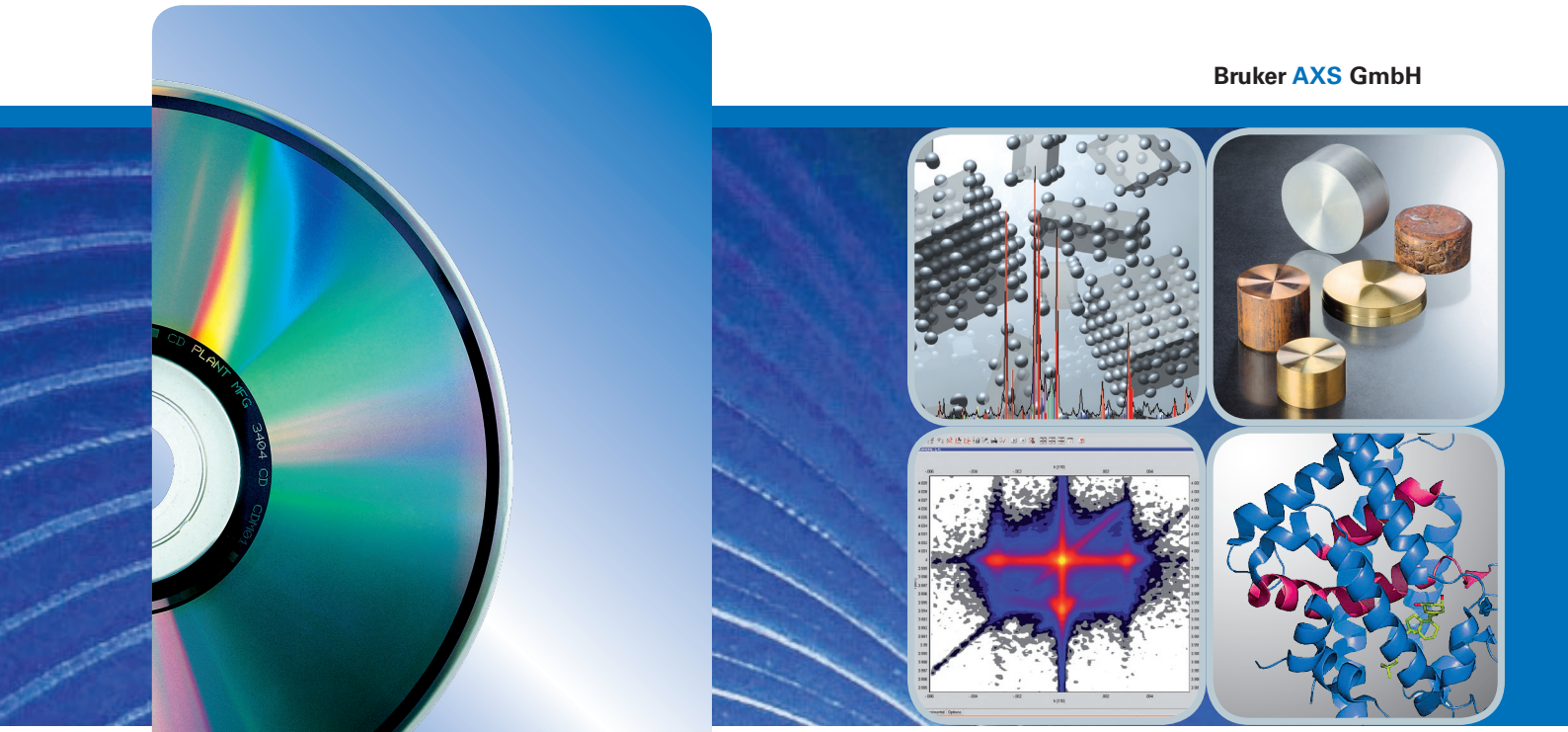
BRUKER

Bruker AXS GmbH



DIFFRAC^{plus}
TOPAS

TOPAS 4.2 What's New

think forward

XRD

Order no. DOC-M88-EXX067 V4.2. Updated: Jan 15, 2009.

Printed in the Federal Republic of Germany.

Bruker AXS GmbH
Östliche Rheinbrückenstr. 49
76187 Karlsruhe, Germany
Tel. +49 (7 21) 5 95-28 88
Fax +49 (7 21) 5 95-45 87
info@bruker-axs.de
www.bruker-axs.com

CONTENTS

(intentionally left blank)

1 TOPAS V1.0

TOPAS V1.0 is a profile fitting software for single peak, local pattern and whole powder pattern fitting using the analytical profile fitting method as well as the fundamental parameters approach.

