

John D. Roberts: In His Own Words and Those of His Friends**

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In memory of Edith Roberts (August 10, 1918–February 21, 2010)

Abstract: In honor of the 97th birthday of Professor John D. Roberts, the author has assembled a collection of poignant quotes and anecdotes, mostly written by Roberts himself, which embody his philosophies of life and his wide-ranging experiences and interests. A brief summary of Roberts's major scientific accomplishments is also presented.

Born in 1918 and still alive and kicking, John D. „Jack“ Roberts was one of the leaders in the Golden Age of Organic Chemistry (1940s–1990s), along with such luminaries as Derek H. R. Barton, E. J. Corey, Donald J. Cram, Carl Djerassi, Albert Eschenmoser, Rolf Huisgen, Koji Nakanishi, Vladimir Prelog, Gilbert Stork, Saul Winstein, and R. B. Woodward. Roberts's career is well described by the title of his 1990 autobiography, *The Right Place at the Right Time*.^[3] *TRPATRT*, as Jack likes to call this volume, was published 25 years ago, two decades before his research actually slowed down. Roberts has left an indelible mark in chemistry as a researcher and scholar, an author of many textbooks, a vocal and poignant statesman within the scientific community, an academic leader (for example, he served as provost and vice president of Caltech), and a strong public voice for science education and government support of the sciences.

Roberts has collected most of the awards an organic chemist can assemble. He was elected a member of the American Academy of Arts and Sciences 63 years ago (1952) and a member of the National Academy of Sciences 59 years ago (1956). He received the ACS Award in Pure Chemistry (1954), the Roger Adams Award in Organic Chemistry (1967), the James Flack Norris Award (1979), the Arthur C. Cope Award (1994), the Priestley Medal (1987), the U.S. National Medal of Science (1990), the Glenn T. Seaborg Medal (1991), and the American Institute of Chemists Gold Medal (2013), among other marks of achievement and appreciation.

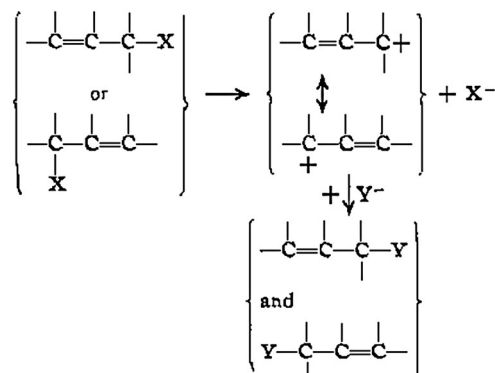
Roberts is a classical physical organic chemist who was one of the earliest practitioners of ¹H, ¹³C, and ¹⁵N NMR spectroscopy. Roberts used these new tools along with standard kinetics measurements to investigate many prob-

lems in physical organic chemistry that are now considered classics in the field. Roberts's research discoveries are on page after page in every organic textbook.

I shall provide a thumbnail sketch of the broad reach of his scientific accomplishments, with a specific emphasis on the many decades of his career and the diversity of his contributions. This will give a taste of Roberts's scientific interests. Reviews of certain depth are found in Roberts's 1990 autobiography^[3] and his 2009 perspective written on the occasion of the centennial of the Division of Organic Chemistry of the American Chemical Society.^[4]

Research Highlights

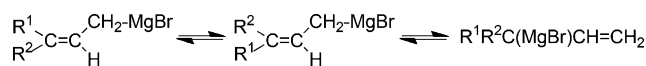
The relationship between structure and reactivity is at its most complex when the reactant exists as multiple, rapidly interconverting compounds (or intermediates or conformations), many of which react in their own unique fashions. Starting in the early 1940s, Roberts examined such systems, namely allyl halides and allyl Grignard reagents. His interest in the mechanism of allyl-X began when he was an undergraduate in the laboratories of Saul Winstein in the early 1940s at UCLA and continued to the 1960s with his own Caltech graduate student George Whitesides. With his own hands, Roberts looked for (and did not find) evidence of an S_N2' reaction by a thorough correlation of kinetics and reaction-product investigations, a study published in 1942 (Scheme 1).^[4,5] With Whitesides and other graduate students, Roberts investigated the structure of allyl Grignard reagents by NMR spectroscopy (Scheme 2). The chemistry is complex, depending on the substituents present. For butenyl Grignard reagent, the primary structure is predominant but there is a very rapid equilibrium between the forms. Whitesides also



Scheme 1. Examination of the reactivity of various allyl compounds to study the occurrence of S_N2' reactions. Reproduced from Ref. [5].

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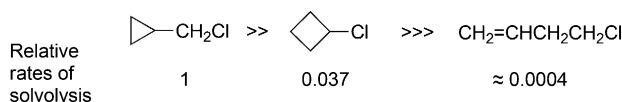
[**] This paper is a sequel to two previously published papers „Gilbert Stork: In His Own Words and in the Musings of His Friends“^[1] and „Carl Djerassi: In His Own Words“.^[2] Those papers celebrated Stork's and Djerassi's 90th birthdays. This paper celebrates John D. Roberts's 97th birthday (born June 8, 1918).



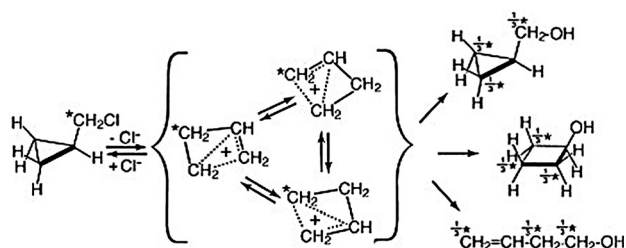
Scheme 2. The structure and reactivity of allyl Grignard reagents.

measured the rate of inversion in $(CH_3)_3CH_2CH_2MgCl$ by examining the AA'BB' (or A_2B_2) spin systems as a function of temperature.

In the 1940s and 1950s, Roberts investigated the chemistry of small-ring compounds including the preparation of cyclopropanol and the reactivity of cyclopropyl and cyclobutyl derivatives. Paper XLIV in his series „Small-Ring Compounds“ confirmed the previously postulated conversion of the cyclopropylcarbinyl Grignard reagent to the allyl carbonyl Grignard reagent.^[6] Roberts's observation that cyclopropylcarbinyl chloride solvolyses 2500 times faster than 3-buten-1-yl chloride (Scheme 3) placed Roberts and his research squarely into the experimental realm of the nonclassical carbocation controversy (Scheme 4).^[4] Indeed, it was Roberts who first suggested the term „nonclassical“ for these three-carbon two-electron moieties.^[7]



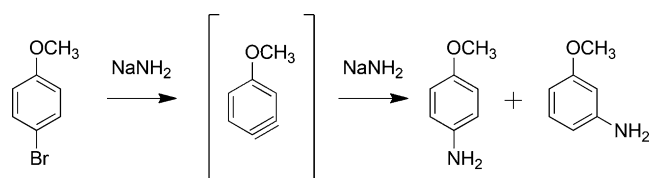
Scheme 3. Demonstration of a major rate enhancement due to the involvement of an unusually stable, nonclassical carbocation in the solvolysis of cyclopropylcarbinyl chloride.



