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Note: 3D render of the alanine peptide molecular model.
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The Chemist

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Editorial

Looking Forward

David Devraj Kumar
Florida Atlantic University

This year, I remain more optimistic than ever before about the future of chemical sciences. Regardless of the pressing global financial situation, chemistry continues to advance. Chemistry research and development (R & D) continue to expand both the theoretical and applied frontiers of science. Chemical education reforms challenge students to think about restoring and sustaining the environment. Growing concerns about public (mis)understanding of chemistry continue to challenge the role of the chemical sciences in society. Increasing public awareness of the role of chemicals in day-to-day technologies calls for a higher level of responsibility of chemical scientists to the general public. In this context, volume 86(1), 2013 of *The Chemist* presents a lineup of informative and thought provoking articles and book reviews dedicated to the continuous progress in chemistry.

Niki Judenary and co-authors are reporting a comparative study of the total, free, and % free prostate specific antigen in the serodiagnosis of prostate cancer in African-American and Caucasian-American males in the US. Their study sheds light on some aspects of prostate cancer providing insight for additional research on this leading non-skin related cancer in men. The study of B. R. Manjunath and co-authors evaluated Cenospheres as fillers for PVC compounds in electrical cable sheathing applications. Abraham George and co-authors report a theoretical modeling of the geometry of 2-Aminophenol optimized using Hartee-Fock (HF) and density functional theory (DTF) methods with the support of the *Gaussian 03™* software. David Manuta describes the chemistry behind a litigation involving the explosion of a lead-acid automotive battery during testing with a battery tester and provides insights about some aspects of chemistry in real-world situations. S. Baroni and B. Holmes point to the need for improving science and technology communication and education between the community of scientists and the general public in order to “create new research opportunities, facilitate broader education initiatives, and foster a more encouraging view of new discoveries.”

John Hill and co-authors address the challenges of chemical education and explores a sustainable chemistry philosophy and practice through green chemistry. Congratulations to John Hill on reaching the 200th mile-mark in refereed publications with this article. Dr. Hill, Professor at La Trobe Institute of Molecular Sciences, Australia, has a distinguished career record in both chemistry and chemical education, and in addition, he serves as an active member of the Editorial Review Board of *The Chemist*. Joshua Strate reflects his experiences as middle school chemistry teacher and argues for making chemistry connections to other content areas as a win-win situation for improving interest in science among middle schoolers.

The book reviews by Margot Hall include informative books on brain science with a “futuristic twist” and books on toxicology. Congratulations to Professor Margot Hall of the University of Southern Mississippi on receiving the Dudley Peeler Award for “outstanding contributions to the Mississippi Academy of Sciences.” She is an active Fellow of The American Institute of Chemists, and a member of the Editorial Review Board of *The Chemist*. The voluntary efforts of reviewers who provided thoughtful feedback in a timely manner are thankfully acknowledged. Finally, I am grateful to Florida Atlantic University for serving as a home base for the editing of *The Chemist*, invaluable in re-establishing this refereed scientific periodical.

Thank you.



A Comparison of Total, Free, and % Free PSA for the Serodiagnosis of Prostate Cancer in African-American and Caucasian-American Males

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Abstract: Although the major types of non-skin cancer among men are prostate cancer, lung cancer, and colorectal cancer, prostate cancer is the second leading cause of cancer death among men. In 2009, there were 192,280 new cases of prostate cancer and 27,360 deaths from this disease in the USA. It has been suggested that there is a disparity in the incidence and recognition of prostatic cancer between African-American males and Caucasian-American males [1]. One of the most widely used approaches for diagnosing prostate cancer involves measuring prostate specific antigen (PSA) serum levels. One objective of this study was to compare normal (healthy) adult PSA levels in African-Americans and Caucasian-Americans to determine if there is racial/genetic bias. A second objective was the comparison of a manual assay with an automated assay for PSA detection. It was hypothesized that the Diagnostic Automation (manual) assays would be superior to the Beckmann Access (automated) assays for the detection of prostate cancer and that there would be a genetic bias. Tumor marker assays were performed according to the manufacturer's directions. Assays used in this study included total PSA and % free PSA (Diagnostic Automation, Inc. and Beckman, Inc.). A total of 1,056 patient samples and 809 healthy adult male subject samples were tested. We concluded that the manual assay was superior to the automated assay for Free PSA detection but not for total PSA. We also concluded that there was genetic bias for African-American males versus Caucasian-American males.

Key Words: Prostate specific antigen, prostate cancer, tumor markers.

INTRODUCTION

In 2012, there will be an estimated 241,740 new cases of prostate cancer and 28,170 deaths from this disease in the USA, according to the American Cancer Society [2]. This makes prostate cancer the leading non-skin cancer among males in the USA. The prostate is approximately the size of a walnut and is located at the neck of the bladder where it surrounds the urethra. It consists of acinar cells which line the prostatic ducts and glands and stromal support cells. The acinar cells secrete nutrients, enzymes, and buffers into the prostatic fluid which forms a portion of semen. The nutrients supply energy to the sperm, the buffers neutralize the pH of the semen, protecting the sperm from the acidic pH of the vagina, and the enzymes lyse the seminal coagulum following

ejaculation, thus permitting the sperm to become motile [3].

The acinar cells are derived from epithelial cells which in turn come from the endoderm. Therefore, the major prostatic cancer is adenocarcinoma. Adeno refers to its glandular nature and carcinoma refers to its embryonic origin in the endoderm [4]. Benign tumors of the prostate are known as benign prostatic hyperplasia or BPH. Benign tumors will remain in situ whereas malignant (cancerous) tumors will eventually invade neighboring tissue and metastasize in blood and lymphatic systems to distant organs. For prostate cancer, the metastasis is usually to the bladder, hipbones, and vertebrae locally, and the lungs distally [4]. Symptoms include difficulty with urination, painful ejaculation, and persistent bone pain. Once symptoms of prostate cancer become noticeable, the tumor is often advanced. The

most widely used approaches for diagnosing prostate cancer involve the use of digital rectal examination (DRE), transrectal ultrasound, prostate biopsy, and prostate specific antigen (PSA) serum levels. Treatment options can include surgery, hormonal replacement, radiation therapy, and chemotherapy [5].

Prostate specific antigen (PSA) is a serine protease and forms a portion of the prostatic fluid. It functions to lyse the seminal coagulum following ejaculation. PSA is highly specific to the prostate. Serum PSA levels are normally very low in healthy males and increase with increasing tumor burden. For these reasons, PSA has been considered an excellent tool for screening, and has been used in combination with other methods for diagnosis, staging, and monitoring for recurrence of disease (relapse). Its one drawback is that serum PSA can be elevated with BPH as well as with prostatic cancer [6].

In serum, prostate specific antigen exists in two forms: free and complexed to alpha-1-antichymotrypsin. Monoclonal antibodies directed at epitopes on free, complexed, and total PSA have been developed and commercial assays exist for each of these [7]. Percent free PSA (% Free PSA) values can be calculated from the free PSA and total PSA results. Normal reference intervals (NRI) are derived for these assays by taking the mean plus or minus two standard deviations ($\bar{x} \pm 2S$) for a set of healthy human subjects. Patient values that fall outside of the NRI are considered to be abnormal. Since a low value for a tumor marker would have no clinical significance, one uses the mean plus two standard deviations ($\bar{x} \pm 2S$) as the "cut-off point" between health and disease. A variety of factors can affect the NRI. Three of the most common effectors are age, gender, and genetics. Examples would include: increasing NRI for cholesterol seen with increasing age, increasing NRI for estrogen seen with females as opposed to males, and decreasing NRI for alcohol dehydrogenase seen in Native-Americans and Asiatics as opposed to Caucasians and Africans [7].

It has been suggested that there is a disparity in the incidence and recognition of prostatic cancer between African-American males and Caucasian-American males [8]. This could be the result of genetic bias or socioeconomic factors. The CDC [9] reported that among all other races, an African-American male has a nineteen percent chance of being diagnosed with prostate cancer and a five percent chance of dying from the disease. In addition, the CDC [10] noted that in 2005 Caucasian males had a higher incidence of prostate cancer than Hispanic males. The UPMC Cancer Center [11] claimed

that Asian men had the lowest incidence of prostate cancer among all other races.

Boyles [12] reported that in a study of 1346 adult males (673 with prostate cancer and 673 without prostate cancer), he observed a slight increase in prostate cancer among those individuals who had a history of prior infection with trichomoniasis. He concluded that there may be a link between STD infection and more aggressive prostate cancer. His study suggests the possibility that a discrepancy between the incidence and/or prevalence of STDs could explain an observed difference in the incidence and/or prevalence of prostate cancer between African-American and Caucasian-American males.

Fowke [13] reported that African-American males, among all other racial groups, were more likely to be diagnosed with prostate cancer at a more advanced stage. He compared 121 African-American males with 121 Caucasian-American males with no prior diagnosis of prostate cancer or diabetes. He observed a correlation between obesity, diabetes mellitus, and PSA levels. PSA blood levels (concentrations) were decreased in obese and diabetic males. This association was more prevalent among obese African-American males but was also observed to some extent among obese Caucasian-American males. This finding could also explain an observed difference in the incidence and/or prevalence of prostate cancer between African-American and Caucasian-American males.

Odedina [14] investigated the relationship between prostate cancer knowledge, cultural beliefs and values, and the incidence and prevalence of prostate cancer among African-American males and West African males. According to Odedina, both West African males and recent immigrants from West Africa to the United States have a lower incidence of prostate cancer than African-American males. In her study, she attributed this to their cultural dissimilarities because they have similar genetic backgrounds. She reported that African-American males suffer disproportionately from aggressive prostate cancer which is often detected at a much later stage. Her data demonstrated that African-American males were more fatalistic in their cancer beliefs than other American ethnic groups and hence were more likely to be diagnosed in late stage disease. She raised the possibility that cultural beliefs may contribute to the higher incidence of prostate cancer among African-Americans.

The purpose of this study was to compare African-American males with Caucasian-American males for healthy adult reference intervals (NRI) for PSA and %

free PSA. One addressed the question of racial/genetic bias and the possibility that one should not continue to use the same PSA cutoff values for different genetic/racial subgroups. Additionally two test methods for PSA (manual vs. automated) were compared. It was hypothesized that the new test (manual test) would prove superior to the in-house test (automated test) and that there would be a significant difference between African-American and Caucasian-American PSA NRI.

MATERIALS

The Beckman Access free PSA and total PSA assay kits were acquired from Beckman Coulter (Faulkner, CA). The intended use of the Beckman Access free PSA is for the quantitative measurement of free prostate specific antigen (PSA) in human serum. The assay should be used in conjunction with the Beckman Access total PSA. The intended use of the Beckman Access total PSA is for the quantitative measurement of total PSA in human serum. The assay is also used as an additional test to aid in the management of cancer. Both of the assays are based on the Microparticle Enzyme Immunoassay (MEIA) technology.

The Diagnostic Automation free PSA and total PSA kits were acquired from Diagnostic Automation, Inc. (Calabasas, CA). The intended use of the Diagnostic Automation free PSA test is for the quantitative measurement of free PSA in human serum. The intended use of the Diagnostic Automation total PSA is for the quantitative measurement of total PSA in human serum. The principle of both assays is based upon a solid phase two-site immunoassay. The kits contain a monoclonal antibody with an attached tracer and another one as a capture antibody. The free (unbound) tracers are removed by washing after certain complexes are made. The assay will produce a colorimetric reaction.

The Beckman Access instrument was acquired from Beckman Coulter, Inc. (Faulkner, CA). For the Diagnostic Automation assay kits, everything is done manually. A Stat Fax 2600 microplate washer was acquired from Diagnostic Automation (Calabasas, CA). The Beckman Coulter AD 340 microtiter plate reader was acquired from Beckman Coulter (Faulkner, CA).

PATIENTS & SUBJECTS

Samples of blood were collected at hospitals (Gulf Coast area) from 1056 male patients seen during a 24-

month period of time. All male patients over the age of 18 years for whom an initial PSA test had been ordered by their physician were included. Prostate cancer was found in 155 of the patients; 901 of the patients did not have cancer. The serum was separated from each blood sample, labeled with a code number, and frozen at -20°C. The hospital pathologists sent the researchers a list of the code numbers with the appropriate diagnoses. All other patient identifiers (e.g. name, social security number, and hospital identification number) were removed to protect the confidentiality of the patients. The sera from 809 healthy adult (>18 years of age) male subjects were also acquired from hospitals for the determination of the normal reference intervals for the assays. Of these five hundred and eighty-four (584) were Caucasian-American males, one hundred and eighty-four (184) were African-American males, and forty-one (41) were Hispanic-American males. These volunteer subjects were determined to be healthy by the pathologists on the basis of their clinical presentations and their pathologic/histological examinations. The University of Southern Mississippi Institutional Review Board approved permission for this study to be conducted and the procedures were in accordance with all ethical standards.

METHODS

The samples of serum were thawed at 37°C and the PSA assay kits for total PSA and free PSA were used according to the manufacturers' instructions. Based on the procedure for the Beckman Access total PSA assay, 150 µL (microliters) of patient's serum were dispensed into each sample well. Then, five drops of the total PSA calibrators and controls were dispensed into the appropriate sample wells. A minimum volume of 250 mL (milliliters) of the MEIA #2 diluent buffer for the Beckman Access total PSA assay kit was also added to the wells. An assay calibration was performed on all new lots of Beckman Access total PSA reagent packs. Once the calibrations were accepted and stored into the Beckman Access instrument, controls were run on the instrument. A minimum of one control per carousel was needed for the run.

Based on the procedure for the Beckman Access free PSA assay, 150 µL of the patient serum was pipetted into each of the wells. Then, five drops of calibrators and controls were dispensed into each appropriate well. A minimum volume of 250 mL of MEIA #2 diluent buffer

was used to properly process each assay run. Calibration was run on all new lots of reagent packs. Once assay calibrations had been accepted and stored into the instrument, controls were run. A minimum of one control per carousel was needed for the run. All of the Beckman Access assay procedures were run on the Beckman Access instrument provided by Beckman Coulter Laboratories.

In accordance with the assay procedure for the Diagnostic Automation total PSA (Figure 1), 50 μL (microliters) of patient serum, standards, and controls were pipetted into the appropriate sample wells. One hundred microliters of zero buffers were also dispensed into each well. The contents of the wells were thoroughly mixed for ten seconds. Then, the wells were incubated at room temperature (18-22°C) for 60 minutes. After 60 minutes, the incubation mixture was removed and discarded properly. The microtiter wells were washed with the STAT FAX 2600 microplate washer and the wells were thoroughly emptied to remove all residual water droplets. Next, 100 μL of enzyme conjugate were dispensed into each well and gently mixed for five seconds. The sample wells were again incubated at room temperature for 60 minutes. The incubation mixture was emptied at the end of 60 minutes, and the microtiter plates were washed with the STAT FAX 2600 microplate washer. After washing, the plates were thoroughly emptied to remove residual water droplets. Then, 100 μL of TMB solution was pipetted into each well and gently mixed for five seconds. After mixing, the wells were incubated for 20 minutes. Then, the reaction was stopped by adding stop solution to each sample well. Next, the contents of the wells were gently mixed until there was a complete color change from blue to yellow and the microliter plates were read on the Beckman Coulter AD 340 microtiter reader at 450 nm within 20 minutes. The absorbance of the assay was directly proportional to the total PSA in each sample.

