

## 3. DUAL BASES IN CRYSTALLOGRAPHIC COMPUTING

starting structure for molecular-dynamics procedures, even though some imperfect geometry is to be expected where each tripeptide joins the next.

## 3.3.3.3. Molecular-modelling systems based on other criteria

Systems described within this section mostly have some form of energy minimization as their objective but some are purely geometrical. The optimization of molecules through empirical force fields has been reviewed by Allinger (1976), Burkert & Allinger (1982) and Boyd & Lipkowitz (1982). Some of these systems are in the academic domain, others are commercial. Most have capabilities exceeding the features referred to here and, of necessity, the list cannot be complete. No attempt at comparative evaluations is attempted or implied.

## 3.3.3.3.1. Molbuild, Rings, PRXBLD and MM2/MMP2

Liljefors (1983) has described a system for constructing representations of organic molecules. The system develops the molecule with plausible geometry and satisfied valencies at all stages of the development with explicit recognition of lone pairs and the various possible hybridization states. Growth is generally by substitution in which a substituent and the atom it is to replace are both nominated from the screen. The bond which is reconstructed in a substitution is generally a single bond. Double and triple bonds are introduced by the substitution of moieties containing them. Atom types may be changed after incorporation in the growing molecule, so that although the menu of substituents includes  $-\text{CH}_3$  but not  $-\text{NH}_2$  the latter may be obtained by incorporating  $-\text{CH}_3$ , then changing C to N and one of the hydrogens to a lone pair. Facilities are also provided for cyclization and acyclization.

van der Lieth *et al.* (1984) have described an extension to this that is specialized to the construction of fused-ring systems. It permits the joining of rings by fusion of a bond, in which two adjacent atoms in one ring are superposed on two in another. It also permits the construction of spiro links in which one atom is common to two rings, or the construction of bridges, or the polymerization of ring systems to form, for example, oligo-saccharides. Again the satisfaction of valencies is maintained during building and the geometry of the result is governed by superposition of relevant atoms in the moieties involved.

*PRXBLD* is a molecular-model-building program which accepts two-dimensional molecular drawings in a manner similar to *Script* (Section 3.3.3.3.2) and constructs approximate three-dimensional coordinates from these. It is the model-building component of *SECS* (Simulation and Evaluation of Chemical Synthesis) (Wipke *et al.*, 1977; Wipke & Dyott, 1974; Wipke, 1974). See also Anderson (1984).

All three of these programs produce output which is acceptable as input to *MM2(82)/MMP2* which are developments of Allinger's geometrical optimization based on molecular mechanics (Allinger, 1976).

## 3.3.3.3.2. Script

This system, described by Cohen *et al.* (1981), is specialized for fused-ring systems, especially steroids, but is not limited to these classes. The system allows the user to draw on the screen (with a light pen or equivalent) a two-dimensional representation of a molecule using single lines for single bonds, double lines for double bonds, and wedges to indicate out-of-plane substituents. The software can then enumerate the possible distinct conformers, each of which is expected to be near an energy minimum on the conformational potential surface. Each conformer may then be annealed to reach an energy minimum using an energy estimate based on bond lengths, bond angles, torsion angles and van der Waals, electrostatic and hydrogen-bonding terms. An example is given of the identification of an unusual conformer as

the most stable one from twelve possibilities for a four-ring system.

The program is a development of similar work by Cohen (1971) in which the molecule was defined in terms of a tree structure and an optimizer based on search techniques rather than gradient vectors was used. The method included van der Waals terms and hence estimated energy differences between stereoisomers in condensed ring systems arising from steric hindrance.

