

Supporting Information of

Solvents and Isotopic effects on Acridine and deuterated Acridine Polymorphism

A. Kupka^a, V. Vasylyeva^a, D.W. M. Hofmann^{b}, K. Yusenkov^c and K. Merz^{a*}.*

^aInorganic Chemistry 1, Ruhr-University Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

^bCRS4, Piscina Manna 1, 09010 Pula, Italy

^csolidchem, Universitätsstraße 136, 44799 Bochum, Germany

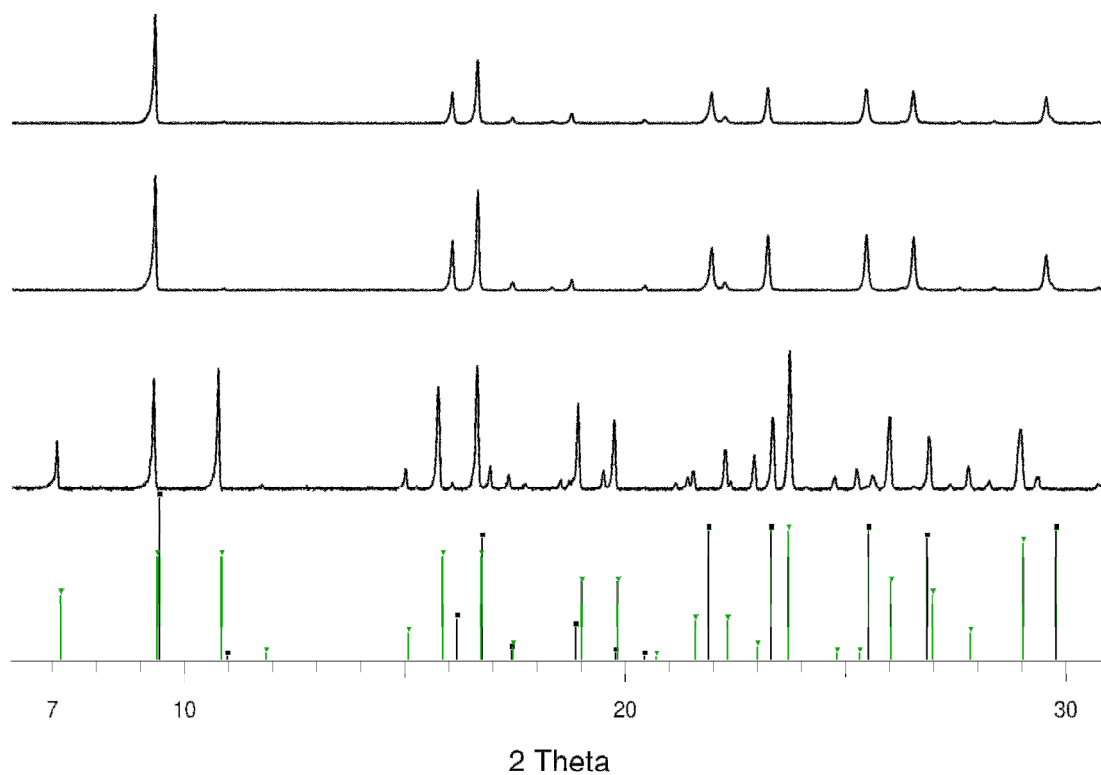
Klaus Merz E-mail: klaus.merz@rub.de

Phone: +49 2343224187 FAX: +49 2343214378

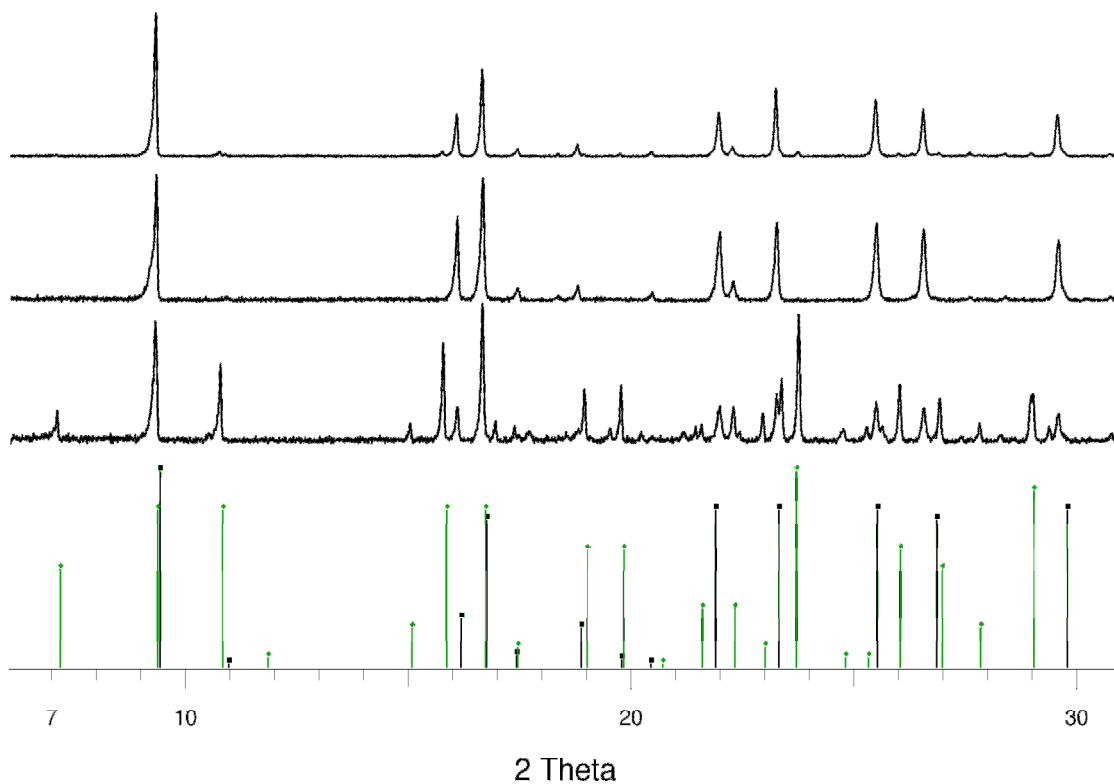
Detlef W. M. Hofmann: E-mail: hofmann@crs4.it

Phone: + 39 0709250369. Fax: + 39 0709250216.

