0.39**	**130.229**	**44.0**	**3.722**	**1.214**	**0.439**	**0.577**
0.210	**0.46**	**129.839**	**56.0**	**3.719**	**0.834**	**0.388**	**0.460**
0.250	**0.50**	**129.580**	**64.0**	**3.717**	**0.692**	**0.364**	**0.413**
0.340	**0.58**	**129.809**	**80.5**	**3.709**	**0.491**	**0.325**	**0.336**
0.420	**0.65**	**128.299**	**96.5**	**3.705**	**0.374**	**0.297**	**0.283**
0.520	**0.72**	**127.543**	**115.5**	**3.698**	**0.286**	**0.271**	**0.240**

*** The capacity measured for solutions are in micro Farrad (μ F) where that of water is equal to 0.18 μ F.**

The association constant K_A of different 1:1 (symmetric) electrolytes can be estimated by applying Fuoss-Shedlovsky equations (9, 10) (equation 5):

$$\frac{1}{\Lambda S(Z)} = \frac{1}{\Lambda_o} + \left(\frac{K_A}{\Lambda_o^2}\right)(C.\,\Lambda.\gamma_\pm^2\ .S(Z)) \ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

where

$$S(Z) = \left[\frac{Z}{2} + \left(1 + \left(\frac{Z}{2}\right)^2\right)^{1/2}\right]^2,\ Z = S.\,(\Lambda_o)^{-3/2}\,(C.\Lambda)^{1/2},$$

$$S = a\Lambda_o + b,\ a = 8.2 \times 10^5\,(\in.T)^{1/2} \text{ and } b = \frac{0.825}{\eta o(\varepsilon T)^{1/2}}$$

Λ, Λ_o are the molar and limiting conductance, $\in$ is the dielectric constant, ηo is the viscosity of the solvent, T absolute temperature and S (Z) is the Fuoss Shedlovsky factor.

With the use of equation (5) for 1:2 electrolytes very low values are obtained for K_A (the association constant). Therefore we are in need of a new equation, which can be derived as follows:

$$A^{+2} + 2\,B^{-} \overset{KA}{\rightleftharpoons} A\,B_2 \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

$$K_A = \frac{(1-\alpha)}{(2\alpha)^2.C_m.\alpha} = \frac{1-\alpha}{4C_m^{\;2}.\alpha^3} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots(7)$$

$$\alpha \text{ (dissociation degree)} = \frac{\Lambda.S(Z)}{\Lambda_o} \ldots\ldots\ldots(8)$$

$$K_A = \frac{1-\dfrac{\Lambda.S(Z)}{\Lambda_o}}{4C_m^{\;2}\left(\dfrac{\Lambda.S(Z)}{\Lambda}\right)^3} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(9)$$

$$K_A = \frac{\Lambda_o^{\;2}\,(\Lambda_o-\Lambda)}{4C_m^{\;2}\,\gamma_{\pm}^{\;2}\;\Lambda^3\,S(Z)^2} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(10)$$

Thus equation (10) can be easily applied for 1:2 electrolytes for diluted solution because this equation is derived from Fuoss-Shedlovsky theory and the Ostwald dilution law, knowing that S (Z) factor for $CoCl_2$ solutions was found to be approximately one. The specific conductance of different $CoCl_2$ solutions were measured and the molar conductance was evaluated by applying equation (11):

$$\Lambda = \frac{K_s.Kcell.1000}{C_m} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(11)$$

K_s is the measured specific conductance, K cell is the cell constant and is equal 0.96 Cm is the molar concentration.

The limiting equivalent conductance Λ_o was obtained by extrapolating the relation between Λ and $\sqrt{C_m}$ for different solutions to zero concentration

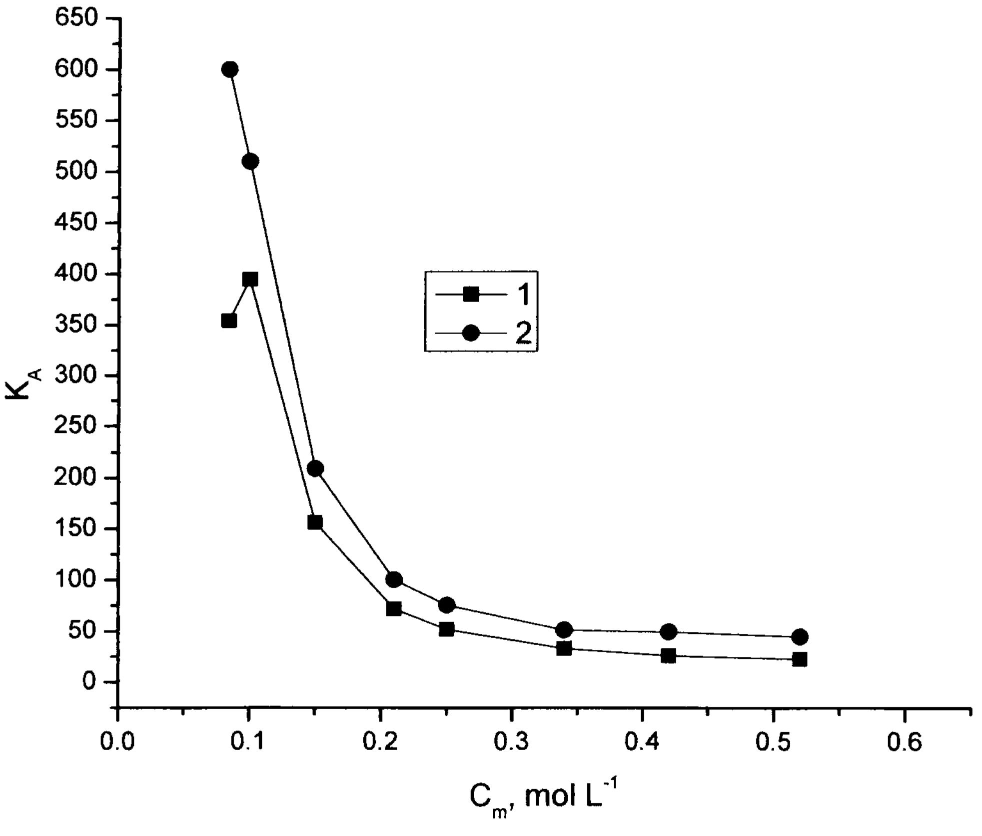


Figure 1. Plot of association constants (K_A) versus concentration (C_m) of $CoCl_2$ solutions in the absence (1) and presence (2) of a magnet at 298.15 K.

The same relation was drawn for $CoCl_2$ solution using a permanent magnet of average power of 0.677 Kilo Gauss and the net results are also illustrated in Fig. 1.

From Λ, Λ_o, the association constants (K_A) for $CoCl_2$ in the absence and presence of magnet were calculated using equation (10) and the results are shown in Table 2.

Table 2. Molar conductance (Λ), limiting molar conductance (Λ_o), dissociation degrees (α) and association constants (K_A) of $CoCl_2$ solutions in the absence and presence of a magnet at 298.15 K.

C_m Molar Conc.	In absence of magnet			In presence of magnet		
	Λ (in mS. cm^2 mol^{-1})	α	K_A (dm^3 mol^{-1})	Λ in (m S cm^2 mol^{-1})	α	K_A (dm^3 mol^{-1})
0.084	7.25	0.764	353.80	8.15	0.741	599.70
0.100	7.05	0.74	394.39	7.80	0.709	509.96
0.15	6.50	0.684	155.99	7.10	0.645	208.61
0.21	5.95	0.626	71.61	6.40	0.582	99.96
0.25	5.65	0.595	51.72	6.00	0.545	75.19
0.34	5.00	0.526	33.06	5.20	0.473	50.98
0.42	4.50	0.474	25.86	4.40	0.400	48.95
0.52	3.95	0.416	22.65	3.80	0.345	44.24

Λ_o = 9.5 m. Siemens (m S cm^2 mol^{-1}) in the absence of the magnet and 11.0 (m S. cm^2 mol^{-1}) in the presence of the magnet.

The dissociation degree, α, was also estimated for the electrolyte studied in the absence and presence of the magnet and the results are also shown in Table 2.

It was concluded that the K_A increases with decreasing $CoCl_2$ concentrations, mainly due to the increase of the degree of dissociation and the activity coefficient, both in the absence and presence of the magnet.

Usingthe magnet, K_A values increase due to the more association near that magnet which attracts the ions near it.

REFERENCES

1.Barthel, J. Krienke, H., Holovko, M. F., Kapke, V. I. and Protsykevick, I., *Cond. Mat. Phys., 3*,637 (2000)

2. Deepa , M., Agnihorty, S. A. Gupta, D., Chandra, R., *Electrochimica Acta, 49*, 373 (2004).

3. Schori, E., Jagur, J., Grodzinski, Z., and Shporer, M.; *J. Am. Chem. Soc., 93*, 7133 (1971).

4. Schori, E., and Jagur, J. and Grodzinski, *Isr. J. Chem. Soc., 11*, 243 (1973).

5. Covington, A. K., and Dickinson, T., "Physical Chemistry of Organic Solvent Systems", Plenum Press, London (1973).

6. Fuoss, R. M. and Accasina, F., "Electrolyte Conductance", Interscience, New York (1959).

7. Gomaa, Esam, A., *Thermochim. Acta, 99*, 128 (1988)

8. Gomaa, Esam, A., *Thermochim. Acta, 152*, 71 (1989).

9. Shedlovsky, T., and Kay, R. L., *J. Phys. Chem., 60*, 151 (1956).

10. Gomaa, E. A., Hafez, M. A. and Moussa, M. N. H., *Bull. Soc. Chem. Fr., 3*, 361 (1986).

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
SOUTH. BRAZ. J. CHEM., Vol. 17, No. 17, 2009

CRISTOFOR I. SIMIONESCU, FOUNDER OF THE ROMANIAN SCHOOL OF MACROMOLECULAR CHEMISTRY

Lavinel G. Ionescu [a,b] *
[a]Scienco Scientific Consulting Services, Viamão, RS, BRASIL
[b]Sarmisegetusa Research Group, Santa Fe, New Mexico, USA

ABSTRACT

Prof. Cristofor I. Simionescu was born in Dumbraveni, County of Suceava, Bucovina, Romania on July 17, 1920 and passed away in Jassy on August 6, 2007. He graduated from the Polytechnic Institute of Jassy in 1944, obtained the Doctoral Degree in Technical Sciences from the same institution in 1948 and served as a faculty member in Jassy for over fifty (50) years. He held various other positions including Rector, Vice-President and President of the Academy of Romania and Director of the "Petru Poni" Institute of Macromolecular Chemistry. He has supervised more than one hundred (100) doctoral dissertations, published over eight hundred (800) scientific papers and authored or co-authored more than twenty seven (27) books. He was a member of many academies and learned societies throughout the world, Editor of many scientific journals and received many prizes and awards. Prof. Cristofor I. Simionescu served on the Editorial Board of many international scientific periodicals, including the Southern Brazilian Journal of Chemistry. He is generally considered the father of macromolecular chemistry in Romania.

KEY WORDS: History of Chemistry, Science in Romania, Macromolecular Chemistry, Polymer Science

RESUMO

Prof. Cristofor I. Simionescu nasceu em Dumbraveni, Contado de Suceava, Bucovina, Romênia em 17 de Julho de 1920 e faleceu em Iasi em 6 de Agosto de 2007. Formou-se em Química Industrial no Instituto Politécnico de Iasi em 1944, obteve título de Doutor em Ciências Técnicas da mesma instituição em 1948 e fez parte do corpo docente em Iasi por mais de cinqüenta (50) anos. Ocupou muitos cargos, incluindo Reitor, Vice-Presidente e Presidente da Academia da Romênia e Diretor do Instituto de Química Macromolecular "Petru Poni".Orientou mais de cem (100) teses de doutorado, publicou mais de oito centos (800) trabalhos científicos e foi autor ou co-autor de mais de vinte sete (27) livros.Ele foi membro de muitas academias e sociedades científicas do mundo inteiro, Editor de muitas revistas científicas e recebeu muitos prêmios e homenagens. Prof. Cristofor I. Simionescu fez parte do Corpo Editorial de muitas revistas científicas internacionais incluindo Southern Brazilian Journal of Chemistry .Ele é geralmente considerado o pai da química macromolecular na Romênia.

PALAVRAS CHAVE: História da Química, Ciência na Romênia, Química Macromolecular, Polímeros

* lavinel@ibest.com.br or lavinel@pop.com.br

DOI: 10.48141/SBJCHEM.v17.n17.2009.43_2009.pdf

Professor Cristofor I. Simionescu was born in Dumbraveni, County of Suceava, Bucovina, Romania on July 17, 1920 and passed away in Jassy on August 6, 2007.

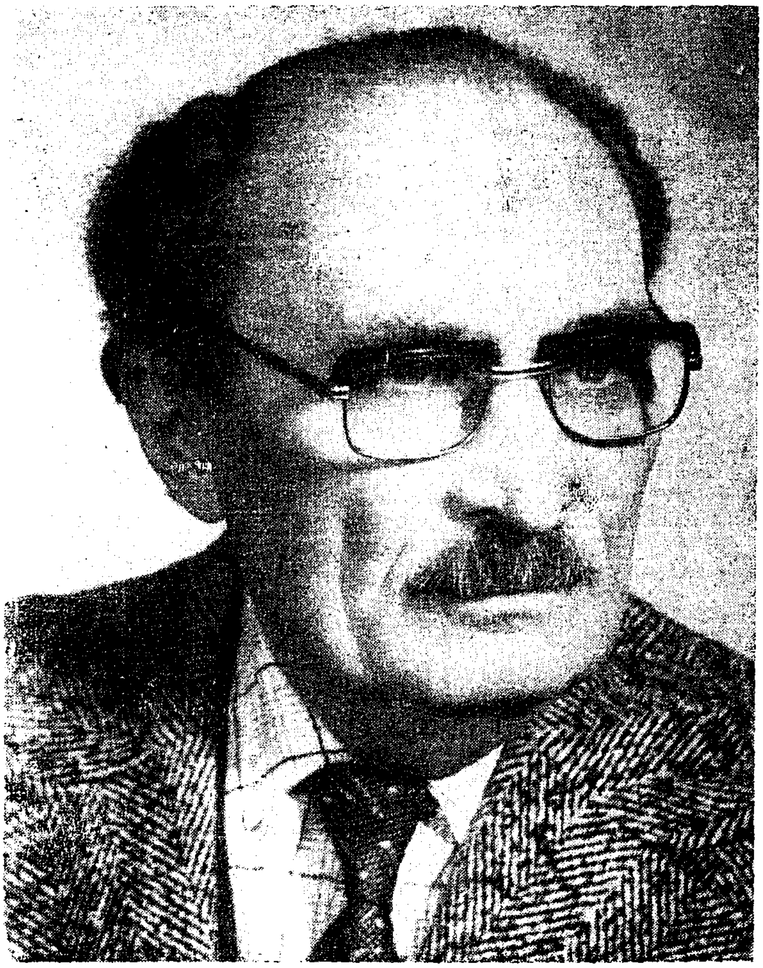
He came from a modest family and both of his parents were school teachers. He attended primary school in Dumbraveni and secondary school in Suceava and the National Lyceum in Jassy.

