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**OBITUARY**

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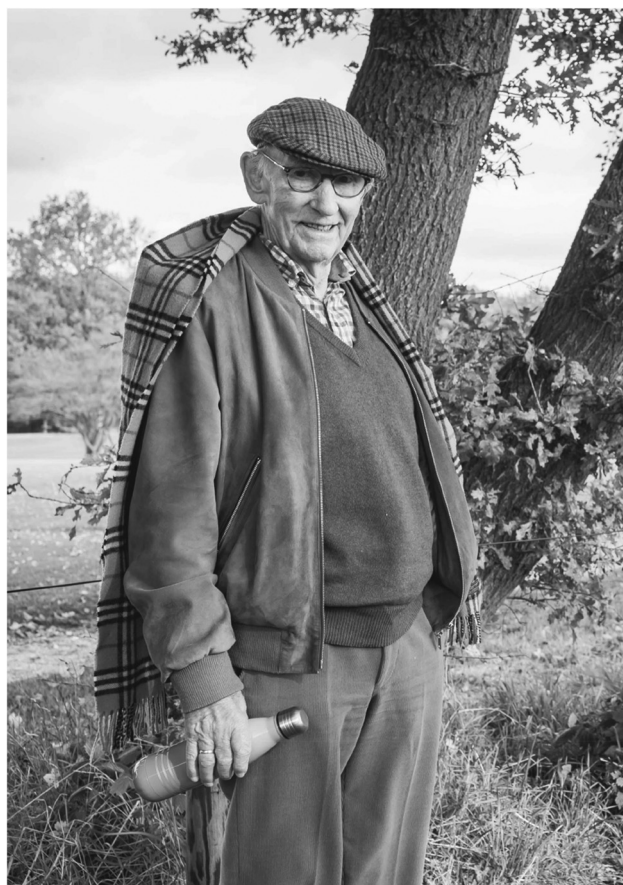


## Obituary: Roger Arthur Sheldon (1942–2025)

 Martyn Poliakoff <sup>a</sup> and Ben L. Feringa <sup>b</sup>

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Portrait of Roger – Frank Sheldon

Roger Sheldon, who died on 6<sup>th</sup> October 2025, was an outstanding scientist

and a pioneering inspirational figure for all of us who work in the field of green and sustainable chemistry. From 1999–2002, Roger served as the founding Chair of the Editorial Board of this journal and thereafter remained a member of the Editorial Advisory Board.

His contribution was neatly summed up in the citation of his 2010 RSC Green Chemistry Award. “*In recognition of the*

*role that he has played as one of the founding fathers of green chemistry and in particular for his work on the development of clean, catalytic technologies for waste minimisation and elimination of toxic/hazardous materials in chemicals manufacture*”. For decades, he has been a travelling ambassador for green chemistry, widely recognized as an excellent and inspiring lecturer. This has been

<sup>a</sup>School of Chemistry, University of Nottingham, Nottingham, NG7 2RD, UK

E-mail: [martyn.poliakoff@nottingham.ac.uk](mailto:martyn.poliakoff@nottingham.ac.uk)

<sup>b</sup>Advanced Research Centre CBBC, Stratingh Institute for Chemistry, Faculty of Science and Engineering, University of Groningen, Nijenborgh 4, Groningen, 9747 AG, Netherlands. E-mail: [b.l.feringa@rug.nl](mailto:b.l.feringa@rug.nl)



reflected by his family receiving messages of condolence from across the world (Australia, Japan, China, Ethiopia, Russia, South Africa, Europe and the Americas). This obituary aims both to give a flavour of Roger's scientific work and to act as an introduction to the virtual collection of his papers, published by the Royal Society of Chemistry.

A turning point in Roger's scientific career came while he was working in the Netherlands in the 1980s where he was involved in a somewhat hair-raising industrial process to manufacture phloroglucinol from TNT (Fig. 1).<sup>1</sup> He realised that only 5% by weight of the starting materials ended up in the desired product. The rest was waste and Roger laconically said words to the effect "The waste was loaded onto a lorry and sent to

East Germany". Even so, disposal of the waste cost nearly as much as the value of the product. This led him to a lifetime's interest in quantifying chemical waste and how best to eliminate or valorise it. As shown in Fig. 1, Roger began using "atom utilisation", a concept that he invented essentially simultaneously with Trost's Atom Economy.<sup>2</sup> However, his real breakthrough came with his environmental or *E*-factor, kilos of waste per kilo of product. Although a very simple metric, the *E*-factor has stood the test of time and its use is widespread throughout green chemistry.

