cRy

Statistical Applications in Macromolecular Crystallography

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Imperial College London

diamond

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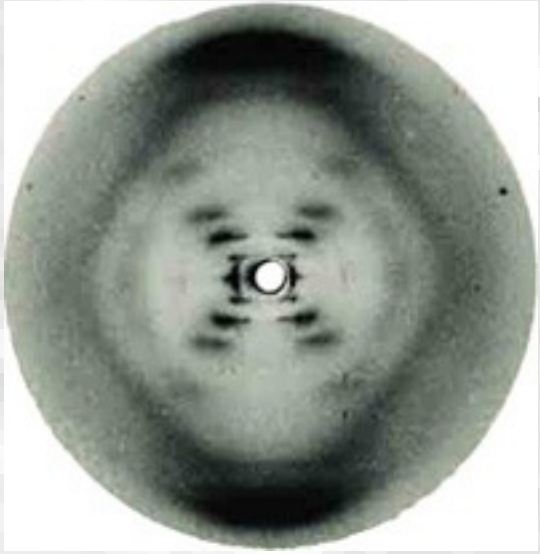
Why cRy ?

c is for … crystallography



The X-ray diffraction from a crystal sample produces a well-ordered diffraction pattern

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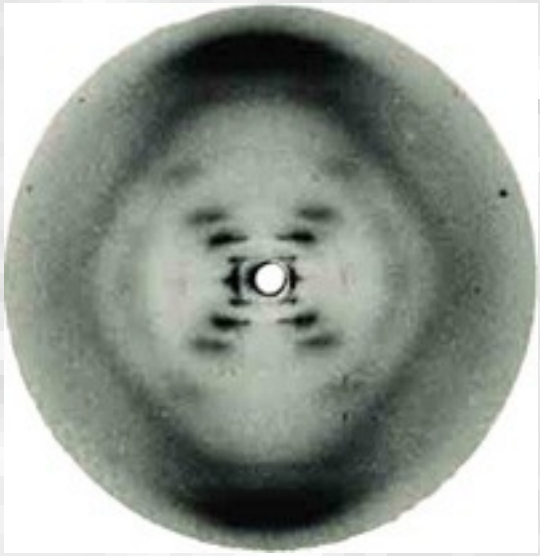

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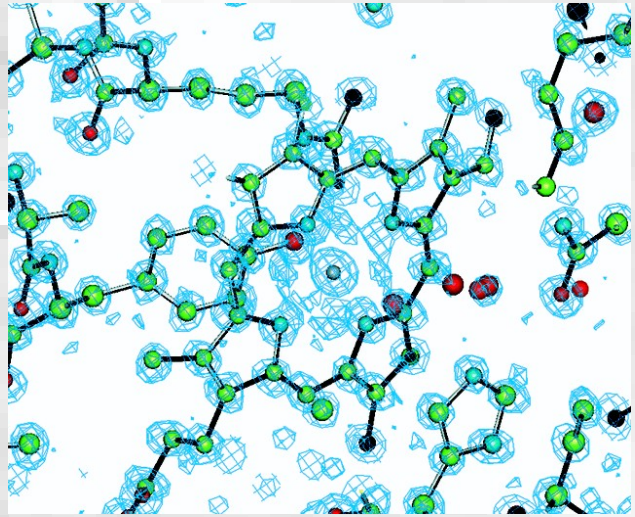
The statistical processing of data and their probabilistic interpretation, allows crystallographers to calculate 3D maps of electron density in which a model of the molecule can be built.



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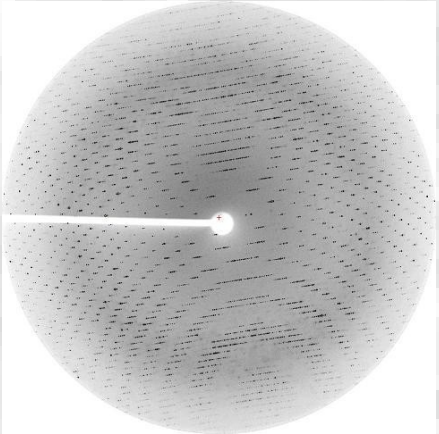
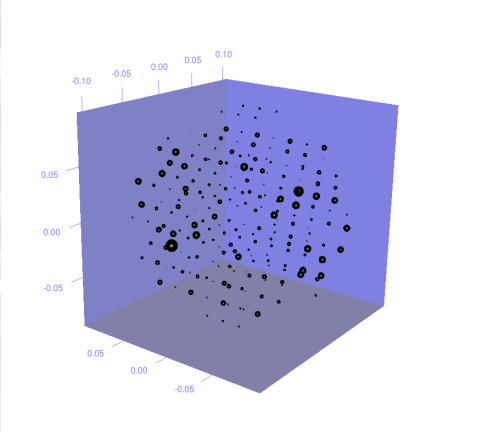
Statistical procedures are needed for
data processing and data extraction