## 3.3.3.3.3. CHARMM

This system, due to Brooks *et al.* (1983), is primarily concerned with molecular dynamics but it includes the capability of model-building proteins and nucleic acids from sequence information and values of internal coordinates (bond lengths, bond angles and dihedral angles). The resulting structure (or a given structure) may then be optimized by minimizing an empirical energy function which may include electrostatic and hydrogen-bonding terms as well as the usual van der Waals energy and a Hookean treatment of the covalent skeleton. Hydrogen atoms need not be handled explicitly, groups such as  $-\text{CH}_2-$  being treated as single pseudo atoms, and this may be advisable for large structures. For small or medium proteins hydrogens may be treated explicitly and their initial positions may be determined by *CHARMM* if they are not otherwise known.

## 3.3.3.3.4. Commercial systems

A number of very powerful molecular-modelling systems are now available commercially and we mention a few of these here. Typically, each consists of a suite of programs sharing a common data structure so that the components of a system may be acquired selectively.

The *Chem-X* system, from Chemical Design Ltd, enables models to be developed from sketch-pad input, provides for their geometrical optimization and interfaces the result to *Gaussian80* for quantum-mechanical calculations.

*MACCS*, from Molecular Design Ltd, and related software (Allinger, 1976; Wipke *et al.*, 1977; Potenzzone *et al.*, 1977) has similar features and also has extensive database-maintenance facilities including data on chemical reactions.

*Sybyl*, from Tripos Associates (van Opdenbosch *et al.*, 1985), also builds from sketches with a standard fragment library, and provides interfaces to quantum-mechanical routines, to various databases and to *MACCS*.

*Insight II* (Section 3.3.3.1.7) is available from Biosym and *GRAMPS* (Section 3.3.3.1.4) is available from T. J. O'Donnell Associates.

## 3.3.4. Graphics software for the display of small and medium-sized molecules

By L. M. D. CRANSWICK

## 3.3.4.1. Introduction

In the age of the Internet, a wide variety of software can be easily obtained for the display of small and medium-sized molecules. An obvious question to ask is 'which software is the best?'. It can be 'best' to try all the relevant available software quickly before settling on two to three programs that are found to be most suitable. Not relying on just a single program can be important for visual and numeric cross validation of the resulting structural plot, as bugs (if present) can be quite subtle in their effect, but moderately easy to find by comparing plots made by different programs.

Most software can import crystallographic data in some format. The IUCr CIF format [see *International Tables for*

### 3.3. MOLECULAR MODELLING AND GRAPHICS

Table 3.3.4.1. *Functionality of software for crystal structure display*

Program	Ball and stick	ADPs	MSDA	Polyhedral display	Cartesian coordinates	Comparison/ overlay of multiple structures	Extended structures/ topology analysis	Magnetic structures	Incommensurate structures
<i>ATOMS</i>	Yes	Yes		Yes	Yes			Yes	
<i>Balls&amp;Sticks</i>	Yes			Yes					
<i>BALSAC</i>	Yes				Yes				
<i>Cameron</i>	Yes	Yes							
<i>CaRIne</i>	Yes			Yes	Yes				
<i>Crystallographica</i>	Yes	Yes		Yes					
<i>CrystalMaker</i>	Yes			Yes	Yes			Yes	
<i>Crystal Studio</i>	Yes	Yes		Yes	Yes				
<i>CrystMol</i>	Yes	Yes			Yes	Yes			
<i>Diamond</i>	Yes	Yes		Yes	Yes			Yes	
<i>DrawXTL</i>	Yes	Yes		Yes				Yes	
<i>FpStudio</i>	Yes	Yes						Yes	Yes
<i>GRETEP</i>	Yes	Yes					Yes		
<i>Mercury</i>	Yes				Yes				
<i>MolXtl</i>	Yes	Yes			Yes				
<i>OLEX</i>	Yes				Yes		Yes		
<i>ORTEP-III</i>	Yes	Yes							
<i>ORTEP-3 for Windows</i>	Yes	Yes	Yes		Yes				
<i>ORTEX/Oscail X</i>	Yes	Yes							
<i>PEANUT</i>	Yes	Yes	Yes						
<i>Platon/Pluton</i>	Yes	Yes			Yes				
<i>PowderCell</i>	Yes								
<i>PRJMS</i>	Yes								Yes
<i>SCHAKAL</i>	Yes				Yes				
<i>STRUPLO</i>	Yes			Yes					
<i>STRUPLO for Windows</i>				Yes	Yes				
<i>STRUVIR</i>				Yes					
<i>VENUS</i>	Yes	Yes		Yes	Yes			Yes	
<i>XmLmctep</i>	Yes	Yes							
<i>X-Seed</i>	Yes	Yes			Yes				
<i>Xtal-3D</i>	Yes	Yes		Yes				Yes	
<i>XtalDraw</i>	Yes	Yes		Yes					