Most important features:

- Refines simultaneously on any number of powder patterns with any number of datapoints
- Peaks can be assigned to crystallographic phases for further processing such as phase dependent crystallite size and strain determination, quantitative analysis, and much more
- Choice of profile fit method: Analytical profile fitting and / or fundamental parameters
- Analytical profile fitting method:
  - Choice of profile function: Gauss, Lorentz, Pseudo-Voigt, Pearson VII
  - Split versions of any of the above to best handle peak asymmetry
  - Crystallite size determination by Scherrer method
- Fundamental parameters approach:
  - Full convolution based synthesis of line profiles
  - Full handling of instrument geometry and instrument parameters as well as sample properties
  - Refinable instrument parameters allow for instrument alignment checks
  - Standardless crystallite size and strain determination
  - Determination of mean sample absorption coefficient and sample thickness possible
- All profile and instrument parameters can be fixed, refined or constrained
- Any linear and non-linear constraints. Constraints are provided by means of equations.
- Batch profile fitting capability

2 TOPAS V2.0

TOPAS V2.0 is a graphics based profile analysis program built around a general non-linear least squares fitting system, specifically designed for powder diffraction line profile analysis. TOPAS integrates various types of X-ray and neutron diffraction analyses by supporting all profile fit methods currently employed in powder diffractometry:

Profile Fitting Methods:

- Single line up to whole powder pattern fitting
- Whole powder pattern decomposition (Pawley method, LeBail method)
- Rietveld structure analysis
- Structure determination

Measurement Data and Refinement Parameters:

- Laboratory and synchrotron X-ray data, and constant wavelength neutron data
- Single crystal data
- Combined refinement of powder and single crystal data
- Non dependence on X-ray data (all kinds of XY data can be fitted)
- Support of non-equidistant x-axis steps
- Support of negative x-axis values
- Refines simultaneously on any number of diffraction patterns with any number of peaks, any number of datapoints, and any number of parameters
- Refines on any number of structures per diffraction pattern with any number of sites per structure and atoms per site
- All parameters can be fixed, refined, constrained and restrained

Peak Shape Models:

- Analytical profile fitting:
  - Profile functions:
    - PVII, Modified PV, Voigt
  - Asymmetry:
    - SPV, SPVII (for single line fitting)
    - Simple and Full Axial Models
  - Crystallite size determination by Scherrer method
- Direct convolution approach
  - Measured instrument functions
  - Fundamental Parameters Approach
    - Standardless crystallite size and strain analysis
    - Refinable instrument parameters

  - Determination of mean sample absorption coefficient and sample thickness
  - Tube tails correction
- Support of user-defined convolutions

Background Models:

- Chebychev polynomial of any order
- Single peaks (PV, SPV, PVII, SPVII, Gauss, Lorentz, Voigt, FPA)
- 1/x-type background
- Modulated background

Preferred Orientation Models:

- March-Dollase
- Spherical Harmonics

Anisotropic Refinement Models:

- Peak broadening
- Peak shifts
- Preferred orientation
- Temperature factors
- Occupancy factors

Constraints and restraints:

- Any linear and non-linear constraints
- Penalty functions. Can be applied to all refineable parameters
- Bondlength restraints (Anti-Bump, Parabola, lattice energy minimization, user-defined)
- Rigid and soft bodies with all parameters refineable

Minimization procedures:

- Marquardt
- Line minimisation
- Extrapolation
- Sparse matrix methods

Miscallenous:

- Simulated annealing
- Support of user-defined fit models
- Batch profile fitting capability

3 TOPAS V2.1

3.1 Bug fixes

- A bug has been fixed, which prevented loading of PRO files with the PVII function. The specific error message read:

  Cannot find match for macro: PVII_h
  Number of arguments: 2
  Mangled name: PVII_h_~2