Scheme 4. The solvolysis of cyclopropylmethyl chloride via the nonclassical carbocationic route. Reproduced from Ref. [4].

As the quotes from Roberts later in this article will show, he is a powerful yet practical scientist. He can be both charming and forceful, often simultaneously. As a reviewer of this paper stated, „Roberts was very combative, and it was a combative time“. The nonclassical ion controversy, as a topic, and Herbert C. Brown (Purdue) and Saul Winstein (UCLA), as protagonists, provide the most vivid examples of Roberts's combativeness. This slice of Roberts's life—one that he intentionally kept narrowly focused and, with time, avoided—will be dealt with in a subsequent publication by this author.

Roberts and his students provided the explanation of and experimental proof for the mechanism of nucleophilic aromatic substitution reactions which involved rearrangement products (Scheme 5). This elimination–addition reaction is now well known by the name of the reaction



Scheme 5. The elimination–addition (benzyne) reaction.

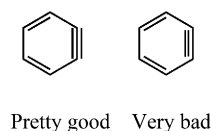
intermediate, benzyne. While the intermediacy of benzyne was first postulated by Georg Wittig in 1940, it was experimentally confirmed by Roberts in 1953.^[8]

This article primarily consists of excerpts from Roberts's writings and those of his friends and colleagues about Roberts. These excerpts will appear below this short summary of Roberts's major scientific interests and achievements. Nevertheless, two excerpts will be placed here because of their immediate relevance.

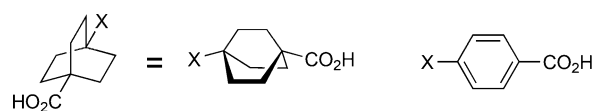
As stated by Georg Wittig: „During a lecture tour of the United States in 1959, my wife and I were invited by Roberts to his home for dinner. In the course of conversation, I noticed some pictures on the wall, among them an impressive portrait of a woman. ‘That's my mother; her maiden name was Dombrowski.’ ‘My mother was also a Dombrowski,’ I answered, amazed. Thereupon Roberts concluded tersely: ‘So then we're cousins.’ With this amusing coincidence of a Polish name, a friendship was sealed between Jack and myself.“^[9]

As recalled by Roberts: „What I found out was that there is a matter of semantics regarding benzyne... If you draw [the extra bond] outside the ring, people don't complain anywhere near as much as if you draw it inside. [laughter]“^[3,10]

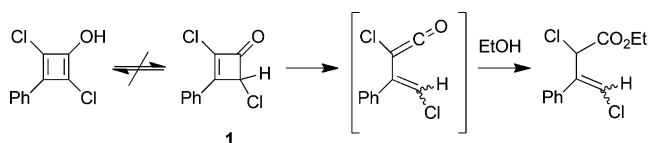
According to Roberts, chemists response to these representations of benzyne:



Fundamental to the understanding of organic chemistry is the effect of substituents on structure and reactivity. Much research was performed in the 1940s, 1950s, and 1960s on the Hammett σ_p relationships, the Taft equation that included steric effects, and extensions thereof. Roberts published a number of papers examining the electrical effects of substituents in the absence of varying steric effects. His most important contribution in this area was to study a series of 4-substituted bicyclo[2.2.2]octane-1-carboxylic acids and compare the results with similarly substituted 4-X-substituted benzoic acids. „The goal was to separate out the benzene resonance contributions to the σ -constants by using a saturated scaffolding with very nearly the same geometry.“^[4] In 1953, Roberts demonstrated that electronic effects were efficiently transmitted through σ -bonds.^[11]

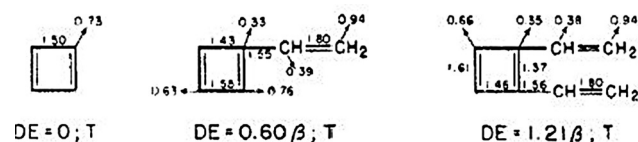


Related to his work on electronic effects and small-ring chemistry, in the early 1960s, Roberts examined halogenated cyclobutanes as possible precursors to substituted cyclobutadiene (CBD). CBD was an important synthetic target in the 1950s and 1960s, following William von Eggers Doering's conceptualization^[12] of the „ $4n+2$ “ rule and Breslow's description of antiaromaticity^[13] based on Hückel's and others' publications. The optically active cyclobutenone **1** was prepared, and it did racemize but not by enolization, as established by the lack of hydrogen–deuterium exchange. Rather, reversible ketene formation occurred (Scheme 6).^[14]



Scheme 6. Roberts's attempt to prepare a derivative of cyclobutadiene led to racemization via ring opening. Reproduced from Ref. [14].

Roberts was one of earliest practitioners of molecular orbital theory in organic chemistry. He may rightfully be considered one of the earliest computational chemists. In 1950, Roberts announced in his first lecture to his organic class at MIT that „resonance would be abandoned and the course would be taught solely on the basis of molecular orbital theory.“^[3] Together with his postdoctoral student Andrew Streitwieser, who would become an eminent experimental and computational chemist,^[15,16] Roberts published a landmark paper, „Molecular Orbital Calculations of Properties of Some Small-Ring Hydrocarbons and Free Radicals.“^[17] One finding involved the lack of delocalization energy of cyclobutadiene (Scheme 7). In 1962, to help organic chemists become familiar with MO theory, Roberts published his handbook *Notes on Molecular Orbital Calculations*.^[18]

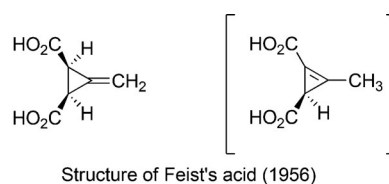


Scheme 7. Three structures illustrating the use of MO theory to demonstrate the lack of aromaticity in cyclobutadiene. Reproduced from Ref. [18].

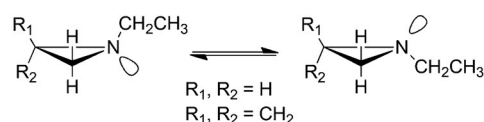
Knowledge transfer can be a two-way street, the teacher, or the chemical consultant, often being the one who learns more than the student! This was often the case for Jack Roberts and the DuPont Company. Roberts—a consultant for DuPont for some six decades—describes that on one of his consulting trips in 1954, DuPont spectroscopist William D. Phillips described his recent experiments with ¹H NMR spectroscopy. „I was surely hyperventilating with excitement,“^[3] summarizes Roberts. Certain of the value of NMR, Roberts convinced then Department Chair Linus Pauling to provide the funds, and the first Varian 40 MHz NMR spectrometer installed in a university was located at Caltech.

Soon thereafter, Roberts's ¹H, ¹³C, and ¹⁵N NMR studies provided incentive for the entire community to develop NMR technology. Some of Roberts's early NMR studies are summarized in Scheme 8. (It is likely that Roberts's research on small rings and halogens, especially fluorinated organics, also benefited from his consulting with DuPont, topics of interest to both the consultant and the company.)

