

George M. Sheldrick (1942–2025)

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Figure 1

George M. Sheldrick and the diffractometer Quaternmass (in the background), which was designed and built from components from many manufacturers to boost its functionality. George had a broad interest in science and occupied his bright mind with problem solving in structural chemistry. Possibly, he was a scientist from his birth in Huddersfield, Yorkshire. He was certainly a chess player before becoming a chemist.

George Michael Sheldrick was not only the brilliant mind behind all that is *SHELX*, and an original scientist, enthusiastic for problem solving, but also an ideal collaborator, mentor and professor, with a wonderful sense of humour and deep humanity. George has touched the lives and careers of so many scientists, extending success, providing a sheltered and free work environment. He was always receptive to new ideas, encouraging independence, supportive and fair in his recognition of credit and ownership. His *SHELX* software has transformed crystallography, empowering researchers across chemistry, mineralogy and biology.

1. Success for all

Success for all was the motto of Huddersfield New College, George's school in the town where he was born, which had been led from 1909 to 1936 by the chess master Henry Ernest Atkins. George not only learned chess and German there, he



Figure 2

Cruickshank Symposium, UMIST, in September 1984. Front row, from left to right: Professor J. D. Dunitz FRS, Professor G. A. Jeffrey, Professor Dorothy Hodgkin FRS, Professor D. W. J. Cruickshank FRS, Professor Mary R. Truter. Behind: Professor K. N. Trueblood, Professor F. L. Hirshfeld, Dr J. S. Rollett, Professor J. E. Boggs, Professor A. C. T. North, Professor O. Bastiansen, Dr G. S. Pawley, Dr J. R. Helliwell, Professor G. M. Sheldrick (FRS 2001).

graduated in a much larger number of courses than was needed, or indeed usual, obtaining nine O-levels, six A-levels and two S-levels. At A-level, he achieved a distinction (the highest grade) in physics, mathematics and chemistry. George was awarded a Major Scholarship to study at Jesus College, Cambridge; at the time he was the only student in Jesus College to come from a non-private school. The school seems to have had a lasting influence. If the motto encapsulates a school's ethos and guiding principle, George took it with him throughout his career.

2. You have to choose between playing chess and playing chemistry

At Cambridge University, George continued to pursue his interest in chess and he took the natural sciences courses, common for a number of terms in mathematics, physics and chemistry. He specialized in the latter in his final year, attracted by structural chemistry and the cutting-edge methods being developed in Cambridge. Structure was providing invaluable information to understand the versatile chemical bonding displayed in inorganic compounds. George worked on various modern structural methods when these were still in their early stages, writing computer programs for all the required calculations. Later on, as a professor, his structural chemistry lectures in Göttingen were exceptionally inspiring: George had been present at the beginning of modern structural methods and his course proposed puzzles and exercises along with the illustration of principles.

His PhD thesis entitled *NMR Studies of Inorganic Hydrides* (1966) was supervised by Evelyn Ebsworth, who influenced his career by confronting him with the need to choose his focus. Fortunately for crystallography, he decided against becoming a professional chess player. As part of his PhD, George prepared silyl phosphines and arsines, the structures of which were unknown. The difficulties associated with this study of extremely poisonous and pyrophoric compounds may not be obvious to modern chemists. The absence of certain signals in the $\text{P}(\text{SiH}_3)_3$ infrared and Raman spectra led to the conclusion that the experiment was consistent with a planar configuration of the heavy atoms.

After his thesis, he took the opportunity to reinvestigate the structures using electron diffraction in the gas phase, contacting Durward Cruickshank at the University of Glasgow. Cruickshank generously shared his equipment and notes on refinement routines, later acknowledged by George for providing the nucleation point to start his *SHELX* work. Electron diffraction established the pyramidal instead of planar environment at the central atom and the paper by Beagley *et al.* (1968) adds to this conclusion: *The structural results do demonstrate the dangers of making geometrical predictions on the basis of the absence of bands in i.r. or Raman spectra, since these may simply be too weak to be observed.*

After his PhD in 1966, George was elected a Fellow of Jesus College. When Ebsworth left Cambridge to become Professor in Edinburgh, George, just 25 years old, shouldered the weighty responsibility of supervising his remaining PhD students during the completion of their work.