*Crystallography* Volume G (2005)] is slowly becoming a standard in this regard, displacing the single-crystal *SHELX* INS format, which has been a *de-facto* standard file format for much crystallographic data exchange. Entering crystallographic data by hand is slow and often introduces errors *via* typographical mistakes. Such mistakes can be minimized by importing structures using a known file type, or reformatting using a text editor or spreadsheet program into a known file type. A variety of software programs can be used for translating crystallographic structure files; however, the output (especially the handling of the symmetry operators and the space group) should be carefully checked. The CCP14 website (Cockroft & Stephenson, 2005) lists a variety of programs that can be used for this, of which a specialist program is *Cryscon* (Dowty, 2005).

#### 3.3.4.2. Types of crystal structure display and functionality

The following information was current at the time of writing, but most software is continually changing with the insertion of new features. Thus occasional checks for updated functionality can be useful. Most software distributions include an 'updates' file containing new features and bug fixes. Detailed information on the software referred to in this section, including functionality, authorship, source and availability, is given in Tables 3.3.4.1 and 3.3.4.2.

##### 3.3.4.2.1. Ball and stick

This is one of the most fundamental methods of displaying a crystal structure and almost all software supports this. The exceptions are *STRUVIR* and *STRUPLO for Windows* [a port of *STRUVIR* incorporating a graphical user interface (GUI)], which are both optimized for the polyhedral display of crystal structures.

##### 3.3.4.2.2. Anisotropic displacement parameters

A subset of the programs that display ball-and-stick structures can also display surfaces related to anisotropic displacement parameters (ADPs) (also known colloquially as 'thermals', 'anisotropic thermal ellipsoids' or 'ORTEPS'). By default, most programs display the ellipsoid surfaces at a probability of 50% and normally allow this value to be changed to values between 1 and 99%. Programs that can draw ADPs include *ATOMS*, *Cameron*, *Crystallographica*, *CrystalMaker*, *Crystal Studio*, *CrystMol*, *Diamond*, *DrawXTL*, *FpStudio*, *GRETEP*, *MolXtl*, *ORTEP-III*, *ORTEP-3 for Windows*, *ORTEX*, *PEANUT*, *Platon*, *VENUS*, *XmLmctep*, *X-Seed* and *XtalDraw*.

##### 3.3.4.2.3. Mean-square displacement amplitude

When a more thorough investigation of the ADPs would be informative (Hummel, Raselli & Bürgi, 1990), *PEANUT* can be used for plotting the mean-square displacement amplitude (MSDA), root-mean-square displacements (RMSDs) and difference surfaces. MSDA 'peanuts' can be displayed where the ADPs are non-positive-definite and the ellipsoids cannot be drawn. *ORTEP-3 for Windows* also has an option for plotting MSDAs. Care should be taken to ensure the resulting display is correct.