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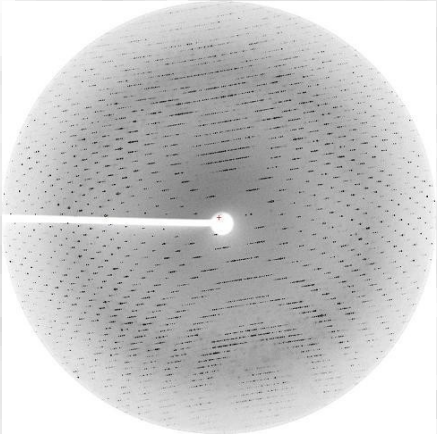

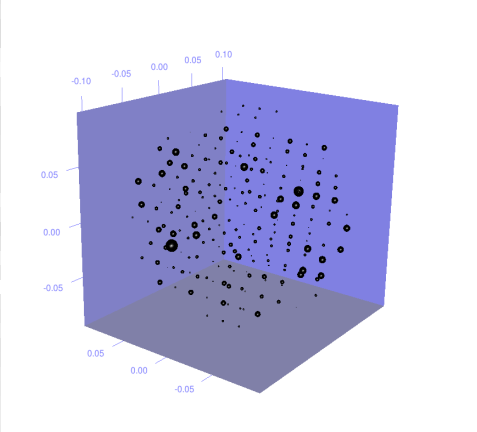

	H	K	L	FP	SIGFP
1	-28	0	2	0.34	0.83
2	-28	0	3	1.89	0.92
3	-28	0	4	3.56	0.86
4	-28	0	5	7.11	0.93
5	-28	0	6	10.59	0.93
6	-28	0	7	5.22	0.87
7	-28	0	8	7.31	0.85
8	-28	0	9	4.12	0.96
9	-28	0	11	10.99	0.94
10	-28	0	12	3.24	0.79
11	-28	0	13	0.82	0.80
12	-28	1	2	0.89	0.70
13	-28	1	3	2.96	0.76
14	-28	1	4	1.49	0.72
15	-28	1	5	0.08	0.65
16	-28	1	6	0.38	0.61
17	-28	1	8	3.29	0.62
18	-28	1	9	1.85	0.60
19	-28	1	10	1.84	0.59
20	-28	1	11	1.13	0.63

A crystallographic data frame

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The well-known crystallographic “phase problem” can be approached, and in many instances solved, using a probabilistic framework known as “direct methods”.

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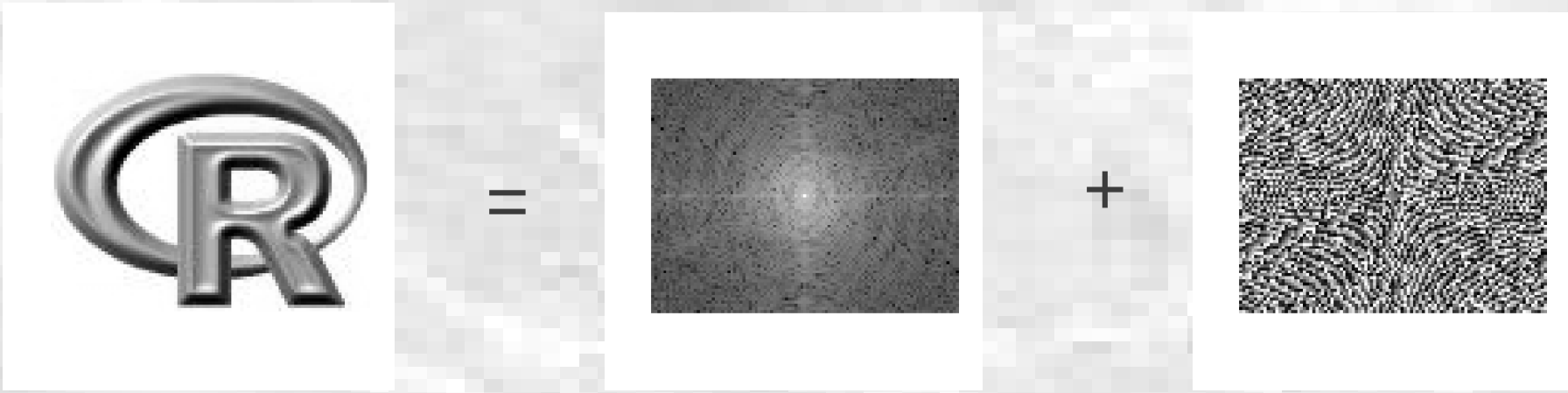