In accordance with the assay procedure for the Diagnostic Automation free PSA (Figure 2), 100 μL of patient serum, standards and controls as well as 100 μL of sample diluent were dispensed into appropriate wells. The contents of the wells were thoroughly mixed for ten seconds and the wells were incubated at 37°C for 60 minutes. After incubation, the mixture was removed

from the wells and discarded. Then, the microtiter plates were washed by using the STAT FAX 2600 microplate washer and the plates were thoroughly emptied of the residual water droplets. Next, 200 μL of enzyme conjugate reagent were dispensed into each well and gently mixed for five seconds. These mixed samples were also incubated for 60 minutes at 37°C. After incubation, the mixture was also removed and washed with the STAT FAX 2600 microplate washer. Then, 100 μL of TMB stop solution were dispensed into each well and gently mixed for five seconds. Next, the wells were incubated in the dark for 20 minutes. After incubation, the reaction was stopped by adding 100 μL of stop solution to each well. The contents of the wells were gently mixed for thirty seconds until there was a complete color change from blue to yellow and the Beckman Coulter AD 340 microtiter plate was used to read the plates at 450 nm within 20 minutes.

Once the patients' specimens for the Beckman Access total and free PSA as well as the Diagnostic Automation total and free values were obtained, a calculation for the % free PSA was performed. The % free PSA was calculated by obtaining the total PSA and free PSA values. The free PSA value was divided by the total PSA value and that Quotient was multiplied by 100.

$$\text{Equation 1: } (\text{Free PSA}/\text{Total PSA}) \times 100 = \% \text{ free PSA}$$

Statistics

All statistical calculations were performed by using the computer SP software package.

RESULTS

Precision

Quality control samples (included in the kits), analyzed over a 3-month period, were used to determine intra- and inter-assay precision (Tables 1A and 1B). The coefficient of variation results were less than 10% for all but the between run precision, which was less than 20%.

Table 1A. Comparison of Diagnostic Automation and Beckman Access Assay Precision for Total PSA using Control Sera

	n	\bar{X} (ng/mL)	SD (ng/mL)	CV (%)
Within-Run				
Diagnostic Automation	4	3.89	0.10	2.48
Beckman Access	2	1.00	0.02	2.00
Between-Run				
Diagnostic Automation	52	3.87	0.71	18.30
Beckman Access	40	1.00	0.02	2.20

Table 1B. Comparison of Diagnostic Automation and Beckman Access Assay Precision for Free PSA using Control Sera

Assay	n	\bar{X} (ng/mL)	SD (ng/mL)	CV (%)
Within-Run				
Diagnostic Automation	4	2.25	0.09	4.10
Beckman Access	2	1.04	0.02	1.79
Between-Run				
Diagnostic Automation	52	2.08	0.40	19.23
Beckman Access	40	1.04	0.04	3.40

Linearity

Serial dilutions of abnormal pool samples were used to determine the linearity of the assays (Tables 2A and 2B). The R² values were greater than 0.99 for all the assays.

Table 2A. Comparison of Diagnostic Automation and Beckman Access Assay Linearity for Total PSA

Assay	R Squared (R ²)
Diagnostic Automation	0.9981
Beckman Access	0.9996

Table 2B. Comparison of Diagnostic Automation and Beckman Access Assay Linearity for Free PSA

Assay	R Squared (R ²)
Diagnostic Automation	0.9998
Beckman Access	0.9986

Assay Sensitivity

Reference intervals for the zero diluent [analytical sensitivity] are given in Tables 3A and 3B. The results range from 0.000 to 0.008 for the manual and automated assays respectively.

Table 3A. Comparison of Diagnostic Automation and Beckman Access Assay Sensitivity (Analytical Sensitivity) for Total PSA

Analytical Sensitivity	n	\bar{X} (ng/mL)	SD (ng/mL)	Range (ng/mL)
Assay				
Diagnostic Automation	19	0.00	0.000	0-0.000
Beckman Access	20	0.00	0.004	0-0.008

Table 3B. Comparison of Diagnostic Automation and Beckman Access Assay Sensitivity (Analytical Sensitivity) for Free PSA

Analytical Sensitivity	n	\bar{X} (ng/mL)	SD (ng/mL)	Range (ng/mL)
Assay				
Diagnostic Automation	20	0.00	0.000	0-0.000
Beckman Access	20	0.00	0.002	0-0.005

Reference Intervals

Normal Reference Intervals are given in Tables 4 for healthy, adult African-American and Caucasian-American males.

Table 4A. Comparison of Diagnostic Automation and Beckman Access Assay Healthy Adult Reference Intervals for Total PSA

Healthy Adults	n	\bar{X} (ng/mL)	SD (ng/mL)	Range (ng/mL)
Total Males				
Diagnostic Automation	808	1.67	2.86	0-7.39
Beckman Access	809	1.91	6.59	0-17.07
African-American Males				
Diagnostic Automation	184	2.27	4.21	0-10.69
Beckman Access	183	2.69	12.42	0-27.53
Caucasian-American Males				
Diagnostic Automation	582	1.45	2.34	0-6.13
Beckman Access	584	1.70	3.37	0-8.84

Table 4B. Comparison of Diagnostic Automation and Beckman Access Assay Healthy Adult Reference Intervals for Free PSA

Healthy Adults	n	\bar{X} (ng/mL)	SD (ng/mL)	Range (ng/mL)
Total Males				
Diagnostic Automation	808	0.07	0.28	0-0.63
Beckman Access	36	0.90	1.26	0-3.42
African-American Males				
Diagnostic Automation	184	0.12	0.43	0-0.98
Beckman Access	10	1.56	2.24	0-6.04
Caucasian-American Males				
Diagnostic Automation	582	0.05	0.23	0-1.02
Beckman Access	26	0.65	0.43	0-1.51

A Comparison of Normal Adult PSA values by genetic background and by methodology are given in Tables 5-6.

Table 5. Comparison of Normal Adult PSA Values by Genetic Background

Total PSA	n	\bar{X} (ng/mL)	SD (ng/mL)	Probability
Diagnostic Automation				
African-American Males	184	2.27	4.21	0.013*
Caucasian-American Males	582	1.45	2.34	
Beckman Access				
African-American Males	183	2.69	12.42	0.288
Caucasian-American Males	584	1.70	3.37	

Free PSA	n	\bar{X} (ng/mL)	SD (ng/mL)	Probability
Diagnostic Automation				
African-American Males	184	0.12	0.43	0.038*
Caucasian-American Males	582	0.05	0.23	
Beckman Access				
African-American Males	10	1.56	2.24	0.230
Caucasian-American Males	26	0.64	0.43	

% Free PSA	n	\bar{X} (ng/mL)	SD (ng/mL)	Probability
Diagnostic Automation				
African-American Males	184	5.29	6.21	0.014
Caucasian-American Males	582	3.45	7.38	
Beckman Access				
African-American Males	10	5.79	9.13	0.230
Caucasian-American Males	26	3.76	8.94	

*p < 0.05

Table 6. Comparison of Normal Adult PSA Values by Methodology (paired t-test)

	n	\bar{X} (ng/mL)	SD (ng/mL)	Probability
Total PSA - Assay				
Diagnostic Automation	807	1.67	2.86	0.167
Beckman Access	807	1.91	6.59	
Free PSA - Assay				
Diagnostic Automation	36	0.29	0.87	0.000*
Beckman Access	36	0.90	1.26	
% Free PSA - Assay				
Diagnostic Automation	31	3.55	5.59	0.000*
Beckman Access	31	19.06	9.01	

*p < 0.05

There was a significant difference between the values for the two racial groups observed with the manual assay. There was a significant difference between the two assay methods for free PSA and % free PSA. There was no difference between the two assays for total PSA.

Predictive Values

Predictive values for prostate cancer in 1056 patients are presented in Tables 7-8. The diagnostic sensitivity for total PSA was less than 50% for both assays and racial groups (Table 7).

Table 7. Predictive Values of Total PSA for Prostate Cancer in 1056 Patients

Assay Method	Sensitivity (%)	Specificity (%)	PV (+) (%)	PV (-) (%)	Efficiency (%)	Cut-Off (ng/mL)
TOTAL Males						
Diagnostic Automation	10.32	93.11	20.51	85.77	80.95	4.00
Beckman Access	18.71	87.57	20.57	86.23	77.46	4.00
African-American						
Diagnostic Automation	16.67	92.23	36.00	80.85	76.54	4.00
Beckman Access	25.93	86.34	33.33	81.57	73.75	4.00
Caucasian-American						
Diagnostic Automation	6.06	93.09	11.76	86.70	81.60	4.00
Beckman Access	14.14	87.60	14.74	87.06	77.93	4.00

In contrast, the diagnostic sensitivity for % free PSA was greater than 90% in both racial groups by Diagnostic Automation and greater than 75% in both racial groups by the Beckman Access method (Table 8).

Table 8. Predictive Values of % Free PSA for Prostate Cancer in 1056 Patients

Assay Method	Sensitivity (%)	Specificity (%)	PV (+) (%)	PV (-) (%)	Efficiency (%)	Cut-Off (ng/mL)
TOTAL Males						
Diagnostic Automation	97.25	4.27	13.23	91.18	16.41	25.00
Beckman Access	80.00	33.33	5.13	97.37	35.34	25.00
African-American						
Diagnostic Automation	95.00	8.00	19.10	87.50	24.19	25.00
Beckman Access	100.00	30.00	4.50	100.00	32.25	25.00
Caucasian-American						
Diagnostic Automation	98.15	3.13	11.74	94.12	14.16	25.00
Beckman Access	75.00	33.75	5.36	96.43	35.71	25.00

The diagnostic specificity for total PSA was greater than 80% for both assays and both racial groups (Table 7). However, the diagnostic specificity for % free PSA was less than 50% for both assay methods in both racial groups (Table 8).

It is important to note that the Diagnostic Sensitivity of a test is the proportion of individuals with the disease who test positively with the test. Diagnostic Specificity of a test is the proportion of individuals without the disease who test negatively with the test. Predictive Value + is the fraction of positive tests that are true positives. Predictive Value - is the fraction of negative tests that are true negatives. Diagnostic Efficiency of a test is the fraction of all test results that are either true positives or true negatives [15].

DISCUSSION & CONCLUSIONS

Based on the findings of this study, the hypothesis that there would be genetic bias was accepted. In contrast, the hypothesis that the manual test would be superior to the automated test was rejected for Total PSA assays and supported for % Free PSA assays. Analytical parameters were acceptable for all the assays. The normal reference intervals were slightly higher than those cited

by the manufacturers. There was a significant difference between the NRI of African-American and Caucasian-American adult males for Total PSA, Free PSA, and % Free PSA by the manual assay. A comparison of normal adult PSA reference intervals by methodology showed significant difference for Free PSA and %Free PSA, but not total PSA. The Beckman Access results were typically slightly higher than the Diagnostic Automation results.

Using the decision values established by the manufacturers, one obtained diagnostic sensitivities of <50% for Total PSA by both methods. This has been reported in the literature. While our values were in line with those of other researchers, they were disappointing. It is speculated that this may be due to inclusion of patients with prostate cancer who may have been diagnosed and were undergoing treatment. Alternatively the patients may have been diagnosed earlier in the course of the disease. The diagnostic sensitivities for % Free PSA were excellent with a Diagnostic Automation value of 97% and a Beckman Access value of 80%. The other predictive values were as expected and there was no significant difference between the values observed in African-American and Caucasian-American males.

Fowler proposed that there was a genetic bias due to high concentrations of high-grade prostatic intraepithelial neoplasia (HGPIN) that was found more often in African-American males than in Caucasian-American males. This study's data are partially supported by his results [1] [8]. Fowke [13] observed a lower PSA level among diabetic and obese males and especially among African-American males. This introduces the intriguing possibility that dietary considerations may play an important role in the epidemiology of prostate cancer. Fowke's work also partially supports our study's findings. Since there was no data collected on social/lifestyle behaviors for our study, we cannot exclude a social contribution to the observed findings of different PSA NRI among different genetic/racial groups (African-American vs. Caucasian-American males).

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Studies on Cenospheres as Fillers for PVC Compounds for Applications in Electrical Cables

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Abstract: The presented work evaluated the behavior of Cenospheres as fillers for some compositions using PVC resin. Different compositions containing varying amounts of Cenospheres were made using Brabender Plasticorder. The compositions were cured using a Hot Press Tester and sheets prepared. Test specimens were cut from the sheets for the different tests as per requirements. The TGA curves at multiple heating rates were obtained. The glass transition temperatures (T_g) were measured for representative samples. It was observed that when Cenospheres are added to the PVC compositions, there was a decrease in Smoke Density Rating (SDR) values without much affecting Limiting Oxygen Index (LOI) and thermal stability. Also, the mechanical properties appeared to be sufficiently preserved. The results, on the whole, indicate that Cenospheres hold out promise as possible fillers for PVC compounds for use in electrical cable sheathing applications.

Key Words: Cenospheres, filler, PVC compound, thermogravimetry, glass transition temperature.

INTRODUCTION

For over two decades now, Cenospheres, which are lightweight, inert, hollow spheres, comprised largely of silica and alumina and filled with air and/or gases, have been used in a wide variety of products, including insulations, fire and heat protection devices, sports equipment, and automobile bodies. Due to their special characteristics, they are primarily used as high-quality, lightweight fillers. Their physical properties, particularly low density (due to hollow structure) and low thermal conductivity among others have made Cenospheres popular as fillers for polymer compositions for insulation products in the electrical industry [1].

Cenospheres are finding increasing use as substitutes for traditional fillers in sectors as diverse as ceramics, plastics, construction, recreation, automotive, energy and technology. Their use in preparing a fire-retardant coating for building materials has been reported [2]. Use of Cenospheres as reinforcing fillers in the preparation of HDPE lightweight composites has recently been reported [3].

Cenospheres have been in use for more than twenty years for improving the properties of a variety of finished consumer products. First introduced as an extender for plastic compounds (as they are compatible with plastisols, thermoplastics, latex, polyesters, epoxies, phenolic resins, and urethanes), their compatibility with specialty cements and other building materials, such as coatings and composites, was also quickly identified. Since then, Cenospheres have been used in many fields [2].

Cenospheres are formed as a by-product of coal-burning power plants [4]. When pulverized coal is burned at power plants, fly ash is produced. Cenospheres are the lighter particles that are contained within the fly ash. Typically, they have a particle size range of 10 - 600 microns [5]. The composition of Cenospheres is: SiO_2 - 53%, Al_2O_3 - 38%, CaO - 3.6%, K_2O - 1.5%, Fe_2O_3 - 1.3%, TiO_2 - 1.3%, MgO - 0.7%, P_2O_5 - 0.4%, Na_2O - 0.1%, Mn_2O_3 - 0.1% [5]. The main application of Cenospheres has been as inert fillers.

The objective of the present work is to study the influence of Cenospheres on the thermal behavior and flame-retardant low-smoke (FRLS) and mechanical properties of PVC-based compositions.

EXPERIMENTAL

The common chemicals used for the study are purchased locally (AR grade) and are used without further purification. Composite materials such as PVC and Martinal (high-grade) are also purchased and used as such. Cenospheres are obtained from the local plant of CPRI, Bangalore, India.