Phloroglucinol was not the first product that had led Roger to thinking about sustainability. In 1973, he was working at Shell when supplies of crude oil feedstocks were threatened by the Yom Kippur war. As a result, he was involved in research to

establish viable routes to platform chemicals *via* syngas generated from coal. Indeed he later published a book, *Chemicals from Synthesis Gas*.<sup>3</sup> In that book, Roger introduced the concept of 'syngas utilisation' to compare feedstock efficiencies of different routes from syngas to bulk chemicals. With hindsight, this was the seed that later led to his formulation of the concepts of atom utilisation and *E*-factors. Fifty years on, this chemistry has become highly relevant because the coal could be replaced by waste biomass as a source of syngas to provide sustainable non-petroleum-based chemicals (Fig. 2).

Roger was born on the outskirts of Nottingham, UK, in 1942 during World War 2. His father, Arthur, was a soldier in the artillery and was sent before Roger was born to defend Singapore. Arthur was taken prisoner by the Japanese and was tragically killed a year later in captivity on the Solomon Islands. So Roger never met his father. Many years later, Roger made an emotional visit to the war memorial in Singapore. Arthur's name is also inscribed on the war memorial in Stapleford, the Nottingham suburb where Roger grew up.

Aged 16, Roger left school and joined the pharmaceutical company Boots Pure Drug Co. as a laboratory technician. While at Boots he studied *via* what is now called "distance learning" to become, six years later, a Graduate of the Royal Institute of Chemistry. He was

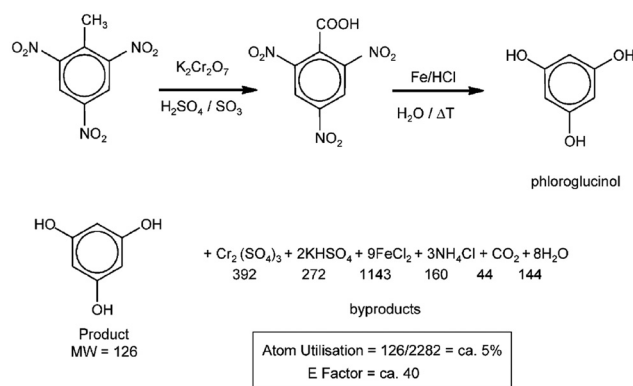


Fig. 1 The process for manufacturing the pharmaceutical ingredient phloroglucinol, which initially triggered Roger's interest in waste. Taken from ref. 1.

### Chemicals from Coal Gasification(Shell Project 1974)

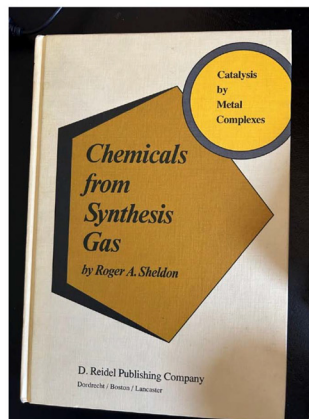
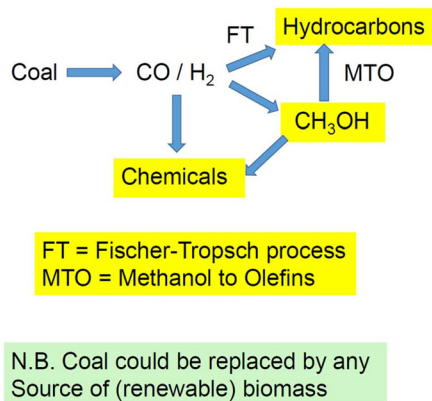


Fig. 2 One of Roger's slides from one of his last lectures, given at the Royal Society, which was subsequently published (taken from a slide deck given to Martyn Poliakoff by Roger).<sup>13</sup>



then supported by the chemical company Albright & Wilson for a PhD in organic chemistry at Leicester University under the supervision of R. S. Davidson and S. Trippett. His thesis, *Some reactions of tetraphenylidiphosphine*,<sup>4</sup> was submitted in 1967.

After his PhD, Roger spent two years as a postdoctoral fellow with Jay Kochi at Case Western Reserve and Indiana Universities working on photochemical and thermal oxidations. Indeed, oxidation chemistry remained an interest for the rest of Roger's career. In 1969 he moved to the Netherlands where, apart from sabbatical leave, he lived and worked for the rest of his life. His first job was as a research chemist at Koninklijke Shell Laboratories, Amsterdam, where the future Nobel Laureate Ben Feringa later became a colleague exploring new catalytic oxidations. Ben vividly remembers numerous discussions with Roger who was working in the Exploratory Chemistry Group at Shell: *"Catalytic oxidations, often notoriously unselective, were a fantastic playground for Roger to challenge me on atom economy, environmental impact and the waste produced. I will not easily forget his demanding questions and critical analysis. He was a great inspiration to all of us pushing the catalysis frontiers to come up with real sustainable solutions to*

*novel industrially viable transformations. He was a bit of a father figure for us as young scientists, challenging a lot and I learned much from him"*.

