BIOGRAF/POLYGRAF/NMRgraf Release Notes
Version 3.0

These notes summarize the changes made to BIOGRAF, POLYGRAF, and NMRgraf for version 3.0. The notes are divided into three sections. The first section outlines the major enhancements to the program, Section II describes the hardware supported, and Section III contains notes about the use of macros, running the program in the background, the Dreiding II force field, and some miscellaneous topics.

Overview:

The major enhancements and modifications to this version of BIOGRAF, POLYGRAF, and NMRgraf are

- A new user interface and menu layout promoting ease of use and portability to a wide range of platforms.
- Interactive deformation/minimization which allows users to easily push molecules into new conformational states by using mouse motions. This feature allows chemists to manipulate conformations of molecules in an intuitive, instantaneous manner.
- A new host of molecular dynamics algorithms for canonical dynamics under conditions of constant temperature, constant volume, constant stress and constant pressure.
- Output of screen images as encapsulated PostScipt files for incorporation into other documents or for generating hardcopy prints.

In addition to these enhancements a number of new features have been added to improve the construction, visualization, simulation, and analysis of molecular systems as described below.

The installation procedure has been modified to provide an easier installation process.

If you have difficulties with the installation of this release or questions about it, the Molecular Simulations Scientific Support Group can provide assistance. Our Hotline numbers are Phone: (617) 487-7875 FAX: (617) 890-8694.

I. Enhancements

New Graphical User Interface (GUI): The program has a new X-Windows based graphical user interface (GUI), making it highly portable and capable of running on a wider range of platforms (ranging from X Terminals, PCs and Macintoshes to workstations to mainframes). It uses standard X-Windows type widgets including file browsers, dialog boxes, alert boxes, and buttons. The menus are now displayed vertically in a Menu Pad. Advantages of the new interface include faster menu drawing and picking, less cursor motion, simpler menu layouts, increased use of automatic file and group selection, and more visible messages. Extraneous menus and information are no longer displayed and the menu labels use longer more legible names. Commonly used functions are now readily accessible via constantly displayed buttons. File browsers speed up file input and make default directory switching easier. See Introduction in Chapter 1 of the *Reference Manual.*

DISPLAY, TOP MENU, and COMMAND Buttons: Three commonly used functions are now always accessible via buttons that are constantly displayed. The Groups menu appears when group selection is required but can be readily brought up anytime via the DISPLAY button. Similarly, the user can go directly to the top level menu or into command mode via the TOP MENU and COMMAND buttons. See Section 1.4.4 of the *Reference Manual.*

More Functional Menu Organization: The menus have been reorganized into more functional groupings making it easier to locate and use program functions. Functions are now logically divided into seven major categories which make up the top level menu: input/output functions, build operations, visualize functions, simulation operations, analysis functions, utilities, and an exit function. The documentation has also been reorganized accordingly. Menu item names have also been extended or renamed to improve clarity. The major changes are described under the appropriate categories below.

Macros Expand Batch Capabilities: The macro facility now supports running jobs in the background. This enhances and expands batch capabilities. See Section 1.8 of the *Reference Manual.*

NMRgraf Functions Expanded: NMRgraf functionality has been greatly expanded to include many of the features available in BIOGRAF. New features include a Solvent Builder, docking capabilities, RMS matching, plotting capabilities, and several visualization tools such as the ability to make groups, use different rendering techniques, and surface structures. Most of the new features available in the 3.0 release of BIOGRAF are also available for NMRgraf users. These include the enhanced editing tools such as interactive deformation/minimization, the file browser, and the expanded molecular dynamics capabilities. A back calculate function which generates NOE spectra from the 3-D structure of the molecule has also been added. See the *NMRgraf Reference Manual.*

IN-OUT

New File Types (BIOGRAF and POLYGRAF only): Two new types of files are now supported. The program can now write CSSR files (used by the CERIUS program), and it can both read and write force field parameter files. Obsolete file types (OLD BGF and OLD XTLG) do not appear on the menu, although the program still reads these obsolete file types. The INIT file type has been deleted since initialization files have been replaced with macro capabilities. See READ and WRITE in Sections 2.1.and 2.2 of the *Reference Manual.*

CAPTION (BIOGRAF and POLYGRAF only): The way that captions, borders, arrows, and boxes are created has been improved (these functions were formerly under HARDCOPY). See CAPTION in Section 2.4 of the *Reference Manual.*

PRINT SCREEN (BIOGRAF and POLYGRAF only): A new function has been added which allows the user to generate an encapsulated PostScript file of the image on the screen so that it can be imported into other applications or output to a printer. The image output may be black and white, gray scale, or color, and positive or negative. The user may include the full screen or a selected portion. See PRINT SCREEN in Section 2.5 of the *Reference Manual.*