The PVC resin was first compounded (mixed) with Cenospheres as filler at filler concentrations of 0, 6, 12, 18 and 24 parts per hundred parts of resin (phr) (Table 1). The compounding was carried out in a Brabender

Plasticorder (PLE 331) at 20 - 30 rpm for about 30 minutes. The torque developed was 4 - 7 N-m. The mixing temperature was 180 °C. After compounding, the compounded polymer-filler mixes were made into sheet specimens using Hot Press Tester (Labtech Co. Ltd., Seoul, Korea) maintained at a temperature of 175 °C and pressure of 90 kg/cm². The sheet specimens obtained were used for determining various properties.

The samples were subjected to thermal studies at various heating rates using Thermogravimetric Analyzer (Perkin Elmer TGA7 Model) and the data are as given in Table 2.

Table 1. The composition of the samples used for study

Substance	Sample (Concentration in phr units)				
	C1	C2	C3	C4	Blank
PVC	100	100	100	100	100
TOTM	36	36	36	36	36
CaCO ₃	16	16	16	16	16
Martinal	28	28	28	28	28
Mg(OH) ₂	04	04	04	04	04
Sb ₂ O ₃	03	03	03	03	03
TBLS	08	08	08	08	08
Calcium Stearate	0.6	0.6	0.6	0.6	0.6
Paraffin wax	0.4	0.4	0.4	0.4	0.4
Cenospheres	06	12	18	24	--

Table 2. TGA data of the samples

β (°C. min ⁻¹)	Sample									
	Blank		C1		C2		C3		C4	
	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
2	270	286	260	273	263	279	265	280	264	280
4	279	291	272	283	273	288	279	292	280	292
8	294	304	289	299	289	300	288	303	293	303
12	300	310	293	304	298	311	296	310	298	312

(a): t (°C) at 5% wt loss (b): t (°C) at 10% wt loss

RESULTS & DISCUSSION

Energetics of the reaction

Using different heating rates, a series of curves (shown in the Figure 1) are recorded, the 5% loss temperatures and 5% loss temperatures shifting to lower values with reduced scan rate.

The temperatures at 5% weight loss, as noted in Table 2, are used to calculate the E value using the following equation [6]-[8]:

$$-\log \beta - 0.457(E/R) (1/T_p) = \text{constant} \text{ or}$$

$$-\log \beta = \text{constant} + (-0.457 E/R) (1 / 10^3). (1/T_p * 10^3).$$

β = heating rate,
 E = energy of activation,
 R = gas constant,
 T_p = peak temperature (here, 5% loss temperature)

This equation is in the form of $y = c + mx$.
 Thus, slope (m) = $(-0.457 E/R) (1 / 10^3)$
 Knowing the slope, the activation energy, E, is calculated.

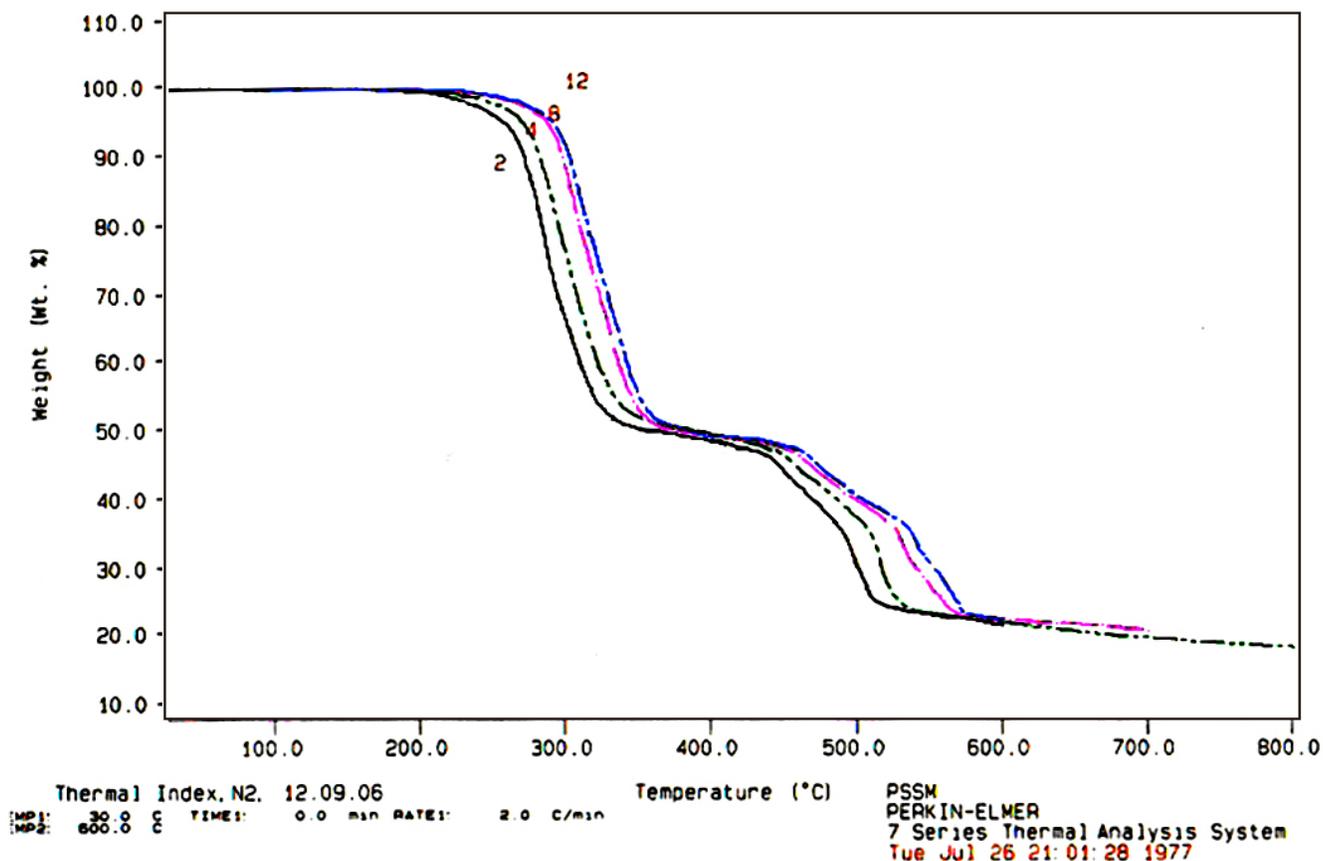


Figure 1. Representative TGA Curves

Evaluation of thermal rating

Reports on the application of thermal analysis for estimation of thermal life of wire enamels from the decomposition reactions are available in literature [7], [9]-[11]. The mathematical expression based on life theory and thermogravimetric theory is given by Toop [7]:

$$\log t_f = (E/2.303 R\theta) + \log [E p(x_i) / \beta R]$$

where $\log p(x_i) = -2.315 - (0.457 E/R T_i)$

E = energy of activation,
 R = gas constant,
 T_f = temperature at which specific change is observed,
 β = heating rate,
 θ = thermal rating and
 t_f = time to condition at temperature θ

Because of the simplicity and reliability, this approach is generally preferred for determining thermal

rating where thermal degradation is the result of simple chemical reaction [12].

The E and the corresponding θ values are given in Table 3.

Table 3. Activation energies and thermal ratings

Sample Name	E (KJ. K ⁻¹ . Mol ⁻¹) (calcd at 5% wt loss)	θ (°C)
C1	129.93	148
C2	133.79	153
C3	147.26	162
C4	162.79	184
Blank	185.48	183

Glass transition temperature studies

The glass transition temperature can be defined as the temperature at which the forces holding the distinct components of an amorphous solid together are overcome by thermally induced motions within the time-scale of the experiment, so that these components become able to undergo large-scale molecular motions on this time-scale, limited mainly by the inherent resistance of each component to such flow [13]. The practical effects of the glass transition on the processing and performance characteristics of polymers are implicit in this definition [14]. The standard T_g value for PVC from literature is 75 - 82 °C [15].

For a few compositions, the T_g values were measured using the thermo mechanical analyzer (TA Instruments: TMA Q400 Model). See Table 4.

Table 4. Glass transition temperatures of the samples

Sample	T _g (°C)
C1	66.55
C3	77.63
Blank	82.13

Effect on properties

The Smoke Density Rating values were measured in accordance with ASTM D 2843 - 99. The lower the SDR value, the better. The Limiting Oxygen Index refers to the minimum amount of oxygen that is required to just

support flaming combustion in a flowing mixture of oxygen and nitrogen and is expressed as volume percent.

The higher the LOI value, the better. The LOI test was performed as per the standard test method ASTM D 2863 - 00. The T.S. values and % elongation-at-break were determined under standard laboratory conditions in accordance with ASTM D 412. See Table 5.

Table 5. FRLS and mechanical properties

Sample	SDR (%)	LOI (%)	Tensile Strength (T.S.) (N/mm ²)	(%) elongation-at-break
C1	68.8	34.4	16.8	139.6
C2	70.6	33.9	16.9	71.0
C3	56.3	33.5	15.0	58.5
C4	56.8	32.9	12.8	53.3
Blank	55.6	32.6	19.0	127.7

CONCLUSION

The possibility of Cenospheres as fillers for PVC-based compositions is explored. In the filler concentration range studied, the 5% and 10% loss temperatures somewhat increase with the filler concentration. The activation energy for decomposition of the compound decreases in presence of Cenospheres, the magnitude of this decrease being maximum at 6 phr of filler and becoming progressively less pronounced at higher filler concentrations. A similar trend is noted for thermal rating values as well.

The T_g value decreases in presence of Cenospheres, again the decrease being maximum at the lowest concentration studied. Lower T_g would mean increased polymer flexibility. The SDR data indicate that the optimal filler concentration may lie in the 18 - 24 phr interval. The LOI values above 30% are acceptable. Decrease in SDR without much affecting LOI values and thermal stability is noteworthy. The mechanical properties seem to be sufficiently preserved, though percentage elongation-at-break needs to be improved.

It appears that there is a critical concentration of the filler content where desired improvements in thermal and FRLS properties become optimal, the advantage being lost if concentration is increased or decreased. More detailed studies are necessary to determine the most appropriate value for Cenospheres concentration for obtaining required levels of change in thermal behavior and other properties of the compositions.

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Notes:

1. TOTM Plasticizer (*Tris (2-Ethylhexyl) Trimellitate*) is a PVC plasticizer for use in applications where low volatility is important. The applications include wire and cable insulation.
2. Martinal, a white powder, is a special grade aluminium hydroxide used as a filler and flame-retardant in polymers, processed at temperatures below 200 °C.
3. TBLS, Tri-Basic Lead Sulfate, is a heat stabilizer for PVC resin. It is popularly used in insulation/sheathing compound for wires and cables.

Computational Studies on the IR and NMR Spectra of 2-Aminophenol

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Abstract: The geometry of 2-aminophenol has been optimized using HF and DFT methods using two basis sets 6-31 G(d) and cc-pVDZ using Gaussian 03™ software. The optimized geometry has been used for calculating the vibrational frequencies and that has been compared with the experimental values. The H¹ and C¹³ NMR have been calculated by the Gauge Independent Atomic Orbitals (GIAO) method and have been found to be in good agreement with experimental values. The relative molecular orbital energies and shapes have been studied.

Key Words: Aminophenol, IR, NMR, GIAO, and Gaussian 03™.

INTRODUCTION

2-Aminophenol is an organic compound with molecular formula C₆H₄(OH)NH₂. It is an amphoteric molecule and a reducing agent useful for the synthesis of dyes and heterocyclic compounds [1]. 2-Aminophenol can be prepared via the reduction of 2-nitrophenol, and it has a rather high melting point due to internal hydrogen bonding (m.p. 174 °C) [2].

A computational study on the enhanced stabilization of aminophenol derivatives by internal hydrogen bonding has been reported [3]. Jose et al. have conducted the density functional theory (DFT) study on the thermodynamic properties of aminophenols [4]. Experimental and theoretical investigation of first hyperpolarizability in aminophenols have been performed and reported by Franzen et al. [5].

In the present study, the vibrational and NMR spectra of the title compound have been calculated and compared with experimental results [10].

COMPUTATIONAL DETAILS

Calculations of the title compound were carried out with Gaussian 03™ software program [6]. The structure of 2-aminophenol has been optimized at two levels of theory using two basis sets. They are RHF/6-31 G (d), RHF/cc-pVDZ, B3LYP/6-31 G(d) and B3LYP/cc-pVDZ [7, 8]. Molecular geometries were fully optimized by Berny's optimization algorithm using redundant internal coordinates. The structural parameters of 2-aminophenol determined by these calculations are listed in Tables 1 and 2 in accordance with the atom numbering scheme in Figure 1.

Tables 1 and 2 compare the calculated bond lengths and angles for 2-aminophenol with those of experimentally available data [10]. Using the optimized geometry, the vibrational frequencies were calculated using the same level of theory and the same basis sets. Harmonic vibrational wavenumbers were calculated using analytic second derivatives to confirm convergence to minima on the potential surface.

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

Atoms	RHF/ 6-31G(d)	RHF/ cc-pVDZ	B3LYP/ 6-31G(d)	B3LYP/ cc-pVDZ
C ₁ - C ₂	1.39	1.39	1.41	1.41
C ₂ - C ₃	1.38	1.39	1.40	1.40
C ₃ - C ₄	1.38	1.39	1.40	1.40
C ₄ - C ₅	1.39	1.39	1.40	1.40
C ₅ - C ₆	1.38	1.38	1.40	1.40
C ₆ - C ₁	1.39	1.39	1.40	1.40
C ₆ - H ₁₅	1.07	1.08	1.09	1.09
C ₅ - H ₁₄	1.08	1.08	1.09	1.09
C ₄ - H ₁₃	1.07	1.08	1.09	1.09
C ₃ - H ₁₀	1.08	1.08	1.09	1.09
C ₂ - H ₁₁	1.43	1.43	1.45	1.45
N ₁₁ - H ₁₂	1.00	1.01	1.02	1.02
N ₁₁ - H ₉	1.00	1.01	1.02	1.02
C ₁ - O ₇	1.34	1.34	1.35	1.35
O ₇ - H ₈	0.95	0.95	0.98	0.98

**Figure 1. Optimized structure of 2- aminophenol**

At the optimized structure (Figure 1) of the examined species, no imaginary wave number modes were obtained, proving that a true minimum on the potential surface was found. The proton NMR and C¹³ NMR of the title compound have been calculated using the gauge independent atomic orbitals (GIAO) method.

