Memories of Giants:
Dick Marsh,
Philip Coppens
and
Howard Flack

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Howard D. Flack (1943-2017)

- Revolutionized the determination of the absolute structure of crystalline materials by X-ray diffraction
- Automatic absorption correction using intensity measurements from azimuthal scans
- Concise intensity statistics of Friedel opposites and classification of the reflections
- Merohedral twin interpretation spreadsheet
- The derivation of twin laws for (pseudo-)merohedry by coset decomposition

You know, PG Wodehouse said that “It is never difficult to distinguish between a Scotsman with a grievance and a ray of sunshine”, and I do recall that it was never very hard to tell if Howard disagreed with you! Of course, he was always right, but especially supportive and generous with ideas too - our absolute structure work would have been quite different without his influence

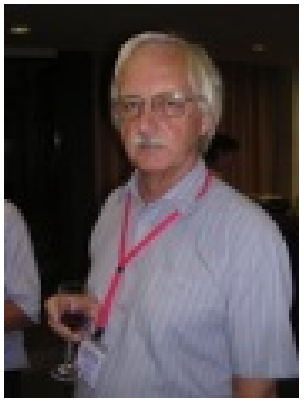
He had a real eye for turning vague ideas into equations. He wasn't happy unless this had been done, even in apparently simple cases, and was able to polish off a quick derivation, with all the contra and co-variant super and sub-scripts in the right places, which would have taken me days of tortured labour! Though they are far from simple, I think his last papers with Shmueli really demonstrate this beautifully, the effect of a centrosymmetric substructure and the FRIEDIF equations are perfect examples.

Simon Parsons

He had a very distinctive lecturing style - he almost seemed to “conduct himself” sometimes - and something of a predilection for cutting up apples 'live' in the coup de roi trick.

Howard loved telling stories, often focusing on humorous events which occurred in hotels and restaurants. It would be difficult to explain to folks how funny these were, as a retelling without Howard's fabulous gestures and funny voices would not work!

Howard was incredibly thorough. I asked his opinion on how F refinement should be weighted if you had reasonable estimates of sigma(F^2). Recall that Unit weights are very suitable if you have no reliable error model, as was the case with photographic data, and might still be the case if you are working with very poor crystals. His reply, without explanation, was a document showing that the mathematical outcome depends upon your prior beliefs. His Method 2 is what you generally find in the literature.



David Watkin

First Method

$G = F^2$

$G + \delta G = (F + \delta F)^2$

$\delta G = (F + \delta F)^2 - G$

$\delta G = F^2 + 2F\delta F + \delta F^2 - F^2$

$\delta G = \delta F\,(2F + \delta F)$

Equate δG with the standard deviation of G and use statistical weights:
$u = 1/(\delta G)^2$, $\delta G = u^{-½}$.

Equate δF with the standard deviation of F and use statistical weights:
$\omega = 1/(\delta F)^2$, $\delta F = \omega^{½}$.

$u^{-½} = \omega^{½}\,(2F + \omega^{½})$

$u = \omega\,/\,(2F + \omega^{½})^2$

Second Method

$G = F^2$

Use a Taylor expansion:

$G + \delta G = F^2 + \delta F\, dG/dF + ½(\delta F)^2\, d^2G/dF^2 + \ldots$

$dG/dF = 2F$; $d^2G/dF^2 = 2$ so

$\delta G = \delta F\, 2F + (\delta F)^2$

which is identical to the intermediate result in the first method.

Third (inverse) method

$F = G^{½}$

$F + \delta F = G^{½} + \delta G\, dF/dG + ½(\delta G)^2\, d^2F/dG^2 + \ldots$

$dF/dG = ½\, G^{-½}$; $d^2F/dG^2 = -¼G^{-3/2}$

$\delta F = \delta G\, ½\, G^{-½} - 1/8\, (\delta G)^2\, G^{-3/2}$

As above use: $\delta G = u^{-½}$ and $\delta F = \omega^{½}$.

$\omega^{½} = u^{-½}\, ½\, G^{-½} - 1/8\, (u^{-½})^2\, G^{-3/2}$

$\omega^{½} = u^{-½}\, ½\, F^{-1} - 1/8\, u^{-1}\, F^{-3}$

$\omega^{½} = ¼\, u^{-½}\, F^{-2}\, (\, 2\, F - ½\, u^{-½}\, F^{-1})$

$\omega = 16\, u\, F^4\, (\, 2\, F - ½\, u^{-½}\, F^{-1})^{-2}$

He asked me to read a draft of a paper. As ever, he did not beat about the bush in telling me what he thought of my reply.

Thank you for your comments on our manuscript. I'm sorry you found it such heavy going. I sent the MS to 16 people and 11 replied. Yours was the most negative of the reports that I received. I have of course corrected all of the funny English according to your counsel.

More interesting are his observations on the presumed enantio-purity of samples. That is why I was particularly determined to get George Tranter, a specialist in optical methods, to contribute to the TETASY Special Edition.