##### 3.3.4.2.4. Polyhedral display

A method for understanding inorganic and intermetallic structures is the use of coordination polyhedra. The faces defined by the outer coordinated atoms generate a polyhedral object that is displayed instead of the individual atoms. This can aid in understanding the structures of polymeric inorganic materials involving both simple and complex tilt systems, and distorted

### 3. DUAL BASES IN CRYSTALLOGRAPHIC COMPUTING

Table 3.3.4.2. Availability of software for crystal structure display

Program	Company or contact person	Contact and/or web address	Reference	Status
<i>ATOMS</i>	Shape Software	521 Hidden Valley Road, Kingsport, TN 37663, USA. <a href="http://www.shapesoftware.com/">http://www.shapesoftware.com/</a>		Commercial
<i>Balls&amp;Sticks</i>	Tadashi Ozawa	<a href="http://www.toycrate.org/">http://www.toycrate.org/</a>	[1]	Freeware
<i>BALSAC</i>	Klaus Hermann	Fritz-Haber-Institut der MPG, Berlin. <a href="http://w3.rz-berlin.mpg.de/~hermann/hermann/bal pam.html">http://w3.rz-berlin.mpg.de/~hermann/hermann/bal pam.html</a> [Copyright (1991–2004) Klaus Hermann. All rights reserved.]		Commercial
<i>Cameron</i>	David Watkin	<a href="http://www.xtl.ox.ac.uk/crystals.html">http://www.xtl.ox.ac.uk/crystals.html</a>	[2]	Freeware
<i>CaRIne</i>	ESM Software	<a href="http://pro.wanadoo.fr/carine.crystallography/">http://pro.wanadoo.fr/carine.crystallography/</a> [Copyright (1989–2005) C. Boudias and D. Monceau.]		Commercial
<i>Crystallographica</i>	Oxford Cryosystems Ltd	<a href="http://www.crystallographica.co.uk/">http://www.crystallographica.co.uk/</a>	[3]	Commercial
<i>CrystalMaker</i>	CrystalMaker Software Ltd	5 Begbroke Science Park, Sandy Lane, Yarnton, OX5 1PF, UK. <a href="http://www.crystalmaker.co.uk/">http://www.crystalmaker.co.uk/</a> ( <i>CrystalMaker</i> 6 for Mac OS X)		Commercial
<i>Crystal Studio</i>	CrystalSoft & Crystal Systems Co. Ltd	PO Box 7006, Wattle Park, VIC 3128, Australia. <a href="http://www.crystalsoftcorp.com/">http://www.crystalsoftcorp.com/</a> [Copyright (1999–2005) Crystal Systems Co., Ltd]		Commercial
<i>CrystMol</i>	David Duchamp	6209 Litchfield Lane, Kalamazoo, MI 49009-9159, USA. <a href="http://www.crystmol.com/">http://www.crystmol.com/</a>		Commercial
<i>Diamond</i>	Crystal Impact	K. Brandenburg & H. Putz, Crystal Impact GbR, Postfach 1251, D-53002 Bonn, Germany. <a href="http://www.crystalimpact.com/">http://www.crystalimpact.com/</a>		Commercial
<i>DrawXTL</i>	Larry Finger	<a href="http://lwfinger.net/drawxtl/">http://lwfinger.net/drawxtl/</a>	[4]	Freeware
<i>FpStudio</i>	Juan Rodriguez-Carvajal	<a href="http://www.ill.fr/dif/soft/fp/">http://www.ill.fr/dif/soft/fp/</a>	[5]	Freeware
<i>GRETEP</i>	Jean Laugier	J. Laugier and B. Bochu, ENSP/Laboratoire des Matériaux et du Génie Physique, BP 46, 38042 Saint Martin d'Hères, France. <a href="http://www.ccp14.ac.uk/tutorial/lmgp/">http://www.ccp14.ac.uk/tutorial/lmgp/</a>		Freeware