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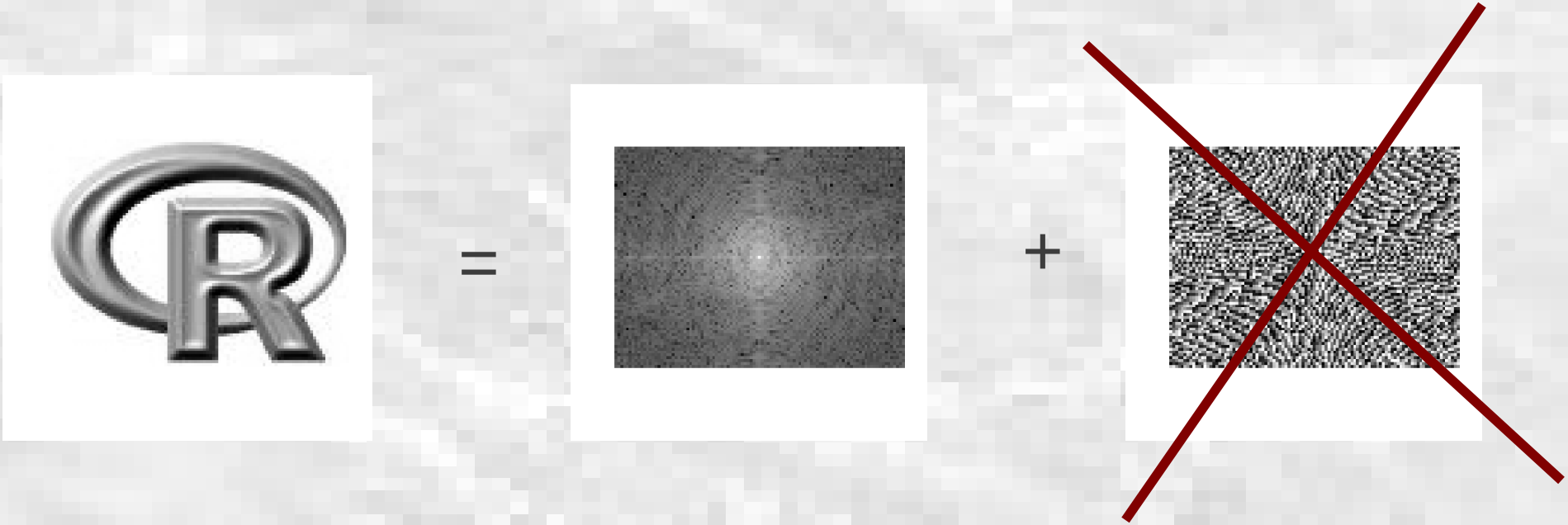

R is for … R

No need to explain what R is and why R is an amazing tool at a UseR conference...

… But in the community of crystallographers R is still not much used, or it is not used at all.

Garib Murshudov

R is for ... R

David Waterman

Gwyndaf Evans

R is for ... R

David Waterman

Gwyndaf Evans

Can we create a package in R to handle crystallography and crystallographic data and formats?

y is for … yes!

We started working on cRy in 2009/2010

With cRy we can carry out simple and complex crystallographic operations

cRy is being developed using S4 classes formalism

cRy

poster in the Bioinformatics/Biochemistry group
Tonight, 20:00

Come and discuss with me details of this new R package

Great potential of fruitful collaborations between
professional statisticians and crystallographers