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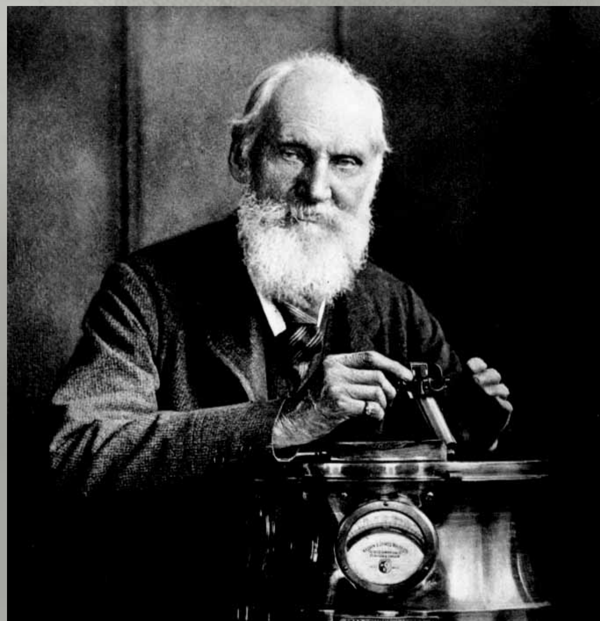
Симметрия и разные определения киральности

www.flack.ch/howard/cristallo/publcns.html

Кельвин



I call any geometrical figure, or group of points, chiral, and say that it has chirality if its image in a plane mirror, ideally realized, cannot brought to coincide with itself.

* I call any geometrical figure, or group of points, *chiral*, and say that it has chirality if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself. Two equal and similar right hands are homochirally similar. Equal and similar right and left hands are heterochirally similar or 'allochirally' similar (but heterochirally is better). These are also called 'enantiomorphs,' after a usage introduced, I believe, by German writers. Any chiral object and its image in a plane mirror are heterochirally similar.

Баррон

True chirality is exhibited by systems that exist in two distinct enantiomorphic states that are interconverted by space inversion but not by time reversal combined with any proper spatial rotation.

... that the hallmark of a chiral system is that it can support time-even pseudoscalar observables.

