M08.0E Difficult Structures

Chair: D.J. Watkin
Co-Chair: P.T. Beurskens

Attendance: 170

The term “ difficult structures “ used to refer to difficulties in solving the phase problem for an otherwise “ normal structure “ , especially in the early days of computer applications for Pattersons (Patterson overlap) and Direct Methods (aberrant phase relations). The tremendously improved modern methodology has almost (but not quit) overcome such problems, and the present session shows that the term “ difficult structures “ now refers to the entire scene of solving crystal structures:

How to get crystals — Roland Boese discussed STRUCTURES FROM (VERY) LOW MELTING COMPOUNDS AND THOSE WHICH FORM PLASTIC OR GLASSY PHASES . The obvious way to overcome difficulties is to get good crystals .... but sometimes craftmanship and devotion are needed! We were happy to observe that the high-level scientific contents of the lecture were not obscured by an extremely splendid presentation.

How to get reflection data — Having crystals, you need intensity data. But for DIFFICULT STRUCTURES: , William Clegg discussed IMPROVING YOUR CHANCES WITH SYNCHRO-TRON RADIATION . With a nice collection of examples he encourages all crystallographers to use synchrotrons. Maybe we need more available facilities!

How to solve the phase problem —At this stage of the structure determination process one sends all available data to one of the many structure solving program packages and hopes that the structure comes out. But we may have a ‘ classical difficult stucture ‘ .... Rene de Gelder showed for small and medium-sized equal-atom structures how to solve unsolvable structures (published as unsolvable!) with CRUNCH: GETTING THE MAXIMUM OUT OF (Karle Hauptman) DETERMINANTS .

How to validate your results — All good structure refinement programs as well as many well-known utility programs supply various ‘numbers’ to prove that the resulting structure is correct. But this may well be the difficulty of the structure determination: is it or is it not ? A hot item: any improvement is very welcome! And so was the talk of Sean Parkin on EXPANSION OF GLOBAL VALIDATION CRITERIA TO 3-D: THE R-TENSOR , which included application to various types of data sets to allow

detection of possible errors in either data or structural results.

How to present the structure — No problems left once the problems of your ‘ problem structure ‘ are solved ..... unless?! Many ‘ problem structures ‘ have some built-in cause for the problem which solution depended on you personal action: is it correct and justifiable? This delicate question must be answered. Anthony Linden in DIFFICULT STRUCTURES: MAKING THEM FIT FOR THE CHEMIST gave some general advices how to answer that delicate question so as to prevent the chemist from drawing incorrect conclusions and allowing the Acta Cryst Editor to accept the paper.

Final comments. Over one hundred abstacts were received on “Methods for Structure Determination”, sixteen of those were assigned for “Difficult Structures”; six of those are described above. The large lecture room was filled early, and remained so during the entire session, showing the interest of the crystallographic community to the essentials of modern structure determinations: what to do if problems are encountered? We enjoyed being Session chairs with such good speakers.

Paul T. Beurskens and David Watkin, August 1999