Howard's international career in Switzerland since 1972

Gervais Chapuis

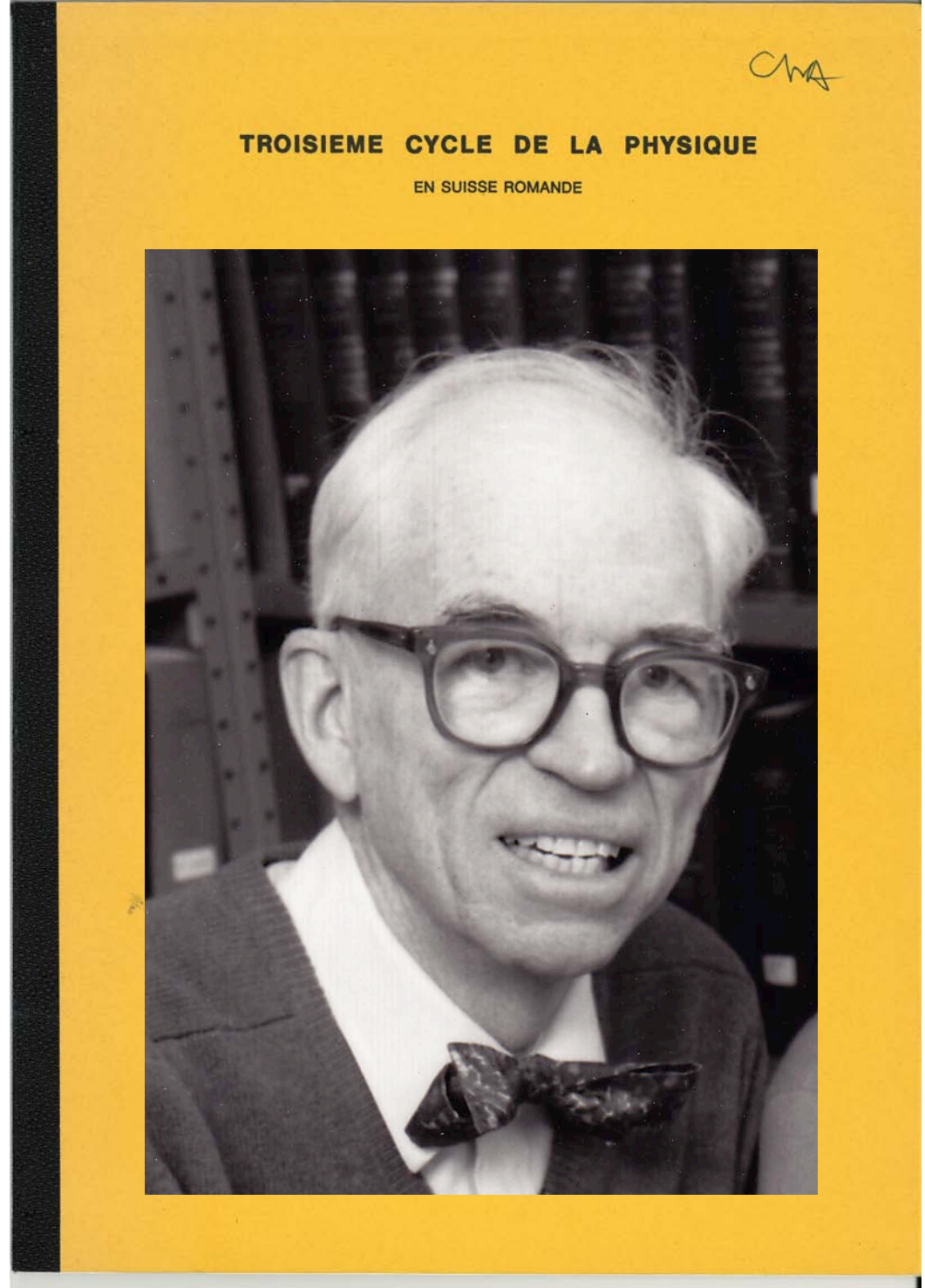
Lausanne

Outline

- The story behind Flack's parameter
- Howard's publications highlights
- The Zurich School of crystallography
- More Howard's pictures