BUILD

Menu Reorganization: The reorganization of the menus has extended the BUILD menu. As before, the BUILD menu includes the Organic Builder plus the other more specialized Builders. These are the Peptide, Lipid, Carbohydrate, DNA-Old, and RNA-DNA Builders for BIOGRAF and NMRgraf users plus the Crystal Builder for BIOGRAF users, and the Polymer, Periodic, Crystal, and Amorphous Builders for POLYGRAF users. The Solvent Builder (formerly under MODEL) is now on the BUILD menu as well as other functions which may be used to complete the building process. These allow the user to rotate bonds (ROTATE BOND), dock two structures (DOCK), convert coordinate files that do not include force field data (CONVERT), and generate connectivity data for input files (CONNECT). One can also add missing hydrogens or change the mass of hydrogens to that of deuterium or tritium (formerly under MODEL, these functions are now under a new option called MODIFY H). See BUILD, Chapter 3 of the *Reference Manual.*

The REPLACE function which is used to replace single amino acid residues with new ones is now on the PEPTIDE menu (it was formerly on the entry-level menu). See Section 3.2.7 of the *BIOGRAF Reference Manual.*

ROTATE is now called DOCK, the ROCK and AUTO ROTATE functions formerly on the ROTATE menu are now under VISUALIZE, and the functions which set the origin of rotation have been placed together with the dials reset functions under a new toggle (SET ORIGIN) on the DOCK menu; they are also located under VISUALIZE. See DOCK, Section 3.10 (Section 3.8 for POLYGRAF users) and VISUALIZE, Chapter 4 of the *Reference Manual.*

Realtime Conformational Distortion/Minimization: This new feature allows chemists to use their intuition for quickly exploring the conformational space of molecules. Most molecular mechanics programs require the user to provide a starting conformation and then use either systematic searching, Monte-Carlo procedures, or molecular dynamics to find a conformation of lower energy. These algorithms proceed without any further direction or input from the user and generally are time consuming. Realtime conformational distortion/minimization on the other hand allows the user to interactively modify the conformation of a molecule while continuously minimizing the structure to remove any highly strained internal coordinates or repulsive steric interactions. For example, the user can grab one atom of a six membered ring and using the mouse drag it to flip the conformation between chair and boat. This process allows the user to push molecules over transition state barriers and quickly test likely low energy conformations. Continuous feedback on the energy of the distorted conformations allows the user to guide the molecule to successively lower energy states. Use of this new feature is described under DRAG-CLEAN in Section 3.1.12 of the *Reference Manual.*

EDIT Improved: The functions for editing molecules have been improved. New features include atom dragging, continuous minimization during molecule deformation as described above, and a SELECT option which speeds up the editing process by allowing the user to specify the atoms to be operated on (individual atoms, substructures, ranges, hydrogens, heteroatoms, lone pairs *etc.* may be specified). See EDIT in Section 3.1.12 of the *Reference Manual.*

SETUP Improved (Organic Builder): The SETUP function for the Organic Builder has been streamlined so that the user is no longer required to enter a residue name, residue number, and chain designator for the file. Default values are automatically used. If the defaults are not wanted, they may be changed using the NEW ATOM IDS function which has been added to the ORGANIC menu. See Sections 3.1.1 and 3.1.2 in the *Reference Manual.*

Crystal Builder (BIOGRAF and POLYGRAF only): An INPUT FILE option has been added to the CRYSTAL menu which allows the user to read in crystallographic data from an input file (previously, this was done using the INPUT COORD option). The file may be selected from listings in the browser box or entered directly. After inputting the crystallographic data, the space group name now appears on the CRYSTAL menu (under SPACE GROUP). The CHARGE option has been moved under DEFAULTS and an INTO CELL function has been added to the DEFAULTS menu which repositions outlying atoms within the unit cell boundaries.

CONNECT Modified: Some changes have been made to the CONNECT option (formerly called CONN PBC). Two CRITERIA are now available for use in determining whether a bond is formed between two atoms: in addition to the scaled van der Waals radii (VDW RADII), the user may now choose to use the equilibrium bond distance (BOND RADII). A DELETE BONDS function has also been added which deletes all bonds. See Section 3.14 of the *BIOGRAF* or *NMRgraf Reference Manual* or Section 3.12 of the *POLYGRAF Reference Manual.*

Improved Solvent Library: The Solvent Builder's library of solvents has been extended to include three additional solvents. See Section 3.8.2 of the *BIOGRAF* or *NMRgraf Reference Manual* or Section 3.6.2 of the *POLYGRAF Reference Manual.*

BOX SOLVENT: The Solvent Builder now includes a BOX SOLVENT toggle. When on, the solvent shell created around the molecule takes the shape of a box. This is useful when working with periodic systems. See Section 3.8.7 of the *BIOGRAF* or *NMRgraf Reference Manual* or Section 3.6.7 of the *POLYGRAF Reference Manual.*