3.2 Most important new features

3.2.1 General

- The overall speed of TOPAS has been improved by about 50%
- Double-Voigt Approach for crystallite size and strain analysis for use with both calculated (FPA) and measured instrument instrument functions. For compatibility issues with respect to V2.0 see section 3.3.
- TCHZ pseudo-Voigt function
- Support of measurement data files in GSAS ("std - const", "alt - ralf"), FullProf and XYE formats
- Definition of program defaults using ".DEF" files
- New scattering data for structure factor calculations
  - anomalous dispersion coefficients:
    http://www-cxro.lbl.gov/optical_constants/asf.html
  - scattering factors:
    http://www.esrf.fr/computing/expg/subgroups/theory/DABAX/dabax.html
  - scattering lengths:
    www.ccp14.ac.uk/ccp/web-mirrors/neutrons/n-scatter/n-lengths/LIST~1.HTM
- Default dynamic limits for all peak parameters (e.g. m1, m2 etc...).
- Site identifying strings may contain the negation character "!"
- An exception is thrown, if reserved parameter names clash with user-defined parameter names

3.2.2 Graphical user interface

3.2.2.1 General

- Graphical options are now saved and reloaded from STARTUP.DEF. These include:
  - The showing of the Peak Edit, Options, Fit and Parameters Windows.
  - The setting of the Scan Chart x and y axis types
  - The showing of Quickzoom and Pie Chart options.
  - The showing of work book pages.
  - The showing of the horizontal scroll bar in scan charts.
  - The showing of hkl tick marks.
- A general defaults mechanism has been implemented for Scan plots. See Right Mouse Button and then “Edit / Print / Chart Options” and then the “Titles/Axies” page. If the “Set as Defaults” button is pressed then the present set of data is saved in STARTUP.DEF and are then used for subsequent plots. Note that “Minimum/Maximum” cannot be kept as defaults.
- Separate MRU ("most recently used") lists with a fixed maximum of 10 items for INP/PRO files in the "File" menu and for INP files in the "Launch" menu. The MRU lists only show up when previous files are loaded.
- MRU list with a fixed maximum of 10 items for measurement data files in the "File" menu. The MRU lists only show up when previous files are loaded.
- The last used file paths (save, load) are now being remembered for the following file types individually: measurement data, INP, PRO, LAM, PAR, DIF, UXD, CIF, and STR.
- The QuickZoom/PieChart speed button now has only two states. The PieChart state has been removed and can be activated/deactivated from the "View" menu.

3.2.2.2 Reporting of results (printing, saving as files)

- TopasEditor program for direct editing and printing of data sent to the clipboard
- The "Text” page has been changed to “Rpt/Text” and the default page after clicking on “Rpt/Text” has been set to the new page “Report Format”
- Report format for refinement results ("Report Format" page)
- The grid text output display ("Text" page) is now color coordinated
- The content of both the "Text" and "Report Format" pages can be printed directly or viewed in launched instances of the TopasEditor or Microsoft Word. For Microsoft Word user-defined document templates (.DOT files) are supported.

3.2.2.3 Scan Window

- Vertical panning; note "View - Fix Y2 to Ymax" must be off

- The "Reset axes to previous" has been included in the context sensitive menu
- "Calculated", "Background", "Difference", and "Single Peaks/Phases" commands have been removed from the context sensitive menu
- The "More" command in the context sensitive menu has been replaced by the "Edit / Print / Chart Options" for direct printing of the scan chart, copying the scan chart to the clipboard, and defining scan chart properties

3.2.2.4 Parameters Window

- Cloning of the parameters window for e.g. viewing different parameters simultaneously (e.g. parameter values and their codes)
- "Use" dependent expand/collapse grid items for "Tube Tails", "Full Axial Model", and "Absorption"
- A list box at the bottom of the tree view displays options available to the currently selected grid page
- Treeview item “Global - Display” providing a general colors mechanism. Settings made in the “Global Defaults” page are saved in STARTUP.DEF.
- User-defined convolutions to describe instrument and microstructure related line broadening have been made into the new "Additional Convolutions" page, and are located under the following tree view items:
  - "Global - Instrument"
  - "Global - All Structures/hkl Phases"
  - "Global - All Peaks"
  - "Range - Instrument"
  - "Range - Structures/hkl Phase"
  - "Range - Structure" / "Range - hkl_Phase" / Range - Peak_Phase"
- The hats convolution has been moved from the "Miscallenous" page to the "Additional Convolutions" page. For compatibility issues with respect to V2.0 see section 3.3.
- The Cagliotti function (UVW parameters) as convolution has been removed from the GUI. For compatibility issues with respect to V2.0 see section 3.3.
- Finger et al. asymmetry correction
- Density and Mass absorption coefficients for structures including errors.
- The "Global - Global Stats" page has been renamed to "Global - Global Stats/Convergence Criterion" and provides access to the convergence criterion.
- Codes with constant equations are displayed in blue in the grid
- d_ls, xo_ls and hkl_ls phases can be saved as files
- "Str Output" treeview item under "Range - Structure" providing
  - Generation of structure data in CIF format
  - Generation of structure factor details in FCF format
  - Calculation of bond lengths and angles incl. errors, which optionally may include lattice parameter errors