Figure 3

It was in Cambridge where George met the love of his life, Katherine Elizabeth Herford. They were married in Jesus College on 13 July 1968.

During this period, the structure of $\text{Fe}(\text{CO})_5$ was determined by electron diffraction in the gas phase and published in *Acta Crystallographica Section B* (Beagley *et al.*, 1969), showing that *Acta Crystallographica* journals were never limited to crystallographic studies alone but have structural questions at heart.

3. *SHELX* before *SHELX-76*

SHELX has transformed crystallography, empowering researchers across chemistry, mineralogy and biology. In one of the most cited papers ever (Sheldrick, 2008), George describes the birth of the *SHELX* programs. While typically our publications are scored by the impact factor of a journal, this paper rocketed the impact factor of the journal *Acta Crystallographica Section A* from 2.05 to 54, surpassing that of *Science*, *Nature* or *Cell* in the years 2009 and 2010. This establishes how many scientific projects must have been aided by George's insightful work and singular solutions. A work that is unstoppable because George has left a legacy not only in his methods and in the achievements they have mediated, but also in training and shaping the next generation of scientists building on his example.

The *Short history of SHELX* (Sheldrick, 2008) relates the technical innovations that were introduced, but understates

the epic quest for solutions to overcome the extreme limitations of computing at the time, when it was not a matter of a program being faster, but whether a given calculation was possible at all.

One example involves the PDP8 computer controlling the Stoe two-circle diffractometer installed in 1969, with its small 4 kb memory. George's program, written to replace the limited one supplied with the machine, filled all the memory, which in the absence of additional physical storage had to hold all the required instructions and data; input and output were on punched paper tape. The issue with filling the memory is that, if written in assembly code and translated by the assembler, this compiler would need to occupy some of the memory itself. Hence George translated his code directly into octal (binary code with bits combined together in threes so that they had a value between 0 and 7), so that each program step was a 4-digit instruction or item of data between 0000 and 7777. Such was the shortage of memory that George used some program instructions to double up as numerical data constants if they happened to have the right value, and so he managed to pack everything necessary for the calculation into the tiny space. At this point, a disclaimer is needed for the benefit of newcomers: this is considered very bad programming practice and should not be emulated... but 'needs must' and under dire straits it worked!

Another trick George used in his Fortran programming at a time when computer memory was limited (the 1970s and 80s with multi-user computers) was a standard option that large programs could be divided into smaller segments with one core section and others that could be called to overwrite each other. These were called overlays and the process was called chaining. Programming the control of a four-circle Syntex P21 diffractometer, George managed to make the program alter itself during execution, something that would not have been possible with a higher-level language such as Fortran, but in binary everything was valid! This allowed him to provide the multiple measurements needed for absorption correction, which would otherwise have required a separate program with the available hardware.

SHELX literally shaped the way in which crystallography was practised, fundamentally changing the routine in a chemical laboratory. A number of laboratories had programs to compute crystallographic operations, but typically they were case-specific calculations for the problem under study, that addressed individual steps involved. This extended calculations as results from one step would be needed for the next one. George contrived generally applicable solutions (*e.g.* valid for all space groups) to all necessary operations, compact enough to fit the limits of computers. The time required for any refinement operation on the fastest, state-of-the-art mainframe computers in Cambridge would occupy at least one night. Integrating the different steps required engendered a routine where the day would be dedicated to setting up experiments, interpreting results, solving problems and designing calculations that would run through the night. His free-variables to encode chosen parameters introduced flexibility. And to top it all they were user-friendly, including