{знак равенства между киральностью и оптической активностью?}

	P	t
Opt. Act.	-	+

Флак

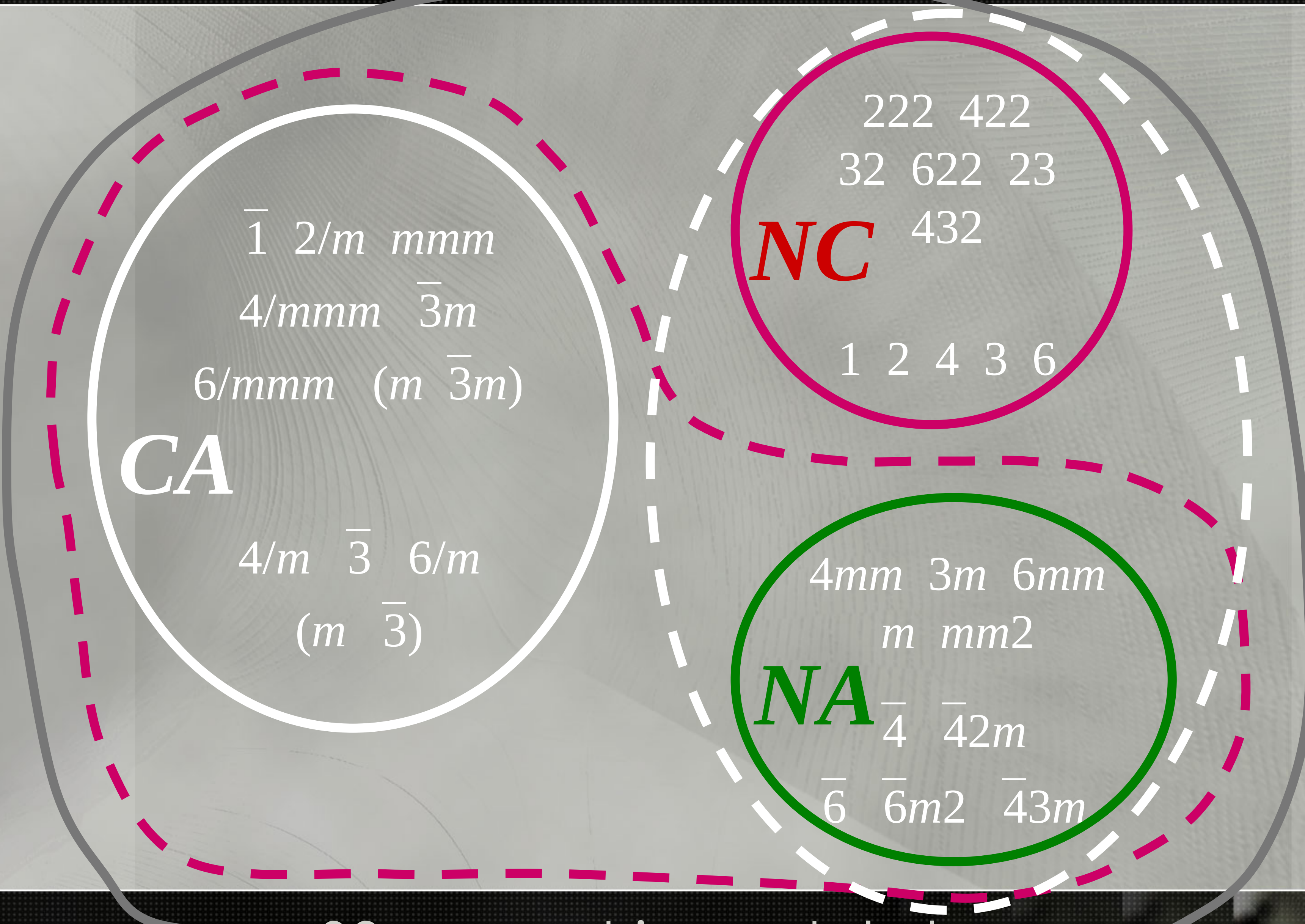
- The geometric property of a rigid object (or spatial arrangement of point or atoms) of being non-superposable by pure rotation and translation on its image formed by inversion through a point; the symmetry group of such an object contains no symmetry operations of the second kind ($\bar{1}$, m, $\bar{3}$, $\bar{4}$, $\bar{6}$). When the object is superposable by pure rotation and translation on its inverted image, the object is described as being achiral; the symmetry group of such an object contains symmetry operations of the second kind.
- True chirality is exhibited by systems that exist in two distinct enantiomorphic states that are interconverted by space inversion by not by time reversal combined with any proper spatial rotation.

1, 2, 3, 4, 6

$\bar{1}$, m, $\bar{3}$, $\bar{4}$, $\bar{6}$

$$\bar{1} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Киральность и симметрия



32 geometric crystal classes

Киральность = оптическая активность?

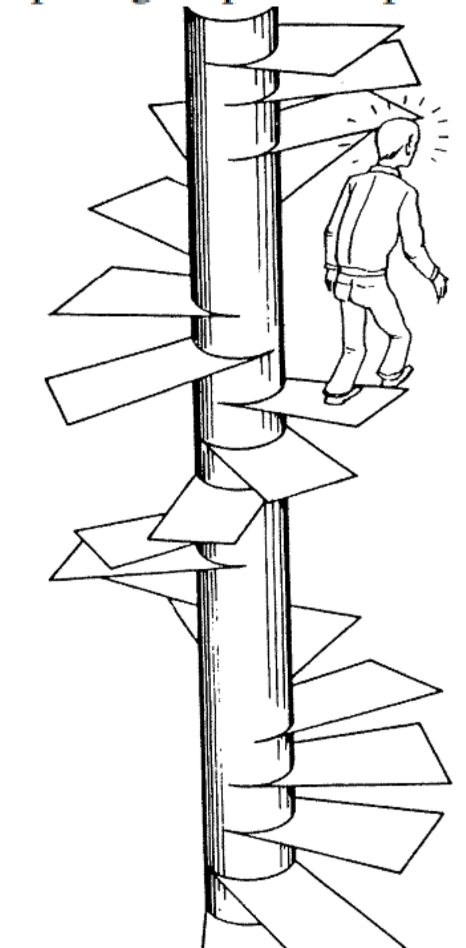
Restrictions on Natural Optical Activity for Crystals and Molecules both Chiral and Achiral.