Table 2. Bond Angles (°) of 2-aminophenol

Atoms	RHF/ 6-31G(d)	RHF/ cc-pVDZ	B3LYP/ 6-31G(d)	B3LYP/ cc-pVDZ
C ₂ -C ₁ -C ₆	120.2	120.1	120.1	120.0
C ₂ -C ₁ -C ₇	120.5	120.5	119.4	119.2
C ₁ -C ₂ -C ₃	119.2	119.2	119.6	119.7
C ₁ -C ₂ -N ₁₁	116.5	116.5	114.9	114.8
C ₆ -C ₁ -O ₇	119.2	119.4	120.5	120.8
C ₁ -C ₆ -C ₅	119.7	119.8	119.4	119.5
C ₁ -C ₆ -H ₁₅	118.8	118.7	119.0	118.9
C ₁ -O ₇ -H ₈	107.3	106.9	103.9	103.4
C ₃ -C ₂ -N ₁₁	124.2	124.2	125.5	125.5
C ₂ -C ₃ -C ₄	120.9	121.0	120.4	120.4
C ₂ -C ₃ -H ₁₀	119.0	118.9	119.2	119.2
C ₂ -N ₁₁ -H ₉	119.9	111.3	111.4	110.9
C ₂ -N ₁₁ -H ₁₂	119.9	111.3	111.4	110.9
C ₄ -C ₃ -H ₁₀	120.1	120.1	120.4	120.4
C ₃ -C ₄ -C ₅	119.2	119.2	119.5	119.5
C ₃ -C ₄ -H ₁₃	120.3	120.3	120.1	120.2
C ₅ -C ₄ -H ₁₃	120.5	120.5	120.4	120.4
C ₄ -C ₅ -C ₆	120.7	120.7	120.9	120.9
C ₄ -C ₅ -H ₁₄	119.9	120.0	119.8	119.8
C ₆ -C ₅ -H ₁₄	119.4	119.4	119.3	119.3
C ₅ -C ₆ -H ₁₅	121.5	121.5	121.6	121.6
C ₂ -N ₁₁ -H ₁₂	107.8	107.0	107.0	106.0

RESULTS & DISCUSSION

Bond Length

All C-C bond lengths in 2-aminophenol have the same value in both HF and DFT methods. The C-H bond length exhibits slight variations when basis set changes from 6-31G (d) to cc-pVDZ in the Hartree-Fock (HF) method. The same bond length has unaltered values in the DFT method. N-H bond length has the same values in DFT method for both basis sets, whereas in HF method bond length increases by 0.01Å as the basis set changes from

6-31G(d) to cc-pVDZ. C=O bond length has same values in the HF and DFT methods. The C=O bond length increases by 0.01Å as the theory changes from RHF to DFT. O-H bond length has same values in HF and DFT method as basis set varies from 6-31G(d) to cc-pVDZ. O-H bond length increases by 0.03Å as theory changes from RHF to DFT. The bond lengths of 2-amino phenol are given in Table 1.

Bond Angles

In 2-aminophenol the bond angle values obtained by RHF and B3LYP calculations exhibit a slight difference in 6-31G(d) and cc-pVDZ basis sets. But in some cases, like C₁-C₂-N₁₁, C₁-O₇-H₈, C₆-C₁-O₇, C₄-C₅-H₁₄, there is much

difference in bond angles of RHF and B3LYP calculations. The bond angles of 2-amino phenol are given in Table 2.

Vibrational Frequencies

The vibrational frequencies were calculated computationally using two basis sets 6-31G(d) and cc-pVDZ and two theories RHF and B3LYP. The DFT hybrid B3LYP tends to overestimate the fundamental modes, therefore scaling factors have to be used for obtaining a considerably better agreement with

experimental data. Therefore, a scaling factor of 0.9613 and 0.8929 was uniformly applied to the wavenumbers calculated using DFT and HF, as suggested in Gaussian 03™ [9]. The vibrational frequency obtained from the calculation using RHF method was multiplied by a factor 0.8929 and by 0.9613 in DFT method for scaling. The frequencies are then being compared with the experimental spectrum obtained from the SDBS website [10]. The computational and experimental frequencies of 2-aminophenol with their assignments are given in Table 3 [11, 12].

Table 3. Infra Red Vibrational Frequencies(cm⁻¹) and their assignments

Modes of Vibration	RHF/ 6-31G(d)	RHF/ cc-pVDZ	B3LYP/ 6-31G(d)	B3LYP/ cc-pVDZ
N-H assym.stretching	3412	3386	3404	3390
O-H stretching	3378	3620	3584	3393
C-H sym. stretching	3093	3013	3031	3080
C-H assym. stretching	3082	3004	3021	3072
C-H assym. stretching	3064	2985	3003	3054
C-H assym. stretching	3051	2973	2990	3041
N-H bending	1626	1608	1636	1642

H¹ NMR

The proton NMR of the title compound has been calculated using the gauge independent atomic orbitals (GIAO) method [13, 14]. From the isotropic values of the molecule and that of TMS we obtain the δ values of the nmr spectrum. The isotropic value of the protons of TMS

is 31.6198 in the RHF calculation and 31.7825 in B3LYP calculation. The proton-nmr spectrum of 2-aminophenol is taken from the website SDBS [10]. The δ values of 2-aminophenol are given in Table 4.

Table 4. δ values of H¹ NMR of 2-aminophenol

Proton	RHF/ 6-31G(d)	RHF/ cc-pVDZ	B3LYP/ 6-31G(d)	B3LYP/ cc-pVDZ	Exeperimental Value [10]
8	4.5343	5.4842	6.9493	7.4618	8.9
9 & 12	0.0959	1.2265	1.2968	1.9253	4.4
	0.0952	1.2272	1.2977	1.9262	4.4
15	5.9322	7.0589	6.6391	7.0936	6.587
10	5.4016	6.5323	6.2952	6.7283	6.543
13	6.0264	7.1094	6.7479	7.1718	6.649
14	5.670	6.7859	6.4479	6.8969	6.400

The proton-nmr spectrum of 2-aminophenol exhibits six peaks. This indicates six types of protons. The computationally calculated values of protons 8, 9, 12, 10,

15, 13 and 14 agree with the experimental values, but the computationally calculated values of protons 9 and 12 are less than the experimental values in both HF and DFT

methods. The chemical shift values calculated by GIAO method show slight difference from the experimental values, but maintain a general trend of chemical shift.

C¹³ NMR

The isotropic value of the C¹³ of TMS is 195.1196 in the RHF theory and 188.7879 in the theory B3LYP. The C¹³ nmr spectrum of the molecule is taken from the

website SDBS [10]. From the isotropic values of the carbon of 2-aminophenol and the TMS we obtain the δ values of their C¹³ nmr spectrum. The δ values of 2-aminophenol are given in Table 5. The C¹³ spectrum of 2-aminophenol reveals 6 peaks, which indicates 6 different types of carbon atoms. From the computational calculations also we have 6 values which agree with the experimental values.

Table 5. δ values of C¹³NMR of 2-aminophenol

C ¹³ type	RHF/ 6-31G(d)	RHF/ cc-pVDZ	B3LYP/ 6-31G(d)	B3LYP/ cc-pVDZ	Exeperimental Value [10]
1	146.123	149.46	151.84	143.13	143.95
2	114.21	117.84	122.64	111.51	116.48
3	123.22	125.91	123.52	119.58	136.40
4	107.86	110.04	112.48	103.71	114.47
5	122.64	125.12	123.65	118.79	119.47
6	106.04	107.86	109.13	101.53	114.44

HOMO-LUMO energy gaps

The relative energy of the molecular orbitals have been calculated and a graphical representation of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of 2-aminophenol are given in Figures 2(a) and (b).

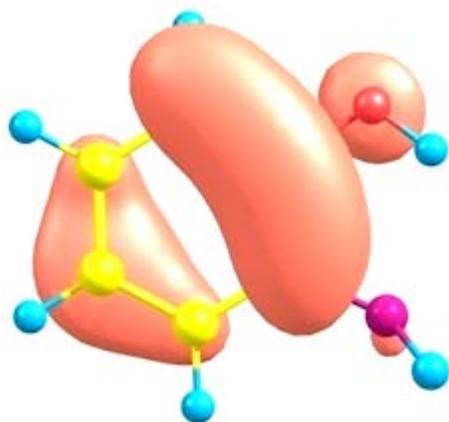


Figure 2(a). HOMO of 2-aminophenol

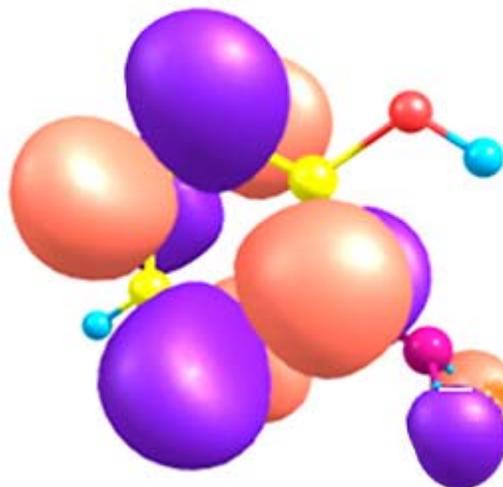


Figure 2(b). LUMO of 2-aminophenol

CONCLUSION

The structure of 2-aminophenol was optimized by the RHF and DFT methods using the basis sets 6-31 G (d) and cc-pVDZ. Using the optimized geometry, the vibrational frequencies, proton NMR and C¹³ NMR of the title compound have been calculated and have been

found to agree well with experimentally reported values. The small differences are due to the fact that experimental values are recorded in the solid state and theoretical calculations belong to the gaseous phase. A plot of the highest occupied molecular orbital (HOMO) and that of the lowest unoccupied molecular orbital (LUMO) is also made.

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The Chemistry Associated with an Exploding Lead-Acid Battery

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Abstract: On April 25, 1997, the Plaintiff was testing an automotive battery with a battery tester when it exploded. He was following his usual practice of ensuring that the battery in a vehicle for sale at his retail store would be sufficiently charged to start the engine. The contact of the inputs from his battery tester to the posts on this battery created a spark that resulted in an explosion. The explosion described by the Plaintiff is indicative of hydrogen gas (H₂) being ignited by available oxygen (O₂) and an ignition source or spark. The force of this explosion was loud enough to cause the Plaintiff's permanent hearing loss.

Key Words: Lead/Acid battery, Hydrogen explosion.

INTRODUCTION

On April 15, 1997, the Plaintiff (of Evans City, PA) went to retrieve an automotive battery (type 24F-50, distributed by MM Battery, Inc.). He placed it on the floor and tested it with a battery tester. As the owner of a retail establishment selling motorized equipment, the Plaintiff generally checked the charge on a battery prior to putting the battery into service. He wanted to ensure that when a customer turned the ignition key, the engine on the purchased vehicle started.

The battery blew up (exploded).

The battery explosion described by the Plaintiff is indicative of hydrogen gas (H₂) being ignited by available oxygen (O₂) [present in ambient air and/or produced with hydrogen by the electrolysis of water (H₂O) in the

battery] and an ignition source or spark. The contact of the battery tester inputs to the actual battery's posts could produce a spark causing hydrogen to explode.

Fundamental Explosion/Flammability Science

Hydrogen is extremely flammable. Two key terms are the lower explosive limit (LEL) and the upper explosive limit (UEL). For hydrogen, the LEL is 4.1% by volume and the UEL is 74.2% by volume. [1] When hydrogen is in this large 70.1% by volume flammability envelope, in the presence of oxygen and an ignition source or spark, it can explode. This scenario is identified in a Material Safety Data Sheet (MSDS) issued by Johnson Controls, the parent company of Interstate Battery. (Table 1)

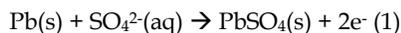
Table 1. Flammability Properties for Lead/Acid Battery (Wetcell)

Flashpoint (for H ₂)	N/A as this is a gas (Test Method: N/A)
Autoignition Temperature (for H ₂)	580°C
Flamable Limits (for H ₂)	LEL - 4.1 UEL - 74.2
Extinguishing Media	Dry chemical, foam, or CO ₂
Special Fire Fighting Procedures	Use positive pressure, self-contained breathing apparatus.
Unusual Fire and Explosion Hazard	Hydrogen and oxygen gases are produced in the cells during normal battery operations, hydrogen is flammable and oxygen supports combustion. These gases enter the air through the vent caps. To avoid the chance of a fire or explosion, keep sparks and other sources of ignition away from the battery.

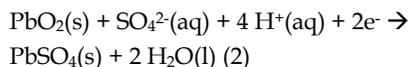
Important Chemical Reactions

The chemical reactions for the lead (Pb) storage battery occur via electron transfer. Important definitions are: an oxidized element has lost electrons and a reduced element has gained electrons.

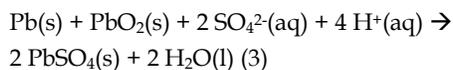
The oxidation reaction for a Pb storage battery is given in equation (1):



The reduction reaction for a Pb storage battery is given in equation (2):



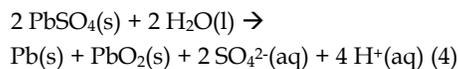
When these chemical reactions are summed, equation (3) results:



The electrochemical potential or voltage from equation (1) is 0.356 Volts, the electrochemical potential or voltage from equation (2) is 1.685 Volts, and the sum in equation (3) is 2.041 Volts. A battery containing six cells as described can produce 6×2.041 Volts or 12.246 Volts. Equation (3) is the discharge reaction in a 12 Volt lead storage battery. [2]

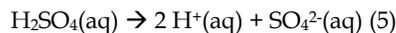
Where: Pb = lead (0) or elemental lead, (s) = solid, SO_4^{2-} = sulfate ion, (aq) = aqueous or water-based solution, PbSO_4 = lead (II) sulfate, e^- = electrons transferred, PbO_2 = lead (IV) oxide, H^+ = hydrogen ion, and (l) = liquid. The chemical reaction in equation (3) as written is favorable since it produces a positive electrode potential or number of Volts. Equation (3) is an example of a galvanic cell chemical reaction.

This also means that, eventually, all of the lead and lead oxide initially present in the battery plates are converted to lead sulfate. At this point, the battery is completely discharged. What makes the lead storage battery unique is that the application of an external electrical source, such as an alternator or generator, reverses the direction in equation (3). The reverse reaction is what happens when a car is running. This is called an electrolytic cell chemical reaction and is shown in equation (4).



Importance of Sulfuric Acid (H_2SO_4) Electrolyte

Sulfuric acid is a very strong acid. This means that it breaks down efficiently to hydrogen ions and sulfate ions as shown in equation (5).



The breakdown of sulfuric acid to its component ions also renders sulfuric acid a strong electrolyte. In the absence of an external source (e.g., alternator or generator), the chemical reaction summarized in equation (3) takes place. The hydrogen ion from the acid reacts with the oxygen from the lead oxide to form water and the sulfate ion from the acid reacts with both lead and lead oxide to form lead sulfate.

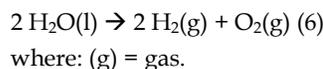
It is very important that the battery does not fully discharge. A fully discharged battery has all of its sulfate present in the lead sulfate. Sulfuric acid must be present for the battery to work properly. This is often tested with a hydrometer or density gauge.

The hydrometer is a syringe with several floating balls. The objective is to draw sulfuric acid into the syringe and to observe how many balls float. The number of floating balls is indicative of the specific gravity of the sulfuric acid.

The specific gravity of water is defined as 1.0 (based on a density of 1.0 gram/milliliter) and the specific gravity of sulfuric acid is about 1.8 (based on a density of 1.8 grams/milliliter). The specific gravity of battery acid is typically in the 1.2 to 1.3 range, indicating that the percent sulfuric acid is about 33%. [1](Table 2)

Battery Charging Can Lead to an Explosion

A charged battery will have water available [on the left side in equation (4)]. The application of electricity from an external source (e.g., alternator or generator) can electrolyze or split water into its component gases hydrogen (H_2) and oxygen (O_2). This chemical reaction is shown in equation (6).



