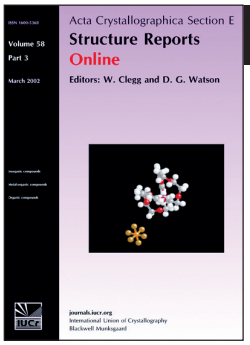


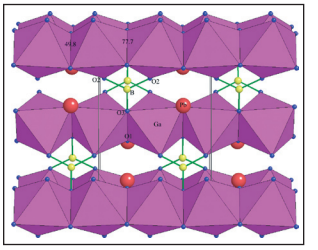
ACTA CRYSTALLOGRAPHICA SECTION E: STRUCTURE REPORTS ONLINE

It has been encouraging, in its first two years of production, to note that Acta Cryst. E has been used for the publication of a great diversity of structures. The three examples reviewed below illustrate this — one a new structure type for an orthoborate, the second a potential building block in supramolecular chemistry and the third a unique β-sheet structure in the form of a 48-membered ring.

$PbGaBO_4$, an orthoborate with new structure type

Hyunsoo Park and Jacques Barbier, *Acta Cryst.* (2001). E**57**, i82–i84

Binary compounds have simple structures with relatively uninteresting properties. Ternary compounds, such as the perovskites, have more complex structures with more interesting properties such as ferroelectricity. Recently, inorganic crystallographers have been studying compounds with four or more elements whose structures are even more complex and continue to stay one step ahead of the ability of theory to predict them or their properties. $PbGaBO_4$ is a good example. It consists of chains of edge-sharing GaO_6 octahedra linked by PbO_4 and BO_3 groups. Because the BO_3 groups share corners with two different GaO_6 octahedra in the same chain, they cause the octahedra to twist (see the figure). One consequence is that the bonds to O3 are stretched leaving O3 underbonded (bond valence sum = 1.79). To compensate, the Ga–O1 bond is shortened, leaving it overbonded (bond valence = 2.23). Although it would be difficult to predict this structure *a priori*, one can at least understand the twists in the chains and the distortions of the GaO_6 octahedra.



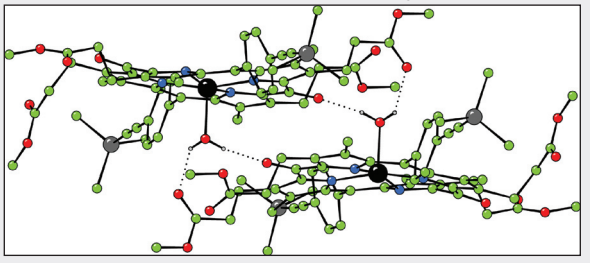
View of the $PbGaBO_4$ structure approximately along the [100] direction. Strong angular distortions are associated with the bridging borate groups.

Reviewed by I. David Brown, Brockhouse Inst., McMaster U. Canada

Aqua{5,15-bis[4-(2-trimethylsilylacetylene)phenyl]-2,8,12,18-tetrakis(2-methoxycarbonylethyl)-3,7,13,17-tetramethyl-10,20-dioxoporphyrinato}zinc(II)

Andrew D. Bond, Neil Feeder, Simon J. Teat, Zoe Clyde-Watson, Nick Bampos and Jeremy K.M. Sanders, *Acta Cryst.* (2001). E**57**, m454–m456

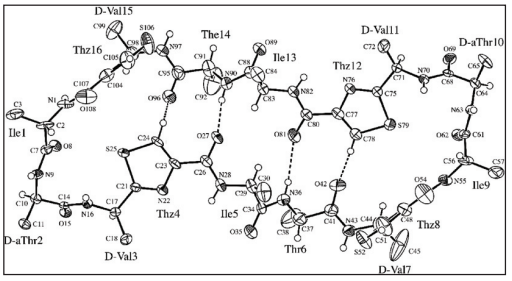
A group from the Cambridge Centre for Molecular Recognition and CLRC Daresbury Laboratory reported the structure of a *trans*-zinc dioxoporphyrin with the other two *meso* positions occupied by the electron-withdrawing group 4-(2-trimethylsilylacetylene). There is a molecule of water occupying an axial site that hydrogen bonds to the carbonyl oxygen of a 2-methoxycarbonylethyl side chain of another molecule to form a centrosymmetric dimer (see figure). The porphyrin adopts a saddle conformation. Adjacent dimers are stacked via laterally shifted porphyrin planes with a Zn···Zn1′ distance of 5.719(1) Å. In adjacent molecules there are edge-to-face interactions. This large structure has 80 non-hydrogen atoms in the asymmetric unit. A small crystal of dimensions 0.02 × 0.06 × 0.07 mm was used to collect a data set at Station 9.8, Daresbury SRS. The radiation employed had λ = 0.6879 Å. An excellent solution and refinement was obtained, illustrating the utility of synchrotron radiation in such instances.