At Shell, Roger performed pioneering research on metal catalysed epoxidations with organic hydroperoxides, laying the foundations for much of the subsequent research in this area, including asymmetric epoxidations. He also played a key role in the development of the heterogeneous Ti/SiO<sub>2</sub> catalysed epoxidation of propylene with alkyl hydroperoxides which formed the basis of the well-known SMPO process for the co-production of styrene and propylene oxide, commercialised in 1974 and still operating today on a multi hundred-thousand-ton scale. The SMPO process constitutes an early example substituting a clean catalytic oxidation in place of a classical stoichiometric oxidation, generating large amounts of waste. Roger was awarded the RSC Award in Hydrocarbon Oxidation (1979) and the Berzelius Medal in Catalysis (1982) in recognition of this pioneering work. He co-authored a book with his postdoctoral supervisor Jay Kochi, *'Metal catalyzed oxidations of organic compounds'*, published in 1981, which is still regarded as a classic text on the subject.<sup>5</sup>

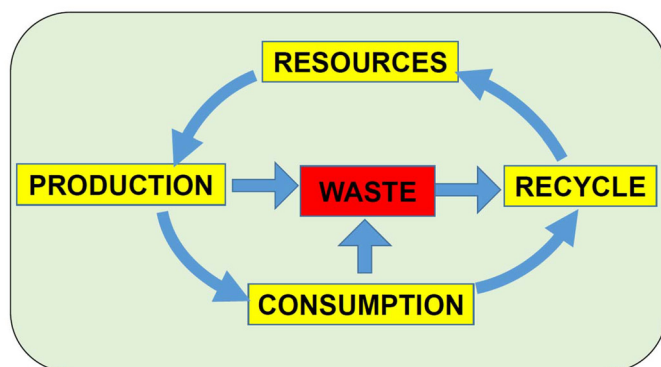
Roger pioneered the application of catalytic technologies in fine chemicals

production, a novel idea back in the 1970s, and subsequently catalysis became a pivotal theme in his research. In 1980, Roger became R&D Director at DSM-Andeno, Fine Chemicals, where his interest broadened to include the application of biocatalysis, in particular for the synthesis of pure enantiomers, on an industrial scale. His third book, *'Chirotechnology: the industrial synthesis of optically active compounds'*, has been used in graduate courses in universities world-wide.<sup>6</sup>

In 1991 Roger moved into academia as the Chair of Organic Chemistry and Catalysis at Delft University of Technology where he continued to promote the concepts of clean chemistry and waste minimisation. In our collection of his papers, you can read many of his original, groundbreaking contributions, including green catalytic oxidations of alcohols, catalysis in novel media and biocatalysis and his invention of a new organo-catalyst (PIPO) for alcohol oxidations in water.<sup>7</sup> He was the first to report biocatalysis in anhydrous ionic liquids and his review *'Catalytic reactions in ionic liquids'*<sup>8</sup> is one of the most highly cited articles in the entire history of Chemical Communications.

Roger invented an extremely effective method for immobilising enzymes as Cross-Linked Enzyme Aggregates (CLEAs)

## Transition to a Carbon Neutral Circular Bio-economy



**Fig. 3** One of Roger's Royal Society lecture slides showing his vision for the defossilisation of chemicals manufacture with waste biomass as the feedstock in a circular economy, with bio-based polymers (e.g. cellulose based polymers and polyhydroxyalkanoates) and enzymatic recycling of polymers back to the monomers (e.g. PET, PEF). This would reduce greenhouse gas emissions and eliminate plastic waste using chemo- and biocatalysis and electro(bio)catalysis. In short, Roger described this as a "new industrial elan" (taken from a slide deck given to Martyn Poliakoff by Roger).



which led, in 2002, to his founding the company, CLEA Technologies, to commercialise this novel technology.<sup>9</sup> He also pioneered enzymatic and chemo-enzymatic cascade processes, a topic of considerable current interest. A prominent example is the development, in collaboration with the company Codexis, of a green, three-enzyme process for the manufacture of atorvastatin,<sup>10</sup> a key intermediate for the cholesterol-lowering agent, Lipitor, currently the world's top selling drug. The process was commercialised and, in 2006, he and Codexis scientists received a US Presidential Green Chemistry Challenge Award for developing this process.