A close relationship between Lausanne and Geneva crystallographers

David Templeton's series of lectures in the University of Lausanne and EPFL (1982) on anomalous scattering



Alternatively, one can say they indicate f'' values less than the true ones. We observed this phenomenon in a crystal of $U(BH_4)_4 \cdot O(C_2H_5)_2$ in which the ratio of the two configurations about 70:30 *(Rietz, Zalkin, Templeton, Edelstein and Templeton, 1978 Inorg.Chem.J ,658)*. Our method was to adjust f'' for uranium as one of the variables in the least-squares refinement of the crystal structure, with a result smaller than the correct value. We used this method because our original objective was to get an experimental value of → f " → from the diffraction data. → *Rogers (Acta Cryst. A37, 734, 1981)* suggested another method: apply a common correction factor → to → f'' → for 'every atom in the crystal and determine it in the least-squares refinement of the structure. The two methods are equivalent when only one kind of atom has an appreciable value of f', but the Rogers method is more logical for the general case. ¶

Rogers contribution

Acta Cryst. (1981). A**37**, 734–741

On the Application of Hamilton's Ratio Test to the Assignment of Absolute Configuration and an Alternative Test

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(*Received* 9 *July* 1980; *accepted* 6 *March* 1981)

ticular problem. A more rigorous justification can be achieved by expressing the atomic scattering factors of all the anomalous scatterers in a crystal in the form $f_{0j} + f'_j + i\eta f''_j$ and refining η, the chirality/polarity parameter. Its standard deviation offers an alternative and more realistic index of the probability of an assignment. A postscript contributed by Professor G. M. Sheldrick reports very encouraging results for η refinement of three structures.

Flack's idea on the enantiomorph polarity parameter

Abstract

The behaviour of Rogers's η parameter for enantiomorph-polarity estimation is examined theoretically and experimentally on simulated intensity data for seven well-assorted compounds. An alternative parameter x, based on incoherent scattering from twin components related by a centre of symmetry, is also considered. It is found that both parameters are very well adapted to implementation in a least-squares program and converge well. The η parameter can give false and over-precise indications of chirality–polarity for structures which are nearly centrosymmetric, whereas the x parameter does not have this fault and converges more rapidly than η.

Acta Cryst. (1983

Laborato *nsermet,*

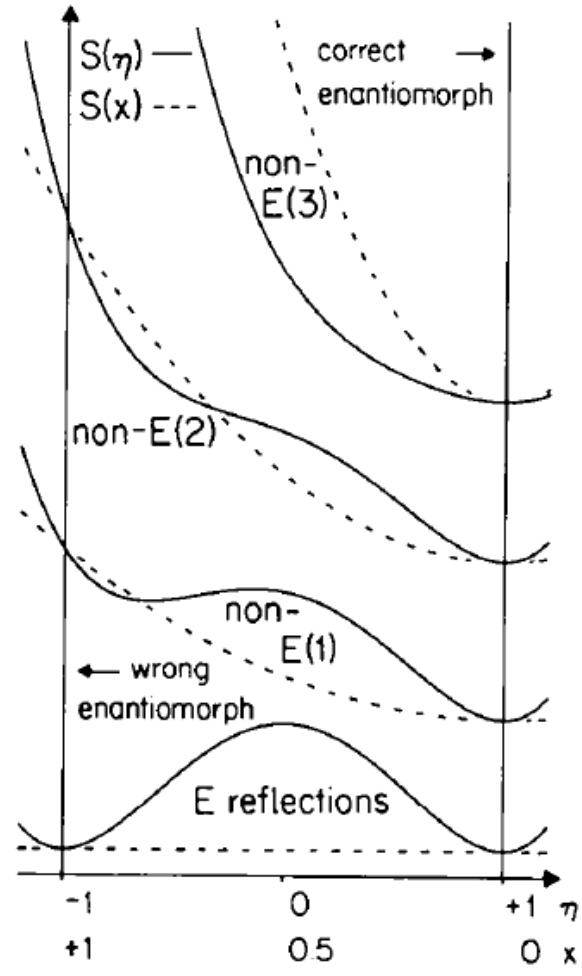
Flack's idea on the enantiomorph polarity parameter