Cristofor I. Simionescu began his university studies at the Faculty of Chemical Engineering of the Polytechnic Institute of Jassy and graduated *"magna cum laude"* in 1944. He obtained the Doctor of Technical Sciences Degree from the same institution in 1948. His doctoral thesis, in the field of organic technology, dealt with properties of oils extracted from plants growing in Romania.

Cristofor Simionescu passed most of his academic life at the Polytechnic Institute of Jassy (now called the "Gh. Asachi" Technical University). He held the positions of Graduate Assistant (1943), Assistant Professor (1944-1948) and Associate Professor (1948-1951). In 1951 he was promoted to Full Professor and appointed to the Chair of Natural and Synthetic Macromolecules. He served as Chairman of the Department for more than thirty five (35) years and retired in 1995.

Professor Cristofor I. Simionescu was the founder of the School of Macromolecular Chemistry and Polymer Science in Romania. He introduced the teaching of formal courses in 1948 and a year later he established the Section of Cellulose, Paper and Artificial Yarns at the Faculty of Chemical Engineering of the Polytechnic Institute of Jassy.

He began studies dealing with wood, lignin, reed from the Danube Delta and special types of paper. Together with his collaborators, he studied the synthesis and modification of polymers through mechanochemical reactions and by plasma induction. Other areas of research included semiconducting polymers, ultrahigh molecular weight polymers, biopolymers, the origin of life, complex macromolecular architecture and biomedical polymers.



CRISTOFOR I. SIMIONESCU (1920-2007)

In 1964, the Institute of Chemistry in Jassy was transformed into an Institute dedicated entirely to research, investigation and application of natural and synthetic fibers, i.e., the **"Petru Poni" Institute of Macromolecular Chemistry.** Prof. Cristofor I. Simionescu served as its Director for 30 years (from 1970 to 2000). It is now an Institute of Excellence of the Academy of Romania.

The studies carried out at the Institute included wood chemistry, reed from the Danube Delta, polysaccharides, synthesis and polymerization (copolymerization) of new monomers, polymer mechanochemistry, photopolymers, semiconducting polymers, chemistry of macromolecular charge transfer complexes, plasmochemistry, multifunctional initiators, polyacetylenes and other polymers with conjugated double bonds and electroinitiated polymerizations.

Prof. Cristofor I. Simionescu was also interested in the origin of life, particularly under the conditions of the reduced atmosphere of primary gases on cold Earth. He published over fifty (50) scientific articles on the subject and also coauthored a book entitled **"Cold Theory of the Origin of Life"**, published in Romanian and Russian.

He has supervised more than one hundred (100) doctoral dissertation of researchers from many parts of the world and some of his former students occupy important positions at universities and research centers in many countries including, Romania, United States, Germany, Canada, Republic of Moldavia, Russia, Bulgaria, Egypt, Pakistan and Algeria.

Prof. Cristofor I. Simionescu is the holder of more than fifty (50) patents, has published more than eight hundred (800) scientific articles and is the author or coauthor of more than twenty seven (27) books written mostly in Romanian, English and Russian. Some of them are the following:

Chemistry of Wood in the People's Republic of Romania (1964)

Chemistry of Reed (1967)

Mechanochemistry of Macromolecular Compounds (1967)

Present Status of the Study of Grafting of Cellulose (1967)

Fractionation of Macromolecular Compounds (1969)

Chemistry of Wood and Cellulose (2 volumes, 1972-1973)

Chemistry of Wood in Romania. Poplar and Willow . (1973)

Treatise of Chemistry of Macromolecular Compounds (4 volumes)
(1973-1993)

Chemistry of Marine Algae (1974)

Biocompatible and Biologically Active Polymers (1980)

Enzymes (1980)

Proteins (1982)

The Origin of Life (1983)

Macromolecular Chemistry (1985)

Polyacetylenes (1987)

Bioenergetic Implications of Dyes (1988)

Aspects of History of Chemistry in Romania (1964)

Relationship between Science and Philosophy

Thoughts (Gânduri , 5 volumes- Essays and Reflections on
Life and Society written during the latter years of his life)

Prof. Acad. Cristofor Simionescu was member of many professional and honorary societies including the American Chemical Society, Société Chimique de France, Société de Chimie Industrielle de Paris, International Society for the Study of the Origin of Life (ISSOL) and others.

He served as Romanian National Representative at the International Union of Pure and Applied Chemistry (IUPAC) and was a member of the Macromolecular Division and the IUPAC Commission for the Teaching of Chemistry.

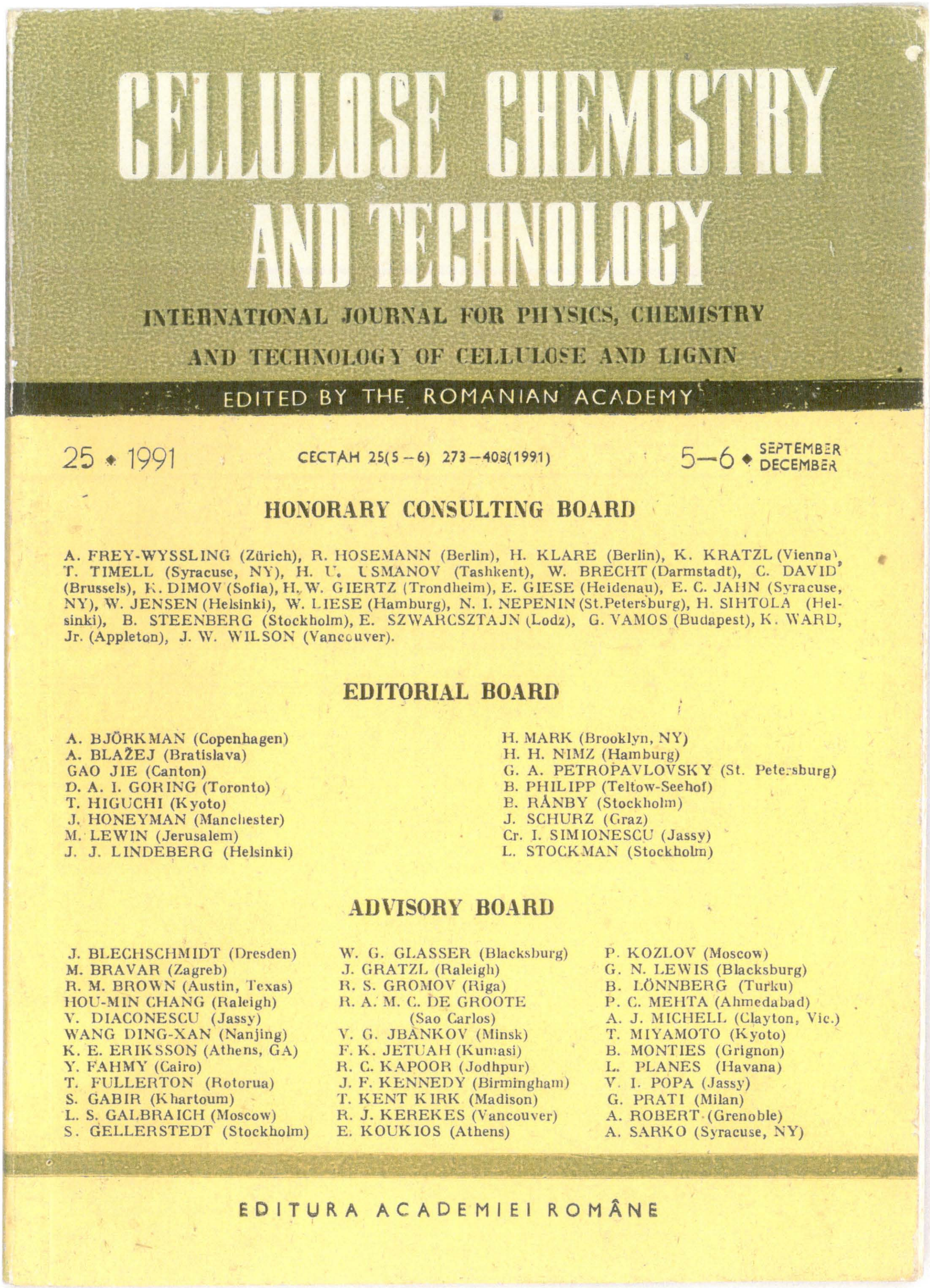
Prof. Acad. Cristofor I. Simionescu was a member, Vice-President and President of the Academy of Romania, member of the International Academy of Wood Science (IAWS), Academy of Sciences of the German Democratic Republic, Hungarian Academy of Science, Academy of Sciences of the Republic of Moldavia, European Academy of Sciences and Arts, New York Academy of Science and others.

He was *Doctor Honoris Causa* of the Polytechnic Institute of Sofia, Bulgaria, was awarded the Gold Medal by the American Chemical Society and 1976 and the National Order *"Star of Romania"* as Grand Officer in 2000.

Prof. Cristofor I. Simionescu was the Editor of several international scientific journals including *Cellulose Chemistry and Technology, Memoirs of the Scientific Sections of the Academy of Romania* and *Fuzzy Systems.*

He also served a member of the Editorial Board of many international journal including *Revue Roumaine de Chimie, Acta Polymerica, Journal of Polymer Science, European Polymer Journal, Journal of Polymer Science- Polymer Chemistry Edition, Polymer Bulletin, Polymers for Advanced Technologies* and the *Southern Brazilian Journal of Chemistry.*

During the early years of publication of the *Southern Brazilian Journal of Chemistry* we had many collaborators from Iasi including Corneliu Oniscu, Adina Dumitrascu, Dan Cascaval, Eugen Horoba, Tinca Onofrei, Cecilia Arsene, Carmen Mita, Radu Tudose, T. Gavriloaiei, Raluca Mocanu, Maria Calistru, R. Olariu and Mircea Constantinescu.



CELLULOSE CHEMISTRY AND TECHNOLOGY

INTERNATIONAL JOURNAL FOR PHYSICS, CHEMISTRY AND TECHNOLOGY OF CELLULOSE AND LIGNIN

EDITED BY THE ROMANIAN ACADEMY

25 ◆ 1991 CECTAH 25(5–6) 273–408(1991) 5–6 ◆ SEPTEMBER DECEMBER

HONORARY CONSULTING BOARD

A. FREY-WYSSLING (Zürich), R. HOSEMANN (Berlin), H. KLARE (Berlin), K. KRATZL (Vienna), T. TIMELL (Syracuse, NY), H. U. USMANOV (Tashkent), W. BRECHT (Darmstadt), C. DAVID (Brussels), K. DIMOV (Sofia), H. W. GIERTZ (Trondheim), E. GIESE (Heidenau), E. C. JAHN (Syracuse, NY), W. JENSEN (Helsinki), W. LIESE (Hamburg), N. I. NEPENIN (St.Petersburg), H. SIHTOLA (Helsinki), B. STEENBERG (Stockholm), E. SZWARCSZTAJN (Lodz), G. VAMOS (Budapest), K. WARD, Jr. (Appleton), J. W. WILSON (Vancouver).

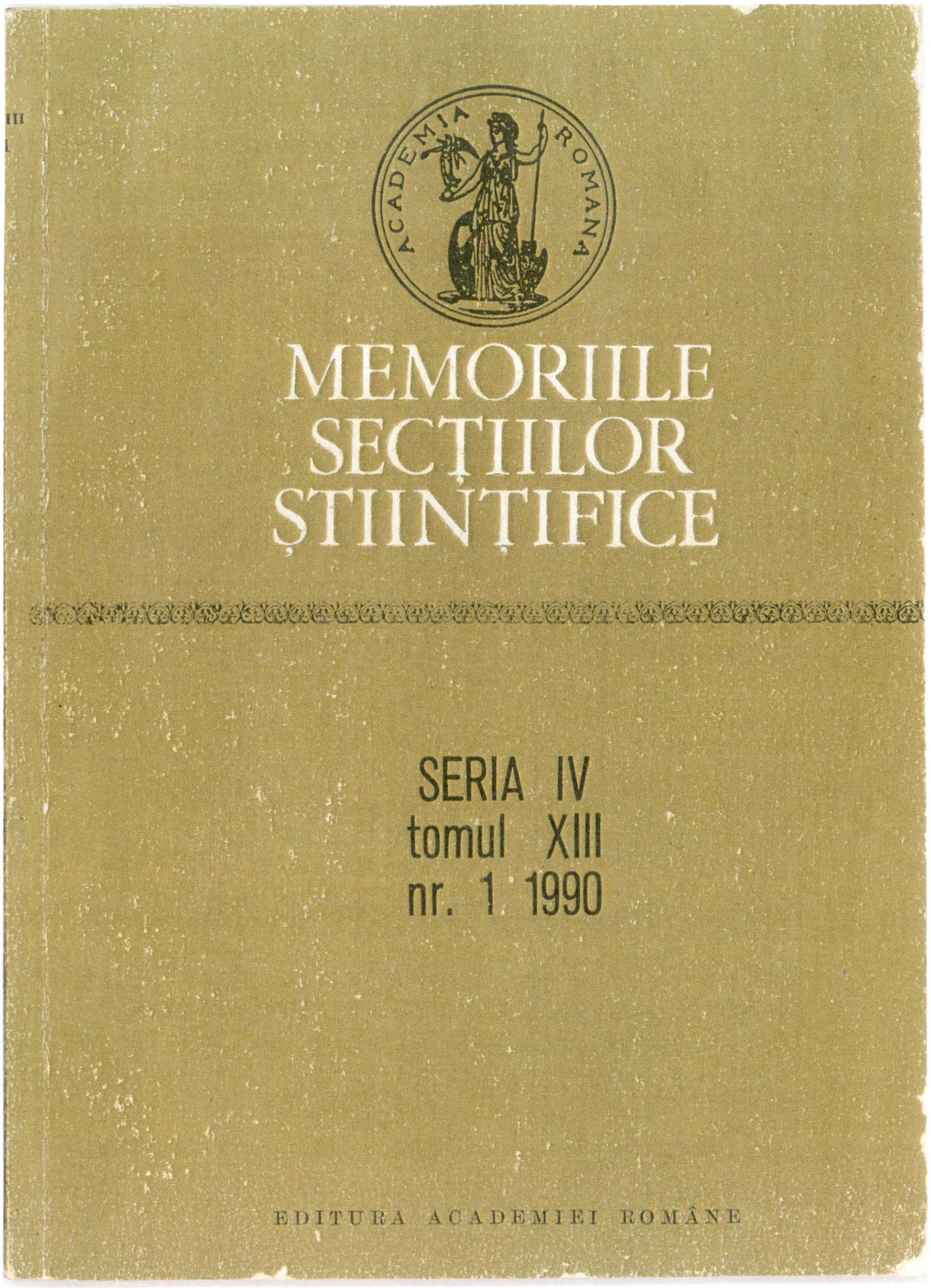
EDITORIAL BOARD

A. BJÖRKMAN (Copenhagen)
A. BLAŽEJ (Bratislava)
GAO JIE (Canton)
D. A. I. GORING (Toronto)
T. HIGUCHI (Kyoto)
J. HONEYMAN (Manchester)
M. LEWIN (Jerusalem)
J. J. LINDEBERG (Helsinki)
H. MARK (Brooklyn, NY)
H. H. NIMZ (Hamburg)
G. A. PETROPAVLOVSKY (St. Petersburg)
B. PHILIPP (Teltow-Seehof)
B. RÅNBY (Stockholm)
J. SCHURZ (Graz)
Cr. I. SIMIONESCU (Jassy)
L. STOCKMAN (Stockholm)

