

# Calculated crystal structure?

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*Source:* <http://sci.tech-archive.net/Archive/sci.physics.research/2005-06/msg00573.html>

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  - *Date:* Tue, 28 Jun 2005 22:48:04 +0000 (UTC)
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Does anybody have software to calculate a probable crystal lattice given only molecular structure?

CrystalG

Acta Cryst. B58 647-661 (2002)

Cryst. Eng. Comm 44 (2001)

Oppositely charged spheres of similar radius usually form close-packed lattices. What crystal lattice will obtain if the spheres are chiral? Consider a 1:1 salt of oppositely charged trivalent three-bladed homochiral propellers. The 1:1 trivalent cations and anions will give a tightly bound crystal lattice (e.g., Madelung energy). What will be the space group of that lattice? It must be one of the 65 chiral space groups.

Please post 'em if you've got 'em.

<http://www.mazepath.com/uncleal/xions.png>

Stereopair images, isolated ions

$\wedge$ -[Co(en)3](3+)  $\wedge$ -[Co(ox)3](3-)

or

$\wedge$ -[Co(en)3](3+) /  $\wedge$ -[Co(ox)3](3-)

<http://www.mazepath.com/uncleal/xsalt.png>

Stereopair images, the salts

Inorg. Syn. 6 186 (1960)

[Co(en)3](3+)

en = 1,2-diaminoethane

Acta Cryst. E57 m448-m450 (2001)

Inorg. Syn. 8 204 (1966)

[Co(ox)3](3-)

ox = oxalate dianion

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Uncle Al

<http://www.mazepath.com/uncleal/>

(Toxic URL! Unsafe for children and most mammals)

<http://www.mazepath.com/uncleal/qz.pdf>

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  - Previous by thread: ***are holonomies arguably observables?***
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