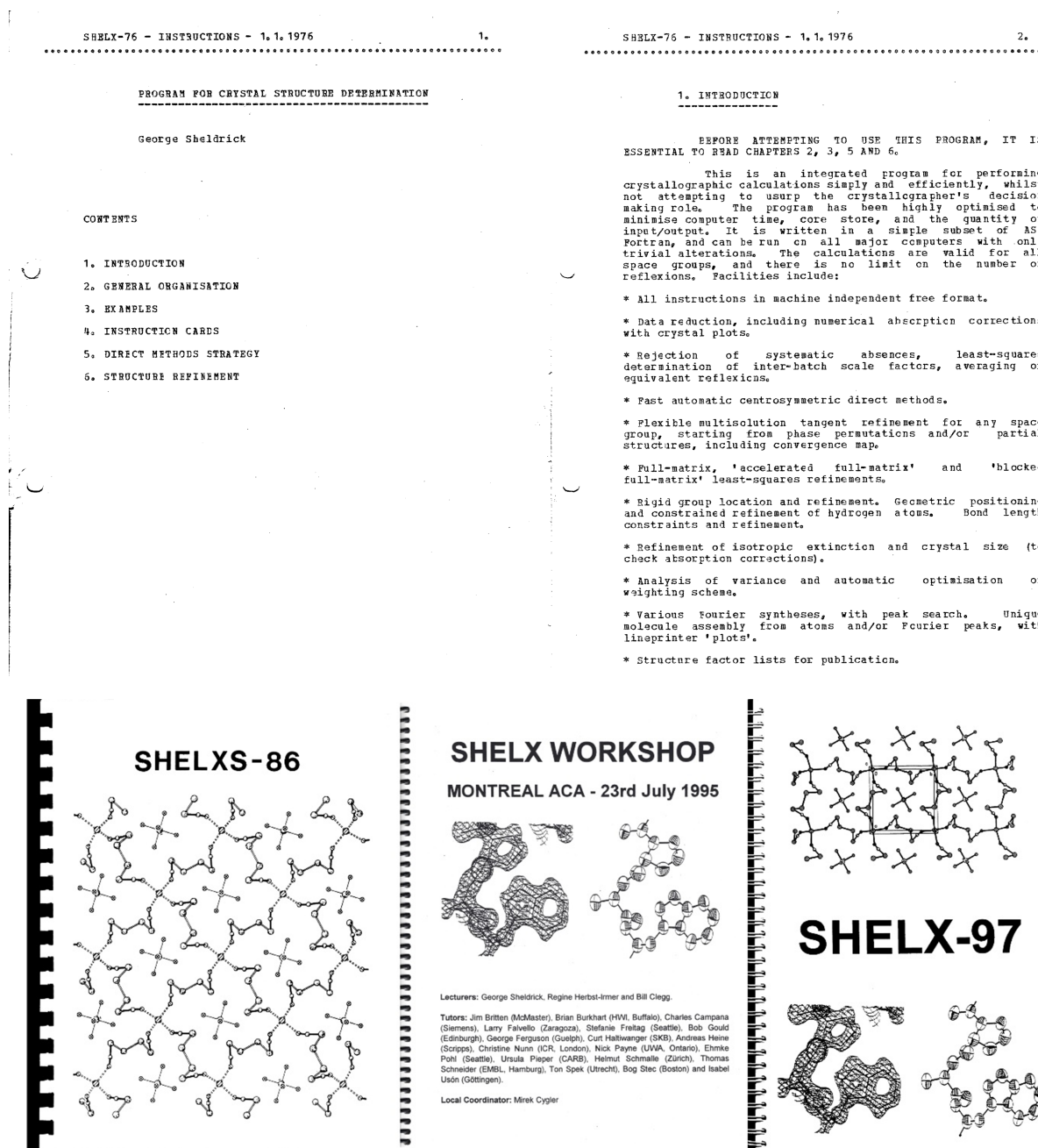


Figure 4

From the start, *SHELX* was user-friendly: well documented and supported. On submitting this manuscript, *SHELX-76* was downloaded from the IUCr website <https://www.iucr.org/resources/commissions/crystallographic-computing/software-museum>. The source was compiled with ifort -f66 SHELXN.FOR (SHELXN.FOR is the shelx76 version extended in 1977 to address neutron scattering) and worked out of the box testifying George's philosophy: zero dependencies and upwards compatibility.

free-format input and were well documented. In the words of many crystallographers, George democratized X-ray crystallography.