MOMENT: A new MOMENT function is now available on the BUILD menu which allows the user to calculate the center of mass and principle axes of a structure and to have the coordinates transformed if desired. This is useful in changing the coordinate system to be aligned with the molecule (*e.g.*, for input to quantum chemistry programs). See Section 3.12 of the *BIOGRAF* or *NMRgraf Reference Manual* or Section 3.10 of the *POLYGRAF Reference Manual.*

Random Copolymers (POLYGRAF only): Random copolymers may be created from selected monomers using the Polymer Builder's new RANDOM COPOLY function. The user specifies the percentage for each monomer included then uses the REPEAT option to specify the overall chain length. See Section 3.2.6 in the *POLYGRAF Reference Manual.*

Molecular Crystal Function Increases Limit on Atoms in Unit Cell (POLYGRAF only): A switch is now available on the PERIODIC menu (MOLXTL ON/OFF) which can be used to treat certain structures as molecular crystals and effectively increase the maximum number of atoms allowed within the unit cell from 1000 to about 20,000 atoms. The unit cell cannot be extended, but periodicity is still implicitly maintained. This option is particularly useful when working with nonpolymeric crystals or large amorphous systems. See Section 3.3.2 in the *POLYGRAF Reference Manual.*

FORM MOLECULE (POLYGRAF only): A FORM MOLECULE function is now available on the PERIODIC menu which uses atom connectivity information to form continuously connected atoms in a given structure. Published crystallographic data often lists atoms only within the unit cell, leaving part of the molecule on the left cell boundary and the remainder on the right. FORM MOLECULE modifies the unit cell atoms to be complete molecules (the whole molecule will be on the left, going across the cell boundary). All calculations are done correctly for full periodic boundary conditions. This is needed for the MOLXTL ON option. See Section 3.3.5 in the *POLYGRAF Reference Manual.*

Multiple Chain Amorphous Polymers or Blends (POLYGRAF only): The Amorphous Builder can now build multiple chain amorphous polymers or blends. Single chain structures are first created using one of the other builders; each structure is saved in a separate file. These files can then be combined into a single file in the Amorphous Builder and used to build a multiple chain homologous polymer or blend. The SETUP function has been modified to allow for this. See SETUP in Section 3.5.1 of the *POLYGRAF Reference Manual.*

VISUALIZE

New VISUALIZE Menu: Functions related to visualizing the images on the graphics display have been placed together under a new VISUALIZE menu. These include the MAKE GROUPS operations which are used to divide a structure into functional groups and the RENDER GROUPS options which are used to change the rendering mode, half-bond/monochrome representation, vector width *etc.* (these functions were formerly under GROUP). Also under VISUALIZE are the SURFACE operations, functions for changing the center of rotation and resetting the dials or mouse (SET ORIGIN), as well as functions for changing group colors (CHANGE COLORS), viewing in STEREO, and automatically rocking or rotating objects about the y axis (ROCK, AUTO ROTATE). See Chapter 4 of the *Reference Manual.*

Slider Bars for Color Selection: A new feature has been added which makes it easier for the user to specify the exact color of a group or structure. The RGB VALUE option on the Colors menu now brings up a dialog box with slider bars which can be used to specify values for the red, green, and blue components as well as hue, saturation, and value. A color box reflects the color as changes are being made. See Section 4.5 of the *Reference Manual.*

Improved Surfacing Algorithms: The algorithms which generate van der Waals and solvent accessible dot surfaces have been improved. Speedups of a factor of ten or more are commonly encountered. Because of the faster execution times, we now use solvent accessible surfaces as the default with a higher density of dots (10.0 dots /Å^2). See Section 4.3 of the *Reference Manual.*

SIMULATE

EEX OPTIONS: A new EEX OPTIONS function is now on the SIMULATE menu which allows the user to set defaults which will be used when setting up the energy expression. Two on/off toggles are provided: FAST SETUP and RIGID MOLECULE, described below.

FAST SETUP: A FAST SETUP toggle has been added under EEX OPTIONS which streamlines setting up the energy expression (SETUP EEX). When on, the energy expression will automatically be set up with all atoms/groups movable. Otherwise, the user must select the movable and updatable groups. See Section 5.1 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.1 of the *NMRgraf Reference Manual.*

RIGID MOLECULE: A new RIGID MOLECULE toggle has been added under EEX OPTIONS. When on, each molecule is treated as a rigid body during minimization and dynamics. This is useful for considering a large number of solvent molecules and for determining packing of molecules (*e.g.*, in liquid crystals). It is also useful as a first step in minimizing the structure when there are a collection of molecules. The algorithms used are based on the quaternion algorithm of Evans and Murad[1]. See Section 5.1 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.1 of the *NMRgraf Reference Manual.*

MODIFY EEX: The OVERRIDE option on the MODIFY EEX menu has been deleted and two new options have been added, FIX ALL and FIX GROUPS, which specify that all atoms be fixed and that selected groups be fixed, respectively. See Section 5.3 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.3 of the *NMRgraf Reference Manual.*

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[1]Evans, D. J. and Murad, S., *Mol. Phys.*, **1977**, 34, 327.