3.2.2.5 Fit dialog / fit options dialog

- Messages "Interface Mode" or "Launch mode" are shown in the Rwp plot to indicate the current mode.
- The message “Fit Zoomed: ON” is shown in the Rwp plot if only the zoomed area is fitted (interface mode only)
- A “Graphics Response Time” option has been added to the Options of the Fit Window. It controls the frequency of graphical updates. The updating of the graphics including the Rwp plot of the Fit dialog can in some cases slow down the refinement process by up to a factor of ten. Increasing the “Graphics Response Time” can significantly increase the speed of the refinement process.
- A warning is shown, if a atomic coordinate is closer than 0.001Å to particular special positions. This helps to avoid input of faulty coordinates by providing values with re-occuring digits instead of an equation, e.g. "0.3333" instead of "=1/3".

3.2.2.6 Miscellaneous

- A version keyword has been included in PRO files
- Peaks can be flagged for "Use" or "no Use" with a "Use" parameter.

3.3 Compatibility issues

Note: Compatibility issues described in the following sections are only relevant for use of TOPAS in GUI mode, when V2.0 PRO or INP files are loaded containing one of the following keywords / macros:

- **Strain**
- **UVW**
- ***hats***

3.3.1 Crystallite size and strain analysis: The Double-Voigt Approach

The implementation of the Double-Voigt Approach significantly improves the TOPAS capabilities for straightforward and more meaningful crystallite size and strain analysis and can be used with both calculated (FPA) and measured instrument functions. It allows the calculation of volume weighted column heights (LVol-IB and LVol-FWHM) and a total strain value (e0), based on individual crystallite size and strain contributions to line profile shapes versus 2θ in terms of Lorentzian and Gaussian type line broadening. For the determination of these contributions the following 4 new profile parameters have been made available, some of which replacing formerly used profile shape parameter / macros:

New profile parameter:	Meaning:	Replaces:
"Size_L"	Lorentzian type crystallite size broadening	"Crystallite Size"
"Size_G"	Gaussian type crystallite size broadening	
"Strain_L"	Lorentzian type strain broadening	"Microstrain"
"Strain_G"	Gaussian type strain broadening	"Strain"

"Size_L" and "Crystallite Size" as well as "Strain_L" and "Microstrain" have identical definitions. If a V2.0 PRO or INP file is loaded into V2.1, the values for "Crystallize Size" and "Microstrain" are displayed as "CS_L" and "Strain_L". These are used for subsequent determination both LVol-IB and LVol-FWHM.

"Strain" has been replaced by the differently defined "Strain_G" parameter. In V2.0 "Strain" is defined as

gauss_fwhm = 2.69129 "Strain" Tan(Th)

In V2.1 "Strain_G" is defined as

gauss_fwhm = "Strain_G" Tan(Th)

As a consequence, "Strain" values obtained with V2.0 are automatically converted to "Strain_G" values (by multiplying by 2.69129). V2.0 PRO or INP files can thus be loaded into V2.1 for direct determination of the total strain parameter ε.

3.3.2 UVW convolution

The Cagliotti function (UVW parameters) as convolution is no longer supported within the GUI and has been removed. Please change the peak_type to PV_TCHZ to continue use of UVW parameters.

3.3.3 Hats convolution

"hats" and "num_hats" as fixed items have been replaced with “Additional Convolutions" at the range scope. "hats"/"num_hats" convolutions loaded from V2.0 INP or PRO files are automatically replaced with equivalent “Additional Convolutions".