The cells in a battery are designed to vent gases such as hydrogen and oxygen. This system works well until

more gas molecules are produced than can be safely vented.

The resulting pressure build-up can (unfortunately) be relieved by a relatively minor jolt, leading to a spark. In the presence of oxygen and a spark (source of ignition) between posts, the hydrogen can explode.

The force of the explosion is sufficient to blow the top off of the battery case. Pieces of the battery case are discharged like shrapnel. The rapid release of hydrogen produces a sound similar to a bomb explosion. [2,3].

Table 2. Physical and Chemical Properties for Lead/Acid Battery (Wetcell)

Physical State	Battery is solid case with solid and liquid internal components.
Appearance and Odor	
Battery Electrolyte (acid)	Clear to cloudy liquid with slight acidic odor.
Acid saturated lead oxide	Dark reddish-brown to gray solid with slight acidic odor.
pH	
Electrolyte	1.0
Boiling Point	
Lead	1755°C
Electrolyte	110-112°C
Melting Point	
Lead	327°C
Solubility in Water	
Electrolyte	100%
Coefficient Water/Oil	N/A
Specific Gravity	
Electrolyte	1.210-1.300
Vapor Pressure	
Electrolyte	11.7
Vapor Density	
Electrolyte	3.4
Percentile Volatile	Not determined
Evaporation Rate	Not determined

DISCUSSION

It is important to have as complete a history of a battery as possible. A discharged battery's plates will contain deposits of lead sulfate. The formation of lead sulfate is indicated in equation (3). While the application of an external electrical source reverses equation (3), the efficiency of equation (4) is reduced. The charging reaction produces fewer electrolytes (sulfate).

The process of lead sulfate plate depositing is called *sulfation*. [4] The problem with sulfation is that the longer the battery sits (without being in service), the more likely equation (3) will proceed; since it is favorable in the absence of an external source of electricity. The effort to recharge the battery can then lead to the explosive scenario previously described. The author of the carblog reference indicates that a consumer should never purchase a battery if it is more than 6 months old. It is unclear whether anyone knows how much time had elapsed from the time of battery manufacture to April 15, 1997, the date of this incident. Due to the ample available knowledge that battery explosions constitute a known hazard scenario, there should have been a manufacture date stamped on the battery, which would have enabled more accurate and precise record-keeping.

CONCLUDING THOUGHTS

To a high degree of scientific certainty, the explosion on April 15, 1997 resulted from the ignition of hydrogen gas in a battery of type 24F-50. The Plaintiff was following his usual practice of ensuring that the battery in a vehicle for sale at his retail store would be sufficiently charged to start the engine. The contact of the inputs from his battery tester to the posts on this battery created a spark that resulted in an explosion.

The force of this explosion was loud enough to cause the Plaintiff's permanent hearing loss, confirmed in a report by Douglas A. Chen, M.D. [5] The explosion seemingly blew the top off of the battery case; a liquid (most likely battery acid) was released onto the floor. A hole was observed in the battery case, presumably from the escaping hydrogen gas. It is helpful to have photographs of the battery in question, but it would have been more helpful to actually have had the opportunity to inspect the battery in question. This is a chain of custody issue. By not adequately maintaining chain of custody, the defendant(s) is (are) unable to determine where the actual battery is located.

There is a record-keeping issue involving the age of the battery. The sulfate, initially present as sulfuric acid and converted upon discharge to lead sulfate, may not have been recharged to a sufficient concentration of electrolyte.

Battery acid is approximately two-thirds water and one-third sulfuric acid on a specific gravity basis. Maintaining the flow of electrons in a recharged battery can electrolyze water. The conditions required for a

hydrogen explosion are well known and, to a high degree of scientific certainty, are met in this incident.

There are several possible defects that may contribute to a battery explosion. We are unable to confirm how these possible defects could have contributed to the explosion at *the Plaintiff's* location. Without the benefit of examining and testing the battery, we can never know if a possible defect could have contributed to the explosion. To a reasonable degree of scientific certainty, the explosion of the battery would not have occurred in the absence of a defect in the battery and/or negligence by the suppliers/manufacturers of the battery. [6]

The Plaintiff was, to a reasonable degree of certainty, counting on the battery to be fresh and not sulfated. He certainly could not have reasonably foreseen that the contact of the battery tester's inputs to the battery posts would have resulted in the hydrogen explosion.

The hydrogen concentration had increased to a level above the battery's pressure venting capacity. Available oxygen and an ignition source (spark) would suffice to create the bomb-like explosion noted by the Plaintiff.

One of the Defendants (owner and president of MM Battery, Inc.) in his Deposition [7] referred to this explosion as a "staged event." The explanations provided in this report indicate, to a high degree of scientific certainty, that a fully charged battery and the subsequent electrolysis of water will produce hydrogen quantities that fall within the 4.1% to 74.2% by volume flammability envelope.

The finding of a hydrogen explosion is a well-established scenario. The Defendant(s) should have identified a possible defect in the now-exploded battery via the age of the battery from the date of manufacture through the date of the explosion.

If there was any doubt about the age of the battery and the potential for an explosion upon charging, the battery should have been removed from the Plaintiff's inventory during "normal" pick-up and delivery "rounds" by one of the Defendant's personnel.

There wasn't any way for the Plaintiff to know that hydrogen was building up inside the battery. As a result, a preventable incident occurred and a man sustained permanent hearing loss. While the Defendant is not a scientist, he should have been aware of the explosion risk associated with hydrogen generation in lead storage batteries and he should have acted in accordance with that knowledge. He failed in his duty to notify the Plaintiff of the explosion risk and he also failed to

mitigate this risk through timely removal of the battery from the Plaintiff's inventory. An event like this one did not need to be staged.

This case was settled favorably for the Plaintiff.

ACKNOWLEDGEMENT

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Challenges for Chemical Education: Engaging with Green Chemistry and Environmental Sustainability

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Abstract: Although sustainability is an abstract concept with many interpretations and ramifications and the metrics thereof are yet to be rationalized, it is becoming increasingly evident that the rapidly advancing degradation of the natural environment, coupled with excessive consumption of natural resources, is threatening the sustainability of humanity.

This paper explores how chemistry and the chemical enterprise are progressing towards a sustainable chemistry philosophy and practice and it also explores the role which sustainable chemistry and, in particular, sustainable chemistry education have in engaging with the wider philosophy of environmental sustainability. It is relevant to note that although chemistry has recently been cited as being of importance in enabling transitions to environmental sustainability, as to how these can be achieved by strategically-structured and targeted chemical education programs has not been debated in the literature to date; hence this paper offers some pioneering suggestions in this context.

Key Words: Green chemistry, sustainability, chemical education, chemistry education.

INTRODUCTION

Although sustainability is a contemporary concept of immense significance, it is an intangible abstract concept, a concise definition of which remains elusive. It essentially represents a paradigm shift in understanding the relationship between humanity and the environment and recognition that the present excessive demands of humanity on natural resources, coupled with excessive waste and pollution generation by human beings, constitute an unsustainable, stressed and threatened global environment. This has been brought into sharp focus over the past decade by increasing awareness of the consequences of global warming, believed to be due to increasing levels of greenhouse gases in the atmosphere derived from anthropogenic sources. However, although there are a number of global initiatives to reduce greenhouse gas emissions, there are by comparison limited initiatives underway to seriously address environmental sustainability. This may be due to a lack of a comprehensive theoretical framework for

understanding 'sustainable development' and its multi-disciplinary complexities, since the range of published definitions is vague and it remains a contested topic, fraught with contradictions [1].

The many definitions of sustainable development are largely benchmarked to the World Commission on Environment and Development (WCED) definition [2]: 'maintaining the needs of the present generation without compromising the ability of future generations to meet their needs'. There is much debate on 'what are the needs (and scale) of present generations' in the context of the 'haves' and 'have-nots' disparity and 'what are the needs (demands) of future generations', as the global population continues to escalate and the 'haves and have-nots' divide widens. Furthermore, there is much concurrent debate on how simultaneous harmonization of the needs of humanity with the needs of the environment can be achieved. It is intuitively obvious that 'sustainable development', and hence 'environmental sustainability', are progressive objectives and that metrics of these concepts need to be established in conjunction with tangible and workable definitions.

In this context, Hill and Mustafa [3] have argued that sustainable development is essentially consistent with sustainable natural resource management (SNRM) that embraces several dimensions including 'social', 'political', 'scientific', 'technological', 'economic', 'research, innovation and development' and, most importantly, 'education', which collectively form a concept framework, as shown in Fig. 1.

It emerges that since environmental degradation is largely due to the excessive needs of humanity, environmental sustainability is the responsibility of humanity, and thus sustainability education is of paramount importance [4]. Science education and chemical education in particular are crucial components of sustainability education [5] since the former informs and enables the climate change debate and the latter emphasizes how green chemistry and green chemical industries enhance the transition to environmental sustainability. Also, the UN declaration of 2011 as the International Year of Chemistry (IYC) [6] established a roadmap for the future of chemistry (and hence chemical education) by defining a series of 'themes', all of which relate to addressing the most critical problems facing humanity in the 21st century, as summarized in Fig. 2, of which 'environmental sustainability' is the primary theme.

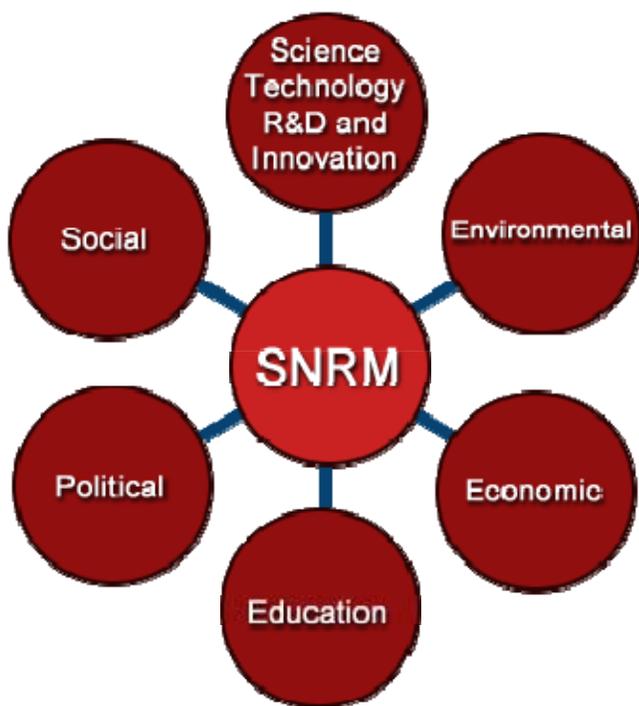


Figure 1. Concept framework of SNRM



Figure 2. The IYC 'themes'

The IYC themes offer significant challenges for chemistry and hence for chemical education. It is evident that the rapid emergence and development of 'green chemistry' over the last decade has dramatically enhanced a positive (social) image of chemistry and the IYC themes not only continue this trend but also enable a transition towards sustainable chemistry. However, although it appears that green chemistry and sustainable chemistry are synonymous terms, Tundo [7] has suggested that there is a subtle difference in that sustainable chemistry has chemical processing connotations involving more energy efficient, less polluting chemical manufacturing processes which may generate greater profit margins, whereas green chemistry is more focused on 'greening' chemical reactions to produce products which are environmentally benign, but are not necessarily of industrial interest or significance. This differentiation of these terms widens the scope and the challenges for chemical education since the sustainability of the chemical enterprise has to be addressed using sustainable chemistry as the major driver.

The aim of this paper is to identify the challenges for chemical education in enabling the transition of the chemical enterprise towards sustainability. Such a paper

is timely since although environmental sustainability is a contemporary concept of immense significance and there are widespread calls to embed sustainability into tertiary curricula, courses emphasizing sustainability are currently limited and tend to be in non-science areas, with emphasis on economic, social and political sustainability [8]. Furthermore, the challenges for science education and chemical education in particular are formidable since embedding sustainability into chemical education involves identification of the major chemical concepts that relate to sustainability of the chemical enterprise and hence to environmental sustainability; consequently, a paradigm shift in chemical education pedagogy is envisaged.

INFLUENCE OF GREEN CHEMISTRY

As for 'sustainable development', there have been many definitions of 'green chemistry' which relate to the synthesis of environmentally benign molecules and materials, new chemical (energy efficient) processes and new quality control technologies which reduce effluent and waste [9]. These definitions imply that 'green chemistry' and 'sustainable chemistry' are closely inter-related since the vision of green chemistry is holistically aligned with environmental sustainability. With its direct linkages to other major science disciplines, such as the life sciences, materials science, chemical engineering and environmental science, and its indirect linkages to economics and ethics, together with its principal aim to provide benefits to society, green chemistry is rapidly changing the negative public image of chemistry which has prevailed for decades.

The guiding principles of green chemistry, as shown in Fig.3, offer significant challenges for chemical education, since the mindset of students and researchers has to be changed to think and learn in terms of environmental sustainability rather than in terms of 'pure chemical sustainability', and the latter has to be addressed with reference to terms and concepts such as 'atom economy', 'waste reduction', 'toxic versus benign', 'energy efficiency', 'renewable feed-stocks', 'quality control' and 'safety management'. Traditionally these terms and concepts have not been included in chemistry education [10]. If the 'benign by design' philosophy is introduced progressively into chemical education pedagogy at all levels, this will greatly assist in the production of trained personnel for sustaining the chemical enterprise.

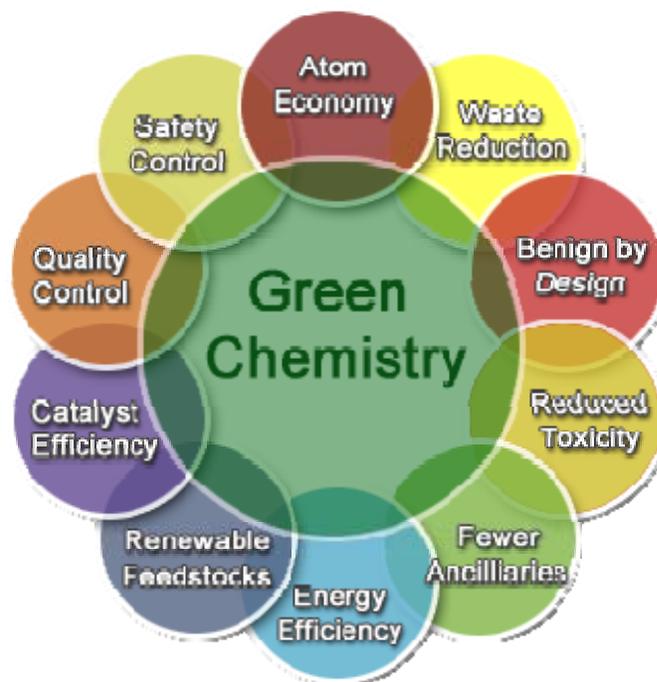


Figure 3. Principles of Green Chemistry.

SUSTAINING THE CHEMICAL ENTERPRISE

The chemical enterprise is an amorphous concept composed of a myriad of interconnected parts, each of which has to be considered from a sustainability viewpoint, as shown in Fig.4.