SHOW EEX: This new function (under SIMULATE) shows how the energy expression has been set up. Movable atoms are indicated with green crosses and fixed atoms are indicated with blue crosses. Other relevant information is shown on the text display. See Section 5.4 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.4 of the *NMRgraf Reference Manual.*

Simulation Results Expanded (POLYGRAF only): The Simulation results menu displayed during the energy calculations for periodic systems now shows the external stress values and unit cell dimensions in addition to the various energy terms. See Section 5.7 of the *POLYGRAF Reference Manual.*

CONVERGENCE, E CONVERGE: Options to set the convergence criteria used in minimizations have been placed directly on the MECHANICS and CONSTRAINED MIN menus so this can be done without going to the MINIMIZE VAR (Minimization variables) menu. See Section 5.7.5 and 5.9.7 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.7.5 and 6.9.7 of the *NMRgraf Reference Manual.*

GEOMETRY PROP: A GEOMETRY PROP function is now available on the MECHANICS menu which provides geometric analysis during energy calculations (for minimizations, the analysis is made at the last step). The user may specify which parameters are to be analyzed (bonds, angles, torsions, inversions, hydrogen bonds, nonbonds) and the cutoff distances to be used for hydrogen bond and nonbond interactions. If desired, parameter values may be averaged according to force field type. Results (distances, angles, atom identification numbers) are shown in the text window. See Section 5.7.8 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.7.8 of the *NMRgraf Reference Manual.*

RESET VELOCITY: A new RESET VELOCITY function has been added to all the dynamics menus which reassigns random velocities before continuing a dynamics run instead of using the last set of velocities as starting velocities. See Section 5.8.1 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.8.1 of the *NMRgraf Reference Manual.*

Nonbond Control: The nonbond switch on the ENERGY VAR menu is now separated into a COULOMB switch for electrostatic interactions and a NONBONDS switch for van der Waals interactions. Two switches have also been added which can force all inversions or all torsions to be included whether they are defined by the force field or not. See Section 5.12.1 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 6.12.1 in the *NMRgraf Reference Manual.*

Charge Equilibration Switch: A switch has been added to the ENERGY VAR menu which allows the user to have charge equilibration done periodically (each time the nonbond list is updated). See Section 5.12.1 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 6.12.1 in the *NMRgraf Reference Manual.*

Canonical Dynamics: Two new options have been added to the DYNAMICS menu which allow the user to perform canonical (Nosé) dynamics. Constant temperature/constant volume dynamics, CANONICAL(TVN), is available to all users, and constant temperature/constant pressure dynamics, CANONICAL(TPN), is available for POLYGRAF users. When using CANONICAL(TVN) dynamics, the user may specify the relaxation time constant and choose the algorithm used (Hoover[2] or Nosé[3]). For the CANONICAL (TPN) method, coupling to external stress/pressure is facilitated through the extended dynamics approach of Andersen-Parrinello-Rahman[4,5]. The strength of the coupling may also be specified. See Section 5.8.6 in the *BIOGRAF Reference Manual*, Section 6.8.6 in the *NMRgraf Reference Manual*, and Sections 5.8.6 and 5.8.7 in the *POLYGRAF Reference Manual.*

Isothermal Dynamics Using Temperature Damping: New options have been added to the DYNAMICS menu which use the Berendsen *et al* approach[6] to perform isothermal dynamics through weak coupling to a thermal bath. Constant volume isothermal dynamics, TEMPDAMP(TVN), is available for all users, and constant pressure isothermal dynamics, TEMPDAMP(TPN), is available for POLYGRAF users. As in canonical dynamics described above, the user may specify the strength of coupling through a damping time constant. Also, for the TEMPDAMP(TPN) method, coupling to external stress/pressure is facilitated through the extended dynamics approach of Andersen-Parrinello-Rahman[3,4]. The strength of the coupling may also be specified. See Section 5.8.7 in the *BIOGRAF Reference Manual*, Section 6.8.7 in the *NMRgraf Reference Manual*, and Sections 5.8.8 and 5.8.9 in the *POLYGRAF Reference Manual.*