It is clear why the cases for which *SHELX* was developed represented milestones: after all, even Julius Caesar had to add the fact that he saw between his coming and conquering! Application of the gaze on chemistry developed by George illustrates the kind of breakthrough that *SHELX* made possible in Cambridge then and later worldwide. Two exam-

ples of important problems solved in collaboration with Olga Kennard should be mentioned. DNA at atomic resolution was seen for the first time in the deoxy-tetranucleotide (dAdT-dAdT) that was phased beginning with only two comparatively light phosphorus atoms from the Patterson analysis and applying tangent expansion, which would eventually become the routine TEXP in *SHELXS* (Viswamitra *et al.*, 1978). A degradation product of the natural antibiotic vancomycin, then and now a last resort antibiotic, would yield a first

characterization, needed to allow chemistry to target synthetic analogues as well as understanding of its mode of action binding to the bacterial cell wall (Sheldrick *et al.*, 1978).

4. *An expert is someone who has made all possible errors once* – George Sheldrick

George was always willing to help with the solution of crystallographic problems, in a way that also transmitted his knowledge and thus promoted the training and independence of the recipient. In addition to sharing his programs with other laboratories, he would provide help at the same time imparting insight and tools on how his solution to a problem was contrived. George was very patient and encouraging, although with particularly catastrophic errors (chemistry getting out of control or a diffractometer collision) he would add *but you do not need to repeat this one*.

George applied for the Inorganic Chemistry university chair in Göttingen in 1975, when he was 33. As usual for such appointments, the process was delayed for a couple of years and, by the time he was offered the chair, Cambridge could not believe that the Sheldricks – who had only recently bought a house and had a young baby – were leaving for Göttingen.

In Göttingen, George had a state-of-the-art computer but it would take a couple of years to acquire a diffractometer. From the start, the mentoring of emergent scientists, supported to develop their own research within the German Habilitation system and other schemes, was an essential part of George's activities. Working with him was inspiring and fun; it covered a broad range of interests in chemistry, geology and biology evolving over the years. He was always receptive to our ideas, encouraging our independence, providing the means to support them and giving us credit for what we accomplished. At the same time, we were spared the financial worries or conflicts that were common in many institutes. If Goethe was right in writing that 'character is built in the tempest of life while talent requires the calm', George shaped the optimal environment to develop our talents. (Some of us were occasionally more proactive than we should have been in generating opportunities to develop character. But George did not interfere in arguments and trusted us to outgrow pointless conflicts.) In Cambridge and Göttingen, George closely supervised more than a hundred theses. He supported attendance of his group at conferences not only as part of their training, but also to assist in achieving their career goals, for instance by meeting possible supervisors in person before applying for a postdoctoral position. This is clearly not to the benefit of the laboratory that loses their members but benefits the scientific community in general. These personal contacts were crucial as any poor choice might be a blow to career expectation.

One unusual trait George had was that he always pondered what people said, not who said it. Experience shows that humans are more ready to value what their friends, allies and authority figures state as being correct and search for reasons why their competition must be wrong! This lack of prejudice may explain why George's research group was always most

diverse: he gave everyone fair opportunities. Listening to colleagues at conferences and reading their papers with impartiality prompted him to try out their ideas in his programs. He would not criticize if such ideas were unsuccessful in his tests but would adopt them if successful and give generous credit to the originators, publicising their work. No wonder that as a member of George's group one enjoyed a generally positive attitude from the community.

Among all collaborations, the prolific co-operation with his colleague in the Institute of Inorganic Chemistry, Professor Herbert W. Roesky, should be highlighted; this continued harmoniously throughout their careers. Their highly successful combination of problem-solving, structural characterization with original, creative synthesis, was recognized with the Gottfried Wilhelm Leibniz Prize, the highest award of the German Deutsche Forschungsgemeinschaft (DFG), in 1988.