The common thread in all of Roger's research has been the drive to achieve precision and elegance in chemical production by applying atom efficient, low *E*-factor and step-economic processes in which a catalyst, if needed, exhibits high activity, selectivity and stability and is readily recovered and recycled. It is clear that Roger was particularly proud of the *E*-factor. What made the *E*-factor particularly valuable was that it included all of the auxiliaries for a process (solvents, spent catalysts, etc.) and also it could be easily applied to multi-step processes. Roger once wrote "*The concept was in essence a flagship of Green Chemistry avant la lettre and its introduction led to a paradigm shift in the concept of process*

*efficiency in organic synthesis, from one based largely on chemical yield of product to one that assigns value to eliminating waste and avoiding the use of toxic and/or hazardous materials*".<sup>11</sup> He wrote a paper, "*The E-factor 15 years on*" to mark his official retirement from Delft and this has been followed by a series of articles marking 25 and 30 years of the *E*-factor. Hopefully, one of our readers will contribute an article to mark 35 years in 2027. It is perhaps fitting that the manufacture of ibuprofen, invented at Roger's first employer Boots, has become one of the most frequently quoted examples to illustrate the use of the *E*-factor.

The key point about the *E*-factor is that it has been instrumental in focusing attention on the problem of waste in the chemical industry and it has had far-reaching consequences. It has been adopted by the chemical industry worldwide, from bulk chemicals to pharmaceutical manufacturers, to assess the sustainability of their processes. Many multinationals, such as Pfizer, L'Oreal and Sumitomo, routinely determine the *E*-factors of their manufacturing processes and use them as the basis for optimisation of their environmental footprint. Over the years, companies and academics have tweaked and refined the concept to produce a bewildering range of metrics to characterise waste. But as Roger put it with characteristic blunt-

ness, "*In our opinion, however, none of these alternative metrics offers any particular advantage over the E-factor for giving a mental picture of how wasteful a process is*".<sup>1</sup>

In his last few years in Delft, Roger published ground-breaking work in the area of catalytic conversions of renewable raw materials, such as triglycerides, carbohydrates and hydroxymethylfurfural, using water-soluble metal complexes, organo-catalysts or enzymes. The impact of this work is being increasingly recognized in the drive towards the widespread use of biomass for the sustainable production of chemicals. Indeed, Roger was the key author in a review on valorising agricultural waste<sup>12</sup> which is still being highly cited.

After retirement, Roger took up a part-time post at Wits University in Johannesburg, where his former co-worker Dean Brady is Professor of Biocatalysis and Director of the Molecular Sciences Institute. In 2015, Roger was elected Fellow of the Royal Society, the UK national academy of science, in recognition of his work in catalysis and green chemistry and, in 2018, he was awarded an Honorary Fellowship of the Royal Society of Chemistry, the highest award of our Society.

Towards the end of his life, Roger became increasingly concerned by the future of the global chemical industry.



Fig. 4 Two photos from Roger's retirement conference in Delft in December 2007. Left Istvan Horvath as the green Santa and right, Roger talking to the parrot at the banquet in his honour (photos by M. Poliakov).



How are we going to provide the chemicals that humanity needs when oil-based feedstocks become prohibitively costly? He crystallised his thoughts in late 2023 in a forceful lecture at the Royal Society.<sup>13</sup> He pointed out that his original version of the *E*-factor did not quantify the energy used by a process because such data were not available at the time. However, now that such data are becoming available, energy can be incorporated *via* the equivalent weight of CO<sub>2</sub> which he estimated as being, typically, 5 kg per kg of product.

His vision was summarised in one of his final slides, Fig. 3. He also criticised the tendency of chemists to over-complicate issues. Many people remember Roger's candid view of the so-called "rainbow of hydrogen", a classification of eight colours depending how the hydrogen is generated, when he said "This is all nonsense! Who thought this up? So, this is my (two-colour) rainbow; green hydrogen is made from electrolysis of water with sustainable energy and black hydrogen is hydrogen from unsustainable fossil resources".<sup>14</sup> Roger repeated his lecture by live video in March 2024 for undergraduates studying sustainable chemistry at the University of Nottingham. The recording of that lecture was shown on October 14<sup>th</sup> 2025 as a tribute to Roger for this year's students. It would probably have greatly pleased Roger to know that he was still teaching sustainability to undergraduates on the day of his funeral!

Finally, it must be stressed that Roger had a lighter side to his character. Ben Feringa remembers that Roger had a great sense of humour and that having a

pint with him was always wonderful after a tough discussion. This aspect of Roger was amply borne out at his retirement conference in Delft in December 2007 when the late Istvan Horvath serenaded Roger in the costume of a green Santa and then one of his co-workers dressed up as a giant parrot at the closing dinner (Fig. 4). Roger is survived by Jetty (Janna), his wife of almost 55 years, his children Annemarie and Frank, his daughter-in-law Myriam, and his five grandchildren, Jason, Femke, Tessa, Thomas and Eva. He will be sorely missed by chemists everywhere. He was irreplaceable.

We thank Frank Sheldon, Mike George, Pete Licence, Jonathan Hirst and Thomas Freese for helpful comments and suggestions.

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