Cristales Líquidos

4.lect.Oettel.pdf:
http://www.soft-matter.uni-tuebingen.de/teaching/vorlesung_atcoma_ss14/4.lect._Oettel.pdf

Introducción a los cristales líquidos

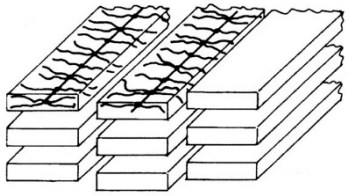
nematic: relating to or denoting a state of a liquid crystal in which the molecules are oriented in parallel but not arranged in well-defined planes.

smectic: denoting or involving a state of a liquid crystal in which the molecules are oriented in parallel and arranged in well-defined planes.

cholesteric o chiral nematic liquid crystals: Of or relating to the chiral nematic phase of some liquid crystals in which the molecules are arranged in parallel planes with adjacent planes rotatedslightly

sanidic….

y más



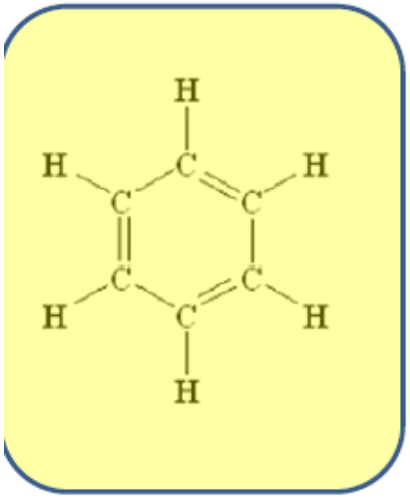
https://www.researchgate.net/publication/283832397_Definitions_of_basic_terms_relating_to_low-molar-mass_and_polymer_liquid_crystals_IUPAC_Recommendations_2001/figures?lo=1

Simetría 2D (excelente divulgación):
http://n.ethz.ch/~nielssi/download/4.%20Semester/AC%20II/Unterlagen/symmetry_2D_3.pdf

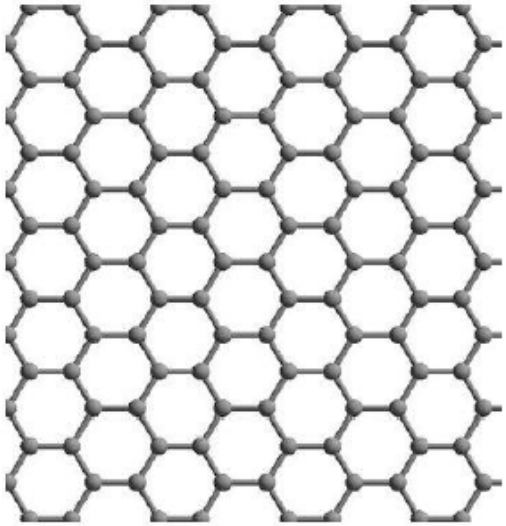
From molecular point group to space groups

Complete consideration of all symmetry elements and translation yields to the space groups

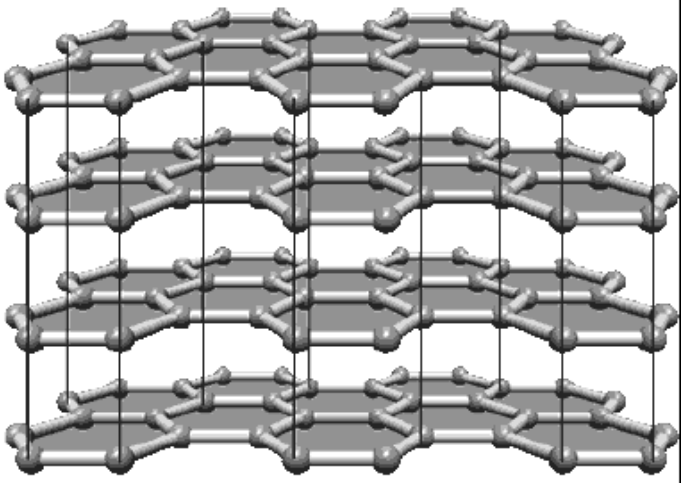
benzene



graphene



graphite



D6h or 6/mmm

Point group

p6mm

Plane group = point group symmetry + in plane translation

$P6_3/mmc$

Space group = point group symmetry + in 3D translation

Simetría 2D (excelente divulgación):
http://n.ethz.ch/~nielssi/download/4.%20Semester/AC%20II/Unterlagen/symmetry_2D_3.pdf

4. Glide Reflections

Glide reflection reflects the asymmetric unit across a mirror and then translates it parallel to the mirror

There are no invariant points under a glide reflection.

A glide plane changes the chirality of figures in the asymmetric unit.

