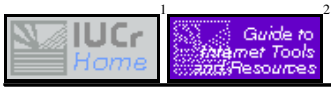

News Example: Want to solve a structure?

```
Newsgroups: sci.techniques.xtallography
From: huffman@indiana.edu (John C. Huffman)
Subject: Want to solve a structure?
Organization: Indiana University Molecular Structure Center
Date: Tue, 26 Apr 1994 16:34:52 GMT
```

I have an interesting problem if someone wants a challenge. A colleague has an organic compound (C28H37O6N) which he has been able to get fairly decent crystals of. Examination of the crystals (thin triangular plates, looking much like an arrowhead) revealed twinning, as evidenced by omega scans. I was finally able to determine that the twinning was parallel to the thin dimension of the crystal and was able to split it into two fragments, one of which no longer shows evidence of twinning. A comprehensive search of reciprocal space locates a set of diffraction maxima indexable as triclinic, with cell parameters suggesting Z=4. Since the material is enantimerically pure (according to the student) there must be four independent molecules present (ca 140 non−hydrogen atoms). I have spent some time trying MULTAN and various options in SHELX to no avail. The data are collected at low temperatures (−173C) and appear to be well−behaved. My lack of success may simply be due to my inexperience with "large" equal atom problems, or there may still be a twinning problem. If someone wants to take a crack at the solution, I have placed SHELX .hkl and .ins files in directory /pub/datasets on our anonymous ftp server. The server is:

```
ftp.chem.indiana.edu
(129.79.136.47)
```

Log in as anonymous with your name as password. In directory /pub/datasets, get (ascii files)

```
94112.hkl
94112.ins
```

Since the best you can get is probably an acknowledgment for your efforts, I am willing to offer one low−temperature data set (up to 4000 reflections, air−stable compound) for the first solution.

If I have any takers and a successful solution, I will post details in case anyone else has problems of interest they would like to share.

```
================================================
John C. Huffman               Senior Scientist
Indiana University Molecular Structure Center
Bloomington, IN 47408-4001                  USA
------------------------------------------------
huffman@indiana.edu             (812) 855-6742
================================================
```

```
Newsgroups: sci.techniques.xtallography
From: a4160007@horus.sara.nl (Milco Numan)
Subject: Re: Want to solve a structure?
Date: 29 Apr 94 13:59:12 +0100
Organization: Lab. for Crystallography, Univ. of Amsterdam
```

Dear Dr Huffman,

We have propably solved your problem structure 94112. Could you please send us some additional information about the positions of the N and O atoms so we can check our solution properly ?

[1] http://www.iucr.ac.uk/iucr−top/welcome.html
[2] int.index.html

FYI : We have used the program CRUNCH (De Gelder, De Graaff & Schenk, Acta Cryst A49, 287–293, 1993) using defaults (R2=0.093 based on E's).

Yours sincerely,

Kees Goubitz (fz@crys.chem.uva.nl) & Milco Numan (milcon@crys.chem.uva.nl)
Lab. voor kristallografie
Universiteit van Amsterdam
Nieuwe Achtergracht 166
1018 WV Amsterdam
Tel. + 31 (20) 525 7038/7041
Fax. + 31 (20) 525 5698

Newsgroups: sci.techniques.xtallography
From: huffman@indiana.edu (John C. Huffman)
Subject: Re: Want to solve a structure?
Organization: Indiana University Molecular Structure Center
Date: Tue, 26 Apr 1994 16:34:52 GMT

And the winner is.....

Milco Numan and Kees Goubitz were able to solve the strucuture I posted earlier. Several different groups had a crack at it–– thanks to all! I would appreciate hearing from others who were trying, and I will post a summary of this rather unusual experiment!
(Instead of saying solved by MULTAN... etc., can I say "solved by Internet....?).

Miloc and Kees are from the Laboratory for Crystallography, Universtiy of Amssterdam, The Netherlands.

==
John C. Huffman Senior Scientist
Indiana University Molecular Structure Center
Bloomington, IN 47408-4001 USA
----
huffman@indiana.edu (812) 855-6742
==

---

[3] int.index.html
[4] http://www.unige.ch/crystal/stxnews/stx/volnteer.htm
[5] http://www.unige.ch/crystal/stxnews/newsgrp/newsexm2.htm