Roger's η parameter

$$F(\mathbf{h},\eta) = \sum_j (f_j^0 + f_j' + i\eta f_j'')$$
$$\times (\cos 2\pi \mathbf{h}^T.\mathbf{x}_j + i\sin 2\pi \mathbf{h}^T.\mathbf{x}_j),$$

Flack's x parameter

$$|F(\mathbf{h},x)|^2 = (1-x)|F(\mathbf{h})|^2 + x|F(-\mathbf{h})|^2.$$



$$S_E = \sum_{\mathbf{h}} w(\mathbf{h})[|F_E(\mathbf{h},\eta)|^2 - |F_E(\mathbf{h},+1)|^2]^2,$$

Flack's idea on the enantiomorph polarity parameter

Conclusion

It would seem, however, that Rogers has erred in his choice of enantiomorph-polarity parameter and that x as defined in (5) is to be preferred as being faster and more reliable than η.

A series of lectures on *Anomalous X-ray Scattering* organized by the Troisième Cycle de la Physique en Suisse Romande and presented by Professor D. H. Templeton in the autumn term of 1982 at the University of Lausanne helped the author immensely in the work described above. The lecturer and the organizers are thanked for their contribution to this paper.

Highlights

- Important contributor to the XRAY72 system of crystallographic software
- Author of the famous CAMEL JOCKEY WITH THREE HUMPS absorption correction software
- Refinement algorithm for absolute structure determination
  - Flack's parameter (1983)
  - Fuitfull collaboration with Gérald (Kiki) Bernadinelli (*e.g.* Acta Cryst. A55, 1999)
- Least-squares restraints for origin fixing in polar space groups (Acta Cryst. 1988)