- Symbol: **g**
- Representation: a dashed line

Zhao, Donnio et al. *J. Mat. Chem. C* (2018) 6, 4471 - 4478

Molecular design of benzothienobenzothiophene cored columnar mesogens: facile synthesis, mesomorphism, and charge carrier mobility

Table S1: Table of indexation†

	d_{meas} (Å) [sh/br/ξ(nm), Intensity]	(*hk*) Peak	d_{calc} (Å)	Mesophase parameters
M1 T = 240°C	20.32 [sh, VS] (11.73) [sh, M] 10.17 [sh, W] 7.67 (sh, W) 14.5 [ξ=6, S] 5.2 [ξ=5, W] 4.5 [br, VS] 3.76 [ξ=5, S]	10 11 20 21 D_1 D_2 h_{ch} h_π	20.32 (11.73) 10.16 7.68	a = 23.5 Å A = 478 Å²

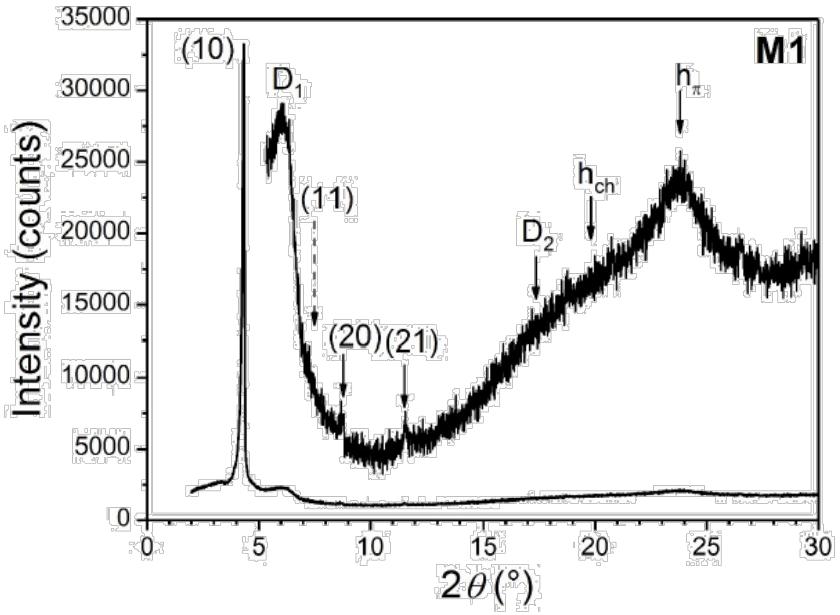


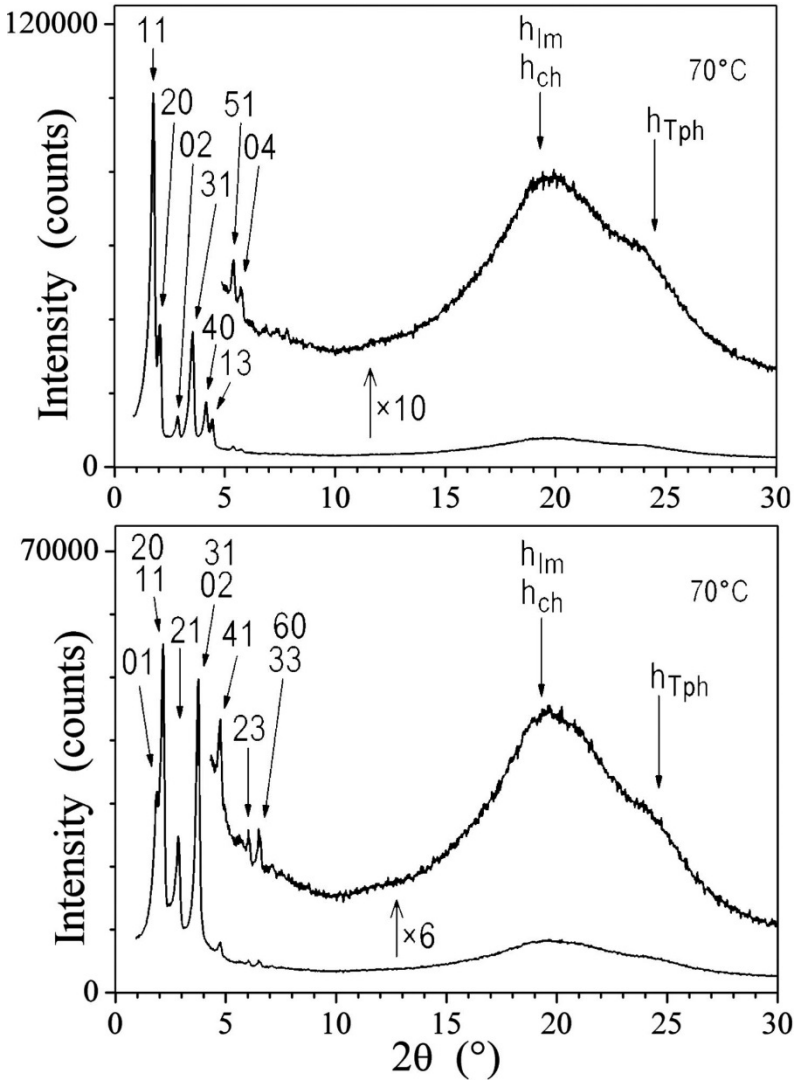
Figure S6. SAXS pattern of compound **M1** at 240°C.