Extended Dynamics Variables (POLYGRAF only): An EXT DYN VAR option has been added to the DEFAULTS menu which sets the variables used when running constant pressure/stress and/or constant temperature dynamics. Options are available which determine the dynamics method used (adiabatic, temperature damping, or canonical), whether the dimensions of the unit cell are kept fixed or allowed to vary, and whether the structure's average coordinates during the course of the dynamics run are saved or not. Options are also available which set the external pressure and the direction and amount of external stress that is applied to the cell during the dynamics calculations. See Section 5.12.5 in the *POLYGRAF Reference Manual.*

Ewald Sums Variables (POLYGRAF only): An EWALD VAR option has been added to the DEFAULTS menu which allows the user to set the Ewald sums variables. These variables apply when using the Ewald sums method for determining nonbond interactions in periodic systems. Included are options for Ewald sums optimization (described below) as well as parameters which specify the accuracy used in the energy calculations, the eta value used for nonbond interactions, the real space and reciprocal space cutoff distances used for electrostatic and van der Waals interactions, and the cutoff distance used for repulsive van der Waals interactions. The user may also specify the time ratio used to optimize eta and whether the geometric mean or arithmetic mean combination rule is to be used when calculating off diagonal van der Waals parameters. See Section 5.12.7 in the *POLYGRAF Reference Manual.*

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2 Hoover, W. G., *Phys. Rev. A*, **1985**, 31, 1695.
3 Nosé, S., *J. Chem. Phys.*, **1984**, 72, 2384.
4 Anderson, H. C., *J. Chem. Phys.*, **1980**, 72, 2384.
5 Parrinello, M. and Rahman, A., *Phys. Rev. Lett.*, **1981**, 52, 7182.
6 Berendsen, H. J., Postma, J. P. O., van Gunsteren, W. I., Di Niola, A. and Haak, J. R., *J. Chem. Phys.*, **1984**, 81, 3684.

Faster Ewald Sums (POLYGRAF only): A new function is now available which automatically optimizes the Ewald sums parameters and thus improves performance when using Ewald sums for evaluating Coulomb and van der Waals dispersion terms of periodic systems. This function uses the accuracy bounded convergence acceleration (ABCA) methodology of Karasawa and Goddard.[7] Three switches are used to implement this function (NEVER OPT EWALD, OPT EWALD NOW, and OPT EWALD AUTO); they appear under EWALD VAR and allow the user to determine if and when Ewald sums optimization occurs. See Section 5.12.7 in the *POLYGRAF Reference Manual.*

Summed Verlet Default Dynamics Algorithm: The summed Verlet is now used as the default dynamics algorithm. The standard Verlet algorithm is no longer available. The DYN ALGOR option which allowed the user to specify which of these two methods was to be used has therefore been removed from the Dynamics variables (DYNAMICS VAR) menu. See Section 5.12.4 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 6.12.4 in the *NMRgraf Reference Manual.*

Improved Minimization Methods (POLYGRAF only): The conjugate gradient and steepest descents minimization methods have been improved to give better results for periodic systems. These new algorithms employ an iterative process which calculates the forces on the unit cells and atoms separately using independent convergence criteria. This leads to lower residual stresses (by a factor of about 10). See MINIMIZE VAR in Section 5.12.2 of the *POLYGRAF Reference Manual.*

Cell Stress Convergence Criterion (POLYGRAF only): A separate convergence criterion for unit cell stress is now available for minimizations of periodic systems (PBC STRSS CVRG). It may be set independently of the convergence criterion for forces on the atoms. See MINIMIZE VAR in Section 5.12.2 of the *POLYGRAF Reference Manual.*

CEL&ATM SEPART/CEL&ATM SIMULT (POLYGRAF only): A two-way toggle has been added to the minimization variables which allows the user to determine whether the unit cell variables will be optimized separately from the atoms in a two-stage cycle which uses independent convergence criteria (CELL&ATM SEPART) or whether they will be optimized simultaneously using RMS FORCE CVRG, the convergence criterion specified for the atoms (CEL&ATM SIMULT). See MINIMIZE VAR in Section 5.12.2 of the *POLYGRAF Reference Manual.*

MODIFY PARAMS: As part of the MSI open-field force field concept, the program has been generalized to allow interactive checking and modification of force field parameters. This allows the user, for example, to change an equilibrium bond angle or force constant and then reminimize to determine whether the values are consistent with experimental or theoretical data. All bond, angle, inversion, torsion, cross-term, and van der Waals parameters are available to be modified. See Section 5.13 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 6.13 in the *NMRgraf Reference Manual.*

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[7] Karasawa, N. and Goddard, W. A., *J. Phys. Chem.*, **1989**, 93, 7320.