	Single crystal	Molecules in solution or as liquid
Achiral	Permitted only in m, mm2, -4, -42m	Forbidden
Chiral	Permitted	Enantiopure: Permitted Racemate: Forbidden Non-racemic mixture: (enantiomeric mixture) Permitted

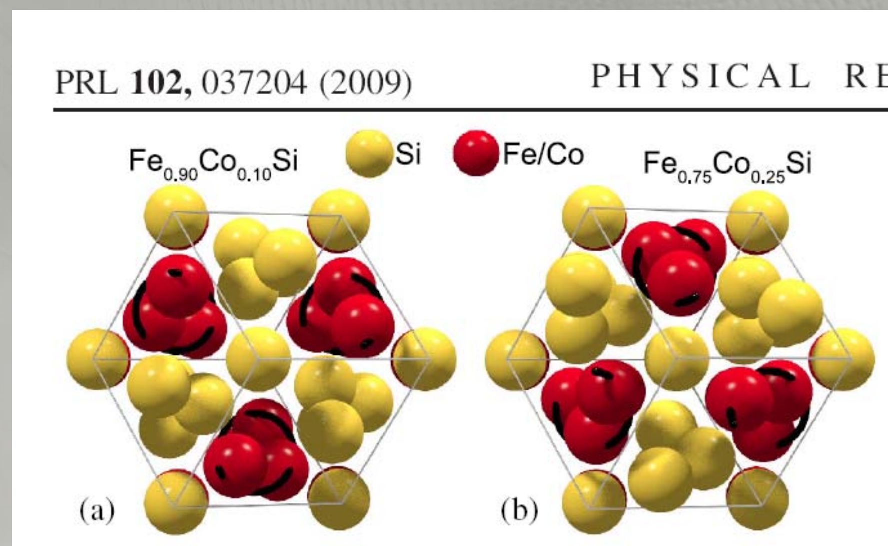
“.. that the hallmark of a chiral system is that it can support time-even pseudoscalar observables”. Isotropic natural optical rotation is such an observable, but anisotropic optical rotation from achiral crystals is not.

Абсолютная структура

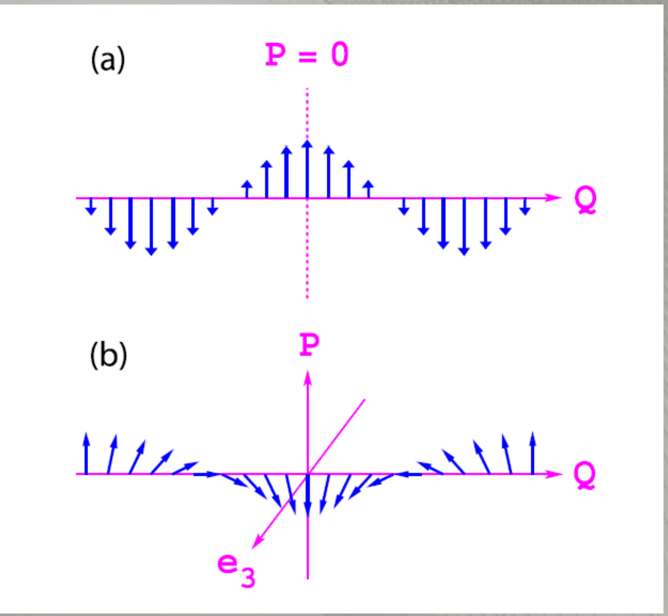
Absolute structure. The spatial arrangement of the atoms of a physically identified noncentrosymmetric crystal and its description by way of unit-cell dimensions, space group and representative coordinates of all atoms.