<i>Mercury</i>	Cambridge Crystallographic Data Centre	<a href="http://www.ccdc.cam.ac.uk/">http://www.ccdc.cam.ac.uk/</a>	[6]	Freeware
<i>MolXtl</i>	Dennis W. Bennett	<a href="http://www.uwm.edu/Dept/Chemistry/molxtl/">http://www.uwm.edu/Dept/Chemistry/molxtl/</a>	[7]	Freeware
<i>OLEX</i>	Oleg Dolomanov	<a href="http://www.ccp14.ac.uk/ccp/web-mirrors/lcells/olex_index.htm">http://www.ccp14.ac.uk/ccp/web-mirrors/lcells/olex_index.htm</a>	[8]	Freeware
<i>ORTEP-III</i>	Carroll Johnson	<a href="http://www.ornl.gov/ortep/ortep.html">http://www.ornl.gov/ortep/ortep.html</a>	[9]	Freeware
<i>ORTEP-3 for Windows</i>	Louis Farrugia	<a href="http://www.chem.gla.ac.uk/~louis/software/ortep3/">http://www.chem.gla.ac.uk/~louis/software/ortep3/</a>	[10]	Freeware
<i>ORTEX/Oscail X</i>	Patrick McArdle	<a href="http://www.nuigalway.ie/cryst/software.htm">http://www.nuigalway.ie/cryst/software.htm</a>	[11], [12]	Freeware
<i>PEANUT</i>	Hans-Beat Bürgi	Laboratorium für chemische und mineralogische Kristallographie, Universität Bern, Freiestrasse 3, CH-3012 Bern, Switzerland. E-mail: <a href="mailto:hans-beat.buergi@krist.unibe.ch">hans-beat.buergi@krist.unibe.ch</a>	[13]	Freeware
<i>Platon/Pluton</i>	Anthony Spek	<a href="http://www.cryst.chem.uu.nl/platon/">http://www.cryst.chem.uu.nl/platon/</a>	[14], [15]	Freeware
<i>PowderCell</i>	Gert Nolze	<a href="http://www.ccp14.ac.uk/ccp/web-mirrors/powdcell/a_v/v_1/powder/e_cell.html">http://www.ccp14.ac.uk/ccp/web-mirrors/powdcell/a_v/v_1/powder/e_cell.html</a>	[16]	Freeware
<i>PRIMS</i>	Akiji Yamamoto	<a href="http://quasi.nims.go.jp/yamamoto/">http://quasi.nims.go.jp/yamamoto/</a>	[17]	Freeware
<i>SCHAKAL</i>	Egbert Keller	<a href="http://www.krist.uni-freiburg.de/ki/Mitarbeiter/Keller/schakal.html">http://www.krist.uni-freiburg.de/ki/Mitarbeiter/Keller/schakal.html</a>	[18]	Freeware
<i>STRUPLO</i>	Reinhadt Fischer	<a href="http://www.brass.uni-bremen.de/">http://www.brass.uni-bremen.de/</a>	[19]	Freeware
<i>STRUPLO for Windows</i>	Louis Farrugia	<a href="http://www.chem.gla.ac.uk/~louis/software/struplo/">http://www.chem.gla.ac.uk/~louis/software/struplo/</a>	[19], [20]	Freeware
<i>STRUVIR</i>	Armel Le Bail	<a href="http://www.cristal.org/vrml/struvir.html">http://www.cristal.org/vrml/struvir.html</a>	[19], [20]	Freeware
<i>VENUS</i>	Fujio Izumi	<a href="http://homepage.mac.com/fujioizumi/visualization/VENUS.html">http://homepage.mac.com/fujioizumi/visualization/VENUS.html</a>	[21], [22]	Freeware
<i>XmLmctep</i>	Alain Soyer	<a href="http://www.lmcp.jussieu.fr/~soyer/Lmctep_en.html">http://www.lmcp.jussieu.fr/~soyer/Lmctep_en.html</a>	[23]	Freeware
<i>X-Seed</i>	Len Barbour	<a href="http://x-seed.net/">http://x-seed.net/</a>	[24], [25]	Commercial
<i>Xtal-3D</i>	Alan Hewat	<a href="http://barns.ill.fr/dif/xtal-3d.html">http://barns.ill.fr/dif/xtal-3d.html</a>	[26]	Freeware
<i>XtalDraw</i>	Bob Downs	<a href="http://www.geo.arizona.edu/xtal/xtaldraw/xtaldraw.html">http://www.geo.arizona.edu/xtal/xtaldraw/xtaldraw.html</a>	[27]	Freeware