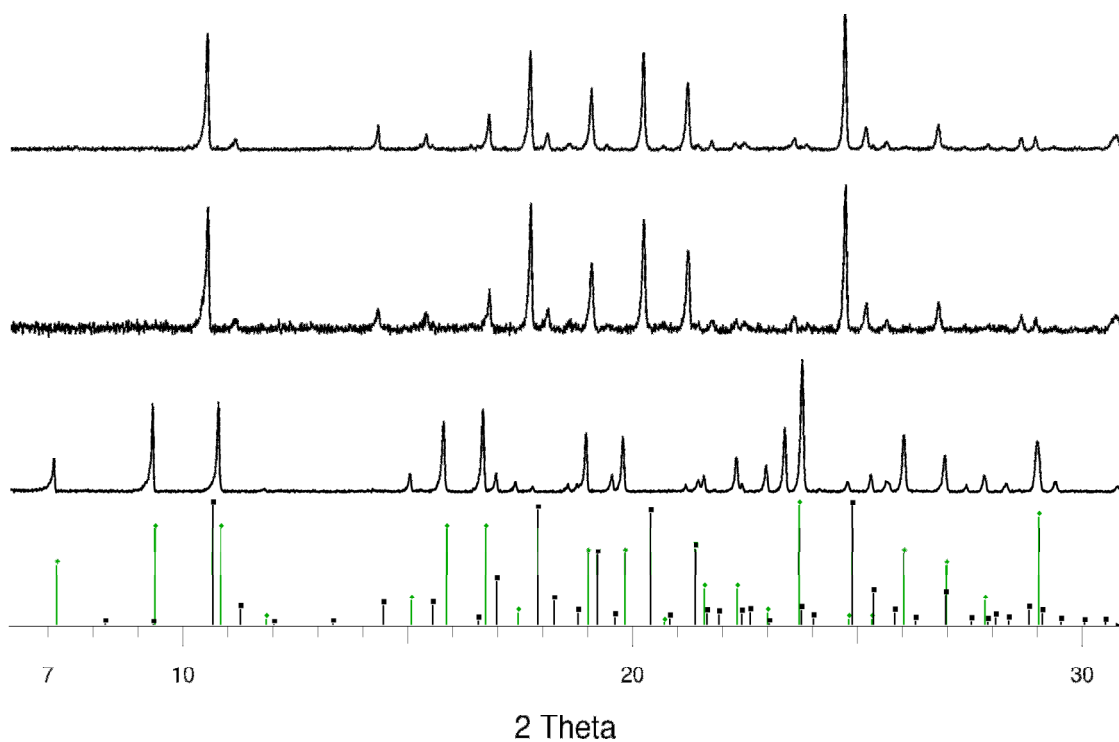
- PXRD of acridine from ethanol p. a.
- PXRD of acridine from ethanol tech.
- PXRD of d₉-acridine from ethanol p. a.
- PXRD of d₉-acridine from ethanol tech.
- PXRD of d₄-acridine from acetone p. a.
- PXRD of d₄-acridine from acetone tech.
- CSD query for deuterated compounds



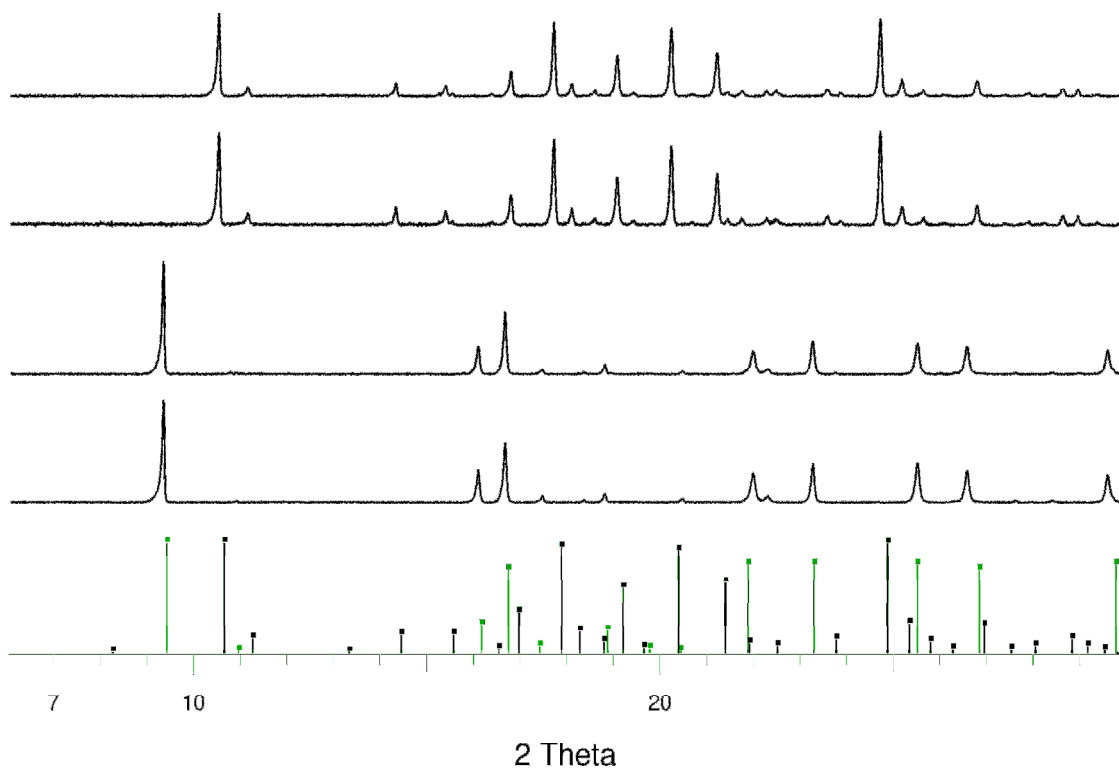
PXRD of acridine from ethanol p.a. show two times form II (black) and once form III (green) in three crystallization experiments.