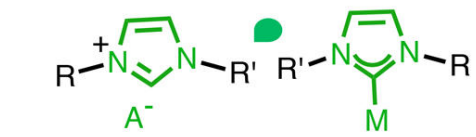
"**SAXS.** Temperature-variation SAXS experiments were performed on a Rigaku Smartlab (3) X-Ray diffractometer equipped with a TCU 110 temperature control unit. The sample temperature was controlled within±1 K. The X-ray sources **(Cu Kα, λ = 0.154 nm)** were provided by 40 kW ceramic tubes."

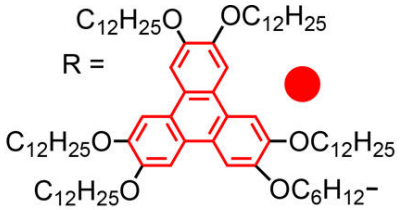
Ec. de Bragg: $\lambda = 2dsen\theta$

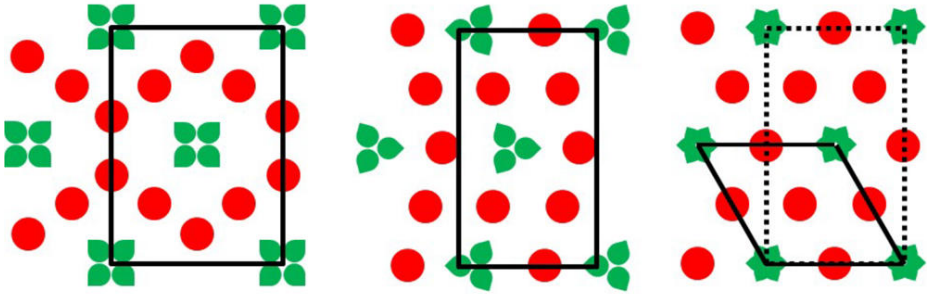
$2\theta = 4.34^{o} \rightarrow d = 20.3$ Å

Inorg. Chem. 2018, 57, 4359–4369









c2mm
$Z_{Tph} = 8$

p2mg
$Z_{Tph} = 6$

p6mm
$Z_{Tph} = 3$

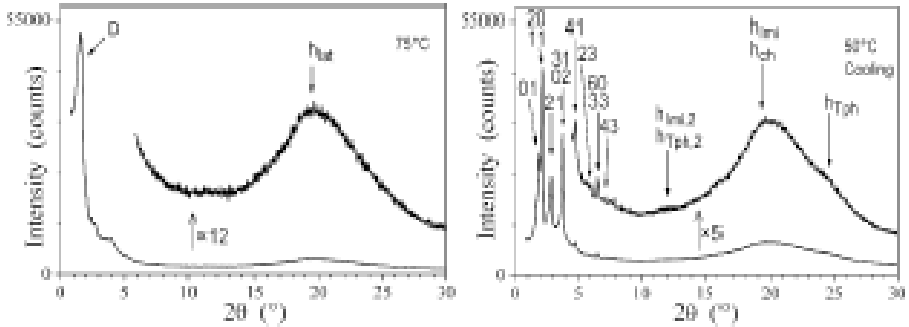


Fig. S41. X-ray diffraction patterns of copper carbenes **5** (left) and **10** (right).

Tutoriales GSAS-II

Tutoriales:
https://subversion.xray.aps.anl.gov/pyGSAS/trunk/help/Tutorials.html

Arrancar GSAS-II
https://subversion.xray.aps.anl.gov/pyGSAS/Tutorials/StartingGSASII/Starting%20GSAS.htm

Refino con datos de rayos X – fluroapatita (Rietveld)
https://subversion.xray.aps.anl.gov/pyGSAS/Tutorials/LabData/Laboratory%20X.htm

Simulaciones
https://subversion.xray.aps.anl.gov/pyGSAS/Tutorials/Simulation/SimTutorial.htm

Preparar datos para resolución estructural
https://subversion.xray.aps.anl.gov/pyGSAS/Tutorials/FitPeaks/Fit%20Peaks.htm
Refino Pawley y Resolución estructural (sacarosa)
https://subversion.xray.aps.anl.gov/pyGSAS/Tutorials/CFsucrose/Charge%20Flipping%20-%20sucrose.htm