Green chemistry strategies target each stage of the lifecycle of a chemical product to continuously enhance its biological and ecological safety, reduce energy consumption associated with its production and eliminate the co-production of waste. Hence, green chemistry offers substantial reductions to the environmental footprint of chemical processes, improvements in the health and safety of those exposed to the manufacture of chemicals and safe handling of hazardous materials [11] leading to greater public recognition of the beneficial significance of the chemical enterprise.

Poliakoff and Licence [12] have argued that although the chemical industry has over recent decades made significant efficiency improvements to the manufacture of 'essential chemicals', finite natural resources will inevitably limit sufficient quantities of essential chemicals to meet the demand of a rapidly increasing global population. Thus, the chemical industry is currently not

sustainable, as shown by 'E-factors' greater than zero. (The E-factor for a chemical process is the ratio of the amount of waste generated compared to the amount of product produced, and thus it is a measure of the 'greenness' of the process.) Since natural resources feed-stocks limit chemical industry E-factors, a sustainable chemical industry depends on achieving E-factors approaching zero by maximizing product yield and minimizing feed-stock input.



Figure 4. Structure of the Chemical Enterprise.

The E-factor metric presents further challenges for chemical education, since most chemical manufacturing processes produce by-products which are typically regarded as waste materials. E-factors can be reduced by recycling and/or reusing such by-products, but this has to be economically viable. Thus, chemical education has to address not only the chemical reactions involved in an industrial manufacturing process, but also reveal the complexities and intricacies of 'stoichiometric economics', which is the basis of the so-called 'measurement science'.

Greening the chemical industry is obviously a progressive exercise. Ananda et al. [13] have proposed a roadmap to a green (sustainable) chemical industry, based on a set of interactive principles broadly termed 'economic', 'social', 'technological', 'cultural', 'political' and 'environmental', which collectively form the 'drivers

of change' in chemical industry policy planning and incorporate green chemical technology. This roadmap has considerable potential for moving the chemical enterprise towards sustainability, and by inference, reducing E-factors.

A definitive and comprehensive study by Grassian and Meyer [14] has proposed that education and basic research in renewable energy resources, green chemistry and the environment play pivotal roles in the quest for sustainability, and have argued that a sustainable future calls for a carbon-neutral economy based on renewable (non-fossil) energy supplies and an enhanced understanding of the environmental impacts of increasing human consumption of natural resources. Thus, to address chemistry sustainability, chemical education has to be multi-disciplinary, encompassing not only new chemical concepts, but also the myriad of connections between these concepts and the chemical enterprise in order to reveal how the latter is linked to environmental sustainability. In view of the complexity and diversity of these connections, the challenges for chemical education are formidable.

SUSTAINABLE CHEMISTRY EDUCATION

The accepted status of chemistry as the central (enabling) science has progressively been augmented by a rich research history dating back over at least a half century. Traditionally, chemical education has been considered as a combination of three major dimensions, as shown in Fig.5.

Over the last two decades, there have been some notable developments of these dimensions. With respect to curriculum design, Atkins [15] has proposed that 'chemistry is based on just a few simple ideas', which has not only led to finalizing the constitution of the long-debated 'core of chemistry knowledge' [16], but also to the re-evaluation of the content and context of secondary and tertiary chemistry courses in conjunction with more effective learning strategies. Also, Fensham [17] has proposed that 'science has social responsibilities', which has been interpreted by Hill [18] from a chemistry perspective. Furthermore, with respect to addressing a new vision for tertiary basic chemistry courses, Hill [19] has designed a curriculum framework for these courses which embraces the proposals of Atkins [15] and Fensham [17] and which leads to defined learning outcomes. However, it should be noted that "chemistry knowledge" alone is not sufficient to resolve issues such

as toxic waste disposal, climate change consequences and nuclear energy concerns [20]. Chemical education is critical as “education is an essential element of all aspects of a transition to sustainability” [21].

With respect to teaching methodologies, Bedgood [22] has asked, ‘Why are we still teaching (Chemistry) the way we were in the 1980’s?’ He has been involved in a pioneering project aimed at enhancing science learning and teaching in Australian universities with a focus on first year science programs, which are characterised by large numbers of student participants, didactic teaching methods and multi-cultural learning environments. This program is piloting student-centred teaching methodologies in conjunction with student group learning strategies, fostering knowledge accumulation and enquiring minds. Further, Reid [23] has asked, ‘What do we know about how students learn in the sciences and how can we make our teaching match this to maximize performance?’ He has proposed new strategies for correlating teaching methods more directly with learning rates and learning outcomes and how well core concepts can be linked to form a meaningful outcome. But such well-intentioned ideas for learning chemistry are often met with challenges in the wake of more computer-oriented online approaches to teaching chemistry [24].

With respect to learning strategies and objectives, Mahaffy [25] has shown that there is an integral connection between chemical reactivity and human activity, and proposed that the traditional three levels of learning chemistry - ‘macroscopic’, ‘symbolic’ and ‘molecular’ - be extended to a fourth dimension ‘human element’. This proposal is consistent with the earlier proposal of Fensham [17] and also, most significantly, links chemical education to the IYC themes and their promulgation.

However, it is timely to examine whether education in chemistry as it is currently practiced is sufficiently equipped to address the IYC themes and hence the sustainability paradigm. In this context, Hill and Mustafa [3] have proposed that the most significant manifestation of ‘sustainability’ is ‘sustainable natural resource management’ (SNRM), which correlates a sustainable environment with human endeavour. Furthermore, SNRM has many dimensions, a major one of which is ‘scientific’. Chemistry, and in particular, environmental chemistry is obviously a central component of the scientific dimension of SNRM, which, when combined with the ‘social’, ‘economic’, ‘technological’ and ‘research, innovation and development’, dimensions becomes a

major driver of SNRM. Further, Hill and Warren [26] have shown that the sustainability theme can be embedded into the curriculum framework which Hill [19] has proposed for the tertiary foundation chemistry course.

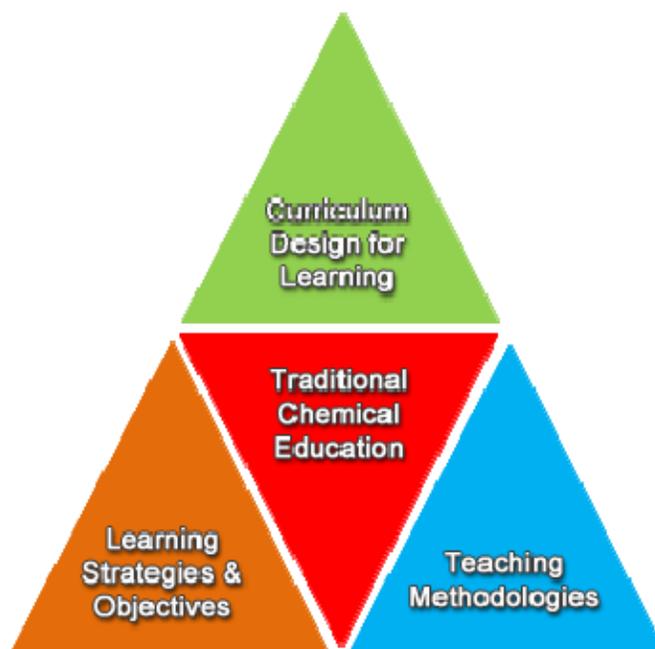


Figure 5. Structure of traditional Chemical Education.

Mahaffy [27] has campaigned for the integration of environmental sustainability into chemical education consistent with chemistry being an integral influence on the global future of humanity in terms of secure energy supplies, and the consequences of climate change and of diminishing food and fresh water resources. Similarly, Nocera [28] has proposed that ‘carbon-neutral energy resources’ and ‘efficient energy use’ are the most pressing issues facing planet Earth in the 21st century, and that chemistry and chemical education have pivotal roles to play in addressing these challenges, since ‘the chemical bond is the currency of energy’. Further, Fanzo, Remans and Sanchez [29] have argued that ‘chemistry’ is the backbone of food and nutrition security and that hunger is one of the greatest threats to the sustainability of humanity; thus, chemical education has a pivotal role to play in revealing how food security is directly related to sustainable agriculture and aquaculture. Also, the cultural dimension of chemical education must not be overlooked. Kumar [30] makes a compelling case in

Wilderer et al.'s [31] collection of essays 'Global sustainability: The importance of local cultures' - that local cultures markedly influence transitions towards sustainability, and in this context, sustainable chemical education plays a most significant role.

Thus, it appears that a new vision for chemical education is required, encompassing many new dimensions, as suggested in Fig.6, if it is to address the challenges inherent in engaging environmental sustainability.

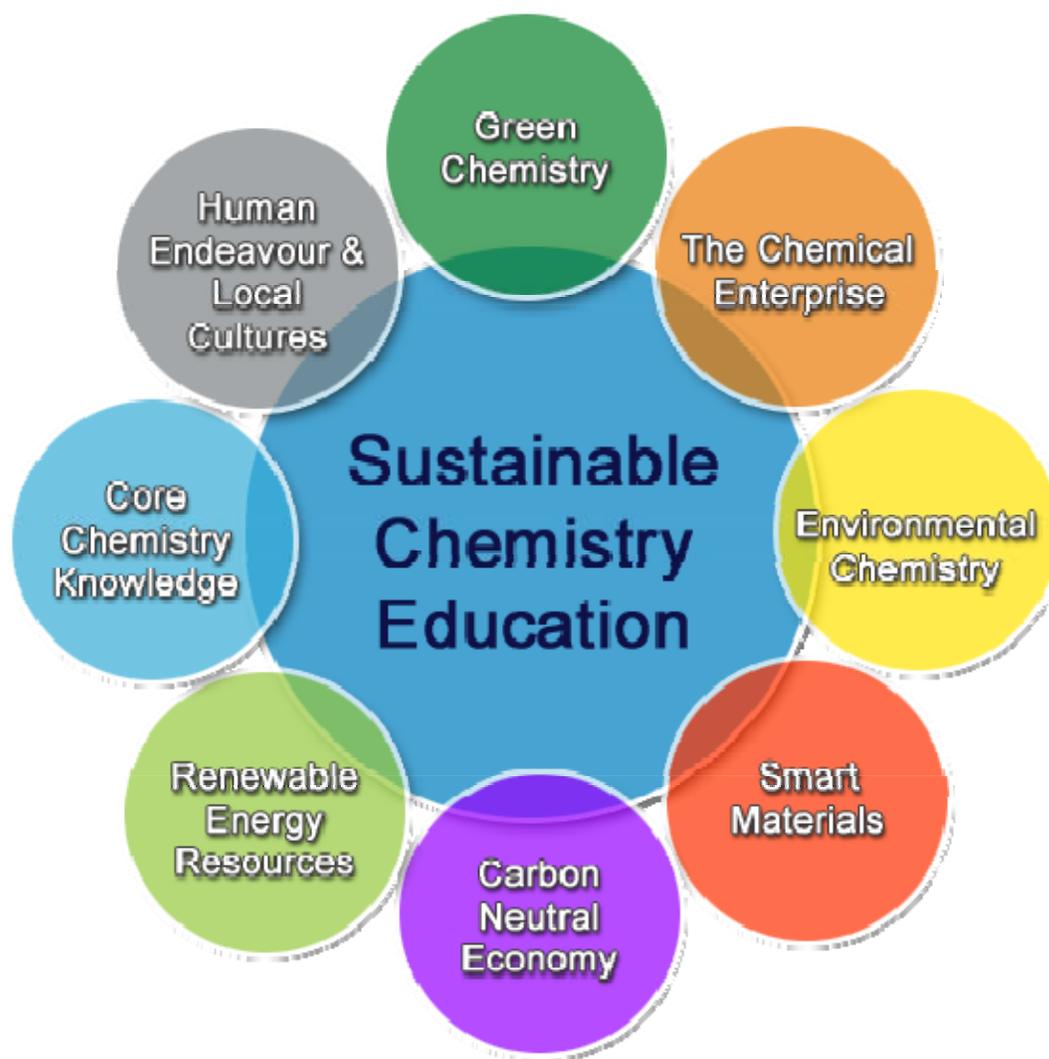


Figure 6. Dimensions of Sustainable Chemistry Education.

It is evident that sustainable chemistry education involves different methodologies in teaching fundamental chemistry concepts, whereby new terms and new philosophies are introduced. For example, chemical systems involving multiple chemical reactions need to be discussed in addition to examples of different types of single chemical reactions. Furthermore, chemical reactions need to be discussed in terms of 'atom economy' to illustrate the principle of chemical efficiency.

The core topic of thermodynamics needs to be discussed in terms of energy efficiency of chemical processing and manufacture in addition to energetics and spontaneity of chemical reactions. The core topic of kinetics needs to be discussed in terms of selective catalysts, which maximise product yield by decreasing by-product formation. Such discussions interlink core chemistry knowledge with green chemistry principles and form the foundation on which sustainability of the chemical enterprise is

progressed. As a consequence of such inclusions in chemistry curricula, a suite of new terms emerges such as 'feedstock' replacing 'reactant' and 'E-factor', which is the ratio of the mass of 'waste' compared to that of 'product'. The latter is a simple empirical measure of the 'greenness' of a chemical process and hence its sustainability [12].

Similarly, a discussion of 'renewable energy resources' must be prefaced by a discussion of present primary energy resources, namely fossil fuels, in order to address climate change; arguing that these have to be replaced progressively by clean, green, renewable energy resources, such as solar energy. However, the dilemma of this challenge must also be discussed, namely that all known commercially viable renewable energy resources combined are unlikely to meet global energy demands over the next two decades, and hence fossil fuels are most likely to dominate the global energy market for the foreseeable future. This leads to a discussion of clean coal technology and the contemporary concept of a 'carbon-neutral economy'; both are outside the scope of contemporary chemical education, but are essential inclusions in the quest to extend chemical education to engage with sustainability.

Sustainable chemistry also embraces environmental chemistry, whereby fundamental chemical concepts such as the p-block elements - C, N, O, P and S - are termed 'nutrients' and 'salts' are responsible for 'salinity' of soils and surface waters. Pollutants disturb the natural nutrient cycles and salinity reduces soil and freshwater quality with overall degradation of the natural environment. Similarly, increasing acidity of rivers and oceans disturbs aquatic ecosystems [32] and is a direct consequence of increased levels of carbon dioxide in the atmosphere. Furthermore, increasing toxicity of the environment due to chemical waste in soils, air and surface waters is of greatest concern in terms of addressing environmental sustainability.

Sustainable chemistry intuitively involves engagement with the generation of new smart materials and hence with nanotechnology and its envisaged linkages to global clean energy requirements. The rapidly advancing nano-chemistry is perhaps the most significant exemplar of leading edge sustainable chemistry with its focus on the development of new smart materials for energy storage, production and conversion, for advancing agricultural productivity, water purification and desalination food processing, building construction, health monitoring and for pest control. Of these applications, rapid advancement in the production of

photo-voltaic devices and carbon nano-tube solar cells [33] is accelerating the solar energy industry. Similarly, the development of nano-catalysts for hydrogen production, coupled with carbon nano-tube hydrogen storage systems are promoting hydrogen as a viable, alternative clean energy resource [26, 33]. Thus, sustainable chemistry via nano-chemistry directly engages with environmental sustainability by providing processes and products which directly benefit humanity without harming the environment.