COULOMB On/Off Switch: A COULOMB on/off switch is now available on the NONBOND VAR menu which determines whether electrostatic interactions are included in the energy calculations. It performs the same function as the COULOMB switch on the ENERGY VAR menu and is provided in both places for convenience. See Section 5.12.6 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 6.12.6 in the *NMRgraf Reference Manual.*

POLYENE Switch: The program has been generalized to allow the bond and angle force constants to depend on bond order. Thus, for 1,3 butadiene, the common bond is longer, with a smaller force constant. Use of this cption is controlled by the POLYENE switch now available under MISC VAR. See Section 5.12.7 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 6.12.7 in the *NMRgraf Reference Manual.*

DEFORM CELL Switch (POLYGRAF only): A DEFORM CELL switch has been added to the MECHANICS and DYNAMICS menus which determines whether the size and shape of the unit cells are allowed to vary during the energy calculations. This allows one to cycle between fixed cells and variable cells without resetting up the energy expression. See Sections 5.7.4 and 5.8.10 of the *POLYGRAF Reference Manual.*

MODIFY CELL Improved (POLYGRAF only): The MODIFY CELL function under MECHANICS has been improved. Strains are now fixed by toggling on a FIX CELL PARAM switch and then selecting the cell parameter to be fixed. A pressure option (P) is also on the menu. P (initially zero) reflects changes in the diagonal elements of external stress and can be modified directly to change the isotropic pressure. See Section 5.7.5 of the *POLYGRAF Reference Manual.*

NO LIST: For smaller molecules, it is convenient to include all nonbond interactions and to avoid calculating a nonbond list. This can now be done using the NO LIST method on the NONBOND VAR menu. See Section 5.12.5 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 6.12.5 in the *NMRgraf Reference Manual.*

Minimum Image (POLYGRAF only): For periodic systems, a minimum image switch has been added to the NONBOND VAR menu. This switch can only be used in conjunction with the NO LIST or SPLINE SWITCH methods. This is faster but less accurate than using the EWALD method, and is faster and more accurate than using the SPLINE SWITCH method. See Section 5.12.5 of the *POLYGRAF Reference Manual.*

Improved Trajectory Analysis: Three new trajectory analysis functions have been added to the ANIMATE menu. The AVERAGE COORDS option does coordinate averaging of all the snapshots read in. RMS COORDS generates RMS fluctuations for these coordinates and displays RMS plots on the screen. An interface has also been provided which allows the user to perform custom statistical analysis using user-written routines (USER TRAJECT). See Sections 5.14.8 - 5.14.10 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Section 6.14.8 - 6.14.10 of the *NMRgraf Reference Manual.*

Mass Definitions: Masses can now be specified on a per atom basis (in the *.bgf* file), on a per atom type basis (in the *.par* file), or on an element basis (in the *.atm* file). This enhancement allows the user complete flexibility in dealing with isotopes.

Vector code (Titan only): Vector mode is now controlled by a logical switch, L_VECTOR, which is read in the defaults file. Setting this switch to YES will enable the calculation of the list-based nonbonded energies to be performed in vector mode. By default the nonbond calculations are performed in scalar mode.

ANALYZE

MATCH moved: The MATCH function which uses least squares fits to match structures is now under ANALYZE (it was formerly located at the top-level). See Section 6.6 in the *BIOGRAF* or *POLYGRAF Reference Manual*, and Section 7.6 in the *NMRgraf Reference Manual.*

New BACK CALCULATE Function (NMRgraf only): A new function has been added which allows the user to back calculate an NOE spectrum from the 3-dimensional structure of the current conformation. The relative NOE peak intensities are calculated as a function of the mixing time, frequency, and correlation time using an iterative relaxation approach as developed by Keepers and James[8]. See Section 7.10.3 in the *NMRgraf Reference Manual.*

UTILITIES

LABEL COLOR, BROWSER: Two new functions have been added under UTILITIES: LABEL COLOR which allows the user to change the color used for menu subtitles and values, and BROWSER which brings up a dialog box listing all the files in the system. The user may browse through the files and/or change the default directory. The toggle to enter command mode is no longer on the UTILITIES menu since it is now available as a global button. Options specific to the E&S PS 300 series graphics stations which is no longer supported have also been deleted. See Chapter 7 of the *BIOGRAF* or *POLYGRAF Reference Manual* or Chapter 8 of the *NMRgraf Reference Manual.*

DOCUMENTATION

BIOGRAF, POLYGRAF, NMRgraf Reference Manuals and Tutorials Rewritten: The *BIOGRAF Reference Manual, POLYGRAF Reference Manual, NMRgraf Reference Manual, BIOGRAF Tutorial* and *POLYGRAF Tutorial* have all been rewritten to reflect changes in the new graphical user interface, menu reorganization, and features for version 3.0. The *POLYGRAF Reference Manual* is no longer a supplement to the *BIOGRAF Reference Manual* but is a complete reference manual for POLYGRAF users.