Molecules of the title compound linked into dimers via hydrogen bonds.

Reviewed by Marilyn Olmstead, U. of California, Davis, USA

A β-sheet structure formed by C–H···O hydrogen bonds between the thiazole rings and amide bonds of a dimeric desoxazoline ascidiacyclamide analogue



Top view of the peptide backbone. Dashed lines represent hydrogen bonds.

Akiko Asano, Taizo Taniguchi, Masahiro Sasaki, Hiroshi Hasegawa, Yoshio Katsuya and Mitsunobu Doi, *Acta Cryst.* (2001). E**57**, o834–o838

This interesting and valuable paper illustrates how much novel information can be derived from one crystal structure and compressed into a small package. The investigators have introduced a non-standard amino acid into a cyclic antibiotic in order to probe the structural determinants of protein folding. In the process, they have elucidated the conformational flexibility of the unusual peptide as well as the cyclic structure, and demonstrated an important role for CH···O hydrogen bonding in the structure. Although the amino acid introduced in the cyclic peptide has not been detected in ribosomally encoded proteins, the recent iden-

IUCr Journals *continued*

tification of the occurrence of pyrrolysine in ribosomally encoded peptides in the Archaea *Methanosarcina barkeri* [*Science*, **296**, 1459 (2002)] and its consequent characterization as the "22nd Amino Acid", raises the possibility that in some species (of the 500,000 or more for which the genetic code has not been unequivocally determined) unusual amino acids such as this may actually be ribosomally encoded in proteins. The CH···O hydrogen bond remains controversial despite numerous observations. This structure presents a very good example of a strong CH···O hydrogen bond involved in defining conformation. Recent observations of such hydrogen bonds in protein structures include cases of stabilization of protein fold, and participation in cofactor binding and protein function.

Reviewed by William L. Duax
Hauptman-Woodward Medical Research Inst., USA

Israeli Scholars: Statement by ICSU

Since its inception in 1931, the International Council for Science (ICSU) has affirmed and vigorously upheld the principle of universality of scientific activity without any discrimination on the grounds of citizenship, religion, creed, political stance, ethnic origin, race, color, age or gender. It has argued that the processes of academic research and scholarship, and the unfettered pursuit of knowledge, are of benefit to mankind as a whole. Moreover, they are dependent for their advance upon the freedom of scholars to converse, to make contact, to travel to conferences, to publish their results and to proffer advice. It is, therefore, in the interests of governments, institutions and above all individuals – whether themselves scholars or not – to support this principle of non-discrimination. Bona fide scholars pursuing academic activities should be free to do so without hindrance.

Recent moves to foster an academic boycott of Israeli scientists and the dismissal of two Israeli scholars from their roles on the editorial boards of two journals published in the United Kingdom are a flagrant breach of this profoundly important principle and have rightly drawn substantial adverse comment from scientists, newspaper columnists and human rights activists in the United Kingdom.

On behalf of the Executive Board of ICSU, we draw attention to these events to remind all our national member academies and research councils and our scientific unions and associates of the critical importance of the principle of non-discrimination and of the need for constant vigil in securing its continuing adoption.

We urge all scholarly communities and not least those in science and technology, to heed the words of the Leader in the *London Evening Standard* on July 10, 2002: "intellectual communities world-wide are in the business of fostering international understanding and co-operation not of penalizing each other for the shortcomings of their governments".

James C.I. Dooge, Chairman and Peter Schindler, Executive Secretary
ICSU Standing Committee on Freedom in the Conduct of Science