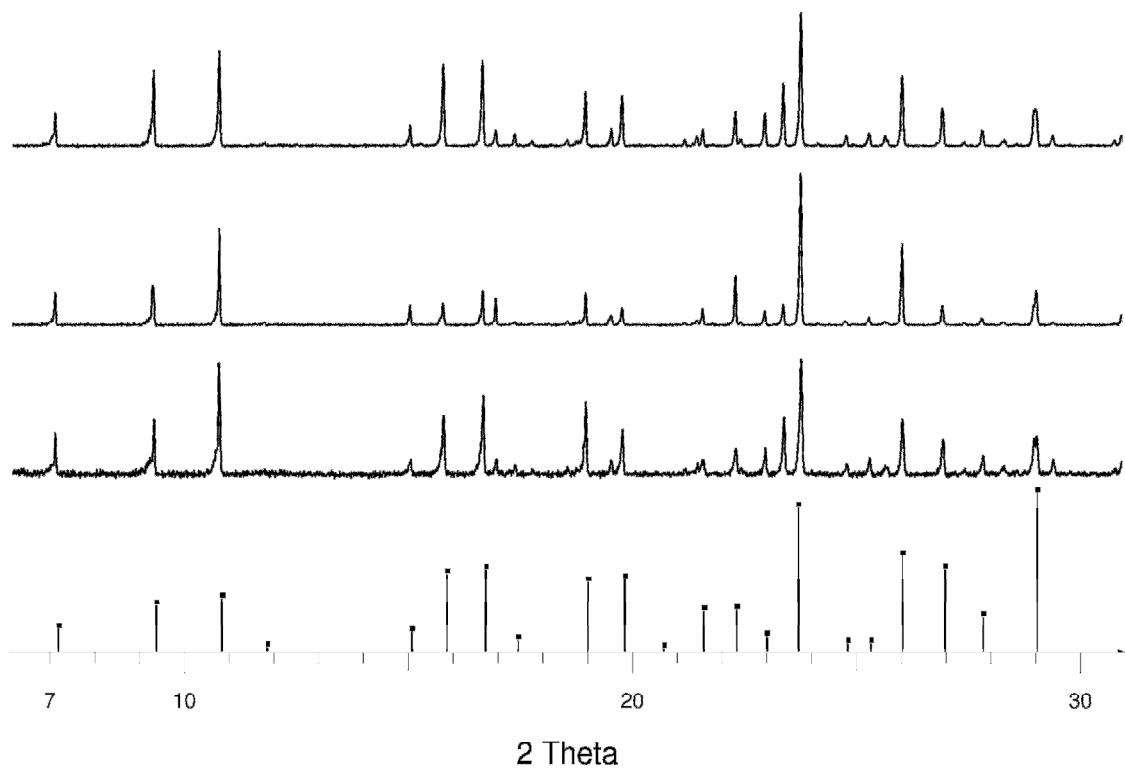
PXRD of acridine from ethanol tech. show two times from II (black) and once form II and from III (green) concomitantly in three crystallization experiments.