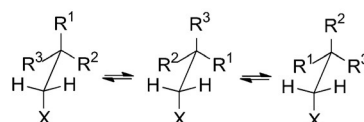
Roberts's textbooks were revolutionary in terms of their early inclusion of spectroscopy, and his texts set the standard as handbooks and reference books for practicing chemists. These textbooks are: *Modern Organic Chemistry*, with Marjorie Caserio, perhaps the first organic text that incorporated NMR and IR spectra (1964); *Modern Organic Chemistry* (1967) and *Organic Chemistry, Methane to Macromolecules* (1971), written with R. Stewart; *Nuclear Magnetic Resonance. Applications to Organic Chemistry* (1959), which



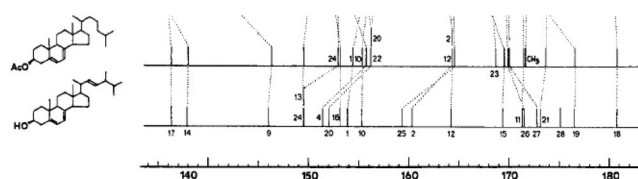
Structure of Feist's acid (1956)



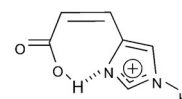
Conformational analysis of aziridines (1956, 1958)



Demonstration of slow rotation about single bonds in ethane derivatives by NMR (1957)



Natural abundance ¹³C NMR spectroscopy, in this instance, derivatives of cholesterol (1969)



"cis-Uric acid but not its trans isomer, shows changes of its ¹⁵N shifts with changes in pH almost identical to those of the histidine of α-lytic protease" (1982)

Scheme 8. Early structural and conformational analyses by Roberts using ¹H NMR (top three examples), ¹³C NMR, and ¹⁵N NMR spectroscopy (bottom example).^[3,4]

may have been the first text with colored graphics; *An Introduction to the Analysis of Spin-Spin Splitting in High-Resolution Nuclear Magnetic Resonance Spectra* (1961); and *Notes on Molecular Orbital Calculations* (1961).

Jack Roberts did not lack for causes. At times, it seemed as if he was interested in nearly everything around him. He was a heavy-weight scientist with clout: as an intellectual and as a chemist; as an educator and a university administrator at the highest levels; as a textbook author; as an influential member of the National Academy of Sciences and the Board of Directors of *Organic Syntheses* for decades; and as a spokesman for science and science funding. His commanding height, strong voice, vigor, and sense of righteousness make him even more of a force to be reckoned with. I also know from many personal experiences that he is a genuine, native Southern Californian „sabra“ (a tenacious, thorny desert plant, with a thick skin that conceals a sweet, soft interior, tough on the outside, delicate on the inside; Wikipedia).

This article celebrates Jack Roberts's life and career as he reaches his 97th birthday. What follows are some of his (and his friends' and colleagues') most profound and entertaining words. I say mine here: Happy Birthday, Jack. Thanks for decades of friendship (Figure 1).



Figure 1. Jack Roberts (right) and Jeff Seeman at the Chemical Heritage Foundation, Philadelphia, March 2012. Photograph courtesy J. I. Seeman.

Unless otherwise attributed, all of the following are excerpts from Roberts's writings.

Who Is John D. Roberts?

As told by George S. Hammond (a colleague for many years at Caltech and the discoverer of the Hammond Postulate): „To debate science with Roberts is a unique experience. He combines the style of a dyspeptic porcupine and the wily cunning of a Las Vegas dealer with fundamental integrity to produce a style that is both frightening and stimulating.“^[19]

As told by W. G. McMillan (fellow undergraduate with Roberts at UCLA and chemical physicist who returned to

teach at UCLA): „My awareness of John Dombrowski Roberts grew like a toothache: at first, a dimly-perceived twinge in the background; then a persistent presence; and finally an inescapable companion.“^[20]

As told by Vladimir Prelog (1975 Nobel Prize in Chemistry): „When I received his *Introduction to Spin-Spin Splitting*... I wrote him, 'I enjoy solving problems from your book... It was an excellent idea to put your photograph on the dust cover, because it is practically impossible to cheat in its presence'.“^[21]

As told by George Whitesides (former graduate student of Roberts): „When J. D. Roberts is displeased, the earth quakes.“^[22]

Responding to Challenges

„I always wanted to know more... Every time there was a teacher who was demanding, I did very well. Every time I got in with some undemanding and usually popular person, I tended to perform badly.“^[10] „I always got along best with the most unpopular, difficult teachers.“^[23]

Moving Science Forward

„Mak[ing] an important, even if approximate step forward... go[ing] in the right direction. This movement may not lead to a complete solution, but you hope to go at least as far as current knowledge and techniques will allow. If the step you make is really in the 'right' direction, others will build on it. Such a step causes people to think and do experiments, even if the direction finally turns out to be a blind alley. Exploring blind alleys and marking them clearly is an important effort in science, even if it earns few 'brownie points' for Nobel prizes.“^[3]

Roberts's Assertiveness

In a 1990 review of a biography of Linus Pauling, Roberts wrote: „One's skepticism of the level of accuracy of a book or news report is definitely aroused when events are described that one has personal knowledge of, or participated in, and these events are incorrectly reported (or are actually non-events). With much of this sort of thing, the whole fabric of a report becomes doubtful. This is a serious problem with [this] book.“^[24]

According to Frank Westheimer (eminent physical organic chemist at Harvard): „When Bill Wheland asked Jack to criticize his chapters on quantum mechanics in *The Theory of Resonance*, Jack did so with gusto. Where Bill wrote, of some mathematical formulation, 'It is obvious that...' Jack appended (in red ink, naturally) 'Obvious to whom? Schrödinger?'“^[25]

What is Success?

„If ‘happiness is a warm puppy,’ what is success? I’ll offer you some definitions:

Success is a Nobel Prize

is working with people you like

is Roger Adams

is a checked Organic Syntheses prep

is friends who will stand with you and help you

is a Harvard professor

is one good paper

is ten good papers

is 100 good papers

is 1000 good papers

is the Editorial Board of Organic Syntheses

„I could go on—however, I think perhaps you get the idea.