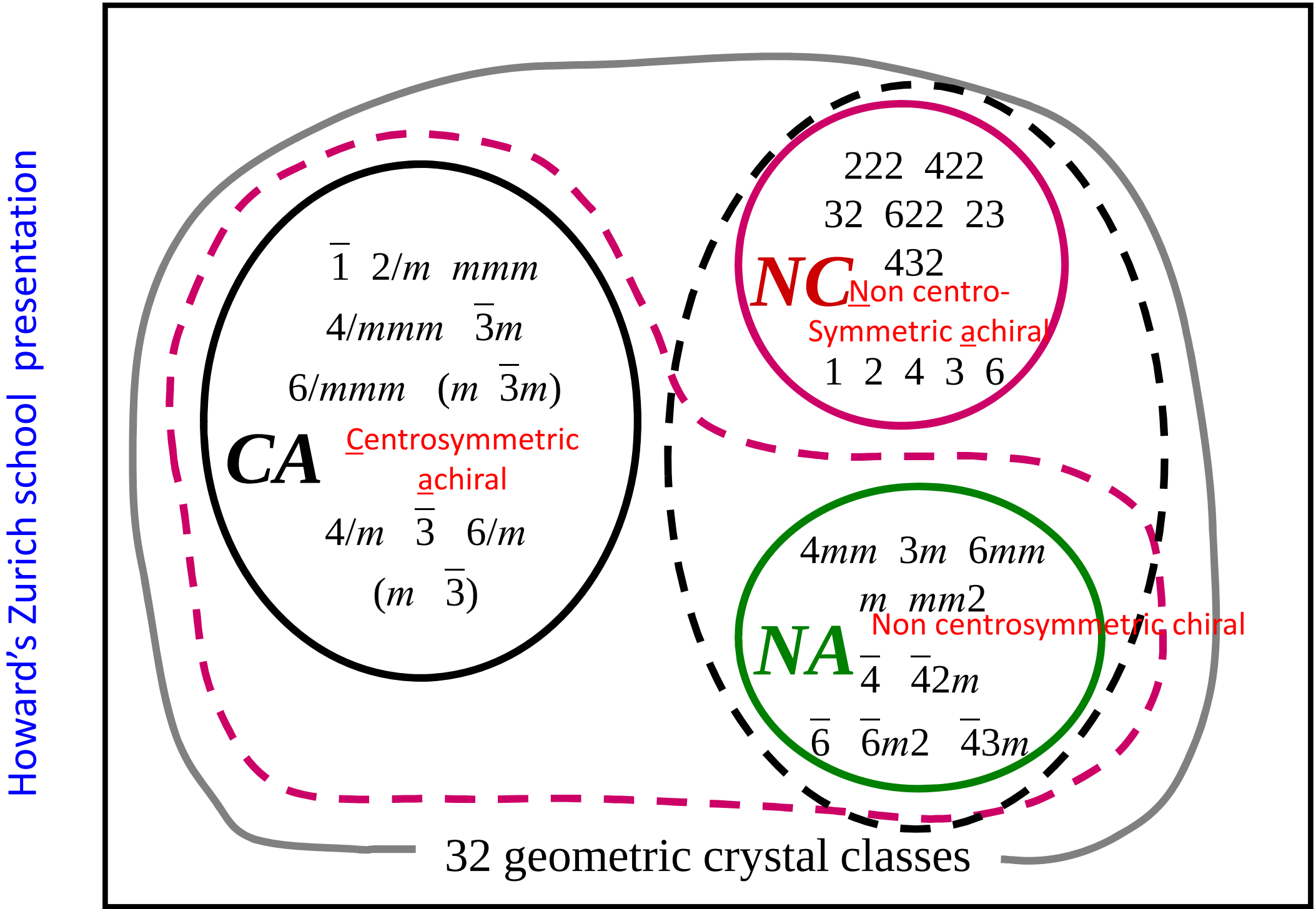
Highlights 2

- Statistical descriptors in crystallography published by an *ad hoc* IUCr subcommittee
  - Report 1 (1989)
  - Report 2 (1995)
- Intensity statistics of Friedel pairs (Shmueli & Flack, 2009)
- Louis Pasteur study (Acta Cryst. A, 2009)
- Merohedral twin interpretation with command lines for SHELXL (Flack & Wörle, 2013)

Other activities linked to Crystallography

- Secretary of the Swiss crystallography society (1981-1990)
  - Introduced the periodic bulletin of the society
  - Principal organizer in Geneva of annual meetings of Crystallography
- Howard interest in the new Internet technology was fondamental to organize what is probably the first conference where abstracts were submitted directly online ! (Aperiodic 1994 in Les Diablerets, Switzerland, organized by the Institue of crystallography at UNIL Lausanne under the responsibility of the IUCr aperiodic committee)
  - WWW was developed at CERN (Geneva). In 1993, only 200 sites were connected
  - NCSA Mosaic was created in 1993
  - Netscape in 1994

The Zurich school of crystallography

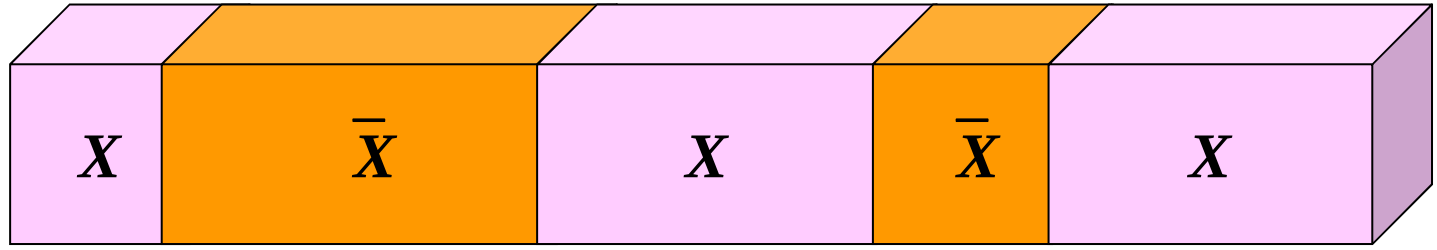

Howard's Zurich school presentation
$\bar{1}$ 2/m mmm
4/mmm $\bar{3}m$
6/mmm (m $\bar{3}m$)
CA
Centrosymmetric achiral
4/m $\bar{3}$ 6/m
(m $\bar{3}$)
222 422
32 622 23
432
NC
Non centro-Symmetric achiral
1 2 4 3 6
4mm 3m 6mm
m mm2
NA
Non centrosymmetric chiral
$\bar{4}$ $\bar{4}$2m
$\bar{6}$ $\bar{6}m$2 $\bar{4}3m$
32 geometric crystal classes