Installation Guide Renamed, Updated: The *BioDesign Installation Guide* has been renamed the *Molecular Simulations Installation Guide.* It now includes installation instructions for Polaris in addition to BIOGRAF, POLYGRAF, and NMRgraf. Installation instructions for the new platforms have also been added.

Programmer's Manual Renamed: The *BioDesign Programmer's Manual* has been renamed the *Molecular Simulations Programmer's Manual.*

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[8] J. W. Keepers and T. L. James, *J. Magn Reson.* **57**, 404-426 (1984).

II. Hardware Supported

X-Windows Based Systems: The new GUI is supported on X-Windows based workstations using the UNIX operating system. These include the Silicon Graphics IRIS-4D and Indigo, Stardent's Titan, IBM RISC System/6000, DEC 5000, and the Evans and Sutherland ESV.

An X-Windows driver is currently under development to support Macintoshes, IBM PCs and other machines capable of running X-Windows. All features currrently available in version 3.0 will be supported with routine X protocol. GKS users should continue using version 2.2 until version 3.0/X-Term is available.

III. Notes

Reading in a File on Startup: A *bgf* or *xtl* file can be specified at the end of the command line used to start up and run the program (*e.g., biograf filename.bgf*). This file will automatically be read in and the structure displayed during program initialization.

Executing a Macro on Startup: A *macro* file can be specified at the end of the command line used to start up and run the program (*e.g., biograf filename.macro*). The commands specified in the macro file are executed until the macro finishes or control is passed to the menus (*i.e.*, program operation is switched to interactive mode).

Running the Program in the Background: All forms of background execution have advantages over the previous manner of running batch jobs in version 2.2. First of all, with version 3.0 the jobs are completely reproducible since they are run from macros. With version 2.2 it was not always easy to recreate the batch submission file since some of the information required to generate it was stored elsewhere. Secondly, macros can be edited to change the conditions of the run. For example, the dynamics temperature or the time of the simulation can easily be modified. All parameters are accessible via macros in version 3.0, whereas only a limited number were available in version 2.2. Finally, macros are programmable and allow the user to run very complicated production jobs. In the batch submission of version 2.2 this would require multiple job submission, a very user-intensive process. The macro programming language is very simple and is logically connected to the menu layout. Most macros are generated initially by an interactive session using menus, where the macro command file is automatically created.

Please spend a few minutes to read through the section on macros presented in Appendix K of the *Reference Manual*. It will greatly increase your productivity in using the program and should require a minimal amount of learning time.

There are a number of ways in which a job can be run offline or in the background. These are outlined below.

1) Begin the job as an interactive session: Setup the time consuming computational part by picking options on the menus. Once you are certain it is executing correctly, iconify the window(s) and let the job run to completion. The execution time will be within a few per cent of running the job as a true background job. This procedure has the advantage of your being able to monitor the progress of the job by simply redisplaying the text or graphics window. Modification of the job or aborting runs can then be done interactively. Typically, file information sent to the text window is lost. If you want to save a copy of the output, redirect output to a file on the command line which is used to execute the program. The stored output file can be followed by running "tail -f" on the output file from another window.

2) Run the job using a previously constructed macro file: Jobs can be executed either in the foreground or background using macros.

3) Run the job as a true batch job: Disable the graphics displays and submit the job in the background to run from a macro file. To disable the graphics and menu displays, add the following line to your defaults file

L_BATCH YES

If you choose "none" as the graphics option when you run COMSTRUCT, the defaults file will automatically be created containing the L_BATCH line to disable the graphics. It is convenient to create separate defaults files for interactive and batch jobs.

Running Multiple Batch Jobs or a Batch Job and an Interactive Session: This can require additional care to make sure the logfiles are not corrupted. When any execution of the program occurs, a file called *logfile.macro* is created in the directory from which the job is run. If two jobs are run simultaneously from the same directory (either interactively or via macros) they will both write to the same *logfile.macro* which may cause problems. There are a number of ways to avoid this.

1) Always run batch jobs from separate subdirectories thereby avoiding the conflict.

2) If the batch job does not require futher use of the *logfile.macro*, change the defaults file to suppress writing this file. This is done with the line

L_LOGFILE NO

3) Change the name of the logfile in the defaults file with the following line

LOGNAME /dir/yourname.macro

Dreiding II - Improved Inversion Potential Algorithm: The energies generated using the Dreiding II forcefield in version 2.2 are reproduced in version 3.0 with one exception. Version 3.0 contains an improved algorithm for calculating the inversion potential and forces near singular points in the potential energy surface. For the protein crambin, this improvement leads to a difference of less than 1 kcal/mol in the total energy.