Success is many things to many people—what looks big to one is small to another and vice versa.“^[26]

„Your path up the mountain of success can’t really be a solitary one—it is full of other people, many of them climbing, many winded and just standing still. When trouble comes, they may do nothing to help, or they may grab you by the seat of the pants and help you up, or they may put their feet in your face. I think you’ll get up faster, and a lot farther than you ever expected to go, by being part of a group and a guy they really want to have along. Fortunately, you can do this without any obligation to give up when any of the others drop out because the way is too steep. What you will almost always find is that they say, ‘I’m tired, you go on ahead.’ I think you want to be known as a man who helps others and wouldn’t disdain a helping hand when it is offered. It’s more human and more fun to operate this way and then, if the avalanche comes before you reached the top, you can say that, at least, you had fun on the way.“^[26]

Advice to a Younger Colleague

„This is a very important paper and one that should be widely known and, at this same time, put you in the best possible magisterial light... the provocation to you over the years has been really intense, but as some have said every really good scientist needs an enemy to do his/her best work and that has indeed been helpful to you. One reason why I think you should take the high road here is because it is more likely to lead to greater appreciation of your overall work... What is important for you is to get it published in good style and get it as widely disseminated as possible. Which journal is best for that I do not know... but it might be a good idea to get quite a few reprints and send them out generously, unsolicited.“^[27]

On Managing One’s Own Academic Career

„I have always had to sell my ideas to somebody to do anything, beyond the most ordinary and trivial... Use internal support to get a program going which is so good that an agency is delighted to avoid the initial investment and is more than willing to sustain and expand it... Continuity is vital and to keep the support coming, we had to be nimble; going from

one nucleus to another and one theme to another, until today virtually nothing recognizable is left of our original thrust. Scrambling for money to make each major move was a scary process, but I have had really great fun, great satisfaction, and no feeling of being coerced into doing other than what I wanted to do; even though from time to time I had to change directions to keep from hitting a stone wall.“^[28]

On Research Projects

„I preferred to keep on dabbling in a multitude of things I found interesting enough to study, especially if each satisfied my desire to confine my research to problems in which I could see no easy solution or involved measurements for which I could not predict the results. Of course, there are limits. As someone said ‘Attention is like butter, if you spread it too thinly, you can’t taste it any longer.’“^[4]

„If somebody becomes convinced that something isn’t going to work, it’s not going to work. I’ve had so many disappointments in that regard. I will want something, and the guy who was involved was sure it wasn’t going to work, and he was right. But others often make some of these things work.“^[10]

On Judgments

„I remember... being sent a proposal to look at. [It] had six reviews on it; and the grades ran from one to six... I pointed out that it was a pioneering sort of proposal by a person who was not terribly thoughtful, who was intuitive in a sense, and who just went into the lab and sort of looked for things. The reviewers who thought it was good were probably the same kind of people, and the people who believed in doing particular kinds of very planned research were the people that didn’t like it.“^[10]

On Raising Funds from NSF

„Shortly before I became division chairman [at Caltech], the NSF had announced a matching program to build buildings. They were willing to entertain the prospect not only of building a building but also of fixing up the space that was vacated... I wrote up the proposal... The NSF sent out some people, and we took them around through the labs. In McConnell’s lab, a board being used as a writing desk had to be moved up out of the way so they could walk through. One of the visitors nudged me on the way out and said, ‘Well, you didn’t really have to put on quite that kind of a show.’ I think we got essentially everything they asked for...“^[23]

On Reproducibility in Science

„One thing also that is not addressed in your article is the nature of the reproducibility problem for experimental results. This seems as though it would be very straightforward, but actually it is not. I have had cases in our laboratory which are illustrative. In two of them, my lab workers claimed not to be able to reproduce the work of two earlier personnel I had

always regarded as reliable as anyone who had ever worked with me, and I was shocked to find that anyone could believe their work to be non-reproducible. ‘How many times did you try? Are you sure you followed the directions *exactly*?’ The answers were so positive that there was a clearly some kind of a problem, and one so vital to continuation of the work that I went into the lab and repeated the procedures myself. In each of these cases what happened was that the people involved did not actually follow the directions *exactly*—what they did was to follow their interpretations of the directions and claim that that was the same thing. I was able to do as well or better than the original workers by doing just what they said they did.”^[29]

On Writing an Autobiography (and Its Validity)

„It is like opening an overstuffed, catch-all storage closet. A mélange of uncorrelated, unresolved, sometimes unpleasant memories comes pouring out. Soon doubt arises as to what, if anything, has historical significance and, even more, what part of the accumulation would be interesting enough for someone else to read about. Finally, there is a nagging possibility that it might be difficult, if not impossible, to stuff the memories back into storage and resume one’s forward tact.”^[3]

On Writing a Book

„When I write a book, I have to have the missionary spirit. I have to feel I’m going to do something that somebody hasn’t done before, cover things that haven’t been covered before, or write about them in a different way than ever before.”^[10]

Roberts’s Style of Communication

William A. Benjamin was owner of W. A. Benjamin, Inc., a major book publisher that began in 1960 and published three of Roberts’s books (Figure 2).

As told by Benjamin: „Roberts’s penchant for moving the actual beyond the normal boundaries was evident in his



Figure 2. Roberts (left) celebrating with W. A. Benjamin at a surprise birthday party for Roberts, at Caltech’s Athenaeum, 1970. Photograph courtesy J. D. Roberts.

publishing ethos. Books needed to appear quickly after manuscript submission. Novel ways of incorporating graphics were constantly being pursued. Roberts published content- and graphics-rich textbooks as well as short but highly pedagogical workbooks, reaching undergraduates, graduate students and his fellow professionals. Benjamin provided the publishing house for Roberts’s vivid imagination and strict standards.

„Correspondence with Professor Roberts was a lesson in corporate communications. He was the first to use the instant-answer device: Jack would fill the margins of your letter or a memo with neat, cryptic, always colorful (!) answers, Thermofax the original, and return the *brown* copy to you. It was positively unnerving to realize that your next salvo was likely to be treated in the same manner. And beware of the use of superlatives, overlooked typographical errors, poor arithmetic, or less-than-absolute recall of prior arrangements. I shall cherish forever the hastily written letter Roberts returned to me, grammatically edited throughout with a red pencil and the grade ‘C+’ firmly printed at the top.”^[30]

Benjamin’s summary of several of Roberts’s principles of professionalism:

„(1) *The Mum Principle:* Never recommend someone if you, or someone you know and trust, have not personally reviewed his work.

(2) *The Dangle Principle:* Never, never put yourself in the position of dealing with a publisher over just one book—always keep another promising title in sight, dangling, just to reinforce your present demands.

(3) *The Squash Principle:* Always challenge your newly made friends, or peers, or subordinates, to compete with you in a sport you know you can beat him at, and never let him forget the score.”^[31]

On Respect for Others

„The future looks wonderful to me. But we must control the seemingly inborn, very stubborn, defense mechanisms, which make us fear, and too often make us wholly intolerant of people who are at all different from the way we are; whether the difference be in language, geographic location, religion, color, political beliefs, or social status.”^[32]

Changing Norms and Political Correctness

Roberts authored an introductory and pedagogical article on the relatively new technique of NMR spectroscopy in the November 1961 issue of the *Journal of Chemical Education* (*JCE*). A rather politically incorrect—by today’s standards—footnote appears on the first page of Roberts’s article (Figure 3). This footnote refers to the cover of that issue of *JCE* reproduced in Figure 4. Marjorie Caserio joined Roberts’s group in 1956 as a postdoctoral fellow and continued in Roberts’s group as a senior research fellow where she published extensively with Roberts, helped lead his burgeoning research group, and co-authored textbooks with him. In 1965, she joined the newly established University of California at Irvine where she became a full professor in 1972.