Howard's Zurich school presentation


1 2 4 3 6
4mm 3m
m mm
NA
4 42
6 6m2

Modelling non-centrosymmetric crystal structures

The macroscopic crystal C is treated as an oriented mixture in variable proportion of a crystal structure X and its inverted structure $\bar{X}$. The model is a crystal twinned by inversion.



$$C = (1 - x)\,X + x\,\bar{X}$$

Modelling non-centrosymmetric crystal structures

$$C = (1 - x)\,X + x\,\bar{X}$$

$(1 - x)$ is the mole fraction of the crystal structure X

x is the mole fraction of the inverted crystal structure $\bar{X}$

X is the crystal-structure model as represented by the set of atomic coordinates, cell dimensions and space group.

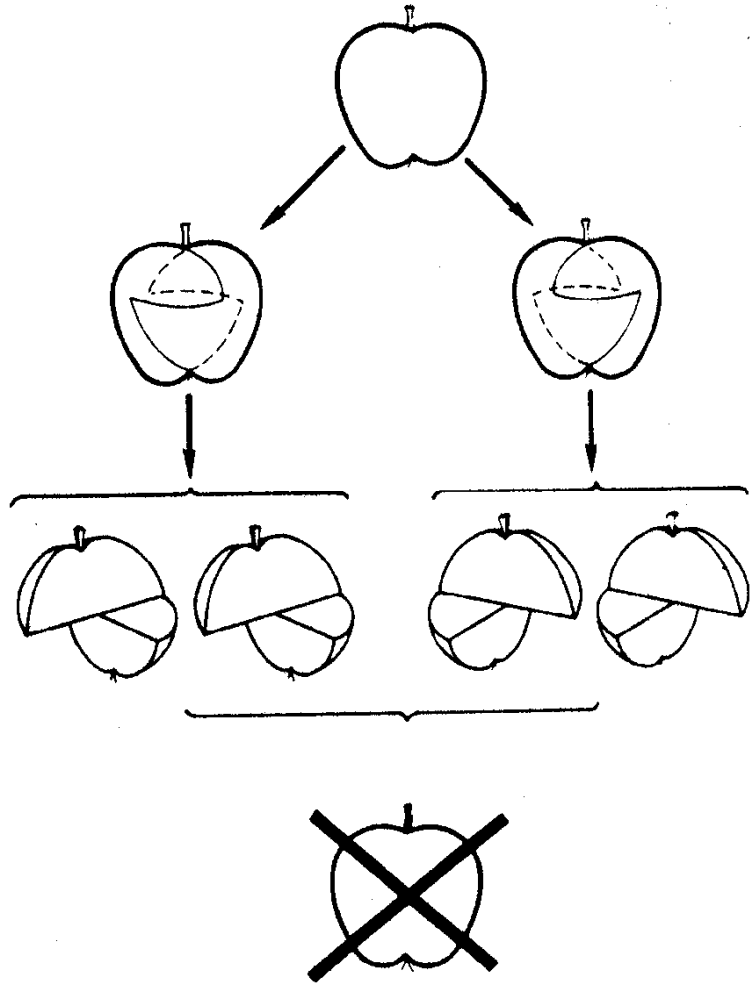
$x = 0$ means the sample C has the crystal structure X,

$x = 1$ means the sample C has the inverted crystal structure $\bar{X}$,

$x = 0.3$ means the sample C is an oriented mixture consisting of 70% of the crystal structure X and 30% of the inverted crystal structure $\bar{X}$.

Howard's Zurich school presentation

La Coupe du Roi




aproz


CARDINAL
Virgin
ICE TEA

A few more pictures from Howard's social and family activities

IUCr 1975
Amsterdam

with Dieter
Schwarzenbach


OMO
AJAX


Esso
LYONS
TEA
WINDSOR


L.N.W.R.

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- Evelyne Flack
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- Dieter Schwarzenbach