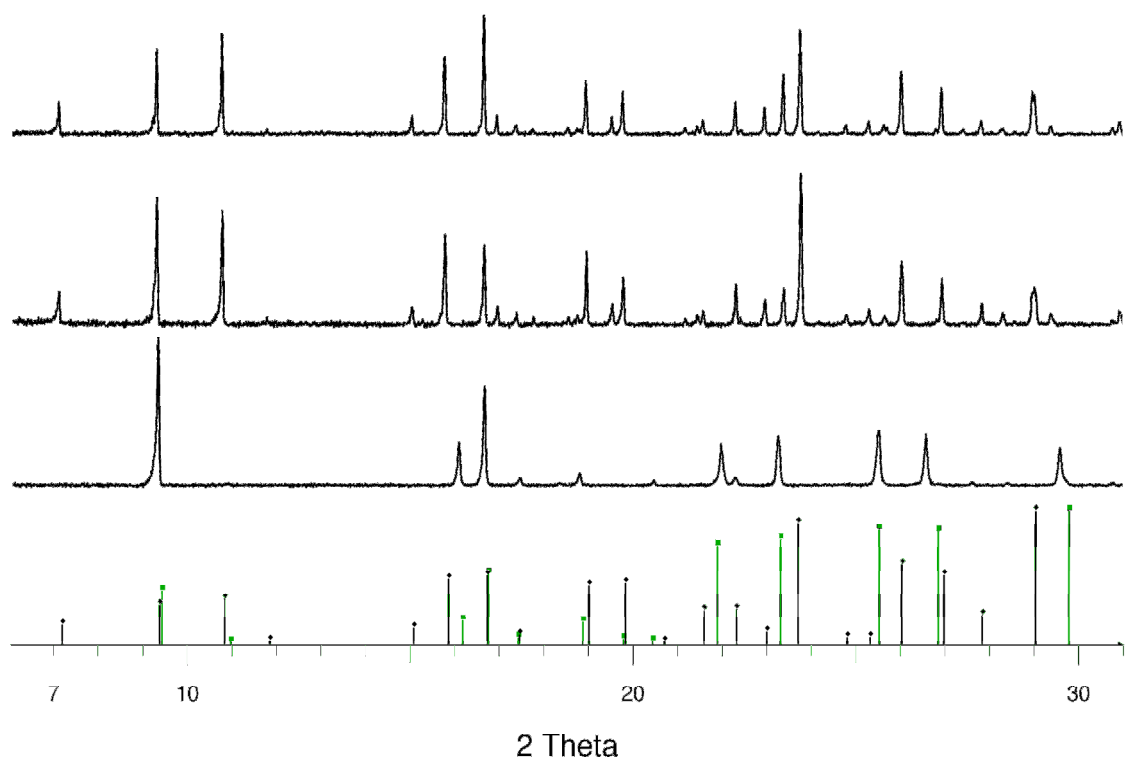
PXRD of d₉-acridine from ethanol p.a. show two times form IV (black) and once form III (green) in three crystallization experiments.



PXRD of d₉-acridine from ethanol tech. show two times form IV (black) and twice form II (green) in four crystallization experiments.



PXRD of d₄-acridine from acetone p.a. show three times form III in three crystallization experiments.



PXRD of d₄-acridine from acetone tech. show two times form III (black) and once form II (green) in three crystallization experiments.

For the calculation of the potentials, the CSD database was searched for small organic molecules consisting of C, N, H / D (except methane). Only those molecules have been considered, for which both the crystal structures of the deuterated, and the non-deuterated form are known.

| deutereuted compounds | non deuterated compounds |
|---|--|
| Hexadeutero-benzene | Benzene |
| Decadeutero-biphenyl | Biphenyl |
| Perdeutero-tetracyanoanthraquinodimethane | 11,11,12,12-Tetracyano-9,10-anthraquinodimethane |
| Octadeutero-naphthalene | Naphthalene |
| Perdeuteronaphthalene | |
| Pentadeutero-pyridinium-1-dicyanomethylid | Pyridinio(dicyano)methylide |
| Perdeuteropyridine | Pyridine |
| Tetradecadeutero-p-terphenyl | p-Terphenyl |
| | 1,1':4',1''-Terphenyl |

CSD query for deuterated compounds