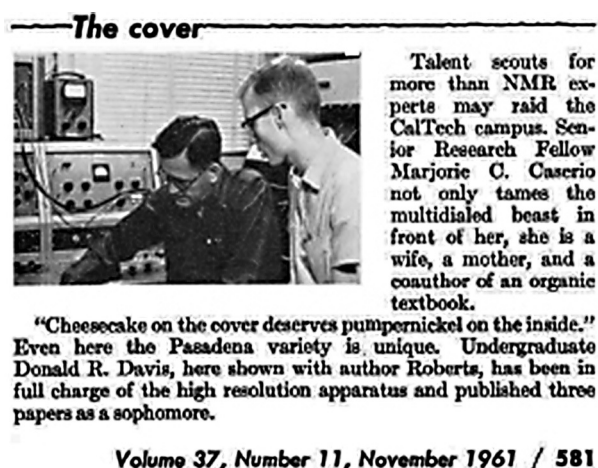


Figure 3. Footnote from the first page of Roberts's 1961 article entitled „Nuclear Magnetic Resonance Spectroscopy“—at that time, a relatively new analytical tool for organic chemists—in the *Journal of Chemical Education*.^[33] See Figure 4 for the cover of that issue of the journal to which Roberts refers as „cheesecake.“ Reproduced with permission from the *Journal of Chemical Education*.

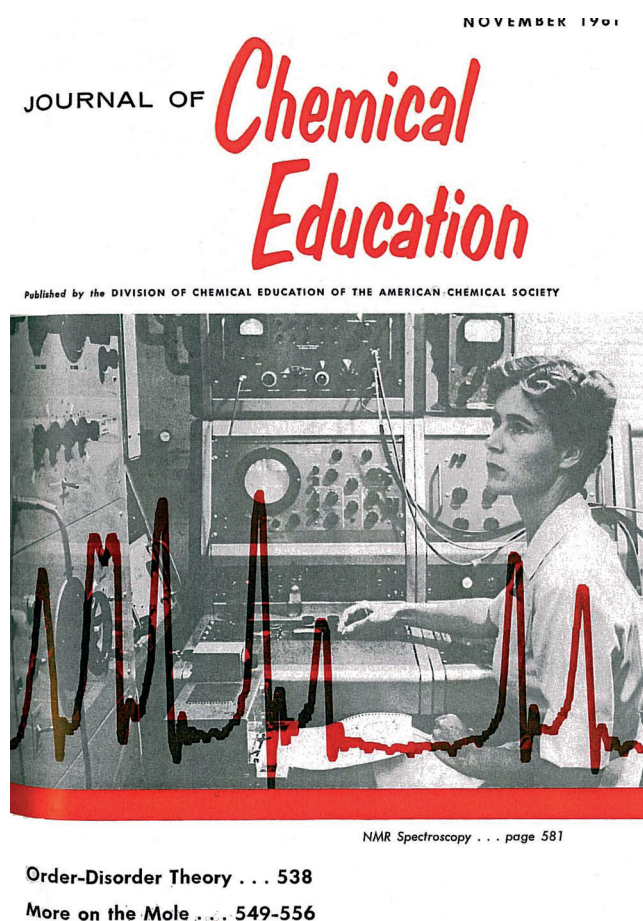


Figure 4. Cover of the November 1961 issue of the *Journal of Chemical Education*.^[34] See Figure 3 for Roberts's caption to this photograph of Marjorie Caserio. Reproduced with permission from the *Journal of Chemical Education*.

Subsequently, Caserio served as vice chancellor of academic affairs at the University of California at San Diego (1990), and in 1995 served as interim chancellor before retiring in 1996.

Roberts's Role in Bringing Women as Graduate Students to Caltech

In a letter to Linus Pauling, then Chair of the Department of Chemistry at Caltech: „Miss Dorothy Semenow, a regularly enrolled graduate student at MIT, is very desirous of permission to transfer to the Graduate School of the California Institute of Technology so that she may continue her doctoral research with me and obtain a degree from Caltech... I realize that the rule of your Institute is not to admit women as graduate students, I should appreciate anything which might be done for Miss Semenow...“^[35] In 1953, Semenow was admitted to Caltech and received her PhD with Roberts.

Early Interest in Science

„Whenever Caltech had an open house, I would get my aunt, the school teacher, to drive over and visit with her friends in Pasadena, and just let me off and let me stay during the day... I was only about thirteen or fourteen. I remember very specially the aromatic smell of the Gates Laboratory. They used to run chemistry demonstrations in the big lab, and those were absolutely fascinating. It was a marvelous thing for a young person to be exposed to that, but it was a tremendous burden on the Caltech staff and students; I never really quite figured out exactly how they got into it or why they gave it up“^[23] (Figure 5).



Figure 5. Roberts „demonstrating an early interest in exploring the radio-frequency spectrum, about 1922.“^[3] Photograph courtesy J. D. Roberts.

Why UCLA for Undergraduate School

„I was working every night, from about seven to about midnight, in the bakery, and all day Saturday. When I went in to sign up for freshman chemistry, the only section that was open at that point had a laboratory section on Saturday morning. And I remember going around to the department's chairman telling him, ‘Well, look, I've got to work; I've got to get into another section. I can't afford it.’ He said, ‘Sorry, I

can't change you.' I said, 'Well, I'm a chemistry major.' He said, 'Oh, if I could get rid of 20 chemistry majors, I'd be much happier. It's Saturday or nothing.'^[23]

„I found that research was the thing I could really do. I wasn't very good in classes, but I could get equipment together and usually made things work.“^[23]

Research in the 1940s

„Before my time, organic research was essentially being done in the same way as it had been done in the previous 50 years. It may seem unbelievable, but in 1938, our best instrument for characterization was the thermometer... Structure determination of any complexity required degradations to smaller compounds of known structure.“^[4]

On Chemistry in 1945

„The 'existence' concept in organic chemistry has changed markedly over my lifetime. When organic chemists characterized their preparations by boiling point, by elemental analysis, and by degradative reactions, many only relatively reactive compounds could not pass muster. In 1945, the idea that substances could be stable and characterized at -80°C was not part of the practicing chemist's thinking“^[3] (Figure 6).

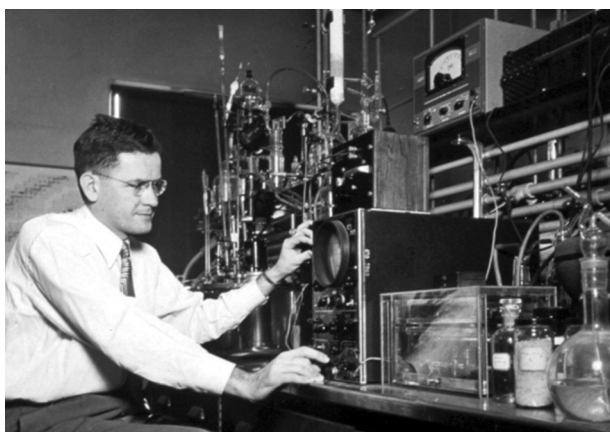


Figure 6. Roberts at MIT, early 1950s. Photograph courtesy the Chemical Heritage Foundation and J. D. Roberts.