Other awards and honours from the scientific, chemical and crystallographic societies include the following: Meldola and Corday-Morgan (Royal Society of Chemistry), Carl-Hermann (DGK), Patterson (ACA), Perutz (ECA), Ewald (IUCr) and Aminoff (Royal Swedish Academy of Sciences), membership of the Niedersächsische Akademie der Wissenschaften zu Göttingen in 1989, and the crowning glory for the British of being elected a Fellow of the Royal Society. While feeling deeply honoured by the recognition of his peers, George would become embarrassed when being thanked or praised. In 2019, at the ECM in Vienna, during the 'Teaching a young dog old tricks' microsymposium, a crystallographer in the audience improvised a concise speech thanking George for the contribution in his programs, which was unanimously backed by a standing ovation. George blushed, but proudly told Katherine about this when they met after the session. Since 2024, the ECA has conferred the Sheldrick Prize to a non-tenured scientist for extraordinary work in the field of structural sciences.

The first major program releases in Göttingen, *SHELXS*-86, *SHELXS*-90 and *SHELXL*-93, greatly extended the power of solution with phase annealing (Sheldrick *et al.*, 1993) and the flexibility of refinement by including a variety of restraints, handling of site substitutions and other well integrated and elegant options to handle complex disorder situations in a versatile and user-friendly way. Introducing refinement based on intensities (rather than structure factors) improved the accuracy of the determinations. *SHELXL*-97 continued this, extending the scope of the program to handle macromolecular structures at atomic resolution.

Twinning, the frequent phenomenon in crystallography whereby several crystal lattices grow intertwined, was also successfully handled. The complications for structure solution and refinement derived from scattering contributed from different lattices, with total or partial overlap were one of the challenges actively addressed in the laboratory in the development of *SHELXL*-93. Twinning – if unaccounted for – could lead to erroneous structural determination. Within mineralogy, this and additional solutions to multiple substitution of ions occupying equivalent sites made it possible to overcome significant hurdles. This is exemplified in the naming of a



Figure 5

Daily meetings and occasional visitors around the coffee table. From left to right: Frank Pauer, Sally Brooker, Thomas Kottke, Ursula Pieper, Kirsten Krahnstöver, Axel Göhr, Regine Herbst-Irmer, Holger Beck, Erhard Irmer, George Sheldrick.

mineral from Mount Saint-Hilaire in Canada to acknowledge the contribution of the *SHELX* methods. Sheldrickite is a sodium calcium carbonate fluoride mineral, named in honour of George M. Sheldrick to acknowledge that determination of the structure of this mineral required the software's capability of handling twinned crystals; thus, recognition of the help woven in the lives of others was also engraved in stone!

The extension of direct methods to solve the phase problem in more complicated structures of macromolecules (larger and without heavy atoms) was implemented in the second half of the 1990s in George's program *SHELXD*. This was developed

in friendly competition with the Shake and Bake method introduced by the group of Herbert Hauptman, who had been awarded the Nobel Prize in the year 1985 for his work on direct methods. Indeed, both groups worked independently but acknowledged each other's merits with remarkable fairness. George increased the radius of convergence by introducing *random omit maps*: discarding one third of the atoms in the current solution at random allowed locked solutions to shake off model bias and proceed into completeness. George would make starts consistent with the Patterson function without solving it, in order to preserve enough randomness to



Figure 6

Group in the early 1990s around the Quaternary diffractometer. Back row left to right: Heinz Gornitzka, Dietmar Stalke, Ludger Häming, George M. Sheldrick, Alexander Steiner, Helmut Dehnhardt, Annja Kuhn, Regine Herbst-Irmer, Andreas Heine. Front row: Ehmke Pohl, Miene Schäfer, Ursula Pieper.



Figure 7

George and his group at the ACA 2011. Left to right: Birger Dittrich, Christian Hübschle, Peter Müller, Kevin Präpper, George M. Sheldrick accompanied by Katherine E. Sheldrick.