ADVISORY BOARD

J. BLECHSCHMIDT (Dresden)
M. BRAVAR (Zagreb)
R. M. BROWN (Austin, Texas)
HOU-MIN CHANG (Raleigh)
V. DIACONESCU (Jassy)
WANG DING-XAN (Nanjing)
K. E. ERIKSSON (Athens, GA)
Y. FAHMY (Cairo)
T. FULLERTON (Rotorua)
S. GABIR (Khartoum)
L. S. GALBRAICH (Moscow)
S. GELLERSTEDT (Stockholm)
W. G. GLASSER (Blacksburg)
J. GRATZL (Raleigh)
R. S. GROMOV (Riga)
R. A. M. C. DE GROOTE (Sao Carlos)
V. G. JBANKOV (Minsk)
F. K. JETUAH (Kumasi)
R. C. KAPOOR (Jodhpur)
J. F. KENNEDY (Birmingham)
T. KENT KIRK (Madison)
R. J. KEREKES (Vancouver)
E. KOUKIOS (Athens)
P. KOZLOV (Moscow)
G. N. LEWIS (Blacksburg)
B. LÖNNBERG (Turku)
P. C. MEHTA (Ahmedabad)
A. J. MICHELL (Clayton, Vic.)
T. MIYAMOTO (Kyoto)
B. MONTIES (Grignon)
L. PLANES (Havana)
V. I. POPA (Jassy)
G. PRATI (Milan)
A. ROBERT (Grenoble)
A. SARKO (Syracuse, NY)

EDITURA ACADEMIEI ROMÂNE

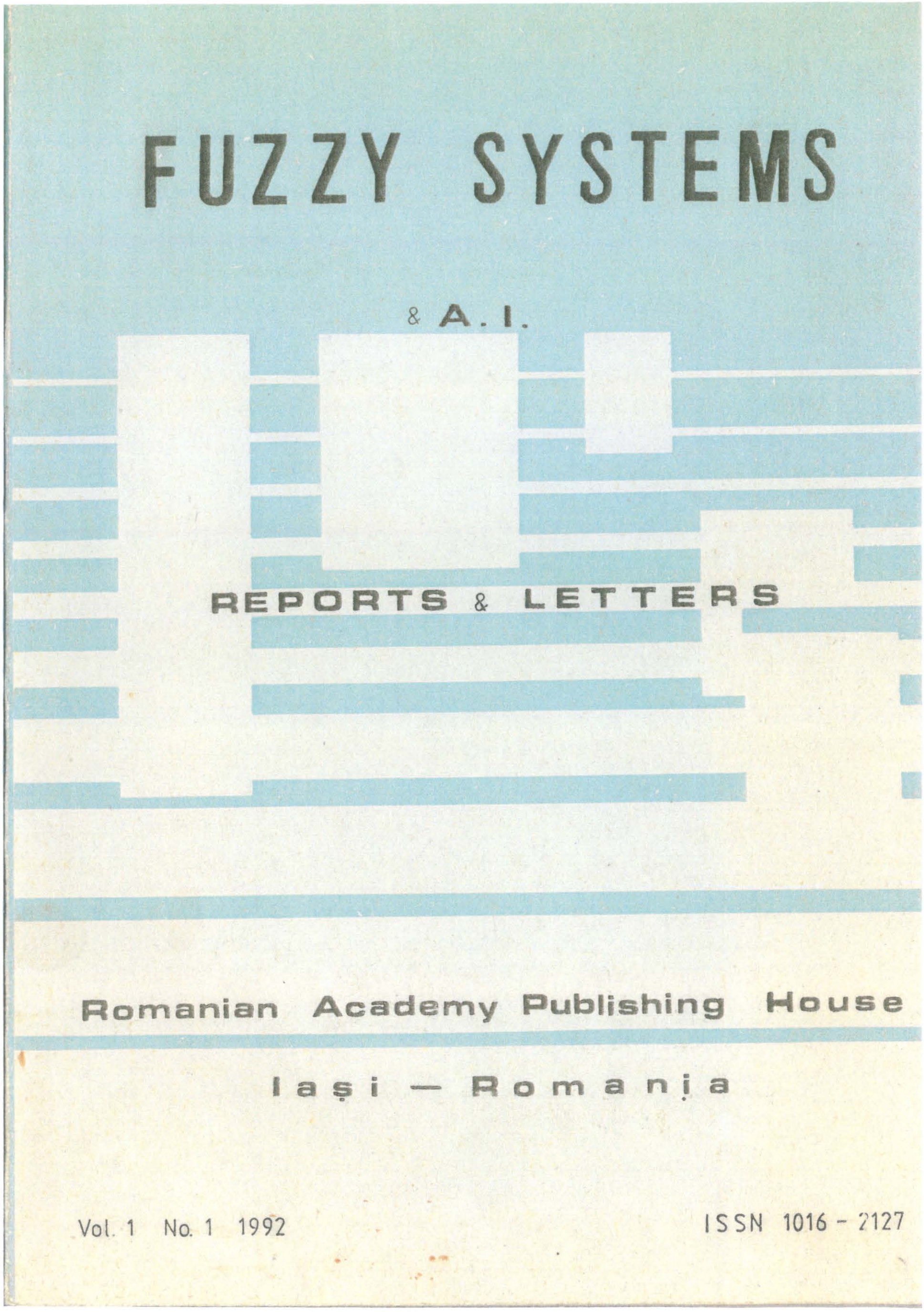


ACADEMIA ROMANA

MEMORIILE
SECȚIILOR
ȘTIINȚIFICE

SERIA IV
tomul XIII
nr. 1 1990

EDITURA ACADEMIEI ROMÂNE



FUZZY SYSTEMS

& A.I.

REPORTS & LETTERS

Romanian Academy Publishing House

Iași — Romania

Vol. 1 No. 1 1992

ISSN 1016 - 2127

FSAI Vol. 1 No. 1 (1992)

EDITORIAL

Romania is well known to have played a major part in the development of fuzzy sets, logic and systems theory. Let us remember here the names of Grigore Moisil, D. Ralescu, C.V. Negoita, D. Butnariu, V. Dumitru.

Following this tradition, both theoretical and applicative consistent researches are currently developed in this country. Although the Romanian school in fuzzy systems is now oriented rather to engineering aspects, the fundamental research is emphasized too.

Today, the main center of research is in Iasi. It is due to the scientific, didactic, and organizatorial efforts of the Managing Editor of this journal. Now, powerful groups involved in fuzzy systems research exists in the Polytechnic Institute of Iasi, in the University of Iaşi and in the Institute for Information Science, Romanian Academy, Iasi Branch. The international symposia organized in Iasi these last three years reflect the high level of research in Romania. I am convinced that these research forces can push the field in this country.

This new journal is aimed to contribute to the dissemination of information in fuzzy systems and in related fields. In the first place, it will reflect the connections fuzzy systems theory has with other recently developed sciences: artificial intelligence, neural networks, chaotic systems. Applications of fuzzy systems in engineering, economics, information science, computer science, medicine a.s.o. will be also emphasized, according to the strategy of the Editors.

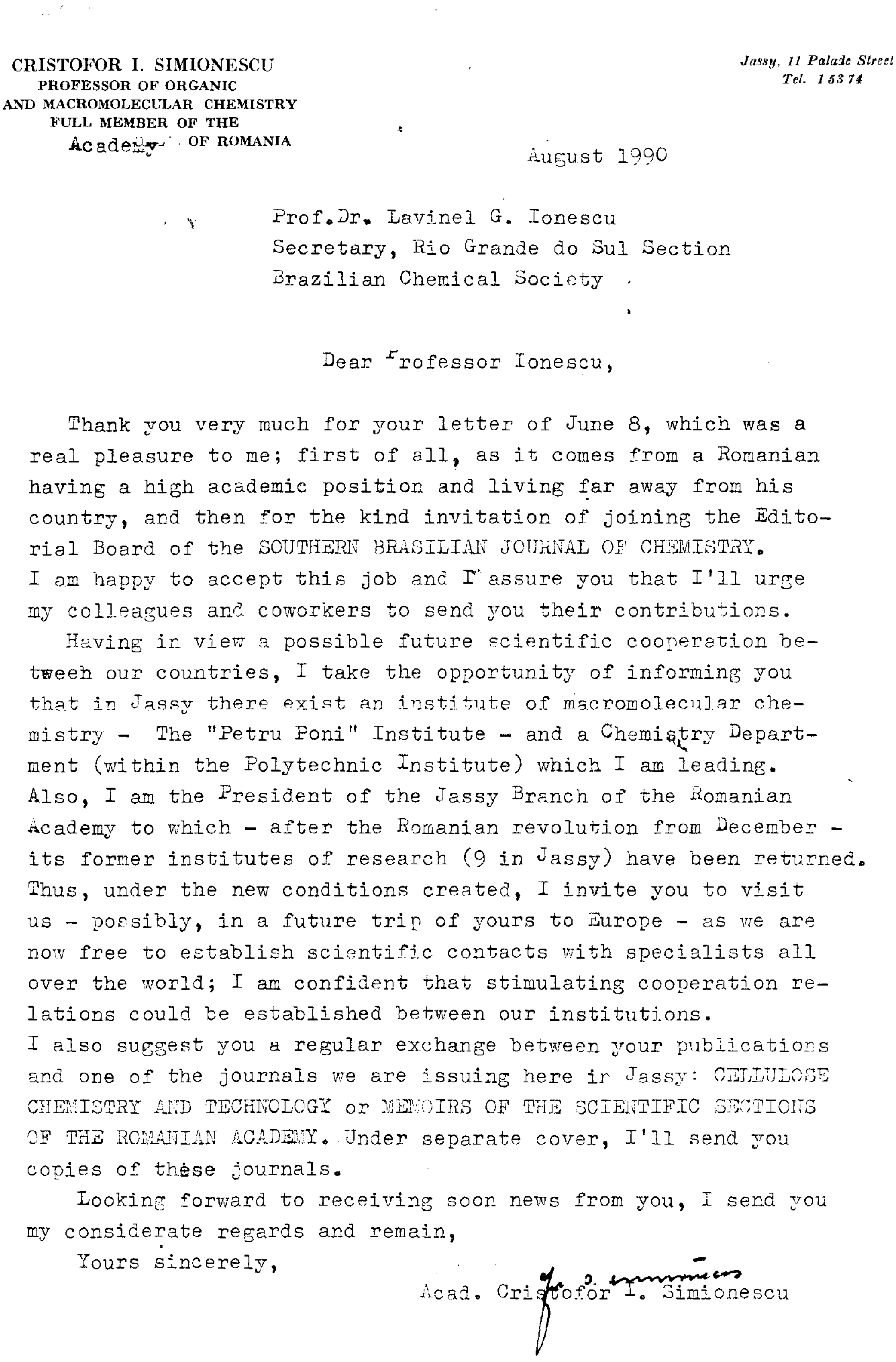
I hope the journal will also reflect the state of the art in research in this country, and that the best papers presented in the symposia organized here will find a suitable publication medium.

The distinguished International Editorial Board offers the guarantee of a top level international journal that will contribute, starting its very first year, to support the impetus of the scientific and technical research in the field of fuzzy systems. I am sure that all the members of the Editorial Board and the referees will help to keep up the scientific level of this journal.

I hope this journal will contribute to the East - West cooperation, as well as to the scientific cooperation at an international scale.

Finally, I hope that this journal will attain his objectives very soon, and it will be soon recognized as a forum for the leading edge researches in fuzzy systems and related fields.

Cristofor Simionescu
President, Iasi Branch of the Romanian Academy



CRISTOFOR I. SIMIONESCU
PROFESSOR OF ORGANIC
AND MACROMOLECULAR CHEMISTRY
FULL MEMBER OF THE
Academy OF ROMANIA

Jassy, 11 Palade Street
Tel. 1 53 74

August 1990

Prof. Dr. Lavinel G. Ionescu
Secretary, Rio Grande do Sul Section
Brazilian Chemical Society

Dear Professor Ionescu,

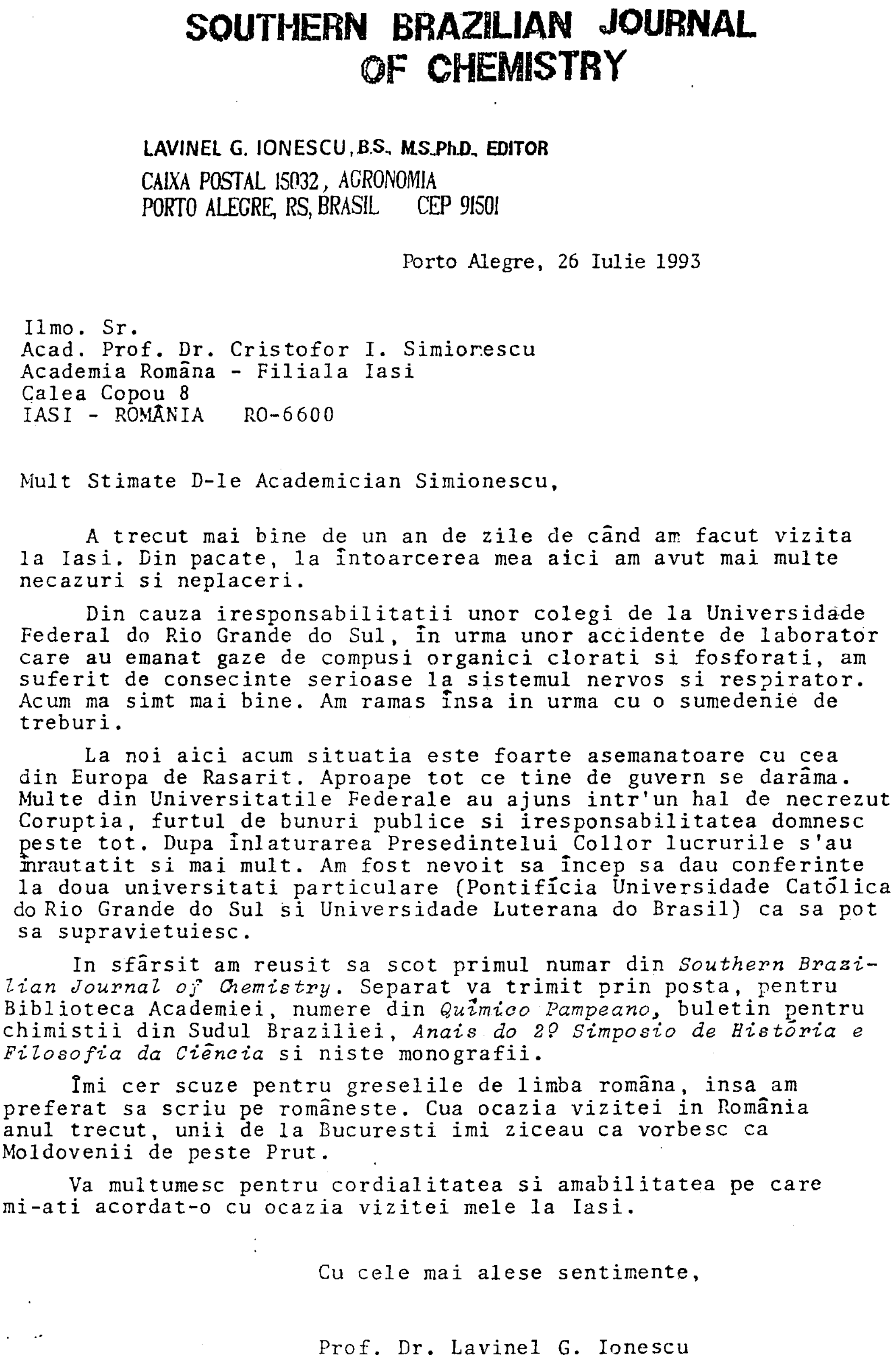
Thank you very much for your letter of June 8, which was a real pleasure to me; first of all, as it comes from a Romanian having a high academic position and living far away from his country, and then for the kind invitation of joining the Editorial Board of the SOUTHERN BRASILIAN JOURNAL OF CHEMISTRY. I am happy to accept this job and I assure you that I'll urge my colleagues and coworkers to send you their contributions.

Having in view a possible future scientific cooperation betweeh our countries, I take the opportunity of informing you that in Jassy there exist an institute of macromolecular chemistry - The "Petru Poni" Institute - and a Chemistry Department (within the Polytechnic Institute) which I am leading. Also, I am the President of the Jassy Branch of the Romanian Academy to which - after the Romanian revolution from December - its former institutes of research (9 in Jassy) have been returned. Thus, under the new conditions created, I invite you to visit us - possibly, in a future trip of yours to Europe - as we are now free to establish scientific contacts with specialists all over the world; I am confident that stimulating cooperation relations could be established between our institutions. I also suggest you a regular exchange between your publications and one of the journals we are issuing here in Jassy: CELLULOSE CHEMISTRY AND TECHNOLOGY or MEMOIRS OF THE SCIENTIFIC SECTIONS OF THE ROMANIAN ACADEMY. Under separate cover, I'll send you copies of these journals.

Looking forward to receiving soon news from you, I send you my considerate regards and remain,

Yours sincerely,

Acad. Cristofor I. Simionescu



SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

LAVINEL G. IONESCU, B.S., M.S., Ph.D., EDITOR
CAIXA POSTAL 15032, AGRONOMIA
PORTO ALEGRE, RS, BRASIL CEP 91501

Porto Alegre, 26 Iulie 1993

Ilmo. Sr.
Acad. Prof. Dr. Cristofor I. Simionescu
Academia Romăna - Filiala Iasi
Calea Copou 8
IASI - ROMÂNIA RO-6600

Mult Stimate D-le Academician Simionescu,

A trecut mai bine de un an de zile de când am facut vizita la Iasi. Din pacate, la întoarcerea mea aici am avut mai multe necazuri si neplaceri.

Din cauza iresponsabilitatii unor colegi de la Universidade Federal do Rio Grande do Sul, în urma unor accidente de laborator care au emanat gaze de compusi organici clorati si fosforati, am suferit de consecinte serioase la sistemul nervos si respirator. Acum ma simt mai bine. Am ramas însa in urma cu o sumedenie de treburi.

La noi aici acum situatia este foarte asemanatoare cu cea din Europa de Rasarit. Aproape tot ce tine de guvern se darâma. Multe din Universitatile Federale au ajuns intr'un hal de necrezut. Coruptia, furtul de bunuri publice si iresponsabilitatea domnesc peste tot. Dupa înlaturarea Presedintelui Collor lucrurile s'au înrautatit si mai mult. Am fost nevoit sa încep sa dau conferinte la doua universitati particulare (Pontifícia Universidade Católica do Rio Grande do Sul si Universidade Luterana do Brasil) ca sa pot sa supravietuiesc.

In sfârsit am reusit sa scot primul numar din *Southern Brazilian Journal of Chemistry*. Separat va trimit prin posta, pentru Biblioteca Academiei, numere din *Químico Pampeano*, buletin pentru chimistii din Sudul Braziliei, *Anais do 2º Simposio de História e Filosofia da Ciência* si niste monografii.

Îmi cer scuze pentru greselile de limba româna, insa am preferat sa scriu pe româneste. Cua ocazia vizitei in România anul trecut, unii de la Bucuresti imi ziceau ca vorbesc ca Moldovenii de peste Prut.

Va multumesc pentru cordialitatea si amabilitatea pe care mi-ati acordat-o cu ocazia vizitei mele la Iasi.

Cu cele mai alese sentimente,

Prof. Dr. Lavinel G. Ionescu

Prof. Acad, Cristofor I. Simionescu was a great scientist, person and human being.[1-7] He never forgot his origins, always helped others and was true citizen of Jassy, Moldavia and Romania.

In retrospect, it is easy to understand why Prof. Acad. Cristofor I. Simionescu was much closer to and a friend of Ilie G. Murgulescu, prominent physical chemist and educator and collaborated and helped him while he was Minister of Education of Romania. It is also easy to understand why he was more distant from Costin D. Nenitzescu, Romania's well known physical organic chemist.[8-9]

Like many great scientists, Prof. Acad. Cristofor I. Simionescu was a modest person, never lost contact with his roots, was a scholar aware of his social responsibility and a patriot.[8-15]

He genuinely believed that school, education and moral values were the key factors in the development of society.

Whether or not he served as Doctoral Thesis Advisor for Elena Ceausescu is not very important and irrelevant at this time, twenty years after her execution. What really matters is that polymer science and macromolecular chemistry developed and reached high standards in Romania.

As Dr. Aubrey D. Jenkins, Emeritus Professor of Polymer Chemistry at the University of Sussex, United Kingdom remarked to us during a visit in Porto Alegre in the 1980's, there were very few international conferences on polymer science that he attended where a President of a Country and his wife were present at the inaugural ceremony, two orchestras played and the scientific level was high.[16]

At the time, Prof. A. D. Jenkins was visiting Brazil and other countries in Latin America on behalf of the British Council to evaluate possible areas of collaboration and cooperation in polymer science.[16]

Prof. Acad. Cristofor I. Simionescu was the main driving force behind the organization of numerous national and international conferences on wood, cellulose and macromolecular chemistry, mainly in Jassy and Bucharest. We cite particularly the International Symposium on Macromolecules (IUPAC Macro 83, Bucharest).

Prof. Acad. Cristofor Simionescu was a very educated and erudite person. Some twenty years ago, when most people were talking about a new era, new paradigms, globalization, other truths and a change of values, Prof. Acad, Cristofor I Simionescu in Jassy and other brilliant minds in Coimbra, Portugal were talking about a crisis of civilization, return to mercantilism and the darkness of the middle ages, imbecilization of the masses and even the imbecilization of the elites (socially superior ruling classes).[16]

Prof. Acad. Cristofor I. Simionescu has left us and gone to other levels and dimensions. His example, his lesssons and his legacy remain for those who may desire to make use of them.

REFERENCES

1. I. I. Negulescu and O. Vogl,"Professor Cristofor Simionescu on His 70th Birth Anniversary", *Mem. Sect. Stiint, Ser.IV, Tom XIII, Academia Romana, Nr. 1,* 8-11 (1990).
2. I.I. Negulescu and O. Vogl, *Cellulose Chemistry and Technology, 24,* 657-659 (1990).
3. I.I. Negulescu and O. Vogl, *J. Macrmol. Sci. Chem., A28(7),* 597-600 (1991).
4. C.I. Simionescu, I.I. Negulescu and O. Vogl,"Polymer Science in Romania", *Polymer News, 13(*11), 351-354 (1988).
5. E. Schab-Balcerzak, *Polimery-Warsaw, 53(6),* 481 (2008).
6. E. Board,"Professor Cristofor I. Simionescu (1920-2007)", *Rev. Roum. Chim., 52(10),* 1007-1008 (2007.
7. E. Chiscop,"Ultimul Tatuc", *Ziarul de Iasi,* 11 Februarie 2002. (A tendentious article about Prof. Acad. Cristofor I. Simionescu and his accomplishments).
8. L. G. Ionescu," Ilie G. Murgulescu, Prominent Scientist and Educator", *South. Braz. J. Chem., 1(1),* 1-4 (1993).
9. L. G. Ionescu, "Costin D. Nenitzescu (1902-1970) -100th Anniversary of His Birth", *South. Braz. J. Chem., 10(1),* 1-10 (2002).
10. L. G. Ionescu and C.A. Perazzolo, "Luis Frederico Leloir – South America's Only Nobel Laureate in Chemistry", *South. Braz. J. Chem. 3(3),* 1-8 1995).
11. L. G. Ionescu, "Ernesto Giesbrecht, Great Chemical Educator and Father of Brazilian Inorganic Chemistry", *South. Braz. J. Chem., 4(4),* 1-8 (1996).
12. L. G. Ionescu, "Andrés Manuel del Rio, Discoverer of Vanadium", *South. Braz. J. Chem., 5(5),* 1-6 (1997).
13. L. G. Ionescu and L.A. B. De Boni, "Theodoro Augusto Ramos – A Brazilian Contribution to the Model of the Atom", *South. Braz. J. Chem., 13(*13), 1-12 (2005).
14. L. G. Ionescu, "Xorge Alejandro Dominguez, Mexico's Foremost Organic Chemist", *South. Braz. J. Chem., 2(2),* 1-4 (1994).
15. L. G. Ionescu and L.A. B. De Boni, "Glimpses of the History of Chemistry in Mexico", *South. Braz. J. Chem., 14(14),* 39-87 (2006).
16. L. G. Ionescu, *Private Reminiscences* (Lembranças), 1980-2000.

The SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY (ISSN: 2674-6891; 0104-5431) is an open-access journal since 1993. Journal DOI: 10.48141/SBJCHEM.
http://www.sbjchem.com.
This text was introduced in this file in 2021 for compliance reasons.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
SOUTH. BRAZ. J. CHEM., Vol. 17, No. 17, 2009

CRISTOFOR I. SIMIONESCU, FUNDADOR DA ESCOLA ROMENA DE QUÍMICA MACROMOLECULAR

Lavinel G. Ionescu [a,b] *
[a]Scienco Scientific Consulting Services, Viamão, RS, BRASIL
[b]Sarmisegetusa Research Group, Santa Fe, New Mexico, USA

ABSTRACT

Prof. Cristofor I. Simionescu was born in Dumbraveni, County of Suceava, Bucovina, Romania on July 17, 1920 and passed away in Jassy on August 6, 2007. He graduated from the Polytechnic Institute of Jassy in 1944, obtained the Doctoral Degree in Technical Sciences from the same institution in 1948 and served as a faculty member in Jassy for over fifty (50) years. He held various other positions including Rector, Vice-President and President of the Academy of Romania and Director of the "Petru Poni" Institute of Macromolecular Chemistry. He has supervised more than one hundred (100) doctoral dissertations, published over eight hundred (800) scientific papers and authored or co-authored more than twenty seven (27) books. He was a member of many academies and learned societies throughout the world, Editor of many scientific journals and received many prizes and awards. Prof. Cristofor I. Simionescu served on the Editorial Board of many international scientific periodicals, including the Southern Brazilian Journal of Chemistry. He is generally considered the father of macromolecular chemistry in Romania.

KEY WORDS: **History of Chemistry, Science in Romania, Macromolecular Chemistry, Polymer Science**

RESUMO

Prof. Cristofor I. Simionescu nasceu em Dumbraveni, Contado de Suceava, Bucovina, Romênia em 17 de Julho de 1920 e faleceu em Iasi em 6 de Agosto de 2007. Formou-se em Química Industrial no Instituto Politécnico de Iasi em 1944, obteve título de Doutor em Ciências Técnicas da mesma instituição em 1948 e fez parte do corpo docente em Iasi por mais de cinqüenta (50) anos. Ocupou muitos cargos, incluindo Reitor, Vice-Presidente e Presidente da Academia da Romênia e Diretor do Instituto de Química Macromolecular "Petru Poni".Orientou mais de cem (100) teses de doutorado, publicou mais de oito centos (800) trabalhos científicos e foi autor ou co-autor de mais de vinte sete (27) livros.Ele foi membro de muitas academias e sociedades científicas do mundo inteiro, Editor de muitas revistas científicas e recebeu muitos prêmios e homenagens. Prof. Cristofor I. Simionescu fez parte do Corpo Editorial de muitas revistas científicas internacionais incluindo Southern Brazilian Journal of Chemistry .Ele é geralmente considerado o pai da química macromolecular na Romênia.

PALAVRAS CHAVE: **História da Química, Ciência na Romênia, Química Macromolecular, Polímeros**

* lavinel@ibest.com.br **or lavinel@pop.com.br**

DOI: 10.48141/SBJCHEM.v17.n17.2009.58_2009.pdf

O Professor Cristofor I. Simionescu nasceu em Dumbraveni, Contado de Suceava, Bucovina, Romênia em 17 de Julho de 1920 e faleceu em Iasi no dia 6 de Agosto de 2007.

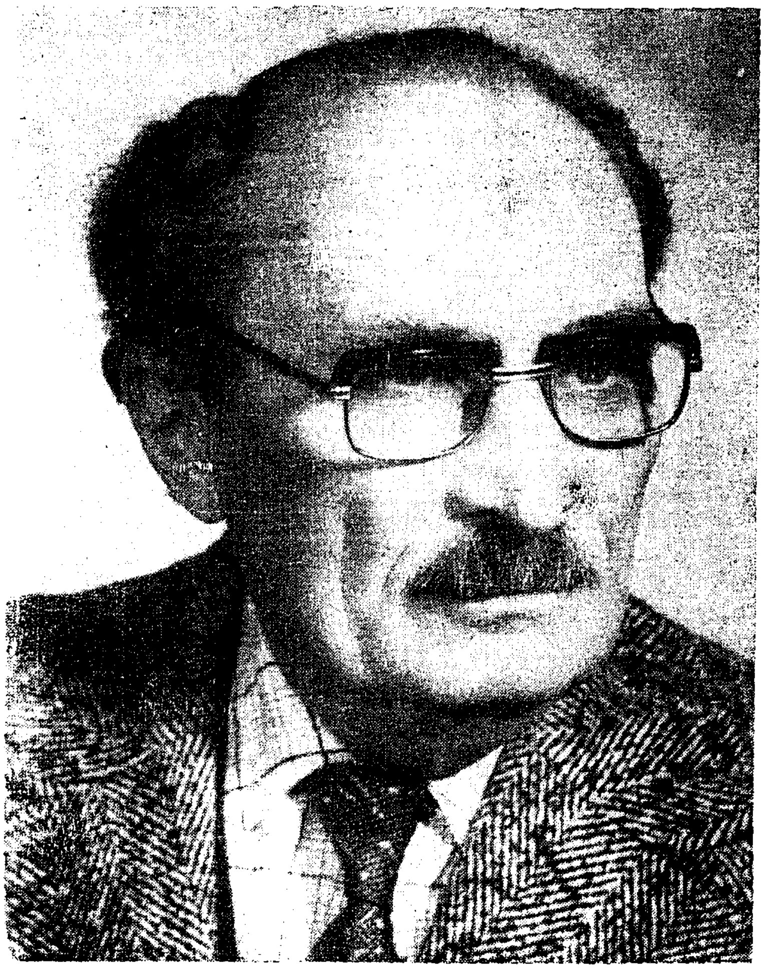
Ele é descendente de uma família modesta e seu pai e sua mãe foram professores. Fez os estudos de primeiro grau em Dumbraveni e completou o segundo grau em Suceava e no Liceu Nacional de Iasi.

Crsitofor I. Simionescu começou os estudos universitários na Faculdade de Química Industrial do Instituto Politécnico de Iasi e formou-se *"magna cum* laude " em 1944. Em 1948 obteve o grau de Doutor em Ciências Técnicas da mesma instituição. A sua tese de doutorado no campo da tecnologia orgânica tratou das propriedades de óleos extraídos de plantas da Romênia.

Cristofor I. Simionescu passou a maior parte da sua vida acadêmica no Instituto Politécnico de Iasi (atualmente denominado de Universidade Técnica Gheorghe Asachi). Ocupou os cargos de Assistente (1943), Professor Assistente (1944-1948) e Professor Adjunto (1948-1951). Em 1951 foi promovido a Professor Titular e Chefe da Cátedra de Macromoléculas Naturais e Síntéticas. Foi Chefe do Departamento por mais de trinta e cinco (35) anos e se aposentou em 1995.

O Prof. Cristofor I. Simionescu foi o fundador da Escola de Química Macromolecular e Ciências dos Polímeros na Romênia. Ele introduziu o ensino de disciplinas formais em 1948 e um ano depois estabeleceu a Secção de Celulose, Papel e Fibras Artificiais na Faculdade de Química Industrial do Instituto Politécnico de Iasi.

Ele começou estudos de pesquisa com madeira, lignina, junco da Delta do Danúbio e tipos especiais de papel. Junto com seus colaboradores, ele estudou a síntese e modificação de polímeros através de reações mecanoquímicas e indução por plasma. Outras atividades de pesquisa incluíram polímeros semicondutores, polímeros com peso molecular muito alto, biopolímeros, a origem da vida, estrutura macromolecular complexa e polímeros de interesse biomédico.



CRISTOFOR I. SIMIONESCU (1920-2007)

Em 1964, o Instituto de Química de Iasi foi transformado num Instituto exclusivamente dedicado à pesquisa, investigação e aplicações de fibras sintéticas e naturais, i.e., o **"Instituto Petru Poni de Química Macromolecular"** e o Prof. Cristofor I. Simionescu atuou como seu Diretor por 30 anos (de 1970 até 2000). Na presente data é um Instituto de Excelência da Academia da Romênia.

Os estudos desenvolvidos no Instituto incluíram a química da madeira, do junco da Delta do Danúbio, polissacarídeos, síntese e polimerização (copolimerização) de novos monômeros, mecanoquímica de polímeros, fotopolímeros, polímeros semicondutores, química de complexos macromoleculares de transferência de carga, plasmoquímica, iniciadores multifuncionais, poliacetilenos e outros polímeros com ligações duplas conjugadas e polimerizações eletroiniciadas.

Prof. Cristofor I. Simionescu também tinha interesse no estudo da origem da vida, particularmente nas condições de atmosferas reduzidas dos gases primordiais na Terra fria. Ele publicou mais de cinqüenta (50) artigos científicos sobre o assunto e também foi co-autor de um livro com título **"A Teoria Fria da Origem da Vida"**, publicado em romeno e russo.

Ele orientou mais de cem (100) teses de doutorado de pesquisadores de muitas partes do mundo. Hoje, alguns dos seus discípulos ocupam cargos importantes em universidades e institutos de pesquisa em muitos países incluindo, Romênia, Estados Unidos, Alemanha. Canadá, República da Moldávia, Rússia, Bulgária, Egito, Paquistão e Argélia.

Prof. Cristofor I. Soimionescu tem mais de cinqüenta (50) patentes, publicou mais de oitocentos (800) artigos científicos e foi autor ou co-autor de mais de vinte e sete (27) livros escritos principalmente em romeno, inglês e russo. Alguns deles são os seguintes:

Química da Madeira na República Popular da Romênia (1964)

Química do Junco (1967)

Mecanoquímica dos Compostos Macromoleculares (1967)

Estado Atual do Estudo do Enxerto da Celulose (1967)

Fracionamento de Compostos Macromoleculares (1969)

Química da Madeira e da Celulose (2 volumes, 1972-73)

Química da Madeira no Romênia. Álamo e Salgueiro. (1973)

Tratado de Química dos Compostos Macromoleculares (4 volumes) (1973-1993)

Química das Algas Marinhas (1974)

Polímeros Biocompatíveis e Biologicamente Ativos (1980)

Enzimas (1980)

Proteínas (1982)

A Origem da Vida (1983)

Química Macromolecular (1985)

Poliacetilenos (1987)

Implicações Bioenergéticas dos Corantes (1988)

Aspectos da História da Química na Romênia (1964)

Relação entre Ciência e Filosofia

Pensamentos (Gânduri, 5 volumes - Ensaios e Reflexões sobre A Vida e a Sociedade, escritos nos últimos anos)

Prof. Acad. Cristofor I. Simionescu foi membro de muitas sociedades professionais e honorárias incluindo a American Chemical Society, Société Chimique de France, Société de Chimie Industrielle de Paris, a Sociedade Internacional para o Estudo da Origem da Vida (ISSOL) e outras.

Ele foi Representante Nacional da Romênia junto a União Internacional de Química Pura e Aplicada (UIQPA) e foi membro da Divisão de Macromoléculas e da Comissão para o Ensino da Química.

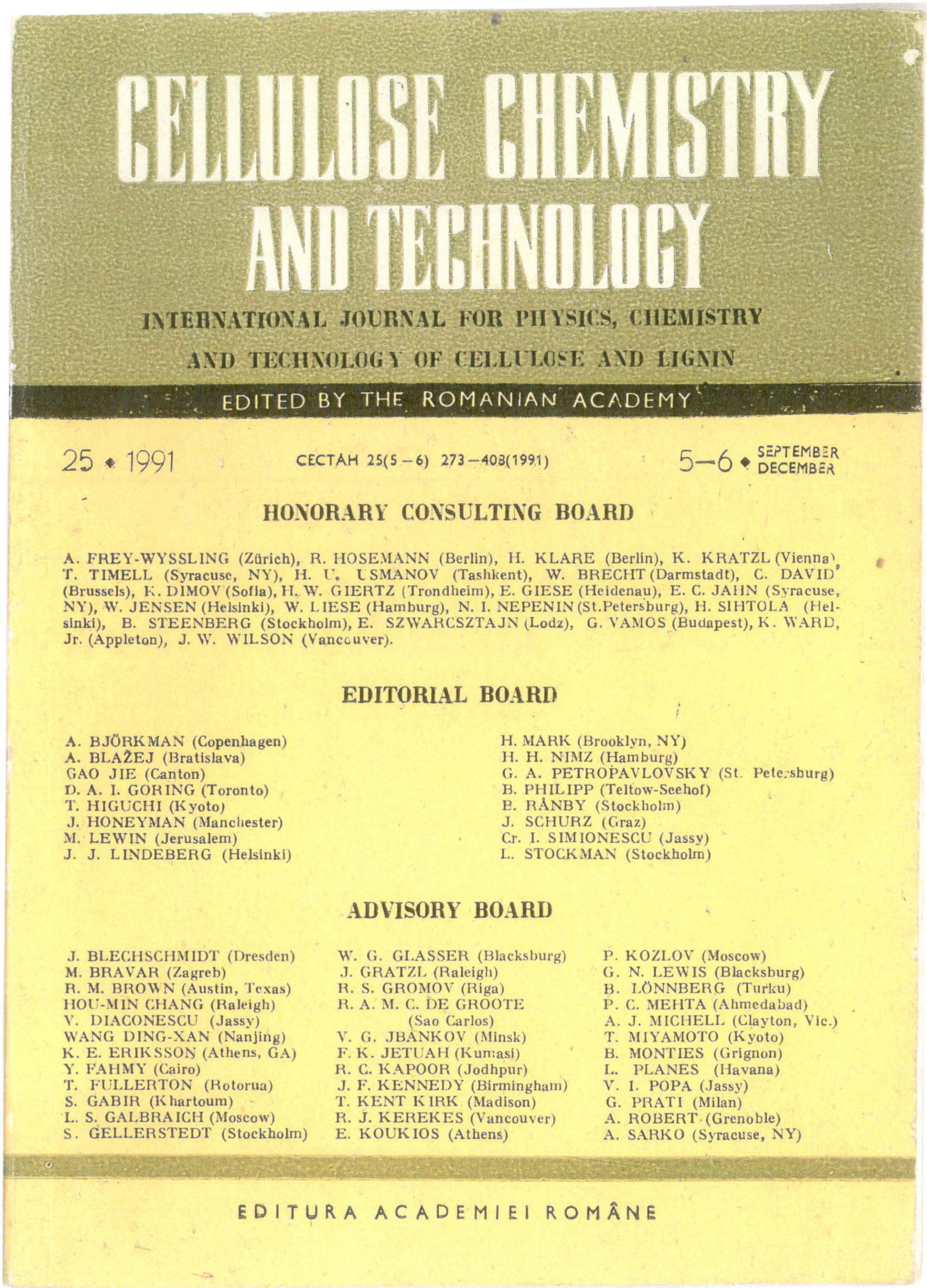
Prof. Acad. Cristofor I. Simionescu foi membro, Vice-Presidente e Presidente da Academia da Romênia, membro da Academia Internacional da Ciência da Madeira (IAWS), Academia de Ciências da República Democrática da Alemanha, Academia de Ciência da Hungria, Academia de Ciências da República da Moldávia, Academia Européia de Ciências e Artes, Academia de Ciências de Nova York e outras.

Ele recebeu o grau de *Doctor Honoris Causa* do Instituto Politécnico de Sofia, Bulgária, a *Medalha de Ouro* da American Chemical Society em 1976 e a Ordem Nacional *"Estrela da Romênia "* como Grande Oficial em 2000.

Prof. Cristofor I. Simionescu foi Editor de várias revistas científicas internacionais incluindo *Cellulose Chemistry and Technology, Memorias das Secções Científicas da Academia da Romênia* e *Fuzzy Systems.*

Ele também fez parte do Corpo Editorial de muitas revistas internacionais incluindo *Revue Roumaine de Chimie, Acta Polymerica, Journal of Polymer Science, European Polymer Journal, Journal of Polymer Science – Polymer Chemistry Edition, Polymer Bulletin, Polymers for Advanced Technologies* e *Southern Brazilian Journal of Chemistry.*

Durante os primeiros anos de publicação do *Southern Brazilian Journal of Chemistry* recebemos o apoio de muitos colaboradores de Iasi incluindo Corneliu Oniscu, Adina Dumitrascu, Dan Cascaval, Eugen Horoba, Tinca Onofrei, Cecília Arsene, Carmen Mita, Radu Tudose, T. Gavriloaiei, Raluca Mocanu, Maria Calistru, R. Olariu and Mircea Constantinescu.



CELLULOSE CHEMISTRY AND TECHNOLOGY

INTERNATIONAL JOURNAL FOR PHYSICS, CHEMISTRY AND TECHNOLOGY OF CELLULOSE AND LIGNIN

EDITED BY THE ROMANIAN ACADEMY

25 ◆ 1991 CECTAH 25(5 – 6) 273 – 408(1991) 5—6 ◆ SEPTEMBER DECEMBER

HONORARY CONSULTING BOARD

A. FREY-WYSSLING (Zürich), R. HOSEMANN (Berlin), H. KLARE (Berlin), K. KRATZL (Vienna), T. TIMELL (Syracuse, NY), H. U. USMANOV (Tashkent), W. BRECHT (Darmstadt), C. DAVID (Brussels), K. DIMOV (Sofia), H. W. GIERTZ (Trondheim), E. GIESE (Heidenau), E. C. JAHN (Syracuse, NY), W. JENSEN (Helsinki), W. LIESE (Hamburg), N. I. NEPENIN (St.Petersburg), H. SIHTOLA (Helsinki), B. STEENBERG (Stockholm), E. SZWARCSZTAJN (Lodz), G. VAMOS (Budapest), K. WARD, Jr. (Appleton), J. W. WILSON (Vancouver).

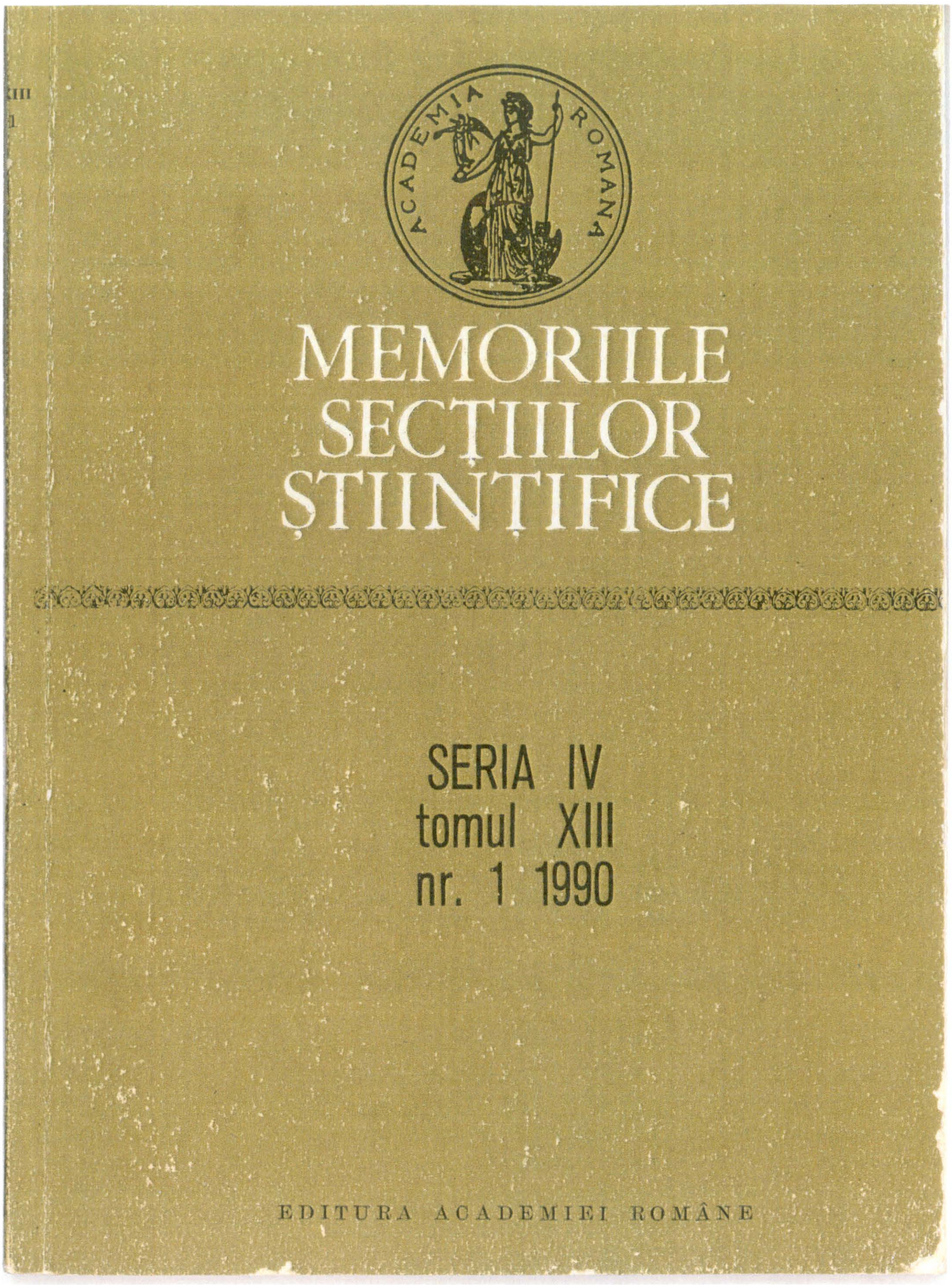
EDITORIAL BOARD

A. BJÖRKMAN (Copenhagen)
A. BLAŽEJ (Bratislava)
GAO JIE (Canton)
D. A. I. GORING (Toronto)
T. HIGUCHI (Kyoto)
J. HONEYMAN (Manchester)
M. LEWIN (Jerusalem)
J. J. LINDEBERG (Helsinki)
H. MARK (Brooklyn, NY)
H. H. NIMZ (Hamburg)
G. A. PETROPAVLOVSKY (St. Petersburg)
B. PHILIPP (Teltow-Seehof)
B. RÅNBY (Stockholm)
J. SCHURZ (Graz)
Cr. I. SIMIONESCU (Jassy)
L. STOCKMAN (Stockholm)

ADVISORY BOARD

J. BLECHSCHMIDT (Dresden)
M. BRAVAR (Zagreb)
R. M. BROWN (Austin, Texas)
HOU-MIN CHANG (Raleigh)
V. DIACONESCU (Jassy)
WANG DING-XAN (Nanjing)
K. E. ERIKSSON (Athens, GA)
Y. FAHMY (Cairo)
T. FULLERTON (Rotorua)
S. GABIR (Khartoum)
L. S. GALBRAICH (Moscow)
S. GELLERSTEDT (Stockholm)
W. G. GLASSER (Blacksburg)
J. GRATZL (Raleigh)
R. S. GROMOV (Riga)
R. A. M. C. DE GROOTE (Sao Carlos)
V. G. JBANKOV (Minsk)
F. K. JETUAH (Kumasi)
R. C. KAPOOR (Jodhpur)
J. F. KENNEDY (Birmingham)
T. KENT KIRK (Madison)
R. J. KEREKES (Vancouver)
E. KOUKIOS (Athens)
P. KOZLOV (Moscow)
G. N. LEWIS (Blacksburg)
B. LÖNNBERG (Turku)
P. C. MEHTA (Ahmedabad)
A. J. MICHELL (Clayton, Vic.)
T. MIYAMOTO (Kyoto)
B. MONTIES (Grignon)
L. PLANES (Havana)
V. I. POPA (Jassy)
G. PRATI (Milan)
A. ROBERT (Grenoble)
A. SARKO (Syracuse, NY)

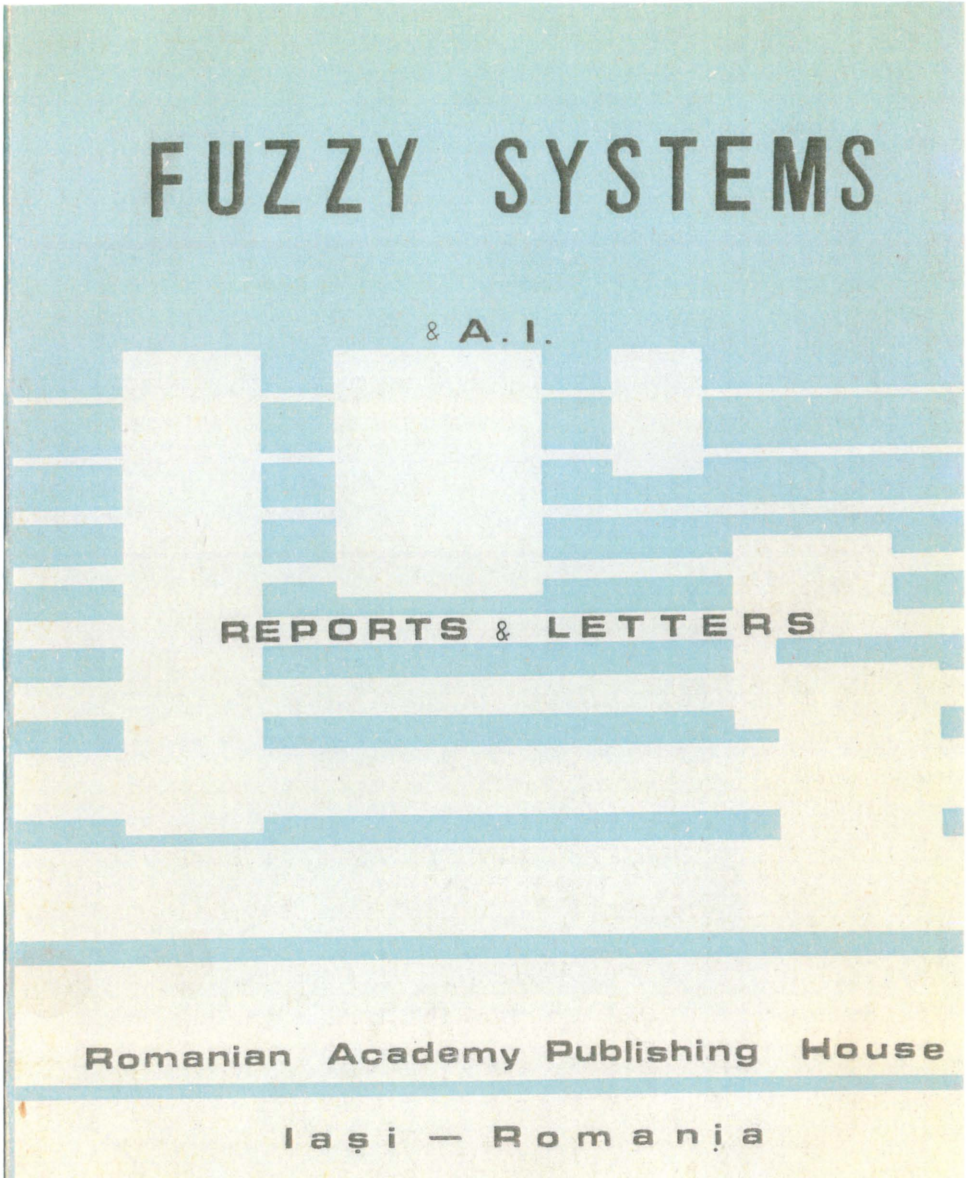
EDITURA ACADEMIEI ROMÂNE



MEMORIILE
SECȚIILOR
ȘTIINȚIFICE

SERIA IV
tomul XIII
nr. 1 1990

EDITURA ACADEMIEI ROMÂNE



FUZZY SYSTEMS
& A. I.

REPORTS & LETTERS

Romanian Academy Publishing House

Iași — Romania

Vol. 1 No. 1 1992 ISSN 1016 - 2127

FSAI Vol. 1 No. 1 (1992)

EDITORIAL

Romania is well known to have played a major part in the development of fuzzy sets, logic and systems theory. Let us remember here the names of Grigore Moisil, D. Ralescu, C.V. Negoita, D. Butnariu, V. Dumitru.

Following this tradition, both theoretical and applicative consistent researches are currently developed in this country. Although the Romanian school in fuzzy systems is now oriented rather to engineering aspects, the fundamental research is emphasized too.

Today, the main center of research is in Iasi. It is due to the scientific, didactic, and organizatorial efforts of the Managing Editor of this journal. Now, powerful groups involved in fuzzy systems research exists in the Polytechnic Institute of Iasi, in the University of Iaşi and in the Institute for Information Science, Romanian Academy, Iasi Branch. The international symposia organized in Iasi these last three years reflect the high level of research in Romania. I am convinced that these research forces can push the field in this country.

This new journal is aimed to contribute to the dissemination of information in fuzzy systems and in related fields. In the first place, it will reflect the connections fuzzy systems theory has with other recently developed sciences: artificial intelligence, neural networks, chaotic systems. Applications of fuzzy systems in engineering, economics, information science, computer science, medicine a.s.o. will be also emphasized, according to the strategy of the Editors.

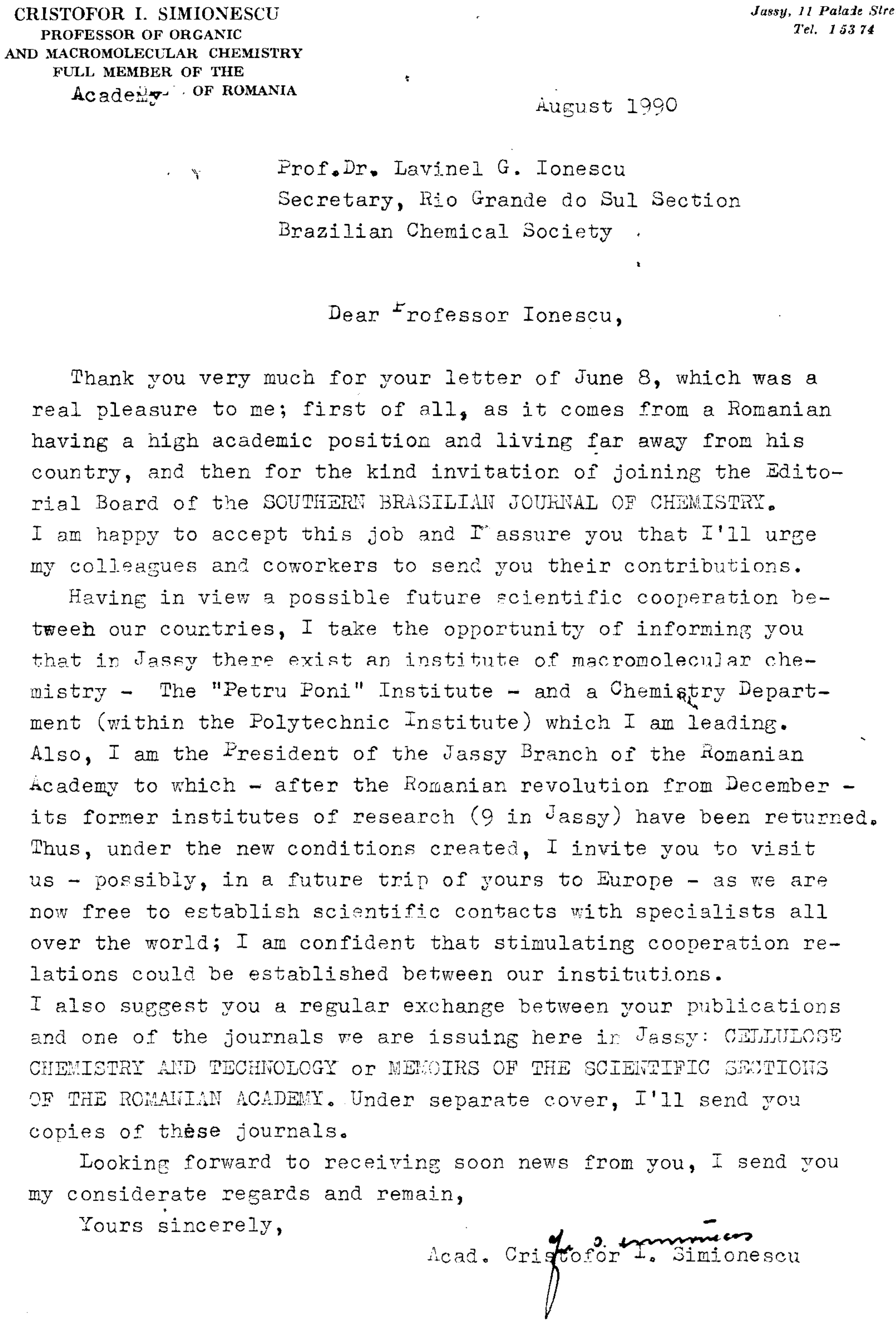
I hope the journal will also reflect the state of the art in research in this country, and that the best papers presented in the symposia organized here will find a suitable publication medium.

The distinguished International Editorial Board offers the guarantee of a top level international journal that will contribute, starting its very first year, to support the impetus of the scientific and technical research in the field of fuzzy systems. I am sure that all the members of the Editorial Board and the referees will help to keep up the scientific level of this journal.

I hope this journal will contribute to the East - West cooperation, as well as to the scientific cooperation at an international scale.

Finally, I hope that this journal will attain his objectives very soon, and it will be soon recognized as a forum for the leading edge researches in fuzzy systems and related fields.

Cristofor Simionescu
President, Iasi Branch of the Romanian Academy



CRISTOFOR I. SIMIONESCU
PROFESSOR OF ORGANIC
AND MACROMOLECULAR CHEMISTRY
FULL MEMBER OF THE
Academy OF ROMANIA

Jassy, 11 Palade Street
Tel. 1 53 74

August 1990

Prof.Dr. Lavinel G. Ionescu
Secretary, Rio Grande do Sul Section
Brazilian Chemical Society

Dear Professor Ionescu,

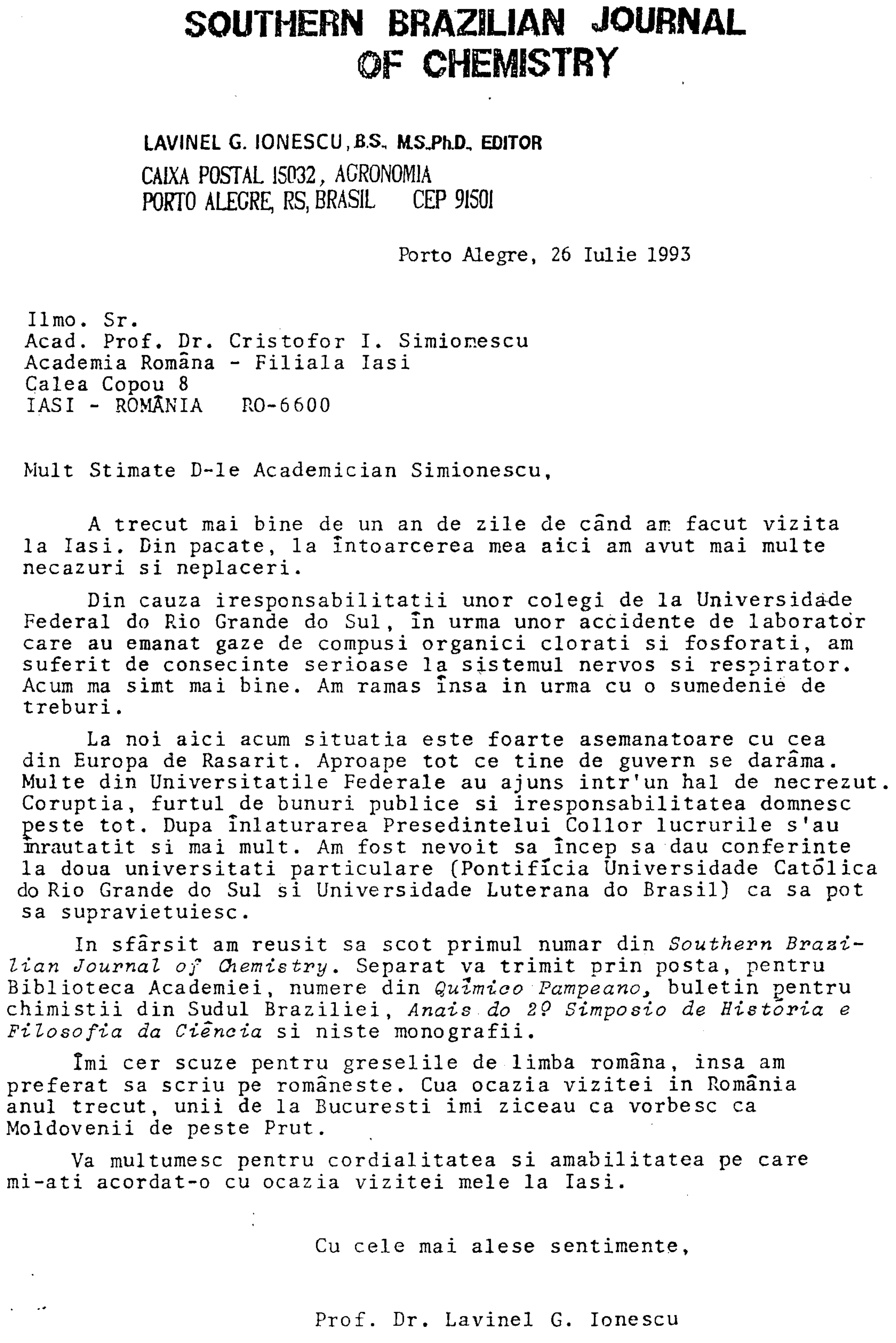
Thank you very much for your letter of June 8, which was a real pleasure to me; first of all, as it comes from a Romanian having a high academic position and living far away from his country, and then for the kind invitation of joining the Editorial Board of the SOUTHERN BRASILIAN JOURNAL OF CHEMISTRY.
I am happy to accept this job and I assure you that I'll urge my colleagues and coworkers to send you their contributions.

Having in view a possible future scientific cooperation between our countries, I take the opportunity of informing you that in Jassy there exist an institute of macromolecular chemistry - The "Petru Poni" Institute - and a Chemistry Department (within the Polytechnic Institute) which I am leading.
Also, I am the President of the Jassy Branch of the Romanian Academy to which - after the Romanian revolution from December - its former institutes of research (9 in Jassy) have been returned.
Thus, under the new conditions created, I invite you to visit us - possibly, in a future trip of yours to Europe - as we are now free to establish scientific contacts with specialists all over the world; I am confident that stimulating cooperation relations could be established between our institutions.
I also suggest you a regular exchange between your publications and one of the journals we are issuing here in Jassy: CELLULOSE CHEMISTRY AND TECHNOLOGY or MEMOIRS OF THE SCIENTIFIC SECTIONS OF THE ROMANIAN ACADEMY. Under separate cover, I'll send you copies of these journals.

Looking forward to receiving soon news from you, I send you my considerate regards and remain,

Yours sincerely,

Acad. Cristofor I. Simionescu



SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

LAVINEL G. IONESCU, B.S., M.S., Ph.D., EDITOR
CAIXA POSTAL 15032, AGRONOMIA
PORTO ALEGRE, RS, BRASIL CEP 91501

Porto Alegre, 26 Iulie 1993

Ilmo. Sr.
Acad. Prof. Dr. Cristofor I. Simionescu
Academia Româna - Filiala Iasi
Calea Copou 8
IASI - ROMÂNIA RO-6600

Mult Stimate D-le Academician Simionescu,

A trecut mai bine de un an de zile de când am facut vizita la Iasi. Din pacate, la întoarcerea mea aici am avut mai multe necazuri si neplaceri.

Din cauza iresponsabilitatii unor colegi de la Universidade Federal do Rio Grande do Sul, în urma unor accidente de laborator care au emanat gaze de compusi organici clorati si fosforati, am suferit de consecinte serioase la sistemul nervos si respirator. Acum ma simt mai bine. Am ramas însa in urma cu o sumedenie de treburi.

La noi aici acum situatia este foarte asemanatoare cu cea din Europa de Rasarit. Aproape tot ce tine de guvern se darâma. Multe din Universitatile Federale au ajuns intr'un hal de necrezut. Coruptia, furtul de bunuri publice si iresponsabilitatea domnesc peste tot. Dupa înlaturarea Presedintelui Collor lucrurile s'au înrautatit si mai mult. Am fost nevoit sa încep sa dau conferinte la doua universitati particulare (Pontifícia Universidade Católica do Rio Grande do Sul si Universidade Luterana do Brasil) ca sa pot sa supravietuiesc.

In sfârsit am reusit sa scot primul numar din *Southern Brazilian Journal of Chemistry*. Separat va trimit prin posta, pentru Biblioteca Academiei, numere din *Químico Pampeano*, buletin pentru chimistii din Sudul Braziliei, *Anais do 2º Simposio de História e Filosofia da Ciência* si niste monografii.

Îmi cer scuze pentru greselile de limba româna, insa am preferat sa scriu pe româneste. Cua ocazia vizitei in România anul trecut, unii de la Bucuresti imi ziceau ca vorbesc ca Moldovenii de peste Prut.

Va multumesc pentru cordialitatea si amabilitatea pe care mi-ati acordat-o cu ocazia vizitei mele la Iasi.

Cu cele mai alese sentimente,

Prof. Dr. Lavinel G. Ionescu

Prof. Acad. Cristofor I.Simionescu foi um grande cientista, uma pessoa fora do comum e um ser humano excepcional.[1-7] Ele nunca esqueceu as suas origens, sempre ajudou os outros e foi um cidadão exemplar de Iasi, da Moldávia e da Romênia.

Em retrospecto, é fácil entender porque o Prof. Acad. Cristofor I.Simionescu se aproximou e foi amigo de Ilie G. Murgulescu, destacado físico-químico e educador. Não foi por acaso que os dois colaboraram quando I.G. Murgulescu foi Ministro da Educação da Romênia. É também fácil de entender o distanciamento entre Cristofor I. Simionescu e Costin D. Nenitzescu, o famoso químico orgânico romeno.[8-9]

Como muitos grandes cientistas, Prof. Acad. Cristofor I. Simionescu foi uma pessoa modesta, nunca perdeu o contato com as suas raízes, estava plenamente consciente da sua responsabilidade social e foi um verdadeiro patriota.[8-15]

Ele, de verdade, acreditou que a escola, a educação e os valores morais são os fatores preponderantes para o desenvolvimento da sociedade.

Se ele serviu ou não como Orientador da Tese de Doutorado de Elena Ceausescu, não parece ser muito importante ou relevante a esta altura, vinte anos após a sua execução. O que é verdadeiramente importante é que a química macromolecular e a ciência dos polímeros atingiu níveis muito altos na Romênia.

Como Dr. Aubrey D. Jenkins, Professor Emeritus de Química dos Polímeros da Universidade de Sussex, Reino Unido, nos confiou durante uma visita em Porto Alegre na década de 1980 , foram poucas as conferências internacionais sobre polímeros das quais ele participou onde o Presidente do País e sua esposa estavam presentes na cerimônia inaugural, duas orquestras tocavam e o nível científico era muito alto.[16]

Na época, o Prof. A. D. Jenkins estava visitando o Brasil e outros países da América Latina a cargo do British Council para avaliar possíveis áreas de colaboração e cooperação na ciência dos polímeros.

Prof. Acad. Cristofor I. Simionescu foi o principal organizador de muitos congressos nacionais e internacionais sobre madeira, celulose e química macromolecular, principalmente em Iasi e Bucareste. Mencionamos, como referência o Simpósio Internacional sobre Macromoléculas (IUPAC Macro 83, Bucharest).

Prof. Acad. Cristofor I. Simionescu foi uma pessoa altamente educada e erudita. Uns vinte anos atrás, quando a maioria das pessoas falavam de uma nova era, novos paradigmas, globalização, verdades diferentes e mudanças de valores, o Prof. Acad. Cristofor I. Simionescu em Iasi e outras mentes brilhantes em Coimbra, Portugal falavam de crise da civilização, regresso ao mercantilismo e obscurantismo da Idade Média, imbecilização das massas e até imbecilização das elites.

O Prof. Acad. Cristofor I. Simionescu nos deixou e subiu para outros níveis e dimensões. O seu exemplo, as suas lições e a sua herança permaneceram para aqueles que gostariam de tirar proveito.

REFERÊNCIAS

1. I. I. Negulescu and O. Vogl,"Professor Cristofor Simionescu on His 70th Birth Anniversary", *Mem. Sect. Stiint, Ser.IV, Tom XIII, Academia Romana, Nr. 1,* 8-11 (1990).
2. I.I. Negulescu and O. Vogl, *Cellulose Chemistry and Technology, 24,* 657-659 (1990).
3. I.I. Negulescu and O. Vogl, *J. Macrmol. Sci. Chem., A28(7)*, 597-600 (1991).
4. C.I. Simionescu, I.I. Negulescu and O. Vogl,"Polymer Science in Romania", *Polymer News, 13(*11), 351-354 (1988).
5. E. Schab-Balcerzak, *Polimery-Warsaw, 53(6)*, 481 (2008).
6. E. Board,"Professor Cristofor I. Simionescu (1920-2007)", *Rev. Roum. Chim., 52(10),* 1007-1008 (2007.
7. E. Chiscop,"Ultimul Tatuc", *Ziarul de Iasi*, 11 Februarie 2002. (A tendentious article about Prof. Acad. Cristofor I. Simionescu and his accomplishments).
8. L. G. Ionescu," Ilie G. Murgulescu, Prominent Scientist and Educator", *South. Braz. J. Chem., 1(1),* 1-4 (1993).
9. L. G. Ionescu, "Costin D. Nenitzescu (1902-1970) -100th Anniversary of His Birth", *South. Braz. J. Chem., 10(1),* 1-10 (2002).
10. L. G. Ionescu and C.A. Perazzolo, "Luis Frederico Leloir – South America's Only Nobel Laureate in Chemistry", *South. Braz. J. Chem. 3(3),* 1-8 1995).
11. L. G. Ionescu, "Ernesto Giesbrecht, Great Chemical Educator and Father of Brazilian Inorganic Chemistry", *South. Braz. J. Chem., 4(4),* 1-8 (1996).
12. L. G. Ionescu, "Andrés Manuel del Rio, Discoverer of Vanadium", *South. Braz. J. Chem., 5(5),* 1-6 (1997).
13. L. G. Ionescu and L.A. B. De Boni, "Theodoro Augusto Ramos – A Brazilian Contribution to the Model of the Atom", *South. Braz. J. Chem., 13(*13), 1-12 (2005).
14. L. G. Ionescu, "Xorge Alejandro Dominguez, Mexico's Foremost Organic Chemist", *South. Braz. J. Chem., 2(2),* 1-4 (1994).
15. L. G. Ionescu and L.A. B. De Boni, "Glimpses of the History of Chemistry in Mexico", *South. Braz. J. Chem., 14(14),* 39-87 (2006).
16. L. G. Ionescu, *Private Reminiscences* (Lembranças), 1980-2000.

BOOKS / LIVROS

HAIDI FIEDLER, **“Homens, terra e água – a relação envolve instintos eternos”**
**“ Mankind, Earth and Water – The Relationship that involves
Eternal Instincts**”, Editora da Autora, Universidade Federal de Santa Catarina,
Florianópolis, SC, Brasil, 2008, 46 páginas .

Disponível on line: http://www.qmc.ufsc.br/lacfi/

Este livro, publicado em português e inglês, conta a história de uma molécula menina chamada Moleculina, com apelido Lina, que nasceu em 4 de Março de 1921. Sua mãe era a Sra. Oxigênio e seu pai era o Sr. Hidrogênio. Lina nasceu e cresceu em conjunto com outras moléculas que formavam um agregado puro e cristalino, um meio superior, chamado “**água pura e cristalina**” em um rio próximo à Cordilheira dos Andes, na fronteira entre Peru, Bolívia e Chile na América Latina.

DOI: 10.48141/SBJCHEM.v17.n17.2009.73_2009.pdf

Com 10 anos de idade, Lina que era cega e sonhadora, se transformou em líquido e foi rio abaixo até a cidade de Santiago. No caminho conheceu muitos lugares bonitos. Na cidade grande porém, sentiu os esgotos domésticos e industriais e decidiu estudar para melhor entender o que estava acontecendo.

Com 17 anos, Lina foi a estudar na Universidade e também no **"Instituto de Estudos Avançados das Moléculas Superiores do Chile".** Sonhava junto com colegas e amigas se transformar em gás, viajar e conhecer o maravilhoso ambiente do país acolhedor chamado Brasil. Foi uma aluna exemplar , criou a "**Teoria da Ondulação Universal**" e como prêmio recebeu uma bolsa de estudos no Programa de Pós-Graduação do Planeta do **"Instituto Avançado do Mar".**

Lina e seu tio cujo nome era Einstein Moleculino de Carbono II, com apelido Emc^2 partem com o consentimento da família e parentes. O tio de Lina explicou para ela que o grande problema dos lugares para onde eles iriam eram os seres chamados **"humanos"** que haviam afetado a **"camada de ozônio**" e provocado o **"Efeito Estufa**".O lucro falava mais alto e as ganância sobrepujou a orgulhosa racionalidade dos humanos.

No **Instituto Avançado do Mar**, Lina e seu tio trabalharam em rede com muitos grupos de pesquisadores com o objetivo de manter o Planeta vivo e saudável. Os estudos estavam relacionados com educação ambiental, sustentabilidade do Planeta, tratamento de resíduos aquáticos e atmosféricos, novos materiais, degradação de fosfatos orgânicos, reflorestamento e outras áreas.

O problema mais sério era um aquecimento demasiado intenso do Planeta, já que os raios do Sol penetraram profundamente através da atmosfera com espessura muito reduzida. Eventualmente, na Terra tudo virou cinza, estava sempre nublado e não dava mais para ver o Sol

Lina desaparece do espaço comum e vai para outra dimensão paralela. Se transforma em gás. No Mar, onde ela se encontra agora passa a se chamar **Àgua** simplesmente, mas com sobrenome **Sólido-Líquido-Vapor.** E **Lina**, ou simplesmente **Molécula Água**, depois de viver um tempo no Mar, quer ir estudar ou trabalhar no Céu nunca desiste de sonhar. "***Deseja fortemente conseguir sentir o Sol mais de perto, ou a luz do seu ou outros Planetas, e dizem ....que foi parar para refletir um pouco mais sobre seu grau de vitalidade em Andrômeda. Mas sempre está querendo chegar mais longe, mais longe, querendo investigar elaborando uma tese indefensável de que o Universo é infinito, ou seja eterno.***

Homens, terra e água

A relação que envolve instintos eternos

Mankind, Earth and Water

Therelationshipthatinvolveseternalinstincts

HAIDI FIEDLER

Ela gostaria de estar PARA SEMPRE presente no Universo".

Lina sabia que a maioria dos Continentes do passado haviam submergido e que agora só existiam poucas ilhas vulcânicas, picos e montanhas.

No Mar, Lina , que nunca casou ou teve filhos, tem muitos alunos e uma casa própria, situada numa região hidrotermal. Ela tem um submersível que ela mesma tripula e procura informações sobre a região, usando ecossondas e outras técnicas.

Lamentavelmente, a região tranqüila perto das "**chaminés hidrotermais**" foi invadida por indústrias multinacionais aproveitadoras. A região, que no passado era um verdadeiro paraíso, virou uma região perigosa para os habitantes com um cinturão de marginalidade.

Lina luta para colocar esta população marginal dentro da sociedade através da **educação** e construir uma sociedade mais justa.

Atualmente, Lina perdeu todos seus familiares, mas não perdeu a sua capacidade contínua de adaptar seus sonhos às diferentes situações de desenvolvimento em que se encontra o seu meio ambiente no momento, porque ela acredita que é um **ser eterno.**

Lina ou simplesmente Água, sofreu muita irradiação devido ao buraco na camada de ozônio, se chama agora **Água Pesada** e possui uma quantidade enorme de deutério. Foi trabalhar em câmaras subterrâneas, abertas nas rochas nas profundezas do mar, onde não deve existir outro tipo de radiação que não sejam os neutrinos. O objetivo de Lina é capturar algum neutrino porque quer estuda-los porque a maioria dos neutrinos são liberados pela combustão nuclear no **Sol**. **Ela pensa que se conseguir saber mais sobre eles, poderá saber mais sobre o Sol para poder "vê-lo mentalmente"**.

Esta é um resumo breve da história de **Lina Moleculina**, também chamada simplesmente de **Água-Sólido-Líquido-Vapor**.

À nível fundamental, pode ser considerada uma história para crianças e uma ficção.

Em nível mais elevado, o livro trata da água, a molécula mais abundante, interessante e importante do Planeta Terra. É um ensaio de pensamentos filosóficos de atualidade, muito graves e difíceis como meio ambiente, aquecimento global, poluição, camada de ozônio, mudanças climáticas, sustentabilidade, novos materiais, teoria da ondulação universal, mecânica quântica, salto com vara, química que é sempre boa, arte e decadência de pessoas, ética e o princípio de responsabilidade e educação.

Como a Professora Dra. Heidi Fiedler, menciona no Prefácio, o livro é o resultado de sua reflexão num périodo difícil da **Vida**. São momentos namo as pessoas pensam seriamente e refletem profundamente sobre a sua trajetória no Planeta Terra. A leitura do livro a este nível não pode e não deve ser um exercício confortável ou uma situação de descontração.

Os pensamentos filosóficos apresentados pela autora devem ser analisados e avaliados por cada leitor individualmente. Cada um deverá tirar as suas conclusões e determinar as trajetórias que deverá seguir.

Recomendamos altamente a leitura deste livro para todos os interessados no Planeta Terra.

Lavinel. G. Ionescu, A.A., B.S., M.S., Ph.D. (Físico-Química/Astrofísica)

HAIDI FIEDLER, **"Mankind, Earth and Water – The Relationship that Involves Eternal Instincts"**, Editora da Autora, Universidade Federal de Santa Catarina, Florianópolis, SC, Brazil, 2008, 46 pages.

This book, published simultaneously in English and Portuguese tells the story of a little girl and molecule, called Moleculina, nicknamed Lina, who was born on March 4, 1921. Her mother was Lady Oxygen and her father was Lord Hydrogen. She was born together with other molecules that formed a pure and crystalline aggregate, a superior environment, called **"pure and crystalline water"** in a river of the Andes Mountain Range, close to the border between Peru, Bolivia and Chile in Latin America.

At the age of ten, Lina who was blind and a dreamer, transformed herself into a liquid and started a journey downstream to the city of Santiago. Along the way, she saw many beautiful places. In the large city, she became disappointed with sewage and industrial wastes and other things and decided to study in order to understand what was going on.

At the age of seventeen, Lina entered the university and also began studies at the **"Chilean Institute of Advanced Studies on Higher Molecules"**. Together with her colleagues and friends she dreamed to transform herself into a gas, travel and get to know the marvelous environment of a friendly country called Brazil.

She was an outstanding student, discovered the "**Theory of Universal Ondulation**" and as a prize she was awarded a scholarship in the Planetary Gaduate School of the "**Advanced Institute of Oceanography**".

Lina and her uncle whose name was Einstein Moleculine Carbon II, nicknamed Emc^2, started a new journey with the consent of the family and friends. Her uncle explained to her that the biggest problem of the places where they will travel were certain beings called **"humans"** that depleted the **"ozone layer"** and caused the **"greenhouse effect"**. Profit was more important and greed overwhelmed the proud rationality of humans.

In the **Advanced Institute of Oceanography,** Lina and her uncle worked in collaboration with many groups of research scientists in order to maintain the Planet alive and healthy. The studies were related to environmental education, sustainability of the Planet, treatment aquatic and atmospheric residues, new materials, decomposition of organic phosphates, reforestation and other areas.

The most serious problem was global warming since the rays of the Sun now passed rather easily through the rarefied ozone layer. Eventually, everything on Earth turned grey, it was always cloudy and the Sun could not be seen anymore.

Lina disappears from common space and goes to a parallel dimension. She becomes a gas. In the Ocean, where she is now, her name is simply **Water,** but now she also has a last name , **Solid-Liquid-Vapor**. And Lina, or simply **Water Molecule**, after spending some time in the **Ocean**, wants to go to study and work in **Heaven** and does not give up dreaming. "**She wants to be closer to the Sun and feel its light or the light of other planets, and they say ...... that she went to reflect about herself and her inner strength somewhere in Andromeda. She wants to reach further and further into Space with the desire to elaborate a thesis that some people think is indefensible that the Universe is infinite and eternal. She would like to be present FOREVER in the Universe".**

Lina knew that the majority of the Continents of the past have been submerged and that now what was left of Mother Earth were a few volcanic islands and mountain peaks.

In the Ocean, Lina who has never married and has no children, but has a lot of students, owns a house in a region near **hydrothermal vents**. She has a high depth submarine (bathyscaph) that she commands and uses to seek information and data about the region using echo probes and other techniques.

Unfortunately, the once calm region of the **hydrothermal vents**, has been invaded by multinational industrial companies that think only about profit and easy money making. The region, that in the past was a true paradise, became a dangerous area for its inhabitants and was transformed into crime and poverty belts with violence, robbery and trafficking of all kinds. Lina works hard and struggles to place this marginal population back into society through **education** and tries to build a society with justice for all.

At the present, Lina lost all her family members but she did not loose the capacity to adapt her dreams to the different conditions of the environment at the time, because she believes that she is an **eternal being.**

Lina or simply Water, was exposed to a lot of radiation because of the depletion of the ozone layer of the atmosphere and she was converted to **Heavy Water** and now she contains a large amount of deuterium. She went to work in subaquatic caves opened in rocks at very large depths where there is no other type of radiation, except neutrinos. Her objective is to capture neutrinos. Since the majority of them are liberated by solar combustion, **she thinks that by studying neutrinos she can understand more about the Sun and mentally visualize it.**

This is a short summary of the story of **Lina Moleculina,** who is also called **Water-Solid-Liquid-Vapor.** In a simple minded way it can be considered a story for children and a fiction.

At a higher level, the books treats of water, the most abundant, important and interesting molecule on Planet Earth. It represents an assay of current , grave and difficult philosophic thoughts such as environment, global warming, pollution, ozone layer, climate changes, sustainability, new materials, theory of universal ondulation, quantum or wave mechanics, pole vault jumping, chemistry that is always good, art and decadence of people, ethics and the principle of responsibility and education.

As Prof. Dr. Heidi Fiedler mentions in the Preface, the book is the result of her reflection during a difficult period of her **Life.** These are moments when people think seriously and reflect profoundly over their trajectory on Planet Earth. The reading of the book at this level can not and should not be a comfortable and relaxing experience.

The philosophic thoughts presented by the author must be analyzed and evaluated by every reader individually. Everyone should draw his own conclusions and determine the trajectories that he should follow.

We recommend highly the reading of this book to all those interested in Planet Earth.

Lavinel G. Ionescu, A.A., B.S., M.S., Ph.D. (Physical Chemistry/Astrophysics)

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

VOLUME SEVENTEEN, NUMBER SEVENTEEN DECEMBER 2009

AUTHOR INDEX / ÍNDICE DE AUTORES

The SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY (ISSN: 2674-6891; 0104-5431) is an open-access journal since 1993. Journal DOI: 10.48141/SBJCHEM.
http://www.sbjchem.com.

INFORMATION FOR AUTHORS

The Southern Brazilian Journal of Chemistry - SBJC will publish review articles, original research papers and short communications dealing with chemistry and interdisciplinary areas such as materials science, biotechnology, bioengineering and other multidisciplinary fields.

Articles report the results of a complete study. They should include an Abstract, Introduction describing the known art in the field Experimental or Materials and Methods, Results and Discussion, Acknowledgments (when appropriate) and References.

Short Communications should be limited to 1500 words, including the equivalent space for figures and/or tables and should include an Abstract and concise Experimental.

Manuscripts may be submitted on-line or in triplicate (original and two copies by registered mail) and are received with the understanding that the original has not been submitted for publication elsewhere. It is implicit that all the persons listed as authors have given their approval for the submission of the paper and that permission has also been granted by the employer, when necessary.

Manuscripts must be written in American or British English, single spaced, on A4 sheets (21 cm x 29.5 cm) and one side only and should be numbered beginning with the title page. Type must be 12 Arial or Times New Roman.

Margins of at least 3 cm should be left at the top and bottom and both sides of each page. The first page of the paper should contain only the title of the paper, the name(s) and addressees) of the author(s), an abstract of not more than 250 words and 4-8 keywords. We reserve the right to translate the abstract in Portuguese. Abstracts are required of all papers including reviews and short communications.

Figures and Tables with short explanatory titles, each on a separate sheet, should be adequate for direct reproduction and identified in pencil on the back of each page by Arabic numerals, corresponding to the order they appear in the manuscript. Tables and Figures (BMP or JPG format) may also be included directly in the text when convenient and the article may submitted in a quasi-final form in order to facilitate editorial work.

References should be numbered in the sequence they appear in the text, cited by superior numbers and listed at the end of the paper in the reference section in the numerical order they appear in the text. The style for references is shown below:

1. L. G. Ionescu and D. S. Fung, *J. Chem. Soc. Faraday Trans. I, 77*, 2907-2912 (1981).
2. K. L. Mittal, Ed., "*Solution Chemistry of Surfactants*", Plenum Press, New York (1984), Vols. 1-3, pp. 1-2173.

IUPAC Rules should be used for the name of chemical compounds and preference should be given to 51 units.

Authors are invited to send manuscripts by registered air mail to the EDITOR - SBJC, C.P. 15032, Agronomia, Porto Alegre, RS BRASIL 91501, or by e-mail to **lavinel@ibest.com.br** or **lavinel@pop.com.br**.

VISIT OUR SITE: http://www.sbjchem.he.com.br

SCIENCO
SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

ISSN 0104-5431

The **SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY** – ***SCIENCO*** **(SOUTH. BRAZ. J. CHEM.)** publishes original research articles in chemistry and related interdisciplinary areas and is intended to fill a gap in terms of scientific information for Southern Brazil.

Occasionally the journal will include review papers and articles dealing with chemical education and philosophy and history of science. It will be published mainly in English, with abstracts in Portuguese and only occasional papers in other languages. At the present there are no page charges and the authors will receive twenty five reprints of their papers free of charge.

We have set high standards for the articles to be published by ensuring strong but fair refereeing by at least two reviewers. We hope that this journal will provide a forum for dissemination of high quality research in chemistry and related areas and are open to any questions and suggestions.

The Editor

SUBSCRIPTION INFORMATION
Brazil and Latin America:
US$ 70.00 per issue,
Other Countries: US$ 100.00 per issue,
including air mail delivery. Persons or institutions outside Brazil should send
subscription fee payable to Dr. L. G. Ionescu,
c/o SBJC, 8532 Howard Circle, Huntington Beach, California
USA 92647

MAILING ADDRESS

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

Lavinel G. Ionescu, B.S., M.S., Ph.D., Editor
C.P. 15032, Agronomia
Porto Alegre, RS, BRASIL 91501-970

Tel. 055 51 3485-1820 / 051 55 3485-1711 / 055 51 995-26616 / 055 51997-64159
E-Mail: lavinel@ibest.com.br lavinel@pop.com.br
VISIT OUR SITE: http://www.sbjchem.he.com.br

FINANCIAL SUPPORT

SARMISEGETUSA RESEARCH GROUP

SANTA FE, NEW MEXICO, U.S.A.

Endless Column, 1937, cast iron
CONSTANTIN BRANCUSI