On Research in the Early 1950s: Prelog, Woodward

„I think that [Vladimir] Prelog's approach to his research is reasonably typical of the hot workers in the natural products field. You can only make a killing if you actually determine *the* structure or carry out *the* synthesis of an important natural material. Fundamental chemistry of a less spectacular source rarely pays off to the same degree. Thus, you can only 'swing for the fences' in these fields and it is a home run or nothing. Naturally, problems of this sort are better delegated to post-doctoral people than graduate students... This is one of the reasons I am not a natural products chemist. We can try to

synthesize pentalene and cyclobutadiene, but the goal is of less importance to us than the fundamental chemistry encountered along the way. Actually, fundamental chemistry on intermediates leading to these compounds is much easier for the average chemist to read about and understand than fundamental chemistry along the routes to and from strychnine.“^[36]



On Teaching MO Theory in the early 1950s

„I had been getting more and more interested in this molecular orbital stuff. And I knew that I wasn't going to sit down and learn it unless I really had to. And so I told the class the first day, that now I am going to teach the course without mentioning resonance at all. I'm going to give the whole course from the standpoint of molecular orbital theory... This was almost my Waterloo... I could see that if somebody asked me certain questions, I was just going to melt into the woodwork because I wasn't going to be able to explain it.“^[23]

„Panic set in. How was I going to understand how those electrons get distributed? I rushed to the library and tried to see what those great works on quantum chemistry had to say about these problems. They said absolutely nothing in words that I could understand...“^[3]

On Obtaining One of the First Commercial NMR Spectrometers

„I started a campaign with my colleagues to get Linus Pauling to help us buy a Varian NMR spectrometer. It was not easy, because Linus knew about NMR and had little faith in its hands-on use by organic chemists who might not even know how the instrument worked... Linus finally seemed to succumb to the lure of using NMR to study resonance vs. tautomerism, but perhaps he actually wanted to get rid of my harassing him about our needs...“^[4]

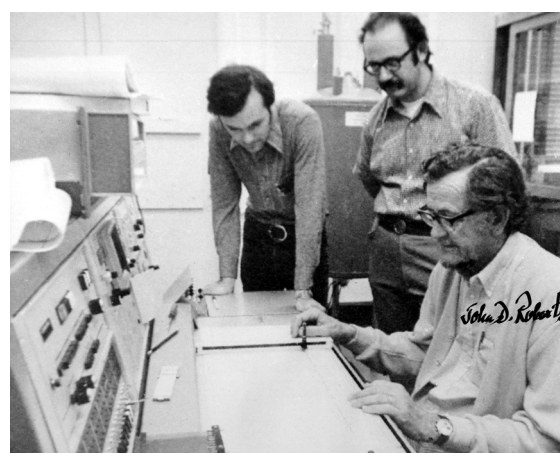


Figure 7. Roberts with (left to right) postdoctoral fellows Devens Gust and Donald Giannini and a Bruker WH-180 NMR spectrometer „wholly dedicated to use for ^{15}N , mostly at the natural abundance.“^[3] Photograph courtesy J. D. Roberts.

„It was often almost as useful, if not more useful, to observe the results of repetitive sweeps on the CRT [cathode ray tube] rather than to record spectra. However, when we did record, we used a relatively high-speed Sanborn recorder, which wrote the output with a hot wire on a narrow strip chart. The normal procedure was to run off a series of seven-second sweeps. We could usually get 15–20 recordings before a major change occurred that would make the spectra unrecognizable. The strip chart was then cut up, and comparisons were made to see if two or more spectra could be found that were the same. If that was not possible, then the probe would be relocated, perhaps the magnet recycled, and the taking of the spectra repeated“^[3] (Figure 7).

On the Installation and Use of Our First NMR at MIT

„The guy from Varian Associates came to install it—Jim Shoolery... I looked over his shoulder, trying hard not to look too ignorant; the machine was covered with dials and lights and switches, really complicated. And the instruction book was frightful; it had the most marginal instructions I've ever seen for a major piece of instrumentation. Jim was adjusting the machine, and finally I said we were doing some stuff in the lab; I had this sample, and I wanted to see how much he could find out about it. So he put it in the machine, and he looked at the spectrum, and he said, 'Oh, that's got a methyl group on a double bond'. And I said, 'No, it doesn't. Your spectra have really got that wrong.' Well, it turned out Shoolery was right. And that was even more impressive; so I became even more eager to get in there and really figure out what was going on.“^[10]

„When we got our first spectrometer, we were turning out spectra every seven seconds... we would run off twenty or thirty [spectra], and we'd try to find two that were the same, because the electronics were not stable, the magnetic field wasn't stable, the temperature wasn't stable—everything was wiggling around.“^[23]

May 3, 1972

TO: H. Brown
FROM: J.D. Roberts

Dear Harold,

I greatly appreciated your letter regarding my promotion to Institute Professor. You did not state whether or not it was necessary to accept this appointment, but I am pleased to do so. I believe that you know how I feel about Caltech, and the very tangible evidence that the feeling is mutual is most satisfying.

At some more leisurely point, I would appreciate knowing more of your ideas about the prerogatives and responsibilities of Institute Professors. For openers, I'll put forth a few possibilities for additional responsibilities.

1. More or fewer haircuts? Beards (Willy Fowler's example)? Wear coat and tie every day?
2. More participation in administration and faculty matters?
3. More statesman-like pronouncements on scientific and public affairs?

Possible prerogatives:

1. Triple salary?
2. More or less unlimited research funds from the Institute?
3. No teaching duties (true of Harvard's University Professorships)?
4. Early retirement on unusually favorable (or unfavorable) terms?

There is no hurry to have a statement of policy on these matters but I received no enlightenment from "Policies and Procedures" about my projected new status and I guess I should know, in case I am expected to undergo a drastic change of life on July 1.

Figure 8. An inter-university message from Roberts to then Caltech President Harold Brown dated May 3, 1972 on the occasion of Roberts's promotion to Institute Professor.^[37]

On Communicating with the President of Caltech

Harold Brown is a physicist (PhD in physics from Columbia University at the age of 21) who served as U.S. Secretary of the Air Force in the Lyndon Johnson administration from 1965 to 1969. From 1969 to 1977, he was president of Caltech. He became U.S. Secretary of Defense (1977 to 1981) under President Jimmy Carter. Brown and Roberts must have had a very warm relationship. In Figure 8, Roberts thanks President Brown for his congratulatory letter on Roberts's promotion to Institute Professor. In another message from several years later (Figure 9), Roberts jokes with Brown on the name of a new „School of Resonance Geology.“