avoid repeating starts. Also, along with starts generated from a random set of atoms it was possible to seed solutions from a randomly placed and locally optimized fragment. The success of *SHELXD* peaked at a conference on direct methods – the famous Erice School – in 1997, during which the structure of the triclinic form of lysozyme was solved. Overcoming the 1000 atom barrier (the structure had 1001 independent atoms) proved the power of *SHELXD* but the impact of this advance is better reflected in the determination of a number of structures, which had remained unsolved for years until then: numerous antibiotics like mersacidin, several actinomycins, balhimycin... culminating in the solution of vancomycin, for which investigation of a subproduct in Cambridge had allowed George a first glimpse 20 years earlier. Vancomycin was solved in parallel by the Shake and Bake team and published independently within a friendly agreement to tie submission time of the respective manuscripts so as not to harm the other group. This is not unheard of, but George's use of his methods to solve the structure of the pumpkin trypsin inhibitor from competitors during a crystallography school in Poland whereas we were working in Göttingen on the very close squash inhibitor was rather remarkable. Their data were better than ours, he fairly acknowledged returning from this trip. Such plant inhibitors, like the antibiotics; some active peptides like octreotide; peptidic toxins from leeches, cone-snails, scorpions or snakes; large cyclodextrins and cycloamyloses mimicking starch had waited decades for these methods to unravel their structures from crystals. Some proteins were also solved *ab initio*: cytochrome *c*₆, HIPIP, ferredoxin. Later on, poly(A) RNA would be solved at atomic resolution, 50 years after its fibre diffraction structure in Alexander Rich's laboratory.

Extension to macromolecules was most effective in experimental phasing; so much so that the application of the *SHELXC*–*SHELXD*–*SHELXE* pipeline for experimental

structure phasing solved too many structures to count or keep track of. Both robust and efficient, they became the standard to calibrate and evaluate performance of synchrotron beamlines.

George Sheldrick should have entered the *emeritus* status in 2011 but received a *Niedersachsenprofessur*, allowing him to extend his chair for six further years. This time was also remarkably productive: a last rewrite in *SHELXL* (Sheldrick, 2015a) allowed him to incorporate features to handle all types of radiation or to read in scattering contributions to address disordered solvent in large supramolecular structures. Unlike previous software, undergoing several cycles of rewriting, *SHELXT* (Sheldrick, 2015b), his dual-space recycling program integrating structure solution with space group determination and element assignment, was written in one sweep as George knew exactly what he wanted to program and, once written, it all worked according to plan.

In lectures, talks or conversations, George would explain complicated concepts making them come across as compellingly simple. His teaching would always prompt critical thinking, as when he faked a nuclear explosion producing a mushroom cloud in his experimental chemistry lecture. This was the 1980s and half of the audience started an *impromptu* demonstration against nuclear power before being absorbed in the debate of why this was impossible and the analysis of what experiment had really taken place. In the 21st century George started a well attended course on environmental chemistry with timely, thought-provoking lectures where he would transmit more chemistry than students realized. Many *SHELX* workshops were organized through the years and enthusiastically attended by students and tutors.

Former students and co-workers would frequently stop in Göttingen and pop by to join the coffee time, where daily group discussions would take place. Many of us have kept in

touch ever since, resorted to him for advice, to share news of personal or professional success or just for the pleasure of discussing science and puzzling problems.

The lasting legacy for those of us lucky enough to have interacted with George is that of having improved ourselves and our work by it: success for all. The appreciation is further seen in the response to the birthday parties (disguised as Christmas parties) that took place in 2012 and 2017. Also, in the surprise movie his whole group made for him in 2002. The plot followed a student in crystallography from the first steps to becoming *big and famous* (*groß und berühmt*), through a large collection of sketches based on true events. For example, there was a blackboard outside George's door where he would write down the details of the next group seminar. On the day where *Seminar über Symmetrie im Reziproken Raum* was announced, two very stressed new students were asking around where the reciprocal classroom was located. After experiencing that George could unexpectedly walk into the film set even at night or at weekends, the schedule was fixed during the time of his lectures!

George mentioned that the better funding opportunities in Germany at the time were not the main incentive to join the excellent University of Göttingen but that he and Katherine truly appreciated the qualities of the school system for raising their children Abigail, Nicola, Peter and Alexander; he also felt that German academia was more open and comfortably untied by class distinction. Not that George minded too much about nationality but when borders returned to Europe, George and Katherine acquired German citizenship, without

becoming less British. Their integration in German society beyond university is seen in Katherine's engagement in music. Their environmental concern motivated the rebuilding of their house, after it burned down in 2008, meticulously designed for energy efficiency with geothermal heat and air recycling, long before climate change became a major topic of public debate.

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