The trouble is the chemists. They are not prepared to quantify correctly (or at all) their prior knowledge concerning the enantiopurity. When one knows how 'enantiopure' substances are produced or enantiopurity is tested, it is clear that the chemists belief concerning the enantiopurity of their compound is totally unrealistic and very very optimistic. A fair number of the people who received our MS came back telling us stories where they had been misled by the information of the chemists. One 'enantiopure' compound crystallized in a centrosymmetric space group. …[the chemists were] finally happy to admit that their enantiopure compound contained 5% of the other enantiomer. So on crystallization, the centrosymmetric racemic compound precipitates first!

David Watkin

Chiroptical spectroscopy and the validation of crystal structure stereochemical assignments George E. Tranter, Delphine D. Le Pevelen, *Tetrahedron: Asymmetry* **2017,** *28,* 1192–1198.

In front of the Pegasus computer examining some 5-hole paper tape (ca. 1966). (from Mike Glazer) in Dame Kathleen Lonsdale's laboratory .

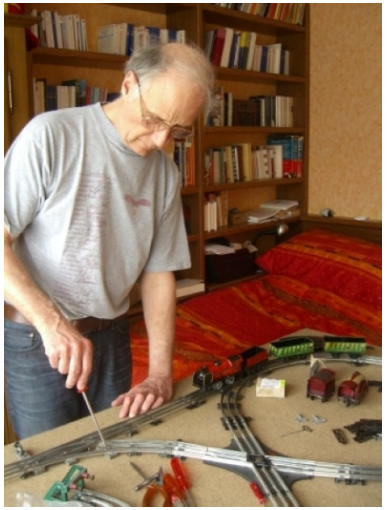
We're cousins!

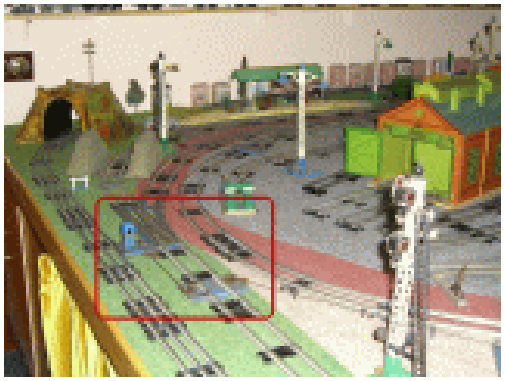
When circumstances in Israel dictated that the 2002 IUCr Congress would have to move to an alternative site, Howard Flack and Hans Grimmer worked extremely hard to make it all happen successfully!!!

Joel Bernstein

In addition to his vast scientific achievements, Howard was devoted to his wife Evelyne and children Patrick and Christine:

And a dedicated train hobbyist (see http://hornby.flack.ch for more!):





He loved traveling and riding with his wife Evelyne and the family:

Howard, I never had a chance to say thanks for your help in the latter part of my career…we never met until 2011, during David Watkin's retirement symposium in 2011.

I was searching for some insight into the thinking behind Yvon LePage's *OBLIQUE* program that predicted twin laws for a given unit cell. Howard was one of few who promised to help, and did!

"You are a lucky boy. I found the source code of the modified version of CREDUC which you need. … What you are looking for is an instruction which limits the maximum absolute value of *hu* + *kv* + *lw* to 2. It is very easy to do when you know exactly what to do and where the relevant instruction is to be found. What is more difficult is to understand why this is the critical criterion. I managed to work it out for myself and when I looked in the software, I found out that Le Page already knew about it for a very long time. This version asks you specifically what maximum value of *hu+kv+lw* you want. When you get the software to work, start with a value of 2 and then rerun with increased values." […emails late 2016]

The current result, *OMEGA,* is available at http://www.xray.chem.brandeis.edu. It is a powerful new program that meets the critiques of *OBLIQUE* set forth by Hans Grimmer. It writes the matrix twin laws for each case, and is an incomplete, evolving work. I can only hope to reach a deep understanding of the theoretical principles as I develop the program.

With Howard, we have not only lost an influential scientist and teacher, we have also lost a widely interested and cultured person. He was well read and familiar with, for example, Tristram Shandy as well as with the lore of Middle-earth. He loved music, opera and concerts. With Evelyne he assembled and restored an impressive collection of vintage toy trains and railway accessories produced by the British firm Hornby between 1920 and 1963. He was a good down-hill skier and horseback rider. And he was a wonderful companion with a fresh humour, funny and fair. He is survived by his wife Evelyne, his son Patrick and his daughter Christine.

David Watkin

Dieter Schwarzenbach

J. Appl. Cryst. 2017, *50*, 666-667

Read Howard's latest brilliant contribution in collaboration with David and Richard here:

HUG and SQUEEZE: using CRYSTALS to incorporate resonant-scattering in the SQUEEZE structure factor contributions to determine absolute structure (R.I. Cooper, H.D. Flack and D.J. Watkin)

Acta Crystallographica, 2017, **C73**, 845–853. [doi:10.1107/S2053229617013304]

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