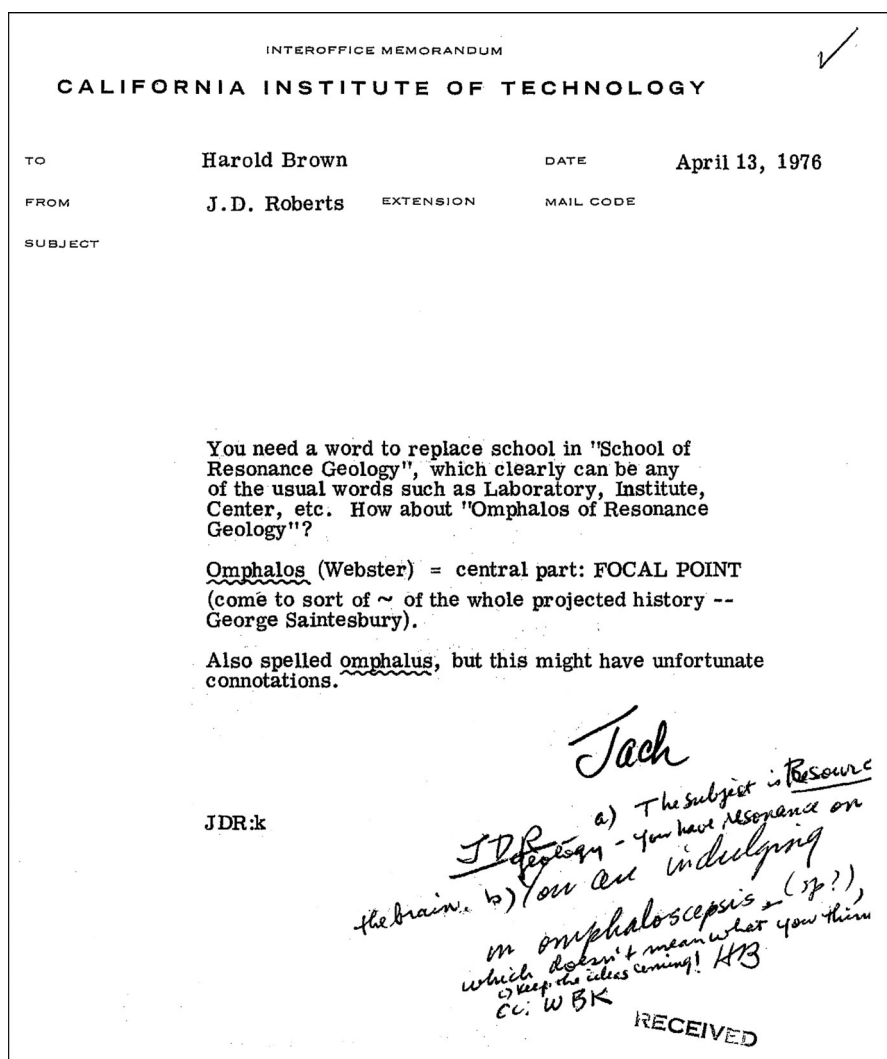


Figure 9. A very playful exchange between Roberts and Caltech President Harold Brown dated April 13 and 21, 1976.^[38] Omphaloskepsis refers to „navel-gazing“ and has been defined as „contemplation of one's navel as an aid to meditation.“

On Pyridine

In a letter to Peter Brook, Roberts wrote, „As for pyridine—Pauling would say it is *p*-hybridized, most people would probably guess it to be *sp*²-hybridized, while I would go on being confused.“^[39]

On Teaching

„[One needs to] explain all or part of the stuff you got so neatly in your head to those who need to know it, in a way they can really understand. Not just give you the ‘yes, yes, I got it,’ but implanted in a way they can use it themselves—and most important, recognize it when seen from the side and not just from the top... getting someone to the point where he/she can apply [it].“^[40]

As told by T. L. Cairns (a chemist at DuPont): „Roberts' approach to teaching and research [and] consult[ing]—no

issue is avoided, no question left unasked, and no sloppy thinking permitted to exist. One research director [at DuPont] commented at the conclusion of an afternoon with Roberts that he didn't really expect to have to take his prelims all over again every time the guy came to visit.“^[41]

Interaction with His Students

As told by Whitesides: „The one avenue of communication that graduate students had with him was strictly one-way: we wrote monthly progress reports, which, in his absence, we left in his office. We never saw the reports again, and their contents elicited no comment. Our emotional condition, as we abandoned these reports on his desk, must have resembled closely that in which earlier and (presumably) more primitive cultures tied offerings of chickens in the forest to be eaten by trolls.

„He compensated by going to considerable lengths to read thesis drafts as rapidly as the students could produce them... As drafts were submitted and returned, it rapidly became obvious that, contrary to popular opinion, he *had* followed the progress of the research. In fact, he knew not only the details that had been included in the progress reports, but also details which he had no earthly reason to know. To this day, I have no idea how he came by some of the information he penciled into the margins of my thesis. Certainly I

never told him; perhaps it was divine revelation, perhaps a priori reasoning. Regardless, although disillusioning at the time, this final exposure to the realities of the situation provided a therapeutic conclusion to the graduate educational process.“^[42]

Roberts Describing His Colleagues and Students

On Arthur C. Cope, eminent physical organic chemistry and discoverer of the Cope rearrangement (MIT): „This man was a tough cookie. Of medium height and strong build, with a long face, curly blond hair, and strong jutting jaw, Art spoke carefully and quietly—indeed, he seemed mild and conciliatory, almost effete. But when you got to know him, you found out that behind that facade, the juices really flowed. When the going got rough, his long, slender white hands seemed to flutter; he would speak more softly and sink deeper into his chair. You learned to watch for those danger signs. His

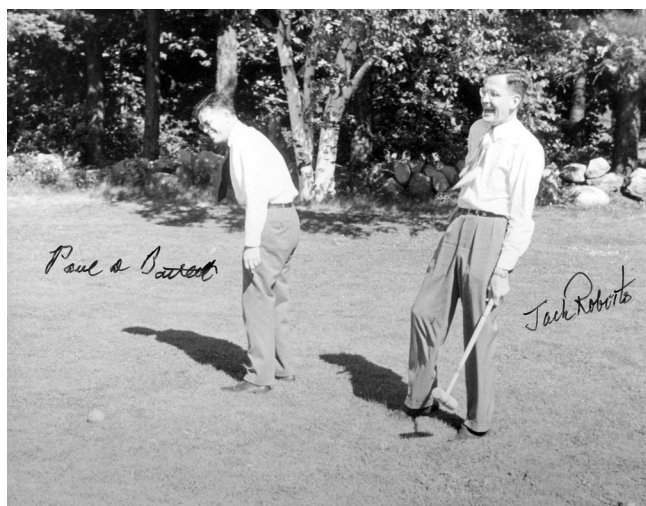
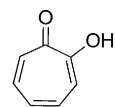


Figure 10. Roberts playing croquet with Paul Bartlett at the 1948 Reaction Mechanism Conference which was part of the Gordon Conference series at that time, Colby College, 1948. Note the formality of the dress in the 1940s. Photograph courtesy J. D. Roberts.

graduate students used to call him ‘the iron fist in the velvet glove’.^[3]

On Paul D. Bartlett (Figure 10), leading physical organic chemist (Harvard): „I always think of him as a typical Vermonter, but in fact, he was born in Butler, Indiana. Of good height, lean but not thin, with rugged features, he could pass as a woodsman, except for his heavy glasses that reflected earlier serious eye problems and severe nearsightedness. He seemed somewhat reserved and often spoke with abruptness, which masked a marvelous sense of humor that could erupt into warm and vigorous laughter. Paul liked to be precise; his words were carefully chosen and his sentences concise. He was not worldly in the fashionable sense, but worldly in the scholarly sense, with broad interests and high ideals.”^[3]

On Michael J. S. Dewar, eminent theoretical, computational and experimental organic chemist (Queen Mary College, Chicago, Texas): „... the era’s Peck’s Bad Boy of chemistry... a genius, broad of interests, quick of intelligence, very outspoken, and possessing a gargantuan humor... achieved instant fame by suggesting the seven-membered ring tropolone structure for colchicine in 1945... Dewar loves to take pot shots at anybody’s sacred cows and then bursts into a sort of shy, nervous, embarrassed laughter. No statement seems too outrageous for him to make. Relatively short, built like one of those round-bottomed, regain-upright dolls, with a profile like New Hampshire’s ‘Great Stone Face’...”^[3]



Tropolone

On Robert S. Mulliken, physicist and chemist, developer of molecular orbital theory, and winner of the 1966 Nobel Prize in Chemistry (University of Chicago): „Mulliken had a hard time making an impression; he was sort of quiet, rather blank-looking, and could never seem to deliver a straight answer to a question.”^[23]

On Linus Pauling, chemist, biochemist, peace advocate, often called one of the founders of quantum chemistry and molecular biology, recipient of the Nobel Prize in Chemistry (1954) and in Peace (1962) (Caltech): „The personal warmth that he expresses when he smiles and his large, luminous eyes beam at you is an unforgettable experience.”^[24] „... how tough, tireless, persistent, and shrewd Pauling was in pursuing his goals against great odds, entrenched dogma, and personal animosities.”^[24]

On Sir Robert Robinson, winner of the Nobel Prize in Chemistry (1947) (Manchester, Sydney, Oxford): „Every time that I met Robinson, he would spend ten minutes telling me how much he hated [Sir Christopher] Ingold and everything he did. Then he would stop and he wouldn’t do what most people in his position usually did and start telling you what they were doing. What he wanted to know as what you were doing. So I would tell him about these things, and he was really complimentary. He was so encouraging. I just couldn’t believe that Robinson was the bitter old man that many people seemed to know of.”^[10]

On John Sheehan, synthetic organic chemist who first synthesized penicillin (MIT): „Sheehan was a first-rate chemist, really Nobel Prize category, and, in fact, he did things that Woodward was not able to do, but his image wasn’t as impressive. He looked a bit like an Irish politician; he just never looked quite smart enough, but he was a very, very clever, very disarming guy... He used theory ably, but his papers seldom reflected the fact, and he resisted presenting *ex post facto* rationalizations as *a priori* reasoning...”^[23]

On Whitesides, chemist and entrepreneur (MIT and Harvard) when he was a graduate student in Roberts’s group: „George was a phenomenon and made many things work... George was so sharp and outwardly sarcastic that he had a somewhat depressing effect on the less intellectually gifted graduate students... Some people find him hard to take. There is another, very different, side to George that many people do not encounter. A warmth and humor... shows up in a special way in his letters. Another facet of George’s other side is seen when he is with his children—the relationship is warm and caring.”^[3]

On R. B. Woodward: „Our postdoctoral group loved to congregate in Woodward’s office after seminars, either for a rehash of the seminar or to listen to his views on current developments. Many of those sessions were Socratic, with problems posed, discussed, and solved. Others were more Delphic. Bartlett accused us of going to the horse’s mouth, and observed (correctly), ‘He will practically neigh for you’ (Figure 11). We generated three axioms about Woodward: He never got drunk, he never got tired, and he never perspired. Each of these became less axiomatic on one occasion or the other, but they held up very well indeed for many years.”^[3]



Figure 11. R. B. Woodward in his sedan chair being transported by his students. At the far left is Stuart Schreiber and in the middle, front is Max Tishler (Merck).

Humor: On Computers and George Whitesides

Whitesides wrote to Roberts (1965): „M.I.T., being as it is a world center of computer application, has just decided to close permanently its only working 7090 [computer]... This admirable trend will soon have me reduced to abacus or toes... I admit that it's comforting to learn these little skills as insurance against my old age. I wonder if key-punch operator would be a step up or down in the academic world?“^[43]

Roberts's response: „Thank you for your letter informing me of your availability as a key-punch operator—the way we are cranking out calculations, we may need you back in that capability very shortly.“^[44]

On Hiring Recommendations for Harvard

In a letter to Woodward: „Needless to say, I am touched, if not overwhelmed, by your intimation that Harvard University—and, in particular, its staff of illustrious professors of organic chemistry—is leaning over breathlessly in anticipation of the sage words of advice which I might offer with regard to Harvard's acute staffing problem in organic chemistry. Now I know full well that you actually only value my opinion when it agrees with your prior firm judgment—indeed, the fact that you have ignored my prior recommendations is excellent evidence of the correctness of this view...“^[45]

Scientists Speaking Out About Public Policy

„I think they ought to speak out... I think that scientists have every right to speak and sound just as infallible as the politicians... And I think scientists often get nervous about making decisions in which they can't be absolutely objective, or can't decide on a scientific basis. But I think they have a duty to speak out. The fact that people listen is what makes [politicians] mad.“^[23]

On Predicting the Future of Chemistry

„I used to tell people that, if I knew where chemistry was going, I'd go and get there first.“^[46]

On the Transience of Fame

„Memory of the titans of any given era of modern chemistry tends to fade rapidly from generation to generation. Unless one is identified by name in connection with some particular discovery or technique, or with the Nobel Prize (and perhaps not even that), one's most important contributions usually become an anonymous part of general chemical knowledge. Even such a titan as G. N. Lewis, who was extraordinarily influential for a long period, could probably only be identified by today's students through widely used 'Lewis electronic structures.' The problem of identifying achievements with people is a very difficult one for textbook writers, because you never know where to draw the line. Every fact or concept is associated with people, and mistakes in attributing priority are never forgiven.“^[3]

Roberts's Wisdom about Aging

„When [Lee A. DuBridge, former president of Caltech] talked, he knew, like most old people don't, when to stop.“^[23]

Roberts Reflecting on His Life

„After many years of being in more or less center stage, it is an odd feeling to run into 'Roberts? Who? Oh, I thought you were much older.' (Perhaps dead?) But that is the inevitable course of history. In this respect, scientists are no different from football or baseball players, and genuine Hall of Famers are very rare indeed. The memories even of many who seemed indelibly engraved on the edifice of organic chemistry in my early days, such as von Baeyer, Wieland, Willstätter, Ruzicka, Karrer, Kohler, and Meerwein, are not well-known, if at all, by today's organic chemistry students.

„In the absence of research immortality, the real joy of accomplishment has to be in the achievements of one's students and postdoctoral associates and, in turn, their students and postdoctoral associates...“^[3]

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