4 TOPAS V3

4.1 Most important new features

4.1.1 General

- Quantification of amorphous phase amounts based on spiking method
- Degree of crystallinity determination
- Animated structure viewer window with many display options
- Rigid body editor window
- Window for inspection of f' and f''
- Surface roughness correction according to Pitschke et al. (1993)
- Surface roughness correction according to Suortti (1972)
- Various new powerful bondlength and angle restraints for structure determination and refinement
- The new keyword *occ_merge* rewrites the site occupancy user defined sites in terms of their fractional atomic coordinates (Favre-Nicolin & Cerny, 2002). This is useful during structure solution for merging of rigid bodies and for identifying special positions.
- The new keyword *adps* generates the *uij* atomic displacement parameters with considerations made for special positions
- Support of TOF neutron data
- A new constrained conjugate gradient minimization routine has been implemented. It considerably improves convergence on big problems (more than 300 parameters) with speed improvements of up to a factor of 10.
- A new memory management routine has been implemented which avoids fragmentation of memory. Memory fragmentation occurs when working on big problems and can affect performance by a factor of 5 or more.

4.1.2 Graphical user interface

4.1.2.1 General

- fit_zoomed is now saved in and loaded from PRO files

4.1.2.2 Parameters Window

- Data grids have been redesigned (where applicable) to allow simultaneous inspection of parameter values, errors and attributes

- Preferred orientation models (March-Dollase and spherical harmonics) have been merged into a single data grid
- Creation of a “hkl_Is" phase from a peaks phase
- Creation of a “str" phase from a “hkl_Is" phase
- Creation of a “hkl_Is" phase from a “str" phase
- General pasting of INP format data from clipboard into the tree nodes or selected grid items
- The Le Bail constant has been visually removed from GUI

4.2 TOPAS I

TOPAS I is a new, optional add-on to DIFFRAC*plus* TOPAS, TOPAS P and TOPAS R for indexing and space group determination of powder diffraction data using the LSI-Indexing and LP-Search methods.

LSI-Index features:

- Iterative use of least squares, Coelho (2003)
- Operates on 2θ or d-values
- Zero-point error consideration
- Automatic spacegroup determination
- Weighting of reflections using observed peak intensities or user-defined weights
- Relatively insensitive to impurity peaks, missing high d-spacings, extreme lattice parameter ratios as well as large d-spacing and zero point errors
- Fully automated fitting of all or user-selected solutions according to Pawley or Le Bail
- Highly sophisticated graphical representation of results such as display of observed versus calculated reflection including assignment of indexed and unindexed reflections, Goodness-of-Fit versus volume plots and much more

LP-Search features:

- Monte-Carlo based Whole Powder Pattern Decomposition
- Independent of 2θ or d-spacing extraction - no d-/2θ values required
- Zero-point error consideration
- Independent of line profile shape
- Particularily suited for indexing of poor quality powder data, where reliable 2θ or d-spacing extraction is difficult or even impossible

5 TOPAS V4

5.1 Product changes

- Because of the big success of the complete TOPAS package, TOPAS R has been discontinued. This eliminates the artifical distinction between full pattern applications (Pawley, LeBail and Rietveld methods) and single line analysis, which is no longer state of the art. All full pattern applications can now take full advantage of single line fitting to model contributions from unknown or amorphous materials. TOPAS R users are entitled to upgrade to the complete TOPAS package.
- All indexing features previously only available in the optional TOPAS I module have been included into TOPAS and TOPAS P, TOPAS I has been discontinued. This eliminates the artifical distinction between the Pawley and LeBail methods versus the LP-Search indexing method, which is no longer state of the art. Also this allows for an improved integration of the LSI indexing method into TOPAS, which significantly improves user-friendlyness.

5.2 Bug fixes

- A bug has been fixed, which prevented loading of PRO files including Pawley or LeBail refinements. The specific error message read:

  "Error loading sstring_in at (ndx_sg), unknown or misplaced keyword..."

- A bug has been fixed, which prevented loading of PRO files including FullPROF or GSAS data. The specific error messages read:

  "Error loading sstring_in at {fullprof_format}, unknown or misplaced keyword..."
  "Error loading sstring_in at {gsas_format}, unknown or misplaced keyword..."

- GUI: If "Convolution Step" had been set to 0 by mistake, the input field freezed and TOPAS had to be restarted. This bug has been fixed.
- On import of CIF files, isotropic temperature factors had been ignored. TOPAS now supports import of isotropic temperature factors in both B_{iso} and U_{iso} notations. Note, that U_{iso} is automatically converted into B_{iso}.
- On import of CIF files, wrong or unusual space group identifiers such as "F 1 D 1" could freeze TOPAS on starting a refinement. This bug has been fixed, an error message will be thrown.
- Loading of CIF files containing the line "### Experimental" had been refused. