Volume 87 • Number 1 • November 2014 Established in 1923 • ISSN 1945-0702



In this Issue

A Dye Sensitized Solar Cell Using Red Sandal Dye And 1,3,5-Triphenylamine Derivatives The Use of EDS Analysis in a Materials Testing Laboratory Improved Corrosion Protection Through Electrodeposition Designing Core Concepts for a Tertiary Basic Chemistry Course

Very Little About Chemistry!

Note: Triphenylamine-3D-balls. This work has been released into the public domain by author Ben Mills, a chemistry Ph.D. student at the University of Bristol in the UK.

Official journal of The American Institute of Chemists, Inc. http://www.theaic.org/pub_thechemist_journals/

The Chemist

Established in 1923, The Chemist is the official publication of The American Institute of Chemists, Inc. (AIC). The Chemist was published quarterly in magazine format up until 2006. The Chemist is currently being set up and formatted as an online journal.

Editor-in-Chief

David Devraj Kumar Florida Atlantic University, USA

Editorial Assistant

Deborah Cate Manuta Chemical Consulting

Art & Web Direction Alberto Fernández

Florida Atlantic University, USA

Editorial Review Board	
John E. E. Baglin	IBM Almaden Research Center, USA
Rodney Bennett	JRF America, USA
Xiongwei Cai	Biogen Idec, USA
Donna Chamely-Wiik	Florida Atlantic University, USA
Jerry Ray Dias	
J. Stephen Duerr	
Lawrence Duffy	
Nwadiuto Esiobu	
Peter D. Fade	
Abraham George	
David Gossman	Gossman Consulting, Inc., USA
Margaret Hall	University of Southern Mississippi, USA
K. R. Haridas	
John Hill	La Trobe University, Australia
Jerry P. Jasinski	
Edward J. Kikta, Jr	
David Devraj Kumar	
Gopendra Kumar	University of Botswana, Botswana
James Kumi-Diaka	
Gary R. List	US Department of Agriculture, USA
Bushan Mandava	
David M. Manuta	
Dayal T. Meshri	Advance Research Chemicals, Inc., USA
E. Gerald Meyer	University of Wyoming, USA
Robert F. Moran	
Wayne A. Morris	
Ronald Persin	
Gary F. Porter	Bergan Community College, USA
Manit Rappon	Lakehead University, Canada
James A. Roe	Loyola Marymount University, USA
David W. Riley	Extrusion Engineers, USA
James S. Smith	
Joy E. Stewart	Broward College, USA
Saligrama Subbarao	Lincoln University, USA
P. V. Thomas	Mar Ivanios College, India
Ranjit K. Verma	Patna University, India
Rock J. Vitale	
Kurt Winkelmann	

The American Institute of Chemists, Inc. does not necessarily endorse any of the facts or opinions expressed in the articles, book reviews, or advertisements appearing in The Chemist. **Subscription:** \$35 per year to members, \$100 per year to non-members. Single copy: \$50. The Chemist (ISSN-0009-3025) is published online by The American Institute of Chemists, Inc.

Volume 87 | Issue 1 | 2014

The Chemist Journal of the American Institute of Chemists

Editorial: Is Chemistry Still the Central Science?	i
ARTICLES	
A Dye Sensitized Solar Cell Using Red Sandal Dye And 1,3,5-Triphenylamine Derivatives Siji Mathew and Karickal R. Haridas	1
The Use of EDS Analysis in a Materials Testing Laboratory Frank Grate	8
Improved Corrosion Protection Through Electrodeposition George E. F. Brewer	11
Designing Core Concepts for a Tertiary Basic Chemistry Course John O. Hill, David Devraj Kumar and Ranjit K. Verma	14
PUBLIC UNDERSTANDING OF CHEMISTRY	
Very Little About Chemistry! Susan Day	23
BOOK REVIEWS	
Nanophysics and Nanotechnology	
Casarett & Doull's Essentials of Toxicology. Edition 2	27 28
	20
Dr. E. G. Meyer	29 30
The AIC Code of Ethica	22
Manuscript Style Guide	32 34
	20
AIC Officers & Board of Directors	40



Editorial

Is Chemistry Still the Central Science?

David Devraj Kumar Florida Atlantic University

I would like to open my editorial with the question – Is chemistry still the central science? It is a common belief among scientists that chemistry is the central science as it helps to bridge the worlds of natural and physical sciences. Chemistry deals with atoms and their interactions, making and breaking of bonds. It is the "science that deals with the properties, composition, and structure of substances (elements and compounds) and the reactions and transformations they undergo, and the energy released or absorbed during those processes. Often called the "central science," chemistry is concerned with atoms as building blocks (rather than with the subatomic domain) with everything in the material world, and with all living things" (1). On the other hand, new discoveries about the universe made by cosmology - the study of the properties of the universe as a whole show that about 4.6% of the universe is made of atoms, while 24% is dark matter and 71.4% dark energy (2). Whether it is possible to gain a thorough understanding of the non-atomic portion of the universe through chemistry is a critical question. While we search for possible answers to this question, let us not forget the fact that chemistry still remains one of most fascinating areas of inquiry as evidenced by the lineup of articles in this issue of The Chemist.

Siji Mathew and Karickal Haridas report the fabrication of dye-sensitized solar cells using 1,3,5-triphenylamine derivatives. These materials are environment-friendly and suitable candidates as hole transporting materials (HTM) for solar cells and solar cell devices. Frank Gate describes the use of Energy Dispersive spectroscopy (EDS) in materials testing, especially useful for detecting basic corrosions in materials. The George Brewer article reprinted from The Chemist discusses electrodeposition of water-dispersed organic coatings used in corrosion protection, anything from toys to automobiles and steel trusses. John Hill and co-authors propose a curriculum framework for a tertiary basic chemistry course design based on Atkins' interrelated core chemical concepts aimed at triggering student interest in pursuing chemistry. Susan Day, under the title, "Very Little About Chemistry!" discusses how her appreciation for chemistry has grown in recent years since chemistry has become more important to her "livelihood," though her terminal degree is in public administration. While Kenneth Abate offers a review of the book Nanophysics and Nanotechnology, Margot Hall reviews the books Brain: The Complete Mind and Casarett & Doull's Essentials of Toxicology (2nd edition). In this issue two long time fellows of The American Institute of Chemists are portrayed, and they are Dr. David W. Riley and Dr. E. G. Meyer. The biography of Dr. Riley and the autobiography ("A wonderful ride") of Dr. Meyer are very impressive portraying a well-balanced life. Without any doubt Dr. Riley and Dr. Meyer are excellent role models, and I wish them the best.

I would like to thank the reviewers on the journal's Editorial Review Board who contributed their valuable time and effort providing thoughtful reviews of manuscripts. Also, I would like to thank Dr. Penelope Fritzer at Florida Atlantic University and Mr. Wade Berstler at Florida Atlantic University for providing thoughtful feedback on book reviews, and Ms Enery Burgos at Florida Atlantic University for providing editorial assistance. Florida Atlantic University continues to provide a home away from home for The Chemist, with the support of Dean Valerie Bristor. Let us not take for granted the support of each and everyone involved in offering various degrees of support for the production of The Chemist because not everyone is a member of The American Institute of Chemists. Collectively their action speaks louder than words that chemistry has an important role to play in contributing to our understanding of the world around and what the journal The Chemist does in this perspective is worth supporting no matter whether chemistry is still the central science or not.

References

1. Merriam-Webster Concise Encyclopedia, n.d. Available at: http://www.merriamwebster.com/dictionary/ chemistry

2. NASA/WMAP Science Team, Universe 101, 2014. Available at: http://wmap.gsfc.nasa.gov/ universe/uni_matter.html

Thank you.



A Dye Sensitized Solar Cell Using Red Sandal Dye And 1,3,5-Triphenylamine Derivatives

Siji Mathew and Karickal R. Haridas*

Kannur University - School of Chemical Sciences / Payyanur Campus, Edat P.O. 670327, Kerala, India (*Email: krharidas2001@yahoo.com)

Abstract: Fabrication of the dye sensitized solar cell (DSSC) using four 1,3,5-triphenylaminederivatives as hole transporting material (HTM) and red sandal natural dye as sensitizer. Performance of cells is measured using current-voltage characteristics. The results obtained indicate that these compounds are prominent candidates as HTM for solar cells and are suitable materials for applications in such devices.

Key Words: Photovoltaic devices, Solar cell, Organic electronics, Titanium dioxide.

INTRODUCTION

The environment-friendly dye sensitized solid state solar cells (DSSC) have attracted much attention since 1991[1] due to their high efficiency and low cost production for practical applications. The past decade has seen great progress in both device fabrication techniques and material development. The typical DSSC is normally in a sandwiched configuration, filled with a HTM in the space between the dye sensitized nanocrystalline TiO₂ photoelectrode and counter electrode. Under the irradiation by visible light, the dye molecules become photoexcited and on an ultrafast time scale, direct electrons into the conduction band of titanium dioxide (TiO₂). Then the oxidized dye sensitizer is effectively scavenged by HTM, which itself is regenerated at the counter electrode by the passing of electrons through the external load.

Usually, synthetic complexes such as ruthenium (II) complexes with carboxylated polypyridyl ligands are employed as molecular sensitizers in DSSC [2]. In order to replace the rare and expensive ruthenium compounds, many kinds of organic synthetic dyes have been actively studied and tested as low cost materials [3] for DSSCs. Some researchers have obtained good solar electric power conversion by testing natural dyes as inexpensive environmentally-friendly alternatives to artificial sensitizers for DSSCs [4]. In nature, some fruits, flowers, leaves, etc. exhibit various colors containing pigments that can be easily extracted and then employed in DSSC for either educational purposes or indoor applications. Therefore, unlike artificial dyes, the natural ones are is easily available, easy to prepare, low cost, non-toxic, environmentally-friendly and fully biodegradable.

We report the fabrication and performance of DSSC using four starburst molecules which we have synthesized as HTM and red sandal dye as sensitizer. In our previous paper, the synthesis, characterization and fabrication of DSSC using N,N,N- Tris- (2-ethoxy-naphthalenen-1-yl) -N,N,N'-triphenylbenzene-1,3,5-triamine [4b] were reported. The conversion efficiency of DSSC is 0.39 [5]. The alkoxyl groups in HTM play an important role for capture of electrons so we change the alkoxyl group to improve the efficiency of solar cell. Here the HTMs are the derivatives of N,N,N-Tris-(4-butoxy-phenyl)-N,N,N-tri-naphthalen-1-yl-benzene-1,3,5-triamine are

- i) N,N,N- Tris-(2-methoxy-naphthalenen-1-yl)-N,N,N'triphenylbenzene-1,3,5-triamine[4a],
- N,N,N- Tris-(2-propoxy-naphthalenen-1-yl) -N,N,N'triphenylbenzene-1,3,5-triamine [4c],
- iii) N,N,N-Tris-(2-butoxy-naphthalenen-1-yl)-N,N,N'triphenylbenzene-1,3,5-triamine[4d], and
- iv) N,N,N-Tris-(2-pentoxy-naphthalenen-1-yl) -N,N,N'triphenylbenzene-1,3,5-triamine[4e].

The synthesis and characterization of N,N,N- Tris-(2methoxy-naphthalenen-1-yl)-N,N,N'-triphenylbenzene-1,3,5-triamine[4a] were also reported [6].

EXPERIMENTAL

MATERIALS

Tetrahydrofuran (THF) was refluxed with sodium and benzophenone, and then distilled. 1, 2dichlorobenzene was dried over CaH₂ and then distilled. All reagents and solvents were purchased from Merck, Loba Chemie and SRL India and used as received unless otherwise stated.

MEASUREMENTS

Infrared (IR) spectra were recorded on a Shimadzu FT-IR 8400 S spectrometer as potassium bromide (KBr) disc. Ultraviolet- visible (UV-Vis) spectra were recorded from diluted solutions in spectroscopic grade ethanol on a Shimadzu 1700 UV-Visible spectrophotometer using a 1.0 cm length quartz cuvette. Proton (¹H) and carbon-13 (¹³C) nuclear magnetic resonance (NMR) spectra were recorded on a NMR-JEOL GSX-400 spectrometer with tetramethylsilane as internal standard Using tetramethylsilane (TMS) as the internal standard and using CDCl3 as solvent in all samples analyzed.

CV measurements were carried out on a Autolab potentiostat PGSTAT 12 at a glassy carbon electrode using millimolar solutions in acetonitrile (ACN) 0.1M containing supporting electrolyte, of а tetrabutylammonium hexafluorophosphate (TBAPF6), in a three electrode cell and potentiostat assembly at room temperature. The CV measurements were carried out at a glassy carbon electrode using millimolar solutions in acetonitrile (ACN) containing 0.1M of the supporting electrolyte tetrabutylammonium hexafluorophosphate (TBAPF6), in a three electrode cell and potentiostat assembly at room temperature. The potentials were measured against platinum as reference electrode and each measurement was calibrated with an internal standard, ferrocene / ferrocenium (Fc) redox system. DSC studies were performed with a NETZSCH DSC 204 thermal analyzer under inert atmosphere. The compounds are analyzed for heating and cooling thermograms (cyclic) in an inert atmosphere from -50°C to 250°C at a rate of 10°C/ min.

SYNTHESIS OF 2-ALKOXY NAPHTHALENE

Alkyl bromide (0.03mol) in toluene (25mL), 2naphthol (4.32g, 0.03mol) in 40% NaOH (20mL) and tetrabutyl ammonium bromide (0.9g, 0.003mol) were refluxed at 70°C for 4.0 hours. After the completion of the reaction which is monitored by TLC, the product is extracted using toluene – water system. Scheme 1 represents the structures and scheme for the synthesis of alkoxy naphthalenes. n-propyl bromides, n-butyl bromides and n-pentyl bromides were used as alkyl bromides to obtain the corresponding alkoxy naphthalene.



Scheme 1: Synthetic procedure for alkoxy naphthalene

2-propoxy naphthalene [1c]:

Appearances: Brown liquid; Yield: 98.2%; Boiling point: 260°C;

UV-Vis. (ethanol,nm): 267, 391; FT- IR (KBr, υ cm⁻¹) 3055, 2974 (Ar-H), 2871, 1456 (-OC₃H₇), 1215 (C-OC); ¹H-NMR (CDCl₃, δ): 0.96-4.04 (-OC₃H₇), 6.97-7.64 (7H, Ar), ¹³C-NMR(CDCl₃, ppm):10.3, 23.4, 74.5(OC₃H₇) 105.8, 118.8, 123.7, 126.8, 127.7, 129.3, 129.5,129.3, 134.6,157.7(Ar-C).

2-butoxy naphthalene [1d]:

Appearances: Brown liquid; Yield: 98.4%; Boiling point: 285°C;

UV-Vis. (ethanol, nm): 314, 260; FT- IR (KBr, υ cm⁻¹)3056, 2932 (Ar-H), 2871, 1387 (-OC₄H₉), 1217 (C-O-C); ¹H-NMR (CDCl₃, δ): 0.98-4.12 (-OC₄H₉), 6.80-7.91 (7H, Ar);¹³C-NMR(CDCl₃, ppm): 14, 19.4, 32.8, 72 (OC₄H₉) 105.5,118.8, 123.7,126.4, 126.8, 127.7, 129.3, 129.5, 134.6, 157.7(Ar-C).

2-pentoxy naphthalene [1e]:

Appearances: Brown liquid; Yield: 98.4%; Boiling point: 290°C;

UV-Vis. (ethanol, nm): 360, 238; FT-IR (KBr, υ cm⁻¹):3057, 2933 (Ar-H), 2859, 1478 (-OC₅H₁₁), 1217 (C-O-C); ¹H-NMR (CDCl₃, δ): 0.89-4.09(33H, -OC₅H₁₁), 6.79-8.5 (7H, Ar). ¹³C-NMR (CDCl₃, ppm): 14, 23.1, 28.8, 30.3, 72.3(OC₅H₁₁), 105.8, 118.8, 123.7, 126.4, 129.3, 126.8, 127.7, 129.5, 134.6, 157.7(Ar-C)

SYNTHESIS OF 2-ALKOXY NAPHTHALENE-1-YL-AMINE

2-alkoxy naphthalene (0.01mol) and conc. H₂SO₄ (5mL) were added in around bottom flask equipped with a condenser. The mixture is cooled and the temperature is maintained at 5 degrees Celsius or less. To this, conc. HNO₃ (4mL) was added drop wise with stirring. The solution was stirred for one hour at 0°C, one hour at room temperature and one hour at 60°C. The contents of the flask were cooled, poured into ice and neutralized with 40% NaOH. The yellow compound obtained is filtered, washed, dried, and recrystallized from ethanol. The product (1.64g, 0.008mol), ammonium ferrous sulphate (1.5g, 0.003mol), ethanol (20mL), water (5mL) and conc. HCl (0.5mL) were heated in around bottom flask on a stem bath for one hour. The product was extracted from the mixture by washing with hot ethanol and then dried. The yellow solid thus obtained was recrystallized from ethanol. Scheme2 represents the structures and scheme for the synthesis of Alkoxy naphthyl amine.



Scheme 2: Synthetic procedure for Alkoxy naphthyl amine

2-propoxy naphthalene-1-yl-amine [2c]:

Appearances: Yellow solid; Yield: 77.9%; Melting point: 80°C;

UV-Vis.(ethanol,nm): 341, 369;FT-IR (KBr, υ , cm⁻¹): 3511, 3417 (-NH₂), 3066, 2968 (Ar-H), 2876, 1368 (-OC₃H₇), 1217 (C-O-C), 1252 (C-N); ¹H-NMR (CDCl₃, δ): 0.96-4.04 (-OC₃H₇), 4.0 (3H, -NH), 6.87-7.59 (7H, Ar); ¹³C-NMR(CDCl₃, ppm): 10.3, 23.4, 74.5(OC₃H₇), 119.8 (C-NH₂)119.1, 119.5, 120.2, 123.4, 124.4, 125.1, 128, 129.9, 141.2(Ar-C).

2-butoxy naphthalene-1-yl-amine [2d]:

Appearances: Yellow solid; Yield: 75.9%; Melting point: 75°C;

UV-Vis.(ethanol, nm):324,308; FT-IR (KBr, υ cm⁻¹):3486, 3395 (-NH₂), 3070, 2940 (Ar-H), 2865, 1353 (-OC₄H₉), 1217 (C-O-C), 1259 (C-N);¹H-NMR (CDCl₃, δ): 0.98-4.07 (21H,-OC₄H₉), 4.0 (3H, -NH), 6.87-7.59 (7H, Ar); ¹³C-NMR(CDCl₃, ppm): 14, 19.4, 32.8, 72 (OC₄H₉), 119.8 (C-NH₂), 119.1, 119.5, 120.2, 123.4, 124.4,125.1, 128, 129.9, 141.2 (Ar-C).

2-pentoxy naphthalene-1-yl-amine [2e]:

Appearances: Brown solid; Yield: 76.2%; Melting point: 77°C;

UV-Vis. (ethanol, nm): 329, 304; FT-IR (KBr, υ cm⁻¹):3454, 3529 (-NH₂), 3085, 2955 (Ar-H), 2871, 1478 (-OC₅H₁₁), 1217 (C-O-C), 1252 (C-N);¹H-NMR (CDCl₃, δ): 0.89-4.09 (33H, -OC₅H₁₁), 4.0 (3H, -NH), 6.79-8.56 (7H, Ar);¹³CNMR (CDCl₃, ppm): 14, 23.1, 28.8, 30.3, 72.3(OC₅H₁₁), 119.8 (C-NH₂), 119.1, 119.5,120.2, 123.4, 124.4, 125.1, 128, 129.9, 141.2(Ar-C).

SYNTHESIS OF

N,N,N'-TRIS-(1-ALKOXYNAPHTHALEN-2-YL)-BENZENE-1,3,5-TRIAMINE

2-alkoxyy naphthalene-1-yl-amine (0.03mol), tribromobenzene (3.30g, 0.01mol), CuCl (0.02g, 0.0002mol) and K₂CO₃ (1.0g, 0.007mol) (dried at 110°C) were refluxed together with 20 ml acetone for 10hours at 60°C. After removal of the solvent by vacuum, ammonia solution (50mL) was added and the mixture was left to stand for 2 hours. Ethyl acetate (150mL) and water (100mL) were added. The organic phase was separated, washed with water (100mL×2) and brine solution (100mL), dried over anhydrous sodium hydrogen sulfate, and concentrated to yield a yellow residue. The yellow residue was purified via column chromatography using ethyl acetate - hexane (4:1) as the eluent. Recrystallisation from ethanol yielded a yellow solid. Scheme 3 represents the structures and scheme for the synthesis of N,N,N'-Tris-(2-alkoxy-naphthalen-1-yl)-benzene-1,3,5-triamine.

N, N, N'-Tris-(2-propoxy-naphthalen-1-yl)-benzene-1, 3, 5-triamine [3c]:

Appearances: Yellow solid; Yield: 42.6%; Melting point: 59°C;

UV-Vis. (ethanol, nm): 397, 331; FT- IR (KBr, v, cm⁻¹): 3461 (N-H), 3071, 2968 (Ar-H), 2876, 1404 ($-OC_3H_7$),1217 (C-O-C), 1256 (C-N); 1 H-NMR (CDCl₃,): 0.96-4.04 (21H, - OC₃H₇), 4.0 (3H, -NH),5.02-7.59 (21H, Ar); 13 C-NMR(CDCl₃, ppm): 10.3, 23.4, 74.5(OC₃H₇) 96.8, 119.1,

119.8,120.2, 123.4, 124.4, 125.1, 128, 129.9, 143.2, 148.1 (Ar-C).

N,N,N'-Tris-(1butoxy naphthalen-2-yl)-benzene-1,3,5triamine [3d]:

Appearances: Yellow solid; Yield: 43.7%; Melting point: 56°C;

UV-Vis.(ethanol, nm): 360, 341;FT-IR (KBr, v, cm⁻¹):3429 (N-H), 3071, 2924 (Ar-H), 2824, 1353 (-OC₄H₉), 1217 (C-O-C) 1259 (C-N); ¹H-NMR(CDCl₃, δ): 0.92-4.14 (27H, OC₄H₉), 4.0 (3H, -NH), 5.02-8.12 (21H, Ar); ¹³C-NMR(CDCl₃,ppm): 14, 19.4, 32.8, 72(OC₄H₉), 96.8, 119.1, 119.5, 120.2, 123.4, 124.4, 125.1, 128, 129.9,141.2, 143.4 (Ar-C).

N,N,N'-Tris-(1-pentoxyynaphthalen-2-yl)-benzene-1,3,5-triamine[3e]:

Appearances: Yellow solid; Yield: 43.6%; Melting point: 60°C;

UV-Vis. (ethanol, nm): 354, 330; FT-IR (KBr, υ cm⁻¹):3461 (N-H), 3083, 2957 (Ar-H), 2871, 1456 (-OC₅H₁₁), 1217 (C-O-C), 1253 (C-N); ¹H-NMR(CDCl₃, δ): 0.89-4.09 (33H, -OC₅H₁₁), 4.0 (3H, -NH), 5.85-7.95 (21H, Ar); ¹³C-NMR(CDCl₃, ppm): 14, 23.1, 28.8, 30.3, 72.3 (OC₅H₁₁), 96.8, 119.1, 119.5, 120.2, 123.4, 124.4,125.1, 129.9, 141.2, 143.4, 151 (Ar-C).



R--- C₃H₇, C₄H₉, C₅H₁₁

Scheme 3: Synthetic procedure for N,N,N'-Tris-(2-alkoxy-naphthalen-1-yl)benzene-1,3,5-triamine

SYNTHESIS OF

N,N,N'-TRIS-(2-ALKOXY-NAPHTHALENEN-1-YL)-N,N,N'-TRIPHENYLBENZENE-1,3,5-TRIAMINE

N,N,N'-Tris-(2-alkoxy-naphthalen-1-yl)-benzene-1,3,5-triamine(0.0071mol), bromobenzene (2.2 mL, 0.0213 mol), CuCl (0.02 g, 0.0002mol) K_2CO_3 (1.0 g, 0.007 mol) (dried at 110°C) were refluxed together with dichlorobenzene(20 mL) 10 hours at 170°C. The progress of the reaction was monitored by TLC. After removal of the solvent in vacuum, ammonia solution (50 mL) was added and the mixture was left to stand for 2.0 hours. Ethyl acetate (150 mL) and water (100 mL) were added. The organic phase was separated, washed with water (100 mL×2) and brine solution (100 mL), dried over anhydrous sodium hydrogen sulfate, filtered and the solvent is removed in vacuum. The product was purified via column chromatography using ethyl acetate – hexane as eluent to obtain a yellow solid which is recrystalized from hexane. Scheme 4 represents the structures and scheme for the synthesis of N,N,N-Tris-(2-alkoxynaphthalenen-1-yl)-N,N,N'-triphenylbenzene-1,3,5triamine.

N,N,N-Tris-(2-alkoxy-naphthalenen-1-yl)-N,N,N'triphenylbenzene-1,3,5-triamine[4c]:

Appearance: Light yellow needles; Yield: 39.2%; Melting point: 70°*C*;

UV-Vis.(Ethanol, *nm*): 396, 331; IR (KBr, v, cm⁻¹): 3070, 2967 (Ar-H) 2876, 1404 (-OC₃H₇), 1217(C-O-C), 1256 (C-N); ¹H NMR (CDCl₃, δ): 0.94-4.35 (21H, -OC₃H₇), 7.51-8.21 (36H, Ar);¹³C-NMR (CDCl₃, *ppm*): 10.1, 22.4, 71.1(OC₃H₇) 108.4, 143, 115.0, 119.4, 123.3, 124.6,125.2, 127.6, 128.4, 129.4, 132.5, 132.5, 132.9, 135.2, 135.7,147.7 (Ar-C).



 $R----CH_{3}, C_{2}H_{5}, C_{3}H_{7}, C_{4}H_{9}, C_{5}H_{11}$

Scheme 4: Synthetic procedure for N,N,N-Tris-(2-alkoxy-naphthalenen-1-yl)-N,N,N'triphenylbenzene-1,3,5-triamine

N,N,N- Tris- (2-butoxy-naphthalenen-1-yl) -*N,N,N'- triphenylbenzene-1,3,5-triamine* [4d]:

Appearance: Light yellow needles; Yield: 39.5%; Melting point: 60°*C*;

UV-Vis.(Ethanol, *nm*): 354, 344; FT-IR (KBr,*cm*⁻¹): 3070, 2958 (Ar-H) 2874, 1342(-OC₄H₉), 1217 (C-O-C), 1259 (C-N); ¹HNMR(CDCl₃, δ): 0.96-4.21 (27H, -OC₄H₉), 7.27-7.92 (36H, Ar); ¹³C-NMR(CDCl₃, *ppm*):14.0, 19.4, 32.8,72.0

 (OC_4H_9) , 108.9, 143.4, 119.1, 119.6, 119.8, 120.2, 121.5, 122.9,123.4,124.4, 125.1, 128.02, 129.4, 129.5, 141.2, 153.2 (Ar-C).

N,N,N- Tris-(2-pentoxy-naphthalenen-1-yl) -N,N,N'- triphenylbenzene-1,3,5-triamine[4e]:

Appearance: Yellow needles; Yield: 38.2%; Melting point: 59°C;

UV-Vis. (Ethanol, *nm*): 327,345; FT-IR (KBr, ∞ cm⁻¹): 3071, 2956 (Ar-H) 2871, 1338 (-OC₅H₁₁), 1217 (C-O-C), 1256 (C-N); ¹H NMR(CDCl₃, δ): 0.84-4.39 (33 H,-OC₅H₁₁) 7.52-9.13 (36H,Ar); ¹³C-NMR(CDCl₃, *ppm*): 14.3,22.1, 27.8, 39.3, 70.6 (OC₅H₁₁),108.4, 143, 115.5, 117.4, 119.8, 121.9, 123.7, 128.8, 129.2,132.9, 133.9, 135.3, 135.6, 135.7, 148.1, 151.4 (Ar-C).

DEVICES FABRICATION

DSSC device comprised of a transparent conducting oxide (TCO) glass electrode coated with porous nanocrystalline TiO₂ (nc-TiO₂), dye molecules attached to the surface of the nc-TiO₂, hole transporting material and a counter-electrode. Fluorinated tin oxide (FTO) coated transparent glass strips (25mm x 25mm) with resistance of 30µ ohms were used for the device fabrication. The structuring of the TCO is done using a chemical etching method. Zinc granulates are spread out on the glass (20 mg/cm²) and reacted with 4 N HCl (1 mL/cm²). Scotch tape is used to mask the TCO area needed for the back contact. The fast reaction between HCl and Zn leads to the removal of the SnO₂. After two treatments of 3 minute reaction time, theSnO2 is completely removed. The structured glass is then cleaned by ultra-sonification in various solvents, such as acetone, ethanol and water, for 10 min in each solvent. Compact TiO₂ (30 nm) were deposited on fluorine-doped SnO₂ (F-SnO₂) glass by spin coating that acts as a blocking layer. The FTO is placed in a chamber for 1 min and accelerated at a speed of1000 rpm. 150 μ l of TiO₂ solution is applied onto the substrate. The substrate is spun up to a speed of 1000 rpm for 30 s with an acceleration of 200 rpm/s. The samples are dried for 30min. After deposition, the prepared TCO/TiO₂ was annealed at 100°C for 1 hour in air with a hot plate to achieve complete pyrolysis of organic species.

Then nanoporous TiO_2 (~2.5µm) film was deposited by tape casting method. The layers were sintered for 30 min at 350°C to consume the organic additives and to obtain mechanically stable samples. Then the sample is cooled down slowly to 80°C and placed into alcoholic solution of red sandal dye overnight. After, the dip coating, HTM in THF (~800nm) deposited on the cell by spin coating method. The organic cells were kept overnight to allow maximum penetration of HTM in TiO_2 . The metal electrode silver (200nm) is coated on HTM of DSSC by thermal evaporation.

RESULT & DISCUSSION

The synthetic strategy employed for the synthesis of N,N,N-Tris-(2-alkoxynaphthalenen-1-yl)-N,N,N'triphenylbenzene-1,3,5-triamine derivatives are described in scheme1. Since the synthesis of the final compound involves multistep organic reaction adding two more wings to the core benzene ring, the overall yield of the synthesis is very low.

THERMAL PROPERTIES

For solar cell application, the thermal stability of the organic material is crucial for device stability and lifetime. The glass forming properties and phase transition of compounds (4a, 4c, 4d and 4e) are studied using DSC. The compounds are analyzed for heating and cooling thermograms (cyclic) in an inert atmosphere from -50°C to 250°C at a rate of 10°C/min. These five compounds differ only in their substitutions at outer naphthalene rings. Due to these differences, we expect only a very few changes in thermal properties. Accordingly, the solubility and density of the compounds may also vary.

The Tg, Tc and Tm values of all synthesized compounds are listed in Table 1. From these data, we recognize that there is only a very small change in thermal properties. This may be due to the change of substitution at the outer naphthalene ring. Well-defined glass transitions are at 65, 59, 50 and 46°C, respectively. Tm values of compounds (4a, 4c, 4d and 4e) are at 95, 70, 60 and 59°C, respectively. All the above compounds are decomposed above 250°C. The compound 4a shows two-phase transitions at 95°C and 115°C. The two transitions in DCS give the possibility of a liquid crystalline nature for the compound.

Table 1: Phase transition temperatures
of N,N,N-Tris-(2-alkoxy-naphthalenen-1-yl)-
N,N,N'-triphenylbenzene-1,3,5-triamine

compounds			
Compounds	Т _д (°С)	T _m (°C)	
4a	65	95, 115	
4c	59	70	
4d	50	60	
4e	46	59	

ELECTROCHEMICAL PROPERTIES

The electrochemical stability is one of the other main conditions to be fulfilled by the materials to find application in various electro-optical devices. The results of electrochemical studies are listed in Table 2. The electron affinity (EA), ionization potential (IP) and band gap of the compounds are calculated from the data. The high-lying HOMO energy level and reversible electrochemical oxidation of 4a, 4c, 4d and 4e suggest that these compounds have high potential for hole transporting material.

Table 2: C V data and HOMO-LUMO values of the compounds N,N,N-Tris-(2-alkoxy naphthalenen-1-yl)-N,N,N'triphenylbenzene-1,3,5-triaminecompounds

Compou nds	Eox vs Fc (v)	HOMO (eV)	Ered vs Fc (v)	LUMO (eV)	Eg (eV)	PI (eV)	EA (eV)
4a	1.5	-6.3	-0.95	-3.85	2.45	6.3	3.85
4c	0.9	-5.7	-1.2	-3.6	2.1	5.7	3.6
4d	1.1	-5.9	-0.9	-3.9	2.0	5.9	3.9
4e	1.0	-5.8	-1.1	-3.7	2.1	5.8	3.7

DEVICE PROPERTIES

The result for photocurrent density (ISC), opencurrent voltage (VOC), fill factor (FF) and corresponding photoenergy conversion efficiency (η) are summarized in Table 3. The efficiency of compound 4b is 0.39 [5]. Different HTM exhibits variable photoconversion efficiencies that are 0.2, 0.7, 0.7 and 0.72 for 4a, 4c, 4d and 4e respectively. Compared with this efficiency, efficiency of 4a is lower and 4c, 4d, 4e are higher. From the result, we can say that as the length of alkyl group increases, the efficiency increases. The low efficiency could be attributed to the poor pore filling of the hybrid nanoporous TiO_2/dye film by the organic HTM, which induces poor dye regeneration and hence low photocurrent.

Table 3: I-V characteristics of DSSC prepared using 4a, 4c, 4d, 4e as HTMs

Hole conductor	voc [V]	VMAX [V]	ISC [A/cm2]	IMAX [A/cm2]	FF [%]	η [%]
4a	0.5	0.25	2	0.5	8	0.2
4c	0.25	0.5	1.75	2	28	0.7
4d	0.5	1	1.75	2	7	0.7
4e	0.9	0.5	4	0.9	8	0.72

CONCLUSION

All five compounds are capable of functioning as DSSC. The efficiency of the devices varies from 0.2% to 0.72%. This may be due to the difference in length of the alkyl group. From these results, we can conclude that as the length of alkyl group increases the efficiency increases. Instead of the ruthenium dye and back electrode gold, we have used the red pigment of red sandal and silver. These are the two major differences we adopted. The low current values we obtained may be due to layer thicknesses of different materials and the possible degradation of natural dye. In the meantime we would like to emphasize the total cost effect of the cell, which will be down to nearly 30-40% of a similar type fabricated cell. The conversion of the non-conventional energy, even if for a very low percentage, is advancement to mankind. The use of a reduced amount of chemicals is an added advantage when the natural dye is applied. This will be an introductory step to the green synthesis. Further studies are being carried out for the optimization of layer thickness of each material and use of different natural dyes to improve the efficiency of DSSC.

REFERENCES

- 1. Regan BO. Graetzel M, Nature, 1991, 353, 737.
- 2. Sauve G, Cass ME, Coia G, Doig SJ, Lauermann I, Pomykal KE, Lewis NS. J. Phy. Chem. B, 2000, 104, 6821.
- 3. Hara K, Tachibana Y, Ohga Y, Shinpo A, Suga S, Sayama K, Sugihara H, Arakawa H. *Sol. Energy Mater. Sol. Cells*, 2003, 77, 89.
- 4. Tennakone K, Kumara GRRA, Kottegoda IRM, Perera VPS, Weerasundara PSRS. J. Photochem. Photobio. A: Chem., 1998, 117, 137.
- 5. Mathew S, Haridas KR. Bull. Mater. Chem. 2012, 35, 133.
- Mathew S, Divia N, Nair TDR, Haridas KR. Ind. J. Chem. B, 2010, 49,1389.



The Use of EDS Analysis in a Materials Testing Laboratory Frank Grate

QC Metallurgical, Inc., 2870 Stirling Road, Hollywood, FL 33020 (E-mail: fgrate@qcmet.com)

Abstract: Application of Energy Dispersive Spectroscopy (EDS) in materials testing is addressed in this paper. EDS analysis is useful for detecting basic corrosion properties and can detect carbon and oxygen. The importance of EDS analysis in materials testing is emphasized along with addressing challenges and limitations. EDS is a very important tool for corrosion analysis.

Key Words: Energy Dispersive Spectroscopy; EDS; Corrosion; Materials Testing.

INTRODUCTION

The energy dispersive spectroscope (EDS) is a key piece of equipment in material testing laboratories. It is an x-ray fluorescence system using energy dispersion rather than frequency (Figure 1). The unit is attached to a scanning electron microscope allowing for very small sample sizes to the analyzed. The data is semiquantitative, but it is essential in some types of analyses.



Figure 1. Energy Dispersive Spectroscope

USES OF EDS ANALYSIS ON MATERIALS

This method is used in many types of analyses. These analyses can include identification of corrosion products, alloys, contamination, structure and homogenous studies. There are many companies that use reverse engineering to produce or to repair products. Determination of the base material becomes necessary.

The EDS system has limitations, as it is semiquantitative and not fully quantitative. Other tests are then utilized to fill in the unknowns. Some of these include hardness and/or conductivity testing. material from a part in which the alloy is not known can be tested non-destructively, as only a small chip or scraping is needed. A small piece is placed into a scanning electron microscope, which magnifies up to 20,000X. Basic materials can then be analyzed to determine the alloy. In other instances, additional analysis such as microstructural and emission spectrograph can be used. These, however, are not nondestructive in nature. The analysis can reveal contamination along with identifying corrosion products. The results can be used to determine the history of the component parts. When someone has an expensive aircraft part, which they plan to reverse engineer or repair, knowledge on the composition of the alloy used is essential. The part can be scraped and a small particle analyzed. The same procedure can be followed for plating or sealants. The parts do not need to be destroyed.

Some materials can present challenges for the individuals performing the analysis. Separating aluminum alloys is one of those challenges. Separation of many stainless steels and low alloy steels can also be a challenge. We have learned over the years that many alloys can be tested by using a somewhat different technique. All analyses performed at QC Metallurgical, Inc. require a minimum 1,000 counts in the spectrum for analysis. There are times that it is necessary to vary the voltage. An example of this is an analysis of aluminum alloy such as 6061. (See Figure 2 for sample scan.) The basic analysis is run at 20 KV in a takeoff angle of approximately 35°. As a sample is usually a chip, the exact takeoff angle is not known. This results in a spectrum in which the lighter elements and the heavier ones can be analyzed, however, for confirmation reasons; the sample is rerun at 30 KV. The confirmation is done in order to excite the copper lines until there is an indication of a peak or no peak. If the copper is present, the alloy is probably 6061; if it's not, then the alloy is likely to be 6063. This technique is used for many different materials, especially those containing columbium, molybdenum, lead and other elements in which the upper peaks are not excited at 20 KV. Other tests can also be used, including hardness and metallurgical analysis. The same type of analysis is used to separate many of the stainless steels, such as 316 or 347 stainless steel.



Figure 2. Sample EDS Scan

The EDS analysis technique can also be used in paint analysis. In South Florida, many structures are coated with paints which have fluorine in them. The same paint may exist without the fluorine, but they do not last nearly as long. The same could be said for Teflon materials. Aluminum alloys which have been anodized have to be sealed in order to prevent corrosion. There are many sealants which are used, including nickel and chromium. The EDS analysis is a tool used to indicate which type of sealant is being used in the samples being examined.

In general, our laboratory uses ASTM A1508; a consensus standard test method. In most cases, a nonstandard method is utilized. There are times when both are used, however, this requires a larger sample. In the aircraft industry, the prime contractors require a vendor to ensure that the materials they purchase are what they have actually received. The semi-quantitative analysis is used to ensure that the vendor has received what he purchased. This is a routine test used to confirm that the correct materials are being used in manufacturing of their components.

The use of ED's analysis for corrosion studies is not only common, but also essential. The EDS analysis will indicate the basic corrosion properties plus EDS can detect carbon and oxygen. These are not typically quantified, however, their presence can be important for the investigator. The EDS analysis will detect all hydrogen, helium, lithium, elements, except for beryllium and boron. Corrosion processes such as dezincification or other parting corrosion mechanisms containing aluminum or nickel can be used. Photographic methods using either dot mapping or line profile analysis can be used. These are very useful tools in corrosion analysis. Diffusion can also be shown graphically using these techniques. These methods are very useful in revealing materials that are not homogeneous.

In general, the use of EDS analysis in a materials laboratory is a very important tool. This laboratory uses this type of analysis almost every day for either material identification or corrosion analysis.



Improved Corrosion Protection Through Electrodeposition

George E. F. Brewer

Coating Consultants, Brighton, Michigan

Abstract: Dr. Brewer was cited as a 1978 Chemical Pioneer for his research in the electrodeposition of water-dispersed organic coatings. This invention is used in over 400 installations for the corrosion protection of automobiles, steel trusses, furniture, toys and many other objects. Advantages include absence of pinholes in the coatings, more efficient use of the paints, and absence of air pollution because no volatile organic solvents are used.

Key Words: Electrodeposition, Electrodeposition, Electropainting, and Elpo.

CHEMICAL PIONEER ADDRESS

One of my ideas, developed with the aid of farsighted men and years of devoted work, evolved into a process used worldwide for improving the corrosion protection of metal products. The process is variously called "Electrocoating," "Electrodeposition", "Electropainting," and "Elpo." It achieved special applications in the automobile industry where rusting was heretofore a continuing problem.

My grandfather's 1912 Ford Model T had lost all of its gloss by 1916, and I received a dime regularly for polishing it; yet it did not show rust when I drove it in 1932. In contrast, rust had eaten some holes into my own 1953 car by 1957, but the rest of the car was as shiny as new. Thus, the 1953 paint itself was more resistant. However, certain areas of the car body failed; a then very puzzling situation. Ultimately, I was able to resolve this puzzle.

In the late 1950s, I went to work for Ford Motor Company trying to develop waterborne paints for prime coating car bodies, and got familiar with the fact that the inner surfaces of spray-painted or dip-coated cars showed an absence of paint in some critical areas, where the rust starts, and destroys the car from the inside out. Actually, wet paint was originally deposited in all these recesses, but was washed off during the bake cycle through the action of condensing vapors, be they solvent or water. What was needed was an essentially solvent-free paint, capable of permanently coating extremely recessed areas: a seemingly insolvable problem. **A new point of view**. Webster's Dictionary defines the term "invention" as the power to conceive and present new combinations of facts or ideas. If so, can we develop a technique of inventing? Yes, through storing and trying to recall vaguely related facts, and through looking at the problem from different vantage points. For instance, if everybody agrees that a zebra is a white horse with black stripes, it may pay to look at it as a black horse with white stripes.

In the case of painting merchandise, I decided that it was not really the paint solvent or carrier fluid per se which were troublesome, but rather the presence of carrier fluid during the bake. Looking at it this way, the problem was to remove the carrier fluid before the bake, and to reuse it, rather than to vaporize solvents during the bake. For about one year I thought and listed all possible ways, and not one seemed to be practical.

One evening while talking about my days in graduate school, I remembered that two classmates had had an explosion. They had tried to make rubber boots by "electrophoretic deposition of natural latex." All of a sudden it dawned on me that this was a separation of a colloid from its carrier fluid.

In 1808 Professor Reuss in Moscow observed that "milky" particles of clay migrate towards the anode in an electrical cell. He called this motion electrophoresis. Off and on the phenomenon was used as an analytical method culminating in Arne Tiselius' work for which he received the Nobel Prize in 1948. There were at least four significant attempts between 1919 and 1936 to use electrophoretic deposition in technical processes by use of naturally occurring products like rubber latex, beeswax, and asphalts. However, the parameters of an effective process for painting by electrophoretic deposition had not been defined, and no attempt had been made to synthesize suitable colloidal materials.

Numerous experiments with film formers such as epoxy resins, alkyds, acrylic, etc., resulted in the definition of parameters, such as range of viscosity, electrical equivalent weight, degree of neutralization, and so forth. The deposition process can be symbolized by the following chemical equations:

THE ELECTROCOATING PROCESS

Electrocoating resembles metal plating inasmuch as direct current is used. The electroplater applies 6 to 30 volts DC, while the typical electrocoater uses from 50 to 500 volts DC. The electrical equivalent weight of metal ions is approximately 30 (1/2 ni+ + = 29.36), while the average film forming macro-ion shows an electrical equivalent weight of 1,600. In other words, to plate out one kg of metal ions requires 34.1 Faradays of electricity, while one kg of electrocoat requires 0.63 Faradays. The electrocoating paint consists of about 90% water plus 10% paint solids, so it has the pumping and other handling characteristics of water. Merchandise is cleaned and prepared in the usual way, and then dipped into the painting tank where electric direct current deposits the paint. The merchandise is lifted from the paint after coating time, which varies from two seconds to three minutes. Droplets and puddles of undeposited paint adhere to the merchandise and are recycled by use of an ultra filtrate rinse.

The development of electrocoating has continued along various lines, and the process is now widely used for the coating of merchandise ranging in size from structural trusses to nuts, bolts, and electronic components. About 70% of all automobile bodies, worldwide, are prime coated by use of the electrocoating process.

The electodeposition of anodic electrocoats increases the life of the car body, and the recently marketed cathodic paints are expected to bring further improvements. In all, the electrocoating process provides four improvements:

- Higher quality of product, largely due to the uniformity of the coat on all surfaces and in all recesses.
- Lower cost due to paint and labor savings.
- Less pollution since water is used as carrier fluid, and the rinsed-off paint is returned to the tank.
- Energy saving through elimination of intermediary drying operations.

Thomas Edison's attribution of success 1% inspiration and 99% perspiration was clearly evident in the efforts to commercially develop an electrocoating process for "painting" automobiles. Before the first car was electrocoated on an assembly line, approximately 150 man years of work were expended by chemists and engineers at Ford Motor Company. More than 75,000 panels were tested; some 10 million wheels were painted on an experimental line; approximately 150 experimental cars went to the test track and were evaluated. In addition, a large amount of work was done by leading paint manufacturers all over the world to provide suitable paints for electrocoating all sorts of merchandise. The technical details were reported in scores of papers and patents over my name as author, co-author, inventor, or co-inventor.

I am grateful to all of those who worked and still work on electrocoating and am proud that they remained my friends through all the pressures of two decades of work. Leading the list are the late Mr. Gilbert L. Burnside, my boss at Ford; Mr. Gordon G. Strasberg, the process engineer, and my wife Maxine, whose plans are frequently interrupted by emergencies in the field of electrocoating. The reward for all this work is the joy of overcoming adversities and the knowledge that I have made some contribution toward improving the quality of consumer goods. Naturally, I am gratified by the recognition of my fellow professionals, especially when it appears in the literature as follows: "Electrocoating... the greatest breakthrough since the invention of the spray gun. ... the 1960's may go down in auto history ... for giving birth to electrodeposition ... "; "... benchmark in Chemistry..."; "...primer and single coats will be applied by electrodeposition almost universally ... " I am thus especially grateful to have been named a recipient of the Institute's 1978 Chemical Pioneer Award.

NOTE

This paper is the 1978 Chemical Pioneer address of Dr. George Brewer, and it originally appeared in *The Chemist*, Volume 55, Number 7, p. 5 (1978). Source: Brewer, G. *The Chemist*, 1978, 55, 5. Copyright The American Institute of Chemists 1978.



Designing Core Concepts for a Tertiary Basic Chemistry Course

John O. Hill^a, David Devraj Kumar^b and Ranjit K. Verma^c

^aLa Trobe Institute of Molecular Sciences (LIMS), La Trobe University, Melbourne, 3086, Australia. ^bCollege of Education, Florida Atlantic University, Davie, Florida 33314, USA. ^cDepartment of Chemistry, Magadh University, Bodh Gaya-824234, India. (^djce.hill@bigpond.com, ^bdavid@fau.edu, ^cprofrkverma@gmail.com)

Abstract: A curriculum framework is proposed for the tertiary 'chemistry fundamentals' course based on Atkins' interrelated core chemical concepts. It is suggested that this course should not only provide a learning platform for 'basic chemistry', but should also show how chemistry exercises a crucial role in sustainable natural resource management and therefore, in sustaining the environment and addressing climate change. Further, it should encompass the principles of 'sustainable chemistry' and how these lead to a sustainable chemical industry and the wider chemical enterprise. The proposed course lends itself to a variety of learning methodologies and assessment procedures in harmony with contemporary pedagogy of 'effective teaching for constructive learning'. It can also easily be constructed into modules and delivered and assessed online. Based on our experience, we believe that the major advantage of this course, compared with most 'basic chemistry' courses previously and currently delivered, is that by acquiring knowledge of a relatively few 'core chemistry concepts', students are able to at least have a superficial understanding of contemporary major advances in chemistry and its associated technological developments and thus, it activates their interest in pursuing 'chemistry' as the main component of a rewarding career.

Key Words: Chemistry, Tertiary Course, Core, Basic, Concept, Design.

INTRODUCTION

The 'core concepts', now called 'cornerstone concepts', of the tertiary 'chemistry fundamentals' course continue to be debated as the diversity of student cohorts taking this course continues to widen both in numbers, educational background and quality. The one semester course is intended for students enrolled in sciences other than chemistry and has to provide knowledge of sufficient basic chemistry to support the needs of many other sciences, most notably, the biological (life) sciences. Also, there has been protracted discussion on the curriculum of the traditional (2 semester) Chemistry 1 course, intended for chemistry majors, with concerns that since this course has not been reviewed in depth in India for at least 15 years (The University Grants Commission did it at national level in 1990's) and in Australia for at least 3 decades, it may no longer be revealing the 'richness' and 'relevance' of chemistry to contemporary



Figure 1. Atkins' core chemical concepts

students. This is evidenced by the unilateral decrease in the number of science students opting to undertake chemistry as a major over the last decade. These concerns initiated the design of an alternative curriculum framework for the tertiary Chemistry 1 course [1], based on three contemporary educational theories – those of Atkins, Lawton and Fensham. The proposed curriculum framework indicated that in addition to delineating the principal concepts of chemistry, it is also important to emphasise that chemistry has social, economic, ethical and environmental responsibilities and accountabilities which, when highlighted, counteract the negative image that chemistry has in the general community and thereby enhance its benefits to society.

Atkins [2] has suggested that nine core concepts form the basis of chemical knowledge (Fig.1).

These are essentially the cornerstone concepts of both the (Australian) one semester 'Chemistry Fundamentals' course and the two semester 'Chemistry Foundation' course for chemistry majors and form the main framework of these curricula [3]. Atkins' core chemical concepts are intended not only to simplify understanding of chemical principles, but also to engage the interest and curiosity of students and people generally in chemistry and to promote understanding and appreciation of the many benefits which it offers to the global society. Also, a wider understanding of these concepts endorses chemistry as the 'central empowering science' and as 'quantifying biology' and forms the basis of understanding 'sustainability science'.

This paper discusses a curriculum framework for the tertiary one semester 'Chemistry Fundamentals' course based entirely on Atkins' core chemical concepts. It is shown that judicious use of examples of each of these nine concepts allows the major areas of chemistry to be discussed at an elementary level. Also, frontier concepts can be introduced as emerging from these basic concepts, so as to project the fascination of chemistry and promote student engagement and interaction. Particular emphasis should be given to those basic concepts which impact directly on the operations of the global chemical industry and empower environmental sustainability.

SCOPE OF CHEMISTRY – THE CENTRAL ENABLING SCIENCE

The introduction to the tertiary 'Chemistry Fundamentals' course should emphasise that chemistry is the central enabling science since it strongly impacts upon many other sciences, most notably biology, biotechnology, and pharmaceutical and materials science. These interactions are shown in Fig. 2.



Figure 2. The scope of Chemistry

Since chemistry is recognised as the foundation molecular science, it impacts on environmental and sustainability science and adds scientific credibility to the present climate change and environmental sustainability debates [4]. Chemistry is the essential precursor of chemical engineering and the reference base of materials science. Chemistry has long had a controversial role in food science, particularly with respect to artificial food additives and, more recently, in conjunction with the genetically modified foodstuffs debate. Chemistry is largely responsible for revolutionising forensic science following the acknowledged success of DNA fingerprinting. Chemistry impacts directly on the health sciences, not only with respect to the perennial quest for cheaper, more effective pharmaceuticals, but also in providing basic chemistry training for health professionals, particularly those involved in MRI scanning diagnosis. Overall, the course introduction should emphasise that studying chemistry and appreciating its richness and rigour can lead to a variety of rewarding careers, both research orientated, chemical industry orientated and teaching orientated. Further, the growing concern for global environmental sustainability [5] and the ever-increasing significance of materials science in the development of cutting edge technologies [6] underline the importance of designing improved foundation studies in chemistry to support student understanding of these developments.

CHEMISTRY: THE PROPERTIES & STRUCTURE OF MATTER

An equally important aspect of the introduction to a 'Chemistry Fundamentals' course is to give a short but concise definition of chemistry as the 'properties and structure of matter', which immediately emphasises that the properties of matter are aligned with its molecular structure and with the extent of intermolecular interactions. Also, chemistry is a quantitative science and is governed by measurements which only have meaning when accompanied by units. This leads to a discussion of the SI unit system, the base SI units and the associated derived units. Special significance must be accorded to the 'mole' as the fundamental unit of chemistry. A brief discussion of 'precision' and 'accuracy' of measurements is also appropriate. Further, it must be emphasised that understanding chemistry requires some knowledge of basic mathematics, particularly 'scientific notation', algebra, rearranging and solving equations and basic calculus.

Like all sciences, chemistry has its own language and a unique nomenclature system, which is used throughout the course and with which students must become familiar and use. Some common words such as 'preparation' have a different meaning in chemistry to that in everyday usage.

Also, it should be emphasised that chemistry is a vast subject which has traditionally been divided into branches: 'inorganic', 'physical', 'organic' and 'analytical'. It is now recognised and accepted that the boundaries between these branches are becoming increasingly blurred and new branches such as 'green chemistry' and 'chemical education' have prominence. Indeed, it can be argued that 'biochemistry' is a branch of chemistry, but because of its prominence in the life sciences, it is generally considered an independent science.

Overall, the introduction to a tertiary 'Chemistry Fundamentals' course must convey to the students not only the richness and rigour of chemistry, but also that chemistry is at the forefront of scientific knowledge and is the enabling force driving technological development of a sustainable future for the environment and for humanity.

The proposed curriculum framework embraces the nine core concepts of chemistry so eloquently, as described by Atkins, and emphasises the connectivity of these concepts so as to provide more than a superficial understanding of chemistry.

ATOMS

Atkins has described 'atoms' as the currency of discourse in chemistry. This is an apt description since the economics of the chemical industry and, more recently, the effectiveness of 'green chemistry' are based on 'atom economy' principles. Atkins points out that 'atoms are chemical accounting devices since is based on their existence stoichiometry and immutability in chemical reactions'. Hence, the 'Chemistry Fundamentals' course must not only highlight the fundamental concept that 'matter is composed of atoms', but also must emphasise the paradox that matter has 'bulk' despite being almost empty space.

An atom is simply described as comprised of a small, dense nucleus made up of positively charged protons and electrically neutral neutrons. Most of the mass of an atom is contained in the nucleus, which is surrounded by much larger extra-nuclear space that contains negatively charged electrons, the number of which is equal to the number of protons in the nucleus. It must be emphasised that it is the number of valence electrons in the outermost shells of atoms that define chemical properties. It is the valence electrons that are involved in chemical bond formation and electron transfer is critical to an explanation of chemical reactions. Thus, the electronic configuration of atoms, particularly with respect to identification of 'core' and 'valence' electrons, is a critical and defining property of atoms and their chemical behaviour.

Some 'frontier science' examples should be discussed based on knowledge of the structure of atoms, such as 'atom splitting' – leading to nuclear energy production, radio-isotope production, radio-carbon dating and nuclear waste production and nano-technology [7, 8] – leading to the production of 'smart materials', semi/super conductors and conducting synthetic polymers (Fig. 3). Also, atomic level manipulation of biological systems is now possible, leading the way to synthetic biology under "controlled conditions" and biodegradable engineered materials that are lighter, stronger and more resilient [9].

NANOTECHNOLOGY – Control of Structure/Specific Properties



Figure 3. Nanotechnology – Control of atomic structure

ELEMENTS

Elements are composed of atoms of the same type and since there are more than 100 types of atoms, there are more than 100 known elements. Atkins has labelled the periodic table as 'the most striking icon of chemistry', since it shows that the elements group into families based on common electronic structures and that trends in physical and chemical properties of the elements and their compounds exist both across periods and down groups. Atkins has quite simply explained the uniqueness of the periodic table in terms of the 'rhythm' in electronic configuration (2:8:8:18:18:32:32), which so aptly explains how the elements cluster into blocks - 's', 'p', 'd', and 'f'. It is important now to emphasise that the most important elements - the elements of life - C, H, N, P, O and S - are in the p block, as are all the gaseous elements, except hydrogen. The most significant value of the periodic table is the prediction and rationalisation of the physical and chemical properties of the elements and their compounds based on their position in the table. In this context, it is appropriate to discuss the properties of Group XV111 the noble gases and the reason why the name of this group has been changed from 'inert' to 'noble' gases due to the discovery of compounds of these elements in the mid- 20th century.

Specific reference should be made to the elements of 'life' – carbon, nitrogen, oxygen, phosphorus and sulphur – since these are the constituents of proteins. Also, a brief discussion should be included of the natural nutrient cycles, particularly the carbon nutrient cycle. The latter can also be used as a template to explain the consequences of increased levels of carbon dioxide in the upper atmosphere.

BONDS

Chemical bonds lead to the formation of molecules. Atkins has proposed that 'sharing of electron pairs' is the core idea of molecular structure and that ionic bonding is the extreme kind of covalent bonding and that metallic bonding is a special type of ionic bonding. It is appropriate to discuss in the 'Chemistry Fundamentals' course some common and important ionic and covalent inorganic compounds together with a selection of organic compounds which show that these are characterised by their 'functional group'. Some examples of organic compounds of biological and environmental significance are worthy inclusions. The important interrelated concepts of 'bond length' and 'bond energy' should be included with reference to covalent bonds. Also, hydrogen bonds should be briefly discussed because of their significance in explaining the anomalous physical properties of water and the folding structures of proteins.

It is appropriate to discuss in this section the unique ability of C to form single, double and triple bonds with itself and to bond to hydrogen, oxygen and nitrogen to form an unlimited range and number of compounds, considered collectively as a separate branch of chemistry known as 'organic chemistry'. Also, it is noteworthy to mention that the main natural source of organic chemicals is 'coal'.

SHAPE

Atkins has emphasised that 'shape' is 'function' in the biological world. However, shape not only relates to molecular architecture, but also to the shape of atoms – leading to the concept of ionic radius and its relationship to ionisation energy and electron affinity and hence, to electronegativity. Further, ionic radius has a major influence on ionic and covalent character of chemical bonds, such that shape determines 'polarity', which in turn influences the magnitude of inter-molecular interactions and solubility of compounds in water.

Since atoms and ions are considered to be spherical in shape, the structures of ionic compounds, such as sodium chloride, are best described in terms of the close packing of spheres with emphasis on the symmetry of the resulting structures. For covalent compounds, the basic principles of hybridisation and VSEPR theories are required to explain the structures of symmetrical molecules, such as methane and asymmetric structures such as water and ammonia. It is also important to relate polarity of molecules to their molecular structures. Further, discussion of the structures of diamond and graphite introduces the concepts of electrical and thermal conductivity and mechanical strength of materials, thus revealing that the properties of bulk matter are defined at the molecular level.

A brief mention of the presence of 'cavities' within structures is important in terms of explaining porosity and absorption properties of bulk materials and also catalytic activity.

INTER-MOLECULAR FORCES

Atkins has described bulk matter as aggregates of molecules formed by inter-molecular attractions. The most important consequence of inter-molecular forces is that the relative strengths of these distinguish the characteristics of gases from those of liquids and solids. The weakest inter-molecular forces are present in gases and the strongest are present in solids with liquids having inter-molecular forces of intermediate strength. Inter-molecular forces should be described in terms of the polarizability of molecules with special emphasis on hydrogen bonding, which explains the structure of ice, the high boiling point of water and its unique solvent property. Also, most significantly, hydrogen bonding plays a critical role in the structure of proteins and hence, in the 'molecules of life'.

Now follows discussion of the properties of gases (Gas laws, Graham's law), solids, liquids and solutions (Raoult's law, Henry's law, osmotic pressure). Special emphasis should be given to the solubility of carbon dioxide in water, since this is a critical stage of the natural carbon cycle and hence, of enormous significance in the present climate change debate.

REACTIONS

Atkins has proposed that chemical reactions can be categorised into just four types: proton transfer (acid/base), electron transfer (redox), electron sharing (radical) and electron pair sharing (Lewis acid/base). Thus, by inference, all reactions involve electrons.

The 'Chemistry Fundamentals' course should therefore contain many examples of acid/base and redox reactions with, perhaps, a few examples of radical and Lewis acid/base reactions. The latter allows a wider, more general definition of acids and bases to be introduced and opens discussion of coordination chemistry and its importance in biochemistry. Of major importance is to show how chemical reactions are described by 'equations', which are different to mathematical equations and that when these are balanced, the stoichiometry of a reaction is defined in terms of the numbers of moles of reactants reacting and the numbers of moles of products formed. Reactions selected for discussion should include not only the common inorganic reactions, but also net ionic reactions, simple organic reactions and reactions of environmental significance, such as the solubility of carbon dioxide in water and the reaction of carbon dioxide with water to give carbohydrates and oxygen under the influence of sunlight and chlorophyll.

ENERGY

Atkins has described 'energy' as 'transactions' associated with chemical reactions which are defined by the 'thermal accounting device' – 'enthalpy'. This is a tangible way of introducing the abstract concept of energy in the 'Chemistry Fundamentals' course – simply that energy 'lost' and 'gained' has to be 'accounted for' and the account must 'balance', which is effectively a simplified statement of the first law of thermodynamics. Indirectly, it is also a definition of state functions such as enthalpy and also a simplified statement of Hess's law.

Since the combustion of fossil fuels is expected to provide the bulk of global energy requirements for at least the next 50 years, a suitable introductory example of the application of the first law of thermodynamics is the 2 – stage combustion of carbon. Similarly, the energy release from typical fuels such as methane (compressed natural gas), propane (liquefied propane gas) and petrol (octane) further illustrate the contemporary dilemma that fossil fuels are not only the (global) primary energy resource but also, are the primary contributor to global warming.

It now needs to be emphasised that if a reaction is exothermic, it is not necessarily 'spontaneous' since the thermodynamic quantity that governs 'reaction spontaneity' is 'free energy' and not enthalpy. This effectively introduces discussion of the second law of thermodynamics.

The need to pursue and develop 'clean energy resources' should be discussed together with the

'advantages' and 'disadvantages' of these by comparison to 'coal' and 'oil' (Fig.4) in addition to exploring energy derived from biological systems.



Figure 4. The quest for 'Clean Energy Resources'

The National Academy of Sciences (NAS) in the United States recommends that research at the intersection of physical and biological sciences is critical to finding solutions to pressing societal issues such as According to the NAS "of the clean energy [9]. opportunities at the intersection of the physical and biological sciences, perhaps none has such intriguing potential as understanding, controlling, and improving photosynthesis, with the goal of decoupling it from plants" (p. 27). This remains a challenge. "Biological systems generate their energy directly in mitochondria at efficiencies of near 90 percent. The energy chemistry in mitochondria is analogous to that in fuel cells, wherein hydrogen and oxygen in the presence of catalysts are converted to water while generating electricity" (p. 28). Chemists working with biologists are capable of finding lasting solutions that lie beyond the traditional boundaries of the chemical sciences.

ENTROPY

Atkins has described 'entropy' as the natural (spontaneous) direction of change from 'order' to

'disorder'. Thus, a decrease in Gibbs free energy of a chemical reaction corresponds to an increase in entropy under constant temperature and pressure conditions. This is a simple explanation of the second law of thermodynamics and also explains why change in free energy and not enthalpy change defines reaction spontaneity. The concept of chemical equilibrium then follows as does the relationship between free energy change and equilibrium constant. Le Chatelier's principle further enhances understanding of chemical equilibrium, particularly with respect to its dependence on temperature. It is important to emphasise that from a chemistry perspective, free energy has greater significance than entropy, despite the latter being the more fundamental thermodynamic quantity.

Since it is widely known that students dislike 'thermodynamics' because of its abstract connotations and mathematical complexity, it is appropriate to show them ways in which nature uses thermodynamics most effectively – as for example in the growth of calcium carbonate structures such as 'shells' and 'bones'. Essentially, the 'local environment' is 'manipulated' by the organism such that the balance between 'enthalpy' and 'entropy' is negative thereby ensuring that development of such structures is spontaneous. The principle of controlling the local environment thermodynamically is the basis of crystal tectonics or 'crystal engineering' whereby crystalline materials are formed under carefully controlled conditions with predetermined physical properties.

KINETICS

Although thermodynamics indicates whether a chemical reaction is spontaneous, it does not reveal the rate at which reactants convert to products. This is the domain of chemical kinetics. In this context, it is noteworthy that biochemical reactions - the life sustaining processes - are kinetically 'slow' whether in 'forming' or 'decaying'. An important initial concept is that for reactions that have attained equilibrium, this means that the rates of the 'forward' and 'reverse' reactions are the same. The central concept to include in the 'Chemical Fundamentals' course is that 'energy barriers' are associated with all chemical reactions, which must be overcome for reactions to proceed. The concept of 'activation energy' follows in conjunction with the relationship between reaction rate and temperature (Arrhenius equation). The critical role of catalysts and the biological counterparts – enzymes in reducing activation energy should be emphasised with special reference to 'molecular shape' in explaining how catalysts function in conjunction with the concept of catalysts 'anchoring' molecules on their surfaces such that the reaction of interest is initiated with reduction of activation energy.

A contemporary example, that of radioactive decay, adequately introduces the concepts of reaction rate, reaction order and half-life, and emphasises the importance of radiocarbon dating and the advantages and disadvantages of nuclear energy.

MODULE STRUCTURE

This course can easily be divided into modules with a 'prologue module' outlining the breadth and depth of chemistry and its central role as an 'enabling science' and an 'epilogue module' outlining the benefits of chemistry to understanding how the world functions, how it benefits humanity and how it contributes to the sustainability of the environment. (These two modules are not assessed.) To illustrate the modular structure of this course, the composition of a proposed 'Intermolecular Forces' module is shown here.

INTER-MOLECULAR FORCES

LEARNING OBJECTIVES

To understand how inter-molecular forces influence the physical properties of liquids and solids.

REVIEW

There are three types of inter-molecular forces: 'dispersion', 'dipolar' and 'hydrogen bonding'. Dispersion forces (induced dipole forces) are the attractions between 'electron clouds' of a molecule and the positively charged nuclei of neighbouring molecules. Dipolar forces are the attractive forces between polar molecules. 'Hydrogen bonding' is a special type of dipolar forces and it can be both inter- and intramolecular in character. Inter-molecular forces are weak compared to the strengths of covalent and ionic bonds, but are greatest for solids and least for gases and of intermediate strength for liquids. The strengths of chemical bonds determine the chemical properties of compounds, but the strengths of inter-molecular forces determine the physical properties of compounds.

Fundamentally, the inter-molecular forces influence the closeness of packing of molecules in gases, liquids and solids. Solids are highly close packed whereas for gases, the molecules are randomly distributed and liquids are less closely packed than solids. Thus, gases can easily be compressed by applying pressure, whereas liquids and solids are incompressible. Effusion and diffusion are rapid for gases, but slow for liquids and non-existent for solids.

Viscosity, surface tension and evaporation rate are important physical properties of liquids. Viscosity is the flow characteristic of liquids. The greater the intermolecular forces, the greater the resistance of a liquid to flow and hence, the greater is its viscosity. A liquid has surface tension due to inter-molecular forces being greater in the bulk than at the surface. Surface tension increases as inter-molecular forces in a liquid increase. Evaporation rate relates to the conversion of a liquid to gas. As inter-molecular forces increase, evaporation rate decreases. Increasing temperature increases evaporation rate. Once the vapour pressure of a liquid is equivalent to the atmospheric pressure, it boils and the temperature at which this occurs is the normal boiling point of the liquid.

It is important to relate inter-molecular forces to molecular structure so as to be able to rationalise the physical properties of liquids and solids. Dipolar forces in general and hydrogen bonding in particular are the primary factors influencing the physical properties of liquids.

WORKED EXAMPLE 1

Which has the greater viscosity and the greater surface tension – ethylene glycol or ethanol?

The structural formula of ethylene glycol is $HO - CH_2CH_2 - OH$, and that of ethanol is CH_3CH_2OH .

Ethylene glycol has two terminal OH groups, whereas ethanol only has one; so the inter-molecular forces are greater for ethylene glycol and hence, it has the greater viscosity and the greater surface tension.

WORKED EXAMPLE 2

For the following pairs of liquids, which has the greater evaporation rate at 298 K?

- (a) $CH_3CH_2CH_3$ or $CH_3CH_2CH_2CH_2CH_3$
- (b) CH₃CH₂CH₂CH₂OH or CH₃CH₂OCH₂CH₃

- (a) Neither propane nor pentane is polar and so only dispersion forces prevail. These are greater for pentane than for propane since the probability for induced dipole formation increases with carbon chain length; so the intermolecular forces are greater for pentane and its evaporation rate is greater than that of propane.
- (b) Butanol has a terminal OH group which leads to hydrogen bonding, and diethylether is polar due to its bent structure. However, intermolecular hydrogen bond strength is greater than that of dipole-dipole attractions, so diethylether has the greater evaporation rate.

WORKED EXAMPLE 3

Arrange the following liquids in order of increasing normal boiling point:

(a) (CH₃)₂CHNH₂ (b) (CH₃)₂CH₂ (c) (CH₃)₂CO

Compound (a) has H - N ---H hydrogen bonding: compound (b) has only dispersion forces since it is non-polar and compound (c) has dipolar forces since it has a C – O permanent dipole; so the order of increasing inter-molecular forces is (a) > (c) > (b) and hence, this is the order of increasing normal boiling point.

Note: Hydrogen bonding is of particular importance in understanding the structures and functions of proteins.

PRACTICE QUESTIONS

1. For the following pairs, which has the stronger inter-molecular attractions?

[Hint: The order of increasing inter-molecular force strength is: Hydrogen Bonding > Dipole/Dipole > Induced Dipole/Induced Dipole.]

 $[\ (a)\ PF_3\ (b)\ SiH_4\ (c)\ CHCl_3\ (d)\ HF\ (e)\ Br_2\ (f) \\ C_6H_{14}]$

- 2. Arrange the following liquids in order of increasing strength of inter-molecular forces present and increasing order of evaporation rate and give reasons:
 - (a) (CH₃)₂CHOH (b) C₃H₈ (c) CH₃COCH₃

[Inter-molecular forces order is a > c > b: (a) has hydrogen bonding: (b) has dipole/dipole interactions: (c) has only induced dipole interactions.]

3. The vapor pressures of the following organic solvents at 20°C are:

CS₂, 294 torr: C₂H₅OH, 44 torr: CH₃OH, 96 torr: (CH₃)₂CO, 186 torr.

Arrange these in increasing order of intermolecular forces operating and increasing order of evaporation rate.

[Hint: The greater the vapor pressure, the lesser are the intermolecular forces.]

 $[CS_2 < (CH_3)_2CO < CH_3OH < C_2H_5OH :$ Evaporation rate is the opposite sequence.]

4. Which has the higher normal boiling point ethylene glycol or ethanol and why?

[The inter-molecular forces are greater for ethylene glycol so it has the lower evaporation rate and hence the higher (normal) boiling point.]

It should be noted that the module structure adopted here follows 'best practice' recommendations, namely commencing with a concise brief overview of the title topic followed by 'worked examples' followed by 'practice exercises'. Answers to the latter are provided. It should also be noted that online structured learning programs could be used to animate modules and to guide and assist problem solving [10].

CONCLUSION

Atkins has shown that 'basic chemistry' can effectively be understood in terms of nine interrelated core concepts, with each given equal emphasis, such that chemistry is revealed as the 'central, enabling science'. However, the 'Chemistry Fundamentals' course should also emphasise that chemistry has 'social', 'environmental', 'economic' and 'ethical' responsibilities and accountabilities and therefore, has a critical role to play in the contemporary challenge of sustainable natural resource management (SNRM), which is inclusive not only of remediating climate change, but also of sustaining the environment for future generations. It is vitally important that the 'Chemistry Fundamentals' course not only discuss the fundamental concepts of chemistry, but also portray these in a sustainability context in line with contemporary pedagogy of embedding sustainability in tertiary curricula [11]. This has the added advantage of showing that chemistry is fulfilling its responsibilities to the chemical industry, the wider chemical enterprise, and society at large and to preservation of the environment. It also emphasises that chemical education is an enabling force in understanding and remediating climate change, and that chemistry 'solves' rather than 'creates' problems for humanity.

RECOMMENDED REFERENCE TEXT

A. Blackman, S. Bottle, M. Mocerino, S. Schmid and U. Wille, *Chemistry*, 2nd Edn., John Wiley & Sons (Australia) Ltd., 2012.

REFERENCES

- 1. Hill JO, *Scientific literacy and the reform of science education in Australia: A chemistry perspective,* Unpublished doctoral dissertation, University of Melbourne, Australia, 2005.
 - <a>https://repository.unimelb.edu.au/10187/15337>
- 2. Atkins P. Chem Ed NZ, 2010, 120, 8-12.
- 3. Hill J, Warren D. Chem Ed NZ, 2007, 115, 4-9.
- 4. Hill J. Chem Ed NZ, 2010, 118, 9-13.
- Hill J, Kumar DD, Verma RK. *The Chemist*, 2013, 86(1), 24-31.
- 6. Hill J, Verma RK, Kumar DD. J Mater. Educ., 2013, 35(1-2), 1-16.
- 7. Kumar DD. The Chemist, 2006, 83(1), 7-10.
- 8. Kumar DD. Australian J Ed Chem, 2007, 68, 20-22.
- 9. National Research Council, *Research at the intersection of the physical and life sciences*, The National Academies Press, Washington, DC, 2010.
- 10. Tobias K, Kumar DD. The Chemist, 2006, 83(2), 6-9.
- 11. Mustafa S, Hill J in *Green world order: Delaying the doom in a changing climate,* Lambert Academic Publishing, Saarbrucken, 2011, p. 110.

Public Understanding of Chemistry



Public Understanding of Chemistry: Chemistry and its social-political-economic context continue to change.

Chemistry and chemistry-based technology that impact our lives make for the complexity and controversy of life and set the stage for thinking about public understanding of chemistry. The Public Understanding of Chemistry section will try to address chemistry in real life context with original contributions (articles/position papers/policy briefs) and/or published articles and columns in reputable sources (used with permission).

Founding Section Editor: David Devraj Kumar, Section Co-Editor: David M. Manuta

VERY LITTLE ABOUT CHEMISTRY!

Susan Day

Florida Atlantic University

I know very little about chemistry. My terminal degree is in public administration, which aligned with my ambition to solve community problems, particularly those involving high risk youth. I'm pretty sure it was my disinterest in learning the periodic table of elements that thwarted my parents' dream of their youngest daughter becoming a medical doctor. I readily admit that much of my most recent thoughts about chemists have been strongly influenced by Walter Hartwell White (a.k.a. Heisenberg on the popular AMC series *Breaking Bad*). Walter is a high school chemistry teacher who fails to interest his students in the study of change while radically transforming into a master meth cook to fund his cancer treatments.



A perusal of an edition of *The Chemist* leaves me awed. From the comparison of CA 242 with twelve other cancer antigens for use in the diagnosis of pancreatic, gastric, and other gastrointestinal cancers to green chemistry techniques for carrying out organic synthesis, I am profoundly grateful for the work chemists do to enhance our quality of life and the quality of our natural environment. I also appreciate what chemists have to teach us about creating a great mix.

My appreciation has grown in recent years for chemists and chemistry because they have become more important to my livelihood. After almost twenty years as a program director/ research faculty for university community service and research efforts in colleges of nursing and urban and regional planning, I am now employed as a grant facilitator for a research university with high research activity, as classified by The Carnegie Foundation for the Advancement of Teaching. I share my own personal experience as an exemplar of many professionals working in the social and behavioral sciences. My tenure as research faculty came to a gradual end in part due to a tightening of soft money for public sector service initiatives between 2007 and 2009 – years in some way defined by the recent Great Recession. Since 2012, my career has gained new life as a grant

facilitator and I have been fortunate to work on a number of STEM (Science, Technology, Engineering, Mathematics) education pipeline/ broader impacts initiatives designed to better prepare, recruit and retain underrepresented minorities for STEM degrees.

At the federal level, the increased focus on STEM performance and accountability has resulted in increased financial support, making STEM funding programs a great target for grant facilitators. The 2011 federal budget for STEM includes \$3.7 billion invested into STEM education [1]. Additionally, \$4.3 billion was earmarked for the *Race to the Top* competition with STEM as the sole competitive preference priority. About \$1.1 billion has as its primary goal targeting populations underrepresented (such as African-Americans, Hispanics, and females) in the STEM fields, according to a recent White House report [2].

Significant numbers of today's women and underrepresented minority chemists and chemical engineers (40 percent) say they have been discouraged from pursuing a STEM career [3]. U.S. colleges are cited as the leading place in the American education system where discouragement happens (60 percent) and college professors as the individuals most likely responsible for the discouragement (44 percent). Not only are underrepresented populations facing barriers to STEM graduation, but only 33 and 42 percent of white and Asian American students who begin their studies aspiring to complete a STEM major are successful [4]. The K-12 experiences of these students cannot explain these low completion rates. Surprisingly, students at more prestigious institutions are often more likely to be discouraged in early STEM courses and to switch majors [5].

Designing a transformative and cutting-edge STEM education pipeline proposal generally requires some inclusion of problem-based learning. Engaging underrepresented minorities in the application of STEM science, how STEM is "done" in real life, is a principal strategy for increasing interest and engagement. The most important modern conception of STEM education might be the notion of integration—meaning that STEM is the purposeful integration of the various disciplines as used in solving real-world problems [6]. Although the chemist may self-identify as a chemist, she/he must have an in-depth understanding of other science disciplines, technology, and math to create "real life" applications that solve problems [7].

It is the integration and alchemy of disciplines converging that often create new innovative perspectives and new ways of solving old problems. The learning and social sciences have something to contribute to the U.S. STEM education problem and social and behavioral scientists can help develop more competitive STEM education grant proposals. Understanding education from a complex adaptive systems approach requires interdisciplinary and trans-disciplinary collaborations that include government, concerned citizens, industry, communities and academia [8]. In this conversation, social and education scientists are critical to developing new, more productive models of STEM education, particularly for underrepresented minorities.

In addition, like an experienced chemist recognizing dangerous combinations in the laboratory, an experienced social/ behavioral scientist can prevent experiments in STEM education from doing harm to a vulnerable populations. In my field-work and research in youth and family violence involving grandparents and abandoned, abused and neglected children, I was always aware of the capacity for our interventions to backfire, causing more physical and emotional harm to vulnerable individuals. In my field, well-intended interventions developed for one population may be inappropriate and even profoundly counterproductive when applied to cases involving a different population [9].

In the quest for increasing sponsored funding for STEM education, university scientists are developing new models of education. In some cases (far too many), STEM faculty are creating mentoring and education programs for underrepresented minorities without the benefits of experienced social and behavioral scientists – scientists who have first-hand experience working with at-risk populations. Engaging experienced social and learning scientists may be the best defense in preventing potential harm to at-risk populations derived from failed mentor matches or failed education experiments.

Post Script

- 1. Breiner, JM, Harkness SS, Johnson CC, Koehler CM. School Science and Mathematics, 2012, 112, 3–11.
- 2. "A Report from the Federal Inventory of STEM Education Fast-Track Action Committee: Committee on STEM Education National Science and Technology Council," The Federal Science, Technology, Engineering, and Mathematics (STEM) Education Portfolio, December 2011.
- 3. Anonymous. *The Hispanic Outlook in Higher Education*, 2010, 20, 30. Retrieved from http://ezproxy.fau.edu/login?url=http://search.proquest.com/docview/375598278?accountid=10902
- Hurtado S, Pryor J, Tran S, Blake LP, DeAngelo L, Aragon M, "Degrees of success: Bachelor's degree completion rates among initial STEM majors." Los Angeles: Higher Education Research Institute, University of California. 2010
- 5. Chang MJ, Cerna O, Han J, Saenz V. Review of Higher Education, 2008, 31, 433-464.
- 6. Labov JB, Reid AH, Yamamoto KR. CBE Life Science Education, 2010, 9, 10–16.
- 7. Bennett SW, O'Neale K. University Chemistry Education, 1998, 2, 58–62.
- 8. Stephens R, Richey M. Journal of Engineering Education, 2011, 100, 3, 417-423.
- 9. Davis RC, Medina-Ariza J, "Results from an elder abuse prevention experiment in New York City," Research in Brief, National Institute of Justice, September 2001.

IMAGE ACKNOLEDGMENT: The image was created by Alberto Fernandez.

Book Reviews



Nanophysics and Nanotechnology

Reviewed by Dr. Kenneth Abate

Kenneth Abate, PhD Consulting, Maple City, MI 49664

Nanophysics and *Nanotechnology* is an upper undergraduate/ master's degree textbook covering the basics of nanophysics and nanotechnology. The book is broken into 8 chapters over 174 pages. The print is on the small side and the overall quality of the paper and print is The book has many diagrams, figures, satisfactory. drawings, and pictures that are satisfactory in quality and clarity. At the end of each chapter is a reference section that cites literature to primarily the late 1990's. After the last chapter, there is a series of exercises pertaining to the subject matter discussed in each of the chapters. No answers are given and some of the questions are aimed at general discussion.

I found that the chapters used the theme of "nano" to mean anything of extremely small dimensions. Although this is true to the definition of the prefix nano, items, such as quantum descriptions of the state of matter, chemical orbital and the various bonding schemes and their mathematical descriptions, friction, viscous forces, harmonics, etc., are not typically what is meant by the subject of nanotechnology. The author seems to cover many of the standard physics and chemical theoretical concepts concerning the nature of things and their interactions as if they were uniquely nano, rather than the classical way of describing/detailing them simply as part of the nature of physics and chemistry. To me, the use of



"nano" was aimed at trying to capture the attention of the modern student by using a new and perhaps more in-vogue description of the standards, even classical materials that have been taught for decades. Some attempts were made to relate nano-scale materials to biological entities, such as nano-motors and single celled organisms, which I again found to be stretching the use of the prefix of nano.

Overall, I found the book to be a too brief description of classical physical chemistry and physics with a scattering of examples of nano-scaled materials within the more normally taught subject matter. Although I am reviewing the book several years after its initial publication, I found it to be the same old stuff being presented under the guise of the new nanotechnology field. Also, I know that the cost of textbooks is always climbing, but feel that the book is too costly for the information presented.

Casarett & Doull's Essentials of Toxicology - Edition 2

Reviewed by Dr. Margot Hall

University of Southern Mississippi, Hattiesburg, MS 39406

This is an excellent textbook for an undergraduate survey course on toxicology. In a nutshell, this book is a shortened version of *Casarett & Doull's Toxicology: The Basic* Science of Poisons. It covers the same material, but without quite so much detail and as such, is an easier read for the novice student. The textbook has 2 editors, 72 contributing authors, 533 pages, numerous tables and figures, a table of contents, and an index. The same authors who wrote the corresponding chapter for Casarett & Doull's Toxicology: The Basic Science of Poisons, a simplified version of the original, wrote each chapter. The appendix found in the original is missing from Casarett & Doull's Essentials of Toxicology and this accounts for the fact that there is one less author. Added features in the simplified book include a list of key points at the beginning of each chapter and a set of 155 selfassessment questions and answers at the end of the book.

Each of the 34 chapters has a chapter outline and its own list of references (approximately 5-25 per chapter). Some terms are defined within the chapter, but there is no glossary of terms. The book is divided into seven parts: 1) general principles of toxicology, 2) disposition of toxicants, 3) non-organ-directed toxicity, 4) target organ toxicity, 5) toxic agents, 6) environmental toxicology, and 7) applications of toxicology. Unit (part) one includes 4 chapters detailing basic principles of toxicology and toxicological testing. It includes the history of toxicology,



general principles of toxicology (e.g., classes of toxicants with spectrum of undesired effects, tolerance, dose response, descriptive animal toxicity tests etc.), mechanisms of toxicology, and risk assessment. Unit two consists of 3 chapters detailing 1) the absorption, distribution and excretion of toxicants, 2) the biotransformation of xenobiotic, and 3) toxicokinetics. Unit three consists of three chapters including 1) chemical carcinogenesis, 2) genetic toxicology, and 3) developmental toxicology. Unit four has eleven chapters detailing the toxic responses of : 1) blood, 2) the immune system, 3) the liver, 4) the kidney, 5) the respiratory system, 6) the nervous system, 7) the ocular and visual system, 8) the heart and vascular system, 9) the skin, 10) the reproductive system, and 11) the endocrine system. Unit five has six chapters describing the toxic effects of toxic agents including: 1) pesticides, 2) metals, 3) solvents and vapors, 4) radiation and radioactive agents, 5) animal venoms and poisons, and 6) plants. Unit six has only two chapters, one on air pollution and one on ecotoxicology. Unit seven contains five chapters describing applications of toxicology including: 1) food toxicology. The book is a user friendly version of the original designed for undergraduate level (300-400) students. It is also recommended for the graduate student or scientist who wants a really good overview

without the extent of detail. This book is highly recommended for teaching, but not recommended as a reference book.

Brain: The Complete Mind

Reviewed by Dr. Margot Hall

University of Southern Mississippi, Hattiesburg, MS 39406

This is a remarkable photographic journey through the brain and its activities. Written for a lay audience, it has hundreds of color images taken directly from nature and from PET scans, MRI scans, electron microscopy, and x-ray crystallography of the nervous system and of drugs.

This excellent book has 342 pages divided into a foreword by Dr. Richard Restak, a table of contents, 10 chapters, a glossary, an index, a bibliography of further reading, and a list of photo credits. Each chapter has its own glossary in addition to fast facts boxes detailing scientific facts and side bar boxes detailing unique scientific breakthroughs in our understanding of neurology.

Chapter 1 (The Amazing Brain) includes: Knowing Itself, Nerve Cells, Anatomy, and Looking Inside. Chapter 2 (The Nervous System) includes: In Harmony, Messengers, and Delicate Balance. Chapter 3 (Brain Development) includes: Evolution, A New Brain, Waves of Changes, and Maturity. Chapter 4 (The Senses) includes: Perception, Sights and Sounds, Smell and Taste, Touch, and Integration. Chapter 5 (Motion) includes: Brain in Action, Silent Running, Shared Roles, and Motion Sickness. Chapter 6 (States of Mind) includes: Daily Routines, Awareness, Brain at Rest, and Altered States. Chapter 7 (The Feeling Brain) includes: Emotions, Dark Emotions, Good Feelings, and Impacts of Loss. Chapter 8 (Learning and Memory) includes: Learning, A Memory Forms, and



Language. Chapter 9 (The Aging Brain) includes: Mature Minds, Brain Changes, and Living Longer. Chapter 10-Epilogue (Future of the Brain) includes: New Intelligence, Social Shifts, Better Brains, Brain Medicine, and Next Steps.

The value of this book is in its wonderful color photography, color illustrations, and its straightforward presentation of complex neuroscience in language that a secondary school student and/or lay person can easily understand. From explanations of seizures to descriptions of the effects of diabetes mellitus, diabetes insipidus, and drug addiction on the brain, this book holds the readers interest. This is not a substitute for a textbook but belongs in every school library to excite the inquisitive student.

Longtime Fellows of the AIC



Dr. David W. Riley

Dr. David W. Riley is Vice Chair of the Board of Directors and Past President of The American Institute of Chemists. Dr. Riley is also the founding President of Extrusion Engineers, specializing in plastic processing, polymer defect technology, and co-efficient friction in the feed section of the extruder. He has an illustrious career record starting at Goodyear Research as a research Chemist in the early nineteen forties. Then he moved on to the US Navy as Naval Officer, Deck, Watch and Small Boat Officer, Research Chemist at E. I. DuPont, Research Engineer at Union Carbide Silicones, Senior Development Engineer at Western Electric-Buffalo, Technology Manager at General Cable Research and Production, Friction Research Director at Scientific Process & Research, and Tenneco. Dr. Riley earned his doctorate in and Master's degree in Physical Organic Chemistry from The Ohio State University (1946-51), and Bachelor's degree in Chemistry from Tufts University (1943). He attended the



Western Electric Graduate Engineering Training Center in Sun Times Building, Chicago. He is a Certified Chemist and Chemical Engineer by the National Certification Commission in Chemical and Chemical Engineering.

Dr. Riley's is an expert in the following areas - Expert Witness, Analytical Instrumentation Adaptation to Processing Equipment, Friction Analysis, Melt Rheology, Extrusion Equipment: Design & Analysis of Production, Telecommunication Cables and Insulation, Power Cables and Testing XLDPE, all phases of PVC Compounding & Extrusion, Thermal Stability of Polymers, Surface Chemistry, Metals & Polymers, Polyethylene Analysis, and FTIR & Electrical. He has published in well-regarded journals on topics ranging from extrusion and Methods of Analysis, Friction Properties of Thermoplastic Solids, Rheology of PVC Blends for SPE ANTEC, Elongation Flow Behavior of PVC Melt to Shear Effects on the Molecular Structure of Polymers, PPS, and Problems with Extrusion.

Dr. Riley has invented/designed several noteworthy analytical methods as follows. He invented Analytical Engineering, a term devoted to a scientific analysis of production, primarily in the field of extrusion, and the Extrusion Rate Controller, which cut the product temperature variability by an order of magnitude on a 150 mm extruder, significantly improving the quality control in a \$40 million wire and cable facility. He designed an extruder screw that saved the wire and cable company \$360,000/year in production costs, invented the "Flow Vision", an instrument on-line for inspecting polymer melts for gels, voids, contamination and any other heterogeneity, and invented a rheological tool for measuring the degree of shear damage done to polymers during processing. This includes the level of fragmentation and the incipient crosslinking in processing as function of shear rate. He developed ASTM Methods for analyzing plastics, D 3364 Melt Flow Analyzer, D 3591 Analysis of Formulated PVC, D 5576 Structural Entities in Polyolefins by IR, D 5477 Polymer Layers or Inclusions by FTIR. (For details, visit http://www.extrusionengineers.com/)

Dr. Riley is an active member of several professional organizations. In addition to a leadership position at The American Institute of Chemists noted earlier, he is an Honorary & Life Fellow of the AIC, Fellow of the American Association for the Advancement of Science, Fellow of American Society for Testing and Materials (ASTM International), Emeritus Fellow of the Society of Plastics Engineers (SPE), Life Senior Member of the Institute of Electrical and Electronic Engineers, Emeritus Member of the American Chemical Society. Member, Society of Applied Spectroscopy, Member of the Society of Rheology, Distinguished Member, Past President and Past Councilor of the Palisades Section of SPE, Initiator & Past Councilor and Past Chairman and again Councilor of the Polymer Modifiers and Additives Division of SPE, Past Councilor for the Polymer Analysis Division of SPE, Section Chairman on Molecular Parameters & Spectroscopy for ASTM Committee D 20 on Plastics, Past Chairman, Subcommittee D 20.70 on Analytical Methods, Member for Forty Five Years ASTM Committee G02 on Wear and Erosion Terminology, Member of the American Institute of Chemical Engineers and Member of the American Society for Mechanical Engineers. He is a member of the Editorial Review Board of the refereed AIC journal *The Chemist*.

Dr. Riley is married to Barbara for twenty four years and previously married for thirty nine years. He has two sons, one daughter, three grandchildren and three great-grandchildren. He is an avid tennis player for over 88 years that includes playing No. 1 on the Tufts Team and No. 3 on the Swarthmore Team. He also enjoys golf. He enjoys spending time in Florida during winter and New Jersey during rest of the year. Overall, he is an outstanding chemist and a great mentor to junior colleagues.

Dr. E. G. Meyer

D Z rqghuixoUlgh

There are a lot of stories (and jokes) about bikes and bikers. My favorite is: <u>You won't find a motorcycle</u> <u>parked in front of a psychiatrist's office</u>. And I believe that to be true. Life has many stresses, and one needs to be able to cope. For me riding in the mountains with a sack lunch to ward off hunger is perhaps the best way to cope, and I have employed this cure for many years.

At the start of my academic career, and well into my work career, there wasn't enough money to cover my needs and a motorcycle. But the day came in 1963 when I arrived in Laramie as Dean of the University of Wyoming College of Arts and Sciences. I was able to buy a 150cc kick-start Kawasaki.

Prior to that I had graduated (1940) from Carnegie Tech (now Carnegie Mellon University) and started graduate school. However, WWII caused a change of plans and I ended up in the US Navy. Actually this was a good experience (although it didn't seem so at the time), and provided lifetime benefits. The first was the GI Bill which helped immensely in my returning to graduate school and finishing my Ph.D. at the University of New Mexico in 1950. Having remained in



the active reserve (by necessity while in graduate school), I was not only able to add a few dollars to the bank account, but with 20 years of active and reserve duty I was "retired", and hence became eligible for a pension and medical services. The latter was a great boon as the girl I met at Carnegie Tech and married acquired a lengthy and terminal illness in her later life.

Then there were the ten years at New Mexico Highlands University where I was much too busy (and too poor with a new family) for a bike. But those years were most valuable in that I learned not only how to initiate my own research program, but later how to administer a research institute and a graduate school. I also learned how to build campus buildings, and this proved to be the key to my being hired at the University of Wyoming.

At UW, I finally got the bike and it surely was important in coping. In 1963, UW was a very small state university (about 5000 enrollment) that, frankly, had to be near the bottom of state and land grant universities. The Arts and Sciences college in particular was overworked, had grossly inadequate facilities, and little character of its own. The campus filling station I called it, as its primary duty was to offer courses needed by the other colleges: agriculture, business, education, engineering, and health sciences. Despite generating about 65% of the student credit hours, the faculty numbered about 100. It took 15 years and many headaches (and lots of bike rides) to build the Science Center, the Fine Arts Building, and obtain and remodel buildings for the Humanities, the Social Sciences, and the new department of Computer Science. More headaches and more bike rides were needed to increase the faculty to 300 with quality people. Still more headaches and bike rides were needed to develop solid bachelor, master, and doctoral programs.

At the end of this time I was promoted (actually demoted, as there is no better a job in a multi-purpose university than Dean of Arts and Sciences) to Vice President for Research, a position that did not exist. To establish the University Research Office involved more headaches and more bike rides, but, as with building Arts and Sciences, it was most rewarding.

Then, of course, 1990 arrived and it was time to retire. But fortunately retirement meant moving on to other things. It meant a campus office with fund raising, committee service, and "advisory" duties. It meant more time for important organizations such as the American Institute of Chemists (50 years) and the American Chemical Society (75 years). It meant time to participate in civic activities, such as serving on the City Council and the Airport Board, and being involved with the Chamber of Commerce, the City Museum, the State Territorial Park, etc. And, of course, I had meant more time to ride the bike...to visit Sturgis, to attend the Harley Davidson 100th anniversary in Milwaukee, to ride through Alaska, and to enjoy nature. But that too came to an end two years ago (sold the bike) with the realization that nothing, regardless of how bad or good, lasts forever. It has been a wonderful ride.

The AIC Code of Ethics



Approved by the AIC Board of Directors, April 29, 1983

The profession of chemistry is increasingly important to the progress and the welfare of the community. The Chemist is frequently responsible for decisions affecting the lives and fortunes of others. To protect the public and maintain the honor of the profession, the American Institute of Chemists has established the following rules of conduct. It is the Duty of the Chemist:

- 1. To uphold the law; not to engage in illegal work nor cooperate with anyone so engaged;
- 2. To avoid associating or being identified with any enterprise of questionable character;
- 3. To be diligent in exposing and opposing such errors and frauds as the Chemist's special knowledge brings to light;
- 4. To sustain the institute and burdens of the community as a responsible citizen;
- 5. To work and act in a strict spirit of fairness to employers, clients, contractors, employees, and in a spirit of personal helpfulness and fraternity toward other members of the chemical profession;
- 6. To use only honorable means of competition for professional employment; to advertise only in a dignified and factual manner; to refrain from unfairly injuring, directly or indirectly, the professional reputation, prospects, or business of a fellow Chemist, or attempting to supplant a fellow chemist already selected for employment; to perform services for a client only at rates that fairly reflect costs of equipment, supplies, and overhead expenses as well as fair personal compensation;
- 7. To accept employment from more than one employer or client only when there is no conflict of interest; to accept commission or compensation in any form from more than one interested party only with the full knowledge and consent of all parties concerned;
- 8. To perform all professional work in a manner that merits full confidence and trust; to be conservative in estimates, reports, and testimony, especially if these are related to the promotion of a business enterprise or the protection of the public interest, and to state explicitly any known bias embodied therein; to advise client or employer of the probability of success before undertaking a project;
- 9. To review the professional work of other chemists, when requested, fairly and in confidence, whether they are:
 - a. subordinates or employees
 - b. authors of proposals for grants or contracts
 - c. authors of technical papers, patents, or other publications
 - d. involved in litigation;
- 10. To advance the profession by exchanging general information and experience with fellow Chemists and by contributing to the work of technical societies and to the technical press when such contribution does

not conflict with the interests of a client or employer; to announce inventions and scientific advances first in this way rather than through the public press; to ensure that credit for technical work is given to its actual authors;

- 11. To work for any client or employer under a clear agreement, preferable in writing, as to the ownership of data, plans, improvements, inventions, designs, or other intellectual property developed or discovered while so employed, understanding that in the absence of a written agreement:
 - a. results based on information from the client or employer, not obtainable elsewhere, are the property of the client or employer
 - b. results based on knowledge or information belonging to the Chemist, or publicly available, are the property of the Chemist, the client or employer being entitled to their use only in the case or project for which the Chemist was retained
 - c. all work and results outside of the field for which the Chemist was retained or employed, and not using time or facilities belonging to a client or employer, are the property of the Chemist;
- 12. Special data or information provided by a client or employer, or created by the Chemist and belonging to the client or employer, must be treated as confidential, used only in general as a part of the Chemist's professional experience, and published only after release by the client or employer;
- 13. To report any infractions of these principles of professional conduct to the authorities responsible for enforcement of applicable laws or regulations, or to the Ethics Committee of The American Institute of Chemists, as appropriate.



Manuscript Style Guide

The Chemist is the official online refereed journal of The American Institute of Chemists (AIC). We accept submissions from all fields of chemistry defined broadly (e.g., scientific, educational, socio-political). *The Chemist* will not consider any paper or part of a paper that has been published or is under consideration for publication anywhere else. The editorial office of *The Chemist* is located at: The American Institute of Chemists, Inc. 315 Chestnut Street Philadelphia, PA 19106-2702, Email: aicoffice@theaic.org.

Categories of Submissions

RESEARCH PAPERS

Research Papers (up to ~5000 words) that are original will only be accepted. Research Papers are peer-reviewed and include an abstract, an introduction, up to 5 figures or tables, sections with brief subheadings and a maximum of approximately 30 references.

REPORTS

Reports (up to ~3000 words) present new research results of broad interest to the chemistry community. Reports are peer- reviewed and include an abstract, an introductory paragraph, up to 3 figures or tables, and a maximum of approximately 15 references.

BRIEF REPORTS

Brief Reports (up to ~1500 words) are short papers that are peer-reviewed and present novel techniques or results of interest to the chemistry community.

REVIEW ARTICLES

Review Articles (up to ~6000 words) describe new or existing areas of interest to the chemistry community. Review Articles are peer-reviewed and include an abstract, an introduction that outlines the main point, brief subheadings for each section and up to 80 references.

LETTERS

Letters (up to \sim 500 words) discuss material published in The Chemist in the last 8 months or issues of general interest to the chemistry community.

BOOK REVIEWS

Book Reviews (up to \sim 500 words) will be accepted.

Manuscript Preparation

RESEARCH PAPERS, REPORTS, BRIEF REPORTS & REVIEW ARTICLES

- The first page should contain the title, authors and their respective institutions/affiliations and the corresponding author. The general area of chemistry the article represents should also be indicated, i.e. General Chemistry, Organic Chemistry, Physical Chemistry, Chemical Education, etc.
- **Titles** should be 55 characters or less for Research Papers, Reports, and Brief Reports. Review articles should have a title of up to 80 characters.
- **Abstracts** explain to the reader why the research was conducted and why it is important to the field. The abstract should be 100-150 words and convey the main point of the paper along with an outline of the results and conclusions.
- **Text** should start with a brief introduction highlighting the paper's significance and should be understood to readers of all chemistry disciplines. All symbols, abbreviations, and acronyms should be defined the first time they are used. All tables and figures should be cited in numerical order.
- Units must be used appropriately. Internationally accepted units of measurement should be used in conjunction with their numerical values. Abbreviate the units as shown: cal, kcal, μg, mg, g (or gm), %, °C, nm, μm (not m), mm, cm, cm³, m, in. (or write out inch), h (or hr), min, s (or sec), ml [write out liter(s)], kg. Wherever commonly used units are used their conversion factors must be shown at their first occurrence. Greek symbols are permitted as long as they show clearly in the soft copy.
- **References and notes** should be numbered in the order in which they are cited, starting with the text and then through the table and figure legends. Each reference should have a unique number and any references to unpublished data should be given a number in the text and referred to in the references. References should follow the standards presented in the AIC Reference Style Guidelines below.

REFERENCE STYLE GUIDELINES

References should be cited as numbers within square brackets [] at the appropriate place in the text. The reference numbers should be cited in the correct order throughout the text (including those in tables and figure captions, numbered according to where the table or figure is designated to appear). The references themselves are listed in numerical order at the end of the final printed text along with any Notes. Journal abbreviations should be consistent with those presented in Chemical Abstracts Service Source Index (CASSI) (http://www.cas.org) guide available at most academic libraries.

- **Names** and initials of all authors should always be given in the reference and must not be replaced by the phrase *et al*. This does not preclude one from referring to them by the first author, et al in the text.
- **Tables** should be in numerical order as they appear in the text and they should not duplicate the text. Tables should be completely understandable without reading the text. Every table should have a title. Table titles should be placed above the respective tables.

Table 1. Bond Lengths (Å) of 2-aminophenol

• **Figure legends** should be in numerical order as they appear in the text. Legends should be limited to 250 words.

Figure 1. PVC Melt Flow Characterized by Analytical Structural Method

- Letters and Book Reviews should be clearly indicated as such when being submitted. They are not peer-reviewed and are published as submitted. Legends should be placed after/under the respective figures.
- Journals The general format for citations should be in the order: **author(s)**, **journal**, **year**, **volume**, **page**. Page number ranges are preferred over single values, but either format is acceptable. Where page numbers are not yet known, articles may be cited by DOI (Digital Object Identifier). For example:

Booth DE, Isenhour TL. The Chemist, 2000, 77(6), 7-14.

• **Books** - For example:

Turner GK in *Chemiluminescence: Applications*, ed. Knox Van Dyke, CRC Press, Boca Raton, 1985, vol 1, ch. 3, pp 43-78.

• **Patents** should be indicated in the following form:

McCapra F, Tutt D, Topping RM, UK Patent Number 1 461 877, 1973.

• **Reports and bulletins, etc. -** For example:

Smith AB, Jones CD, *Environmental Impact Report for the US*, final report to the National Science Foundation on Grant AAA-999999, Any University, Philadelphia, PA, 2006.

• Material presented at meetings - For example:

Smith AB. Presented at the Pittsburgh Conference, Atlantic City, NJ, March 1983, paper 101.

• Theses - For example:

Jones AB, Ph.D. Thesis, Columbia University, 2004.

REFERENCE TO UNPUBLISHED MATERIAL

• For material presented at a meeting, congress or before a Society, etc., but not published, the following form should be used:

Jones AB, presented in part at the 20th American Institute of Chemists National Meeting, Philadelphia, PA, June, 2004.

• For material accepted for publication, but not yet published, the following form should be used:

Smith AB. Anal. Chem., in press

• For material submitted for publication but not yet accepted the following form should be used:

Jones AB, Anal. Chem. submitted for publication.

• For personal communications the following should be used:

Smith AB, personal communication.

• If material is to be published but has not yet been submitted the following form should be used:

Smith AB, unpublished work.

Reference to unpublished work should not be made without the permission of those by whom the work was performed.

Manuscript Selection

The submission and review process is completely electronic. Submitted papers are assigned by the Editors, when appropriate, to at least two external reviewers anonymously. Reviewers will have approximately 10 days to submit their comments. In selected situations the review process can be expedited. Selected papers will be edited for clarity, accuracy, or to shorten, if necessary. The Editor-in-Chief will have final say over the acceptance of submissions. Most papers are published in the next issue after acceptance. Proofs will be sent to the corresponding author for review and approval. Authors will be charged for excessive alterations at the discretion of the Editor-in-Chief.

Conditions of Acceptance

When a paper is accepted by *The Chemist* for publication, it is understood that:

• Any reasonable request for materials to verify the conclusions or experiments will be honored.

- Authors retain copyright but agree to allow *The Chemist* to exclusive license to publish the submission in print or online.
- Authors agree to disclose all affiliations, funding sources, and financial or management relationships that could be perceived as potential conflicts of interest or biases.
- The submission will remain a privileged document and will not be released to the public or press before publication.
- The authors certify that all information described in their submission is original research reported for the first time within the submission and that the data and conclusions reported are correct and ethically obtained.
- The Chemist, the referees, and the AIC bear no responsibility for accuracy or validity of the submission.

Authorship

By submitting a manuscript, the corresponding author accepts the responsibility that all authors have agreed to be listed and have seen and approved of all aspects of the manuscript including its submission to *The Chemist*.

Submissions

Authors are required to submit their manuscripts, book reviews and letters electronically. They can be submitted via email at aicoffice@theaic.org with "Submission for consideration in *The Chemist*" in the subject line. All submissions should be in Microsoft® Word format.

Copyright Assignment & Warranty Form for The Chemist

It is the policy of *The Chemist* to require all contributors to transfer the copyright for their contributions (hereafter referred to as the manuscript) to The American Institute of Chemists, Inc. (hereafter referred to as The AIC) the official publisher of *The Chemist*. By signing this agreement you assign to The AIC to consider publishing your manuscript the exclusive, royalty-free, irrevocable copyright in any medium internationally for the full term of the copyright. This agreement shall permit The AIC to publish, distribute, create derivative works, and otherwise use any materials accepted for publication in *The Chemist* will be sent to the author(s) whose manuscript is accepted for publication. The AIC will not publish any accepted manuscript in *The* Chemist without its author(s) fully complying with this requirement.

For further information or if you can any questions please contact the Publisher of *The Chemist* at (215) 873-8224 or via email at publications@theaic.org.

Website: http://www.theaic.org/ Email: aicoffice@theaic.org Phone: 215-873-8224

Announcements

INVITATION TO AUTHORS

Authors are invited to submit manuscripts for *The Chemist*, the official online refereed journal of The American Institute of Chemists (AIC). We accept submissions from all fields of chemistry defined broadly (e.g., scientific, educational, socio-political). *The Chemist* will not consider any paper or part of a paper that has been published or is under consideration for publication anywhere else.

Research Papers (up to ~5000 words) that are original will only be accepted. Research Papers are peer-reviewed and include an abstract, an introduction, up to 5 figures or tables, sections with brief subheadings and a maximum of approximately 30 references.

Reports (up to ~3000 words) present new research results of broad interest to the chemistry community. Reports are peer- reviewed and include an abstract, an introductory paragraph, up to 3 figures or tables, and a maximum of approximately 15 references.

Brief Reports (up to ~1500 words) are short papers that are peer-reviewed and present novel techniques or results of interest to the chemistry community.

Where to Send Manuscripts?

Please submit your manuscripts by email (aicoffice@theaic.org) to the attention of:

The Editor-in-Chief, The Chemist The American Institute of Chemists, Inc. 315 Chestnut Street, Philadelphia, PA 19106-2702 Email: aicoffice@theaic.org

Review Articles (up to ~6000 words) describe new or existing areas of interest to the chemistry community. Review Articles are peer-reviewed and include an abstract, an introduction that outlines the main point, brief subheadings for each section and up to 80 references.

Letters (up to ~500 words) discuss material published in *The Chemist* in the last 8 months or issues of general interest to the chemistry community.

Book Reviews (up to ~ 500 words) will be accepted.





From its earliest days in 1923 to the present, the American Institute of Chemists has fostered the advancement of the chemical profession in the United States.

The Institute has a corresponding dedication "to promote and protect the public welfare; to establish and maintain standards of practice for these professions; and to promote the professional experience through certification as to encourage competent and efficient service."

The AIC engages in a broad range of programs for professional enhancement through the prestigious Fellow membership category, awards program, certification programs, meetings, publications and public relations activities.

The American Institute of Chemists, Inc.

Officers

David M. Manuta	President
E. Gerald Meyer	Secretary
J. Stephen Duerr	Treasurer
Jerry P. Jasinski	. Chair of the Board and Immediate Past President
David W. Riley	Vice-Chair of the Board

Board of Directors

Stanley Edinger Jerry Jasinski (Chair) David Devraj Kumar Edmond Malka Paul E. Mills David W. Riley (Vice Chair) Dayal Meshri Margaret Hall James Smith

Advertising: Send insertion orders and advertising materials to AIC. Visit The AIC Web site for additional information at www.TheAIC.org.

The American Institute of Chemists, Inc.

315 Chestnut Street, Philadelphia, PA 19106-2702. Phone: (215) 873-8224 | Fax: (215) 629-5224 | E-mail: aicoffice@TheAlC.org