Dreiding II - New Naming Convention for Aliphatic and Polar Hydrogens: In version 2.2 of Dreiding II we recommended that all polar hydrogens be included explicitly to correctly incorporate the effects of hydrogen bonding. In naming nitrogen and oxygen atom types, we kept a naming scheme consistent with the earlier Dreiding I forcefield. In this naming convention the number of hydrogens was always appended to the atom type, *i.e.*, N_R1 for the nitrogen in an amide bond. N_R was also an equally correct name for this nitrogen, and both names gave identical results since by convention the hydrogen atom was always included explicitly in the model. This naming convention for polar hydrogens is in conflict with the convention for naming aliphatic hydrogens. In Dreiding II, atoms having a different number of implied *aliphatic* hydrogens use different van der Waals parameters. This is due to the fact that Dreiding II does not need explicit aliphatic hydrogens to generate satisfactory results for carbon centers, and both explicit and implied aliphatic carbons are supported and treated correctly in Dreiding II.

We have chosen to make the conventions for naming both aliphatic and polar hydrogens the same in version 3.0 of Dreiding II. By default only implied hydrogens will be indicated in the fourth character position of the atom type name. This means that in general nitrogen and oxygen will have only blanks in the fourth character position of the atom type name. One advantage of using this naming convention is that the assignment of atom masses is now consistent with the assignment of implied hydrogens. These changes are merely changes in the labeling of atoms and do not affect calculated energies or geometries. All fragment libraries and sample data files that come with the program have been changed to reflect the new naming convention.

Relinking with User Functions: On most platforms in order to save on space, the prelinked object file in the *library* directory has been compressed with the UNIX compress command, resulting in a file with .Z at the end. To restore the file so that it can be relinked, change to the *library* directory and type `uncompress` followed by the filename. Two object files are provided with the Iris distribution, *gv300_iris.o_3.Z* and *gv300_iris.o_4.Z* for use with the 3.3.2 and 4.0.1 operating systems, respectively. There is also a second makefile in the *source* directory for 4.0.1. The object files may be deleted to conserve space if they are not needed.

Tutorial Manuals and Programmer's Manual: The BIOGRAF, POLYGRAF, and NMRgraf Tutorial Manuals and the Programmer's Manual are not yet finished. They will be shipped to you as soon as they are available. The Programmer's Manual is being updated to reflect the changes in the graphical user interface; however, the program can be relinked by following the directions in the Programmer's Manual, version 2.2.

Macro Commands: The "cycle" command in the macro language has been changed from the way that it is described in the documentation. The new syntax is

```
cycle = toggle_string,target_string
```

where toggle_string is the name of the menu item that would be toggled interactively, and target_string is the desired value for that toggle. For example, a valid command for selecting the method for calculating the nonbond list might be

```
cycle = method,no list
```

The following macro commands are described in the documentation but are not functional in this version.

save, restore, define_menu, display_menu, display_info, display_logo, remove_menu

Known Problems: In certain situations using the molecular crystal option with atoms extending outside of the unit cell, the program will generate messages that the nonbond list is inconsistent and the energies and forces will clearly be wrong. In those cases where the number of atoms is less than 1000, the calculation can be performed correctly with the molecular crystal option off.

"Form molecule" was designed for finite molecules. Its use with infinitely long chains will probably not work correctly.

The split screen stereo mode and ribbons are not functional on the IBM RS6000.

[illegible]

[illegible]

[illegible] the program [illegible]

[illegible] However, [illegible] ex- [illegible] If you [illegible] can [illegible]

[illegible]

BIOGRAF/POLYGRAF/NMRgraf Release Notes
Version 3.0 Last Minute Additions

A few last minute additions and changes have occurred which may interest you.

Latest news:

- To all customers currently on maintenance, we are sending a trial of our new software, Polaris, which will expire at the end of May. You will be receiving documentation on Polaris in a couple of weeks. To activate Polaris, you may either start your standard program and toggle on the MSI logo to switch to Polaris or you may run COMSTRUCT, selecting Polaris as the program to be run.
- The `save` and `restore` commands in the macro language have been fixed for 3.0.
- Only one prelinked object file, *gv300_iris.o*, is needed for all Silicon Graphics customers, but two makefiles are supplied. *Makefile_iris_3* and *Makefile_iris_4* should be used with the 3.3.2 and the 4.0.1 operating systems, respectively.
- In interactive mode, if the minimizer encounters problems, the program will send warning messages to the screen, but the minimizer will often recover. However, in L_BATCH mode, the program will call a subroutine, *die*, which will stop execution. If you choose, you can add the line, `L_DIE NO`, to your defaults file. That will make the batch mode behave the same way as the interactive mode.
- "Conformational search" used to skip particular conformations if it determined that the energy would be so high that it might cause the program to stop. In 3.0, those conformations will not be skipped so as to produce better plot files. You may wish to use the `L_DIE NO` line described above to keep the program from quitting in batch mode.