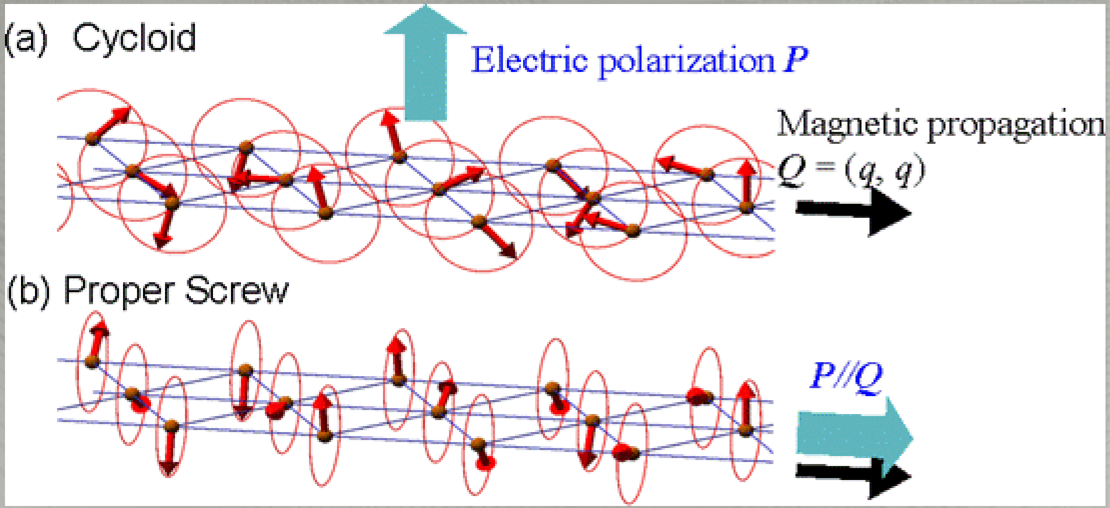


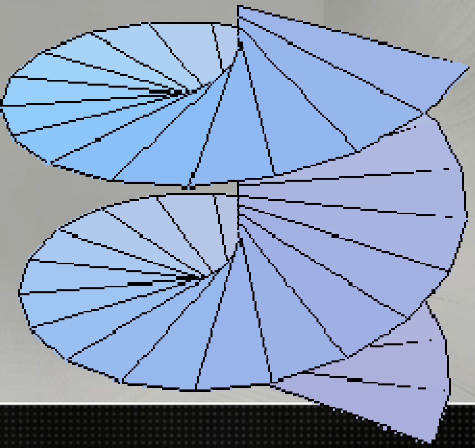
1. Определена ориентация кристалла и задана система координат
2. Выбрана длина волны обеспечивающая резонансный вклад (нарушен закон Фриделя)
3. В заданной ориентации кристалла определены координаты атомов



Магнитная модуляция







$$\frac{d\sigma}{d\Omega} = \left(\frac{rS}{2}\right)^2 \frac{(2\pi)^3}{V_0} \{[1 + (\hat{q}\hat{c})^2 - 2(\hat{q}\mathbf{P}_0)(\hat{q}\hat{c})]\delta(\mathbf{q} - \mathbf{k})$$

$$+ [\mathbf{P}_0 \rightarrow -\mathbf{P}_0]\delta(\mathbf{q} + \mathbf{k})\}\sin^2\alpha,$$

…и циклоида

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Neutron and synchrotron diffraction study of UPtGe

It should be noted that a cycloidal structure does not have an *absolute* chirality since the sense of a cycloid is reversed by rotation of π about its propagation direction. The apparent chirality of the structure is therefore reversed by this rotation and will appear to be opposite for the $h^{+}kl$ and $h^{-}kl$ reflections. Since this is a real rotation one can perform on the crystal it is clear that the "chirality" of the cycloid cannot exist. Changing chirality requires an improper rotation, i.e., one that involves the use of a mirror plane, in the sense that the left hand may be transformed into the right. As discussed earlier, the cycloid is a special case of the helix, but with the angle between the normal to the plane of the moments and the propagation direction equal to $\pi/2$. Any deviation of this angle from $\pi/2$ allows one to talk of chiral domains, but the domains in UPtGe do not have that character. Nevertheless, it seems likely that the formation of a

Проявление киральности в эксперименте

1. difference in Fridel pairs (X-ray)
2. Chiral scattering (polarised neutrons)
3. Optical activity (light)

Управление киральностью?

- Пастер – кристаллизация в магнитном поле
- Кельвин, Фарадей – не будет работать

But what is the scalar chirality physically?

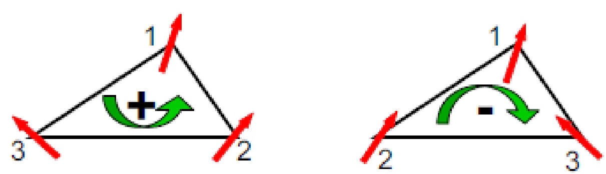
What does it couple to?

How to measure it?

Breaks time-reversal-invariance T and inversion P - like currents!

→ $\chi_{123} \neq 0$ means spontaneous circular electric current $j_{123} \neq 0$ and orbital moment $L_{123} \neq 0$

$$L_{123} \propto j_{123} \propto \chi_{123}$$



Couples to magnetic field:

$$-LH \sim -\chi H$$

http://lns.pnpi.spb.ru/media/pdf/khomsky.pdf

Вопросы

Можно ли наблюдать киральное рассеяние нейтронов на нецентросимметричных но акиральных магнитных структурах?

{да}

Можно ли изменить киральность системы магнитным или электрическтм полем?

{нет}