References: [1] Ozawa & Kang (2004); [2] Watkin *et al.* (1996); [3] Siegrist (1997); [4] Finger *et al.* (2007); [5] Chapon & Rodriguez-Carvajal (2005); [6] Bruno *et al.* (2002); [7] Bennett (2004); [8] Dolomanov *et al.* (2003); [9] Burnett & Johnson (1996); [10] Farrugia (1997); [11] McArdle (1994); [12] McArdle *et al.* (2004); [13] Hummel, Hauser & Bürgi (1990); [14] Spek (1998); [15] Spek (2003); [16] Kraus & Nolze (1996); [17] Yamamoto (1982); [18] Keller (1999); [19] Fischer (1985); [20] Le Bail (1996); [21] Izumi & Dilanian (2002); [22] Izumi (2004); [23] Soyer (1993); [24] Barbour (2001); [25] Atwood & Barbour (2003); [26] Hewat (2002); [27] Downs & Hall-Wallace (2003).

coordination structures. Polyhedral display is provided by the programs *ATOMS*, *Balls&Sticks*, *CaRIne*, *Crystallographica*, *CrystalMaker*, *Crystal Studio*, *Diamond*, *DrawXTL*, *STRUPLO*, *STRUPLO for Windows* (a port of *STRUVIR* incorporating a GUI), *STRUVIR*, *VENUS*, *Xtal-3D* and *XtalDraw*. Nearly all the

programs display polyhedra automatically after the user has defined (i) a central atom, (ii) the coordinated atoms and (iii) minimum (often a default of near zero) and maximum bond distances. One exception is *Balls&Sticks*, where graphical point and click of the mouse is used to define the polyhedra.

### 3.3. MOLECULAR MODELLING AND GRAPHICS

#### 3.3.4.2.5. Cartesian coordinates

Importing Cartesian coordinates can allow the display of incommensurate and quasicrystal structures if the refinement software has this as an output option. Using Cartesian coordinates can sometimes be more convenient for the slight modification of structures for the display of distortions or individual molecules. A structure defined as triclinic with space group *P1* and a cubic cell with edges of unit length would also work for importing a structure or molecule originally defined in a Cartesian frame of reference.

#### 3.3.4.2.6. Comparing or overlaying crystal structures

The graphical comparison of crystallographic structures can be useful and time-saving for comparison of polymorphs or a chemically similar series of small-molecule structures. One program that can perform this function is *CrystMol*, where multiple molecular structures can be compared using a point and click menu or *via* the *CrystMol* scripting system. RMS differences are also listed. Superposition of structures is discussed in Section 3.3.1.2.2.

#### 3.3.4.2.7. Extended structures and topology analysis

Currently, the only available program that rigorously analyses extended structures (involving overlapping or interpenetrating molecules) is *OLEX*. For graphical viewing of extended structures *OLEX* displays particular fragments in a single colour. *GRETEP* also has this display functionality, making it useful for viewing extended structures.

#### 3.3.4.2.8. Magnetic crystal structure display

The software listed in Tables 3.3.4.1 and 3.3.4.2 includes programs that can display graphics representing magnetic vectors without necessarily having the ability to understand magnetic symmetry. Programs that can display magnetic structures include *ATOMS*, *CrystalMaker*, *Diamond*, *DrawXTL*, *FpStudio*, *VENUS* and *Xtal-3D*.

#### 3.3.4.2.9. Incommensurate crystal structures

*PRJMS* and *FpStudio* are currently the only programs that can plot modulated structures in three-dimensional space; *FpStudio* is currently restricted to incommensurate magnetic structures. However, importing Cartesian coordinates can be used to display incommensurate structures when incommensurate refinement software can output coordinates in this format. *BALSAC* provides a good example of software which by default uses Cartesian coordinates, from which plots of incommensurate and quasicrystal structures can be generated.

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