However, all of these dimensions of sustainable chemistry present formidable challenges for chemical education, both in terms of future direction and scope. It is clear that 'sustainable chemistry' cannot be considered as a single academic course, but requires the concept and philosophy of sustainability to be progressively introduced into all chemistry courses, both at the secondary and post-secondary/tertiary levels. Furthermore, the complexity of sustainable chemistry and the diversity attached to its implementation demand flexible teaching methodologies, such as Problem Based Learning supported with multimedia anchors [34], leading to carefully designed learning outcomes (research into which is, at best, embryonic).

In conclusion, since 'sustainability' and 'sustainable development' are complex, multi-dimensional' concepts, sustainable chemistry is also multi-dimensional in character, embracing disciplines not normally aligned with it such as economics, accounting, humanities, sociology, cultural studies, health sciences, food science and agricultural science. Hence, successful engagement of chemical education with sustainability involves developing partnerships with these disciplines to form a united educational platform for moving towards environmental sustainability. Fundamentally, sustainable chemistry education is a powerful philosophy integrating 'chemistry' into the 'sustainable future' syndrome and offers challenging educational opportunities to achieve identifiable sustainable outcomes.

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Chemical Education: Reflections of a Middle School Teacher

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Abstract: From the explosion of idea, formulas, and provisions associated with a practical approach to learning chemistry, chemistry education has become an integral part of science education. Direct uses of chemistry education and instructional practices of chemistry education are trickling down to the middle school science level in hopes to further situate adolescent understanding of chemistry. In a study designed to ascertain the chemistry understanding of middle school science students, more than 60 percent of the students demonstrated understanding of chemistry. The survey “A Survey of Scientific Understandings” included basic chemistry questions such as “What happens to the mass of an iron bar when it rusts, assuming that none of the rust flakes off? [1]” Some of the implications of this survey are that students at the middle school level are more aware of the role of chemistry in the real world around them. Chemistry connections to other content areas could be a part of a win-win situation towards developing interests in the sciences among middle school students.

Key Words: Chemical Education, Middle School.

CHEMICAL EDUCATION

Chemical education involves the teaching and learning of chemistry at all levels of education. In early days the focus of chemical education was to train chemical technicians and chemical scientists for industries, and chemical compounders for pharmacies. Since the later half of twentieth century chemical education has become a vibrant component of science education curriculum and reform not only in the United States, but also in other developed and many developing nations around the world [2, 17]. In the school science curriculum the emphasis of chemical education often ranges from traditional academic preparation in chemistry to chemistry in everyday life [3]. At the K-12 education in the US when junior high schools were phased out in the 1980's, chemical education received a place in the middle school curricula [4].

MIDDLE SCHOOL SCIENCE ENDEAVOR

Middle school science education is a multi-faceted approach to integrate several general science disciplines

with the ultimate intention of instructing students in the basics of science [4, 5]. With this approach, many middle school science teachers have obtained knowledge of many fields of science, including chemistry.

Chemistry concepts that are taught include properties of matter, changes in matter, energy and matter transformation, forms of energy, periodicity of elements, and chemical interactions in matter [6]. These chemistry concepts are taught to enrich students' understanding of the natural world. This instruction also serves the purpose of preparing students who are skilled in performing calculations and would serve the public interest if they pursued science careers.

TEACHING CHEMISTRY TO MIDDLE SCHOOL STUDENTS

Students at the middle school age are in a period of adolescence. As a middle school educator of eight years, it seems to me that the one thing that all middle school students do is test their limits. The nature of learning for most middle school students is based on prior experiences such as learning through elementary school

and home environment [7]. Chemistry to most middle school students, equates to blowing stuff up and seeing reactions. This tends to excite them about something they can usually grasp quite quickly.

Why is chemistry more interesting to middle school students?

As stated previously, students like to see science in action, that is, they appreciate and gain interest in seeing something reacting. Therefore, chemistry is quite often the most interesting subject for middle school students to learn [8]. Chemistry is one of the few subjects that require students to learn through listening, and in most cases

students can learn through seeing interactions between matters by engaging in hands-on chemistry laboratory activities.

The fact that the students in my class are more interested in watching chemicals interact, such as bubbling over of acid-base reactions, fingerprint oil from human hands appearing after super glue is heated, and learning about why certain metals are reactive with water just demonstrates that they want to actively learn about chemistry in middle school. See Table 1 for results of students' chemistry understanding for studied population. The active role that middle school students play in the science classroom may be related to their scientific understanding of chemistry concepts [1, 9].

Table 1. Chemistry Understanding of Middle School Students

Question	Percentage of Students Correct
1. What happens to the weight of an iron bar when it rusts, assuming nothing flakes off?	56
2. After dissolved gases are removed from pure water, the water is heated in a pot to boiling. What gas is inside the bubbles that form as the water boils?	52
3. One pound of salt is added to twenty pounds of water. After all the salt has dissolved, what will be the mass of resulting salt/water mixture?	73
4. The density of mercury at 20 °C is 13.5 gm/cc. Representing density with the letter d, mass with the letter m and volume with the letter v, within the rectangle write an equation with which one can calculate the volume of 27 gm of mercury at 20 °C.	72

Note: Statistical data is derived from reference [1], which consisted of statistical analyses conducted on the scores of 106 students earned on the chemistry component, four questions, of a scientific understanding survey [9]. This survey was approved via the local IRB for FAU and the local school county.

Importance of Learning Chemistry Concepts

The importance of learning chemistry at the middle school level is documented by several research studies. Sheridan et al. [10] from a research study performed with middle school students, identified the importance as a foundation for students to pursue science careers that utilize chemical knowledge. Pharr [11] also supports this idea through research performed via web-based tutorials that enrich middle school student learning about chemistry. Pharr (2009) found that, even though the attitude toward science did not improve with the use of web-based tutorials, content knowledge did improve significantly. Other researchers support this concept as well. In fact, students who learn chemistry, along with other science subjects, at an earlier age on average,

pursue high school science courses, and become scientists upon completing their collegiate studies [10, 12, 13].

Innovative science endeavors have increased the output of students that pursue science careers, as a result, innovative science is the direction that science education is taking in order to remediate, educate, and evaluate student interest in science careers. While middle school students do not have to choose a career path, middle school students in most states have to decide on a high school program that they will follow to in order to pursue a career track. Nanoscience education is an innovative science program that middle school students have experienced in some states. This form of nanoscience education, also known as nanotechnology is focused on the various applications of how nano-sized particles can be utilized to teach students scientific concepts [14].

A middle school teacher's reflection on chemical education

Chemistry is only one of the many subjects that middle school students learn. Middle school students in my county have units dedicated to learn Earth sciences, Life sciences, and physical sciences for them to be considered sufficiently proficient to enter high school [6]. Students are also required to earn a minimum score of 325 out of 500 on the state standardized exam for science. This requirement is undermining the high standards that education should be setting for students that are expected to enter the workforce completely prepared.

The problem for students gets complicated when an unprepared science teacher instructs them in a subject in which they have little background knowledge. Content knowledge is necessary for developing scientific understanding in students [15]. Without this essential background, science, especially the middle school general sciences, is not being communicated to students in a manner in which they will gain interest. It is this very concept that researchers believe effective teaching comes from years of practice. As a teacher who is responsible for educating students in the chemical and physical sciences, one should not blame the subject for a lack of student interest and more appropriately blame the need for quality educators.

SUMMARY & RECOMMENDATIONS

First, students at the middle school level need more than just the topical treatment chemistry taught. Chemistry should be made more interesting to students than other subjects [16]. Therefore, it is strongly recommended that middle school students learn chemistry by actively doing chemistry. As a result, we would expect to find more students pursuing careers in science than we have at the current time. Second, state officials should look into the prospect of chemical education as a means for increasing student interest in middle school science. Middle school students are fascinated with things that are visible and can engage them, so why not give them some extrinsic motivation that serves a dual purpose? They learn while doing chemistry, and at the same time they obtain a better understanding and their connection to other science subjects [17, 18]. The end result is a science-minded generation of individuals who can meet the demands of

an increasingly science and technology dominated workforce and enjoy the benefits of chemistry in their everyday life.

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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-Editors:** David M. Manuta and Kurt Winkelmann

SCIENCE & TECHNOLOGY COMMUNICATION: NANOTECHNOLOGY – A POSITIVE ISSUE

S. Baroni and B. Holmes

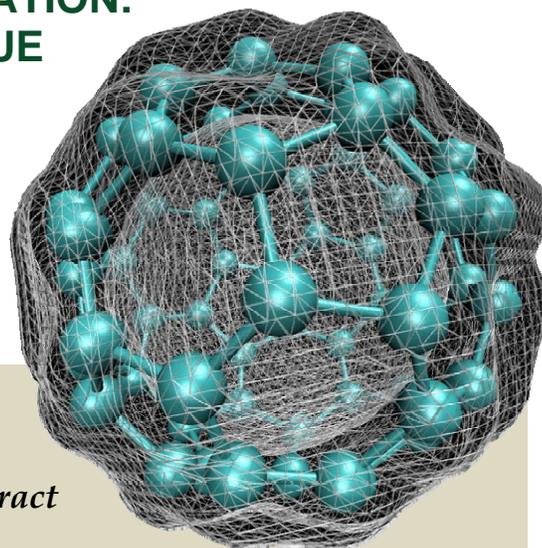
NIU, Washington, DC

Science, Technology and the Public

Science Daily, in *Nanoparticles Against Aging*, examines the development of an intelligent nanodevice consisting of mesoporous nanoparticles with a galactooligosaccharide surface that selectively opens in degenerative phase or senescent cells [1]. Ramón Máñez effectively communicated this scientific breakthrough to the public, reporting that the discovery demonstrates how selected chemicals can be released in some cells and not in others. The use of an intelligent nanodevice to deliver chemicals enables new discoveries and reveals some of the unique capabilities of this technology including treatment delivery systems. Scientists continue to make great strides in applied nanotechnology (e.g., carbon nanotubes [2]) research with breakthroughs in medical delivery, materials technology, manufacturing developments and processing.

Scientists may easily grasp the positive attributes of this nanodevice discovery; however, the public, in general, might not be able to decrypt the scientific jargon or the full potential of its use, often leaving them confounded and/or apprehensive about the ramifications of such a discovery.

Public references to nanotechnology elicit a mixed response. For instance, some environmentalist groups condemn nanotechnology as “nanocontamination.” In 2010, the National



Abstract

Improving science and technology communication between the public and the scientific community is critical. Scientific success and development rest upon the premise of an informed public. Rapid development in fields like nanotechnology, for example, necessitates that the scientific and higher education community reconsider more effective ways to both communicate with and to educate the public sector to facilitate a more positive response and enable new discoveries.

Key Words

Communication, nanotechnology, informed public, science and technology, education

Science Foundation conducted a public assessment of the benefits and harms of nanotechnology study and found that only 37% of adults polled believed that the benefits of nanotechnology will outweigh the harmful results, 43% answered that they simply did not know and 11% responded that the harmful results outweigh the benefits.

Communication is Key

Improving science and technology education and communication between the public and the scientific community is critical in a rapidly changing global environment. Effective communication may create new research opportunities, facilitate broader education initiatives, and foster a more encouraging view of new discoveries. By doing so, one might contextualize nanotechnology research in an easy to understand way that actually affects the connotation.

Scientific success and development rest upon the premise of an informed public. Rapid science and technology development necessitates that we, in the scientific and higher education community, reconsider the best and most effective ways to both communicate with and to educate the public sector on science and technology.



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IMAGE ACKNOWLEDGMENT: The image is a Bucky ball with isosurface of ground state electron density, calculated with DFT and the CPMD code. It was created by Isaac Tamblyn (<http://myweb.dal.ca/itamblyn/site/Home.html>). It is used under the GNU Free Documentation License.



Best of the Brain (1st Edition) from Scientific American

Reviewed by Margot Hall

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This is a nice little neuroscience book with a futuristic twist. Fully one third of the book is directed at future uses and treatments of the brain. The book has 31 contributing authors, 270 pages, numerous figures and color pictures, a table of contents, 21 chapters divided into three sections, and an index. Each chapter has a short bibliography for further reading on the topic and a very short overview of the chapter's author(s). One appendix includes a list of other books and periodicals on this topic and a list of free resources for teachers who wish to introduce the subject of the brain into their class curriculum.

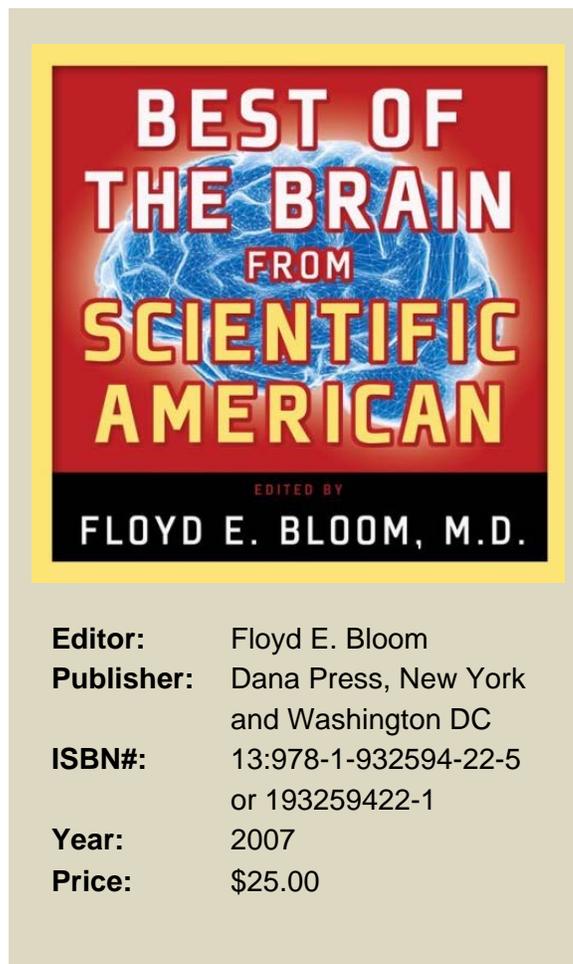
Section 1 (Mind) includes six chapters: Unleashing Creativity, Stimulating the Brain, Freud Returns, The Neurobiology of the Self, How the Brain Creates the Mind, and The New Science of Mind.

Section 2 (Matter) has nine chapters including: Vision: A Window on Consciousness, Rethinking the 'Lesser Brain', Sign Language in the Brain, Hunting for Answers, Brain-Repair Yourself, Diagnosing Disorders, The Addicted Brain, Decoding Schizophrenia, and Turning Off Depression.

Section 3 (Tomorrow's Brain) includes 6 chapters: Treating Depression-Pills or Talk, The Coming Merging of Mind and Machine, Controlling Robots with the Mind, Thinking Out Loud, Neuromorphic Microchips, and The Quest for a Smart Pill.

This book proved most provocative in two ways. First, it defined parallels between the chemistry of certain drugs and chemicals of abuse and the neurochemical pathways affected with the neurochemistry of schizophrenia and other mental disorders. Next, it gave a simple look at how electronic microchips and computers can control and/or be controlled by the nervous systems of people. The robot is no longer mere science fiction.

The strength of this book lies in its brevity and simplicity. The editor has minimized the details while maximizing the images (word and picture) which convey understanding. He points the reader toward tomorrow's neurochemical and pharmacological breakthroughs.



Principles of Toxicology (2nd Edition)

Reviewed by Margot Hall

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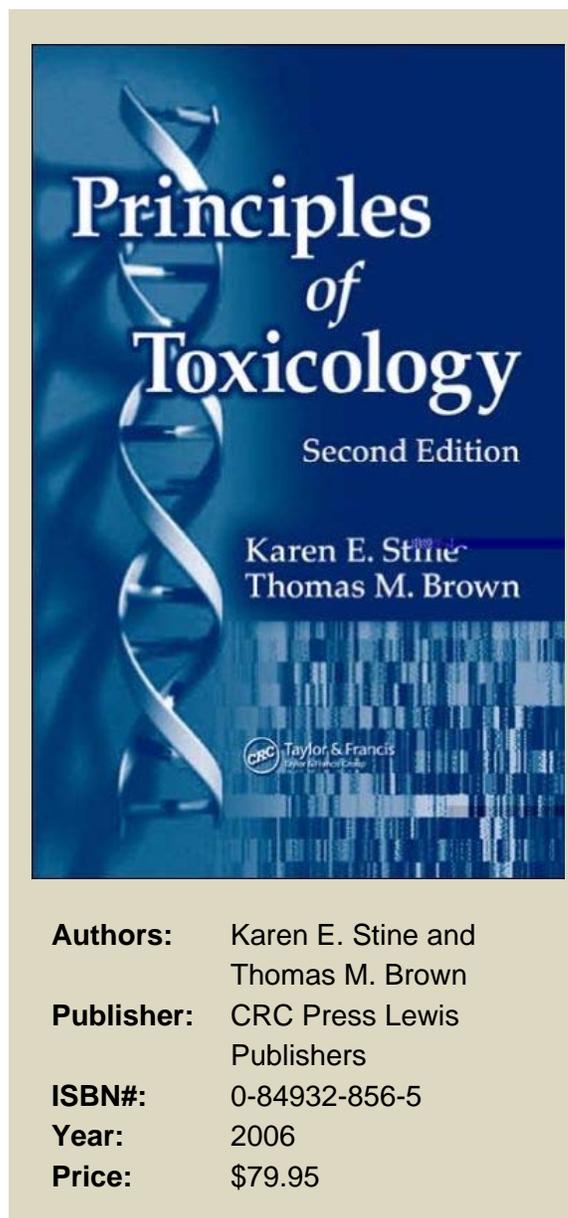
This is an excellent small/short book on toxicology. It evolved from an introductory course which the authors taught at Clemson University. It will serve nicely as a course outline or companion book/textbook for an undergraduate toxicology course.

The book has three especially useful features: 1) extensive cross listing to help the student quickly locate related subject matter, 2) an appendix with a list of selected toxicants including their structures, chemical formulas, physical properties, sources, uses, and toxicity, and 3) a brief summary of important physiology introductory to each chapter to prepare the reader/student for the significance of the toxicological information presented in that chapter.

This textbook has 2 authors, 259 pages, and numerous figures. In addition to the table of contents and the index, there is one appendix and numerous inserts listing page numbers of cross-listed material. Each of the 16 chapters has a list of references (~5-30 per chapter). The book is organized into chapters describing sub-cellular (molecular) toxicity, followed by chapters on cellular, physiological, and environmental/ecological toxicity. Major topics covered in the textbook include:

- 1) Measuring toxicity and assessing risk,
- 2) Toxicokinetics,
- 3) Biotransformation,
- 4) Cellular sites of action,
- 5) Carcinogenesis,
- 6) Reproductive toxicology and teratology,
- 7) Respiratory toxicology,
- 8) Cardiovascular toxicology,
- 9) Neurotoxicology,
- 10) Hepatic toxicology,
- 11) Renal toxicology,
- 12) Immunotoxicology,
- 13) Ecological toxicology,
- 14) Air pollution,
- 15) Water pollution, and
- 16) Toxic wastes.

Overall, this book is an easy read which will be especially appreciated by undergraduate students. There is no glossary of terms but key terms and concepts are italicized in the text to draw the student's attention to them. The book is recommended for an undergraduate survey course.



Authors: Karen E. Stine and Thomas M. Brown
Publisher: CRC Press Lewis Publishers
ISBN#: 0-84932-856-5
Year: 2006
Price: \$79.95

The Human Brain Book

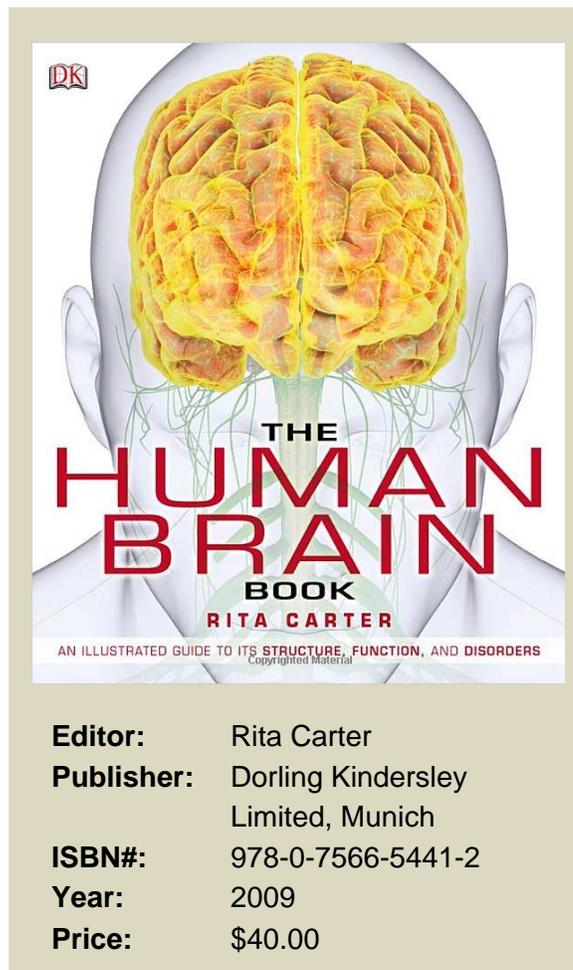
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This is a beautifully illustrated guide to the human brain. Essentially designed as a student aid, this book has 256 pages of color 3-D illustrations and PET scans. An accompanying DVD-ROM allows the student to experience interactive exercises with brain scans and brain anatomy.

The book has a table of contents, 14 sections/chapters, a glossary, an index, and a list of acknowledgments. It lacks a bibliography of further reading. Essentially laid out as illustrations with explanatory text, this book was planned as a manual for health care professionals or a neuroscience/medical reference for the family. Of particular interest is a chapter which presents 50 different brain related diseases and mental disorders with accompanying test scans and explanations.

An introductory section includes: No Ordinary Organ, Investigating the Brain, Landmarks in Neuroscience, Scanning the Brain, and A Journey through the Brain. Section 2 (The Brain and the Body) includes: Brain Functions, Nervous System, The Brain and the Nervous System, Brain Size- Energy Use- and Protection, and Evolution. Section 3 (Brain Anatomy) includes: Brain Structures, Brain Zones and Partitions, The Nuclei of the Brain, The Thalamus- Hypothalamus- and Pituitary Gland, The Brainstem and Cerebellum, The Limbic System, The Cerebral Cortex, Brain Cells, and Nerve Impulses. Section 4 (The Senses) includes: How We Sense the World, The Eye, The Visual Cortex, Visual Pathways, Visual Perception, Seeing, The Ear, Making Sense of Sound, Hearing, Smell, Perceiving Smell, Taste, Touch, The Sixth Sense [Proprioception], Pain Signals, and Experiencing Pain. Section 5 (Movement and Control) includes: Regulation, The Neuroendocrine System, Planning a Movement, Unconscious Action, and Mirror Neurons. Section 6 (Emotions and Feelings) includes: The Emotional Brain, Conscious Emotion, and Desire and Reward. Section 7 (The Social Brain) includes: Sex-Love-and Survival, Expression, The Self and Others, and The Moral Brain. Section 8 (Language and Communication) includes: Gestures and Body Language, The Origins of Language, The Language Areas, A Conversation, and Reading and Writing. Section 9 (Memory) includes: The Principles of Memory, The Memory Web, Laying down a Memory, Recall and Recognition, and Unusual Memory. Section 10 (Thinking) includes: Intelligence, Creativity and Humor, Belief and Superstition, and Cognitive Illusions. Section 11 (Consciousness) includes: What is Consciousness, Locating Consciousness, Attention and Consciousness, Altering Consciousness, Sleep and Dreams, Time, and The Self and Consciousness. Section 12 (The Individual Brain) includes: Nature and Nurture, Influencing the Brain, Personality, and Strange Brains. Section 13 (Development and Aging) includes: The Developing Brain, The Aging Brain, and The Brain of the Future. Section 14 (Diseases and Disorders) includes: The Disordered Brain, and Directory of Disorders. Clear, concise language adds to this book's usability.



Editor: Rita Carter
Publisher: Dorling Kindersley Limited, Munich
ISBN#: 978-0-7566-5441-2
Year: 2009
Price: \$40.00

Casarett & Doull's Toxicology: The Basic Science of Poisons (7th Edition)

Reviewed by Margot Hall

University of Southern Mississippi, Hattiesburg, MS 39406

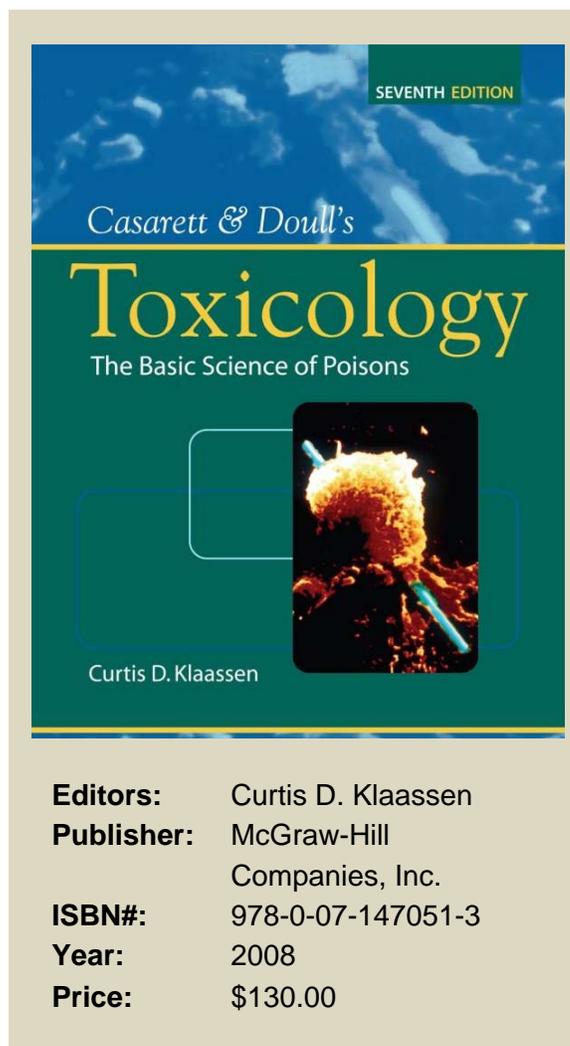
This is an outstanding and very thorough comprehensive textbook on toxicology. It will serve equally well as a reference book or textbook for graduate students.

The 7th edition offers references from the internet as well as from traditional books and journals. It also offers expanded information from molecular biology, oncology, environmental health, risk assessment, and the myriad of new laboratory techniques. This excellent text has 1 editor, 73 contributing authors, 1236 pages, numerous tables, figures, and photographs including medical imaging and karyotyping studies. In addition to the table of contents and the index, there is one appendix. It is arguably the most complete work of its type in the area of basic science toxicology.

Each of the 34 chapters has a chapter outline and its own list of references (approximately 50-250 per chapter). 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 xenobiotics, 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, 2) analytic and forensic toxicology, 3) clinical toxicology, 4) occupational toxicology, and 5) regulatory toxicology. The book has an appendix on recommended limits for occupational exposure to chemicals.

Overall, this book is an authoritative work that will prove exceptionally useful to practicing toxicologists, researchers, and graduate students. A particularly nice feature is the inclusion of short descriptions of the scientific research data/design from which toxicological information was obtained. There is a great deal of depth and detail in each chapter and thus the book can also serve as a reference for the toxicology laboratory. One drawback is the lack of a glossary of terms. The book is most highly recommended for any laboratory involved in toxicological studies and for a graduate (500-600) survey course in toxicology.

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 ~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 ~ 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), %, $^{\circ}\text{C}$, nm, μm (not m), mm, cm, cm^3 , 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.

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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.

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

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



DR. MARGOT HALL RECEIVED THE DUDLEY PEELER AWARD FROM THE MISSISSIPPI ACADEMY OF SCIENCES

Dr. Margot Hall, FAIC is the recipient of the the Dudley Peeler Award from the Mississippi Academy of Sciences. The award is given for “outstanding contributions to the Mississippi Academy of Sciences” (MAS). These included: 1) serving as President-elect, President, Past-president (2000-2003), 2) serving as the Corporate Coordinator (fund raiser) (1999-2005) and developing a data bank for future fund raising efforts, 3) serving as a judge for the Health Sciences Division of MAS (1986-present) and for the Mississippi Junior Academy of Sciences, 4)

serving as a referee (peer-review) for manuscripts submitted to the *Journal of the Mississippi Academy of Sciences*, and 5) supporting students and student research both at University of Southern Mississippi and at the Mississippi Medical Center (1986-present).

CONGRATULATIONS TO DR. JOHN HILL ON REACHING THE 200TH MILE-MARK IN SCHOLARLY PUBLICATIONS!

Dr. Hill is Professor Emeritus of Chemistry at La Trobe Institute of Molecular Sciences, La Trobe University, Melbourne, Australia and an active member of the Editorial Review Board of *The Chemist*. He has a long record of distinguished career. He is former Head of the Department of Environmental Management & Ecology, La Trobe University, Albury/Wodonga campus, and Pro Vice Chancellor and Head of the Albury/Wodonga campus of La Trobe University. He holds three doctorates, a PhD and DSc in Chemistry and a PhD in Chemical Education. He has held postdoctoral appointments in major universities in the USA, UK, Canada and Sweden. He is an internationally recognised authority in the thermal sciences.



His major research interest has been in Thermochemistry and over a period of 40 years he has applied a variety of calorimetric and thermal analysis techniques to study a diverse range of chemical and biochemical systems, with special emphasis on the application of these techniques to coordination compounds and systems of biological and environmental significance. He is also a leader in promoting sustainable chemistry education. He developed and taught the multidisciplinary undergraduate course titled 'Fuels, Energy & Environmental Sustainability' (FEES) at La Trobe University addressing renewable energy resources such as solar, wind and bio-fuels as future primary energy resources towards reducing global warming. His numerous awards and recognitions include election as a chartered chemist and a Fellow of the Royal Australian Chemical Institute and a Fellow of the Royal Society of Chemistry.



American Institute of Chemists

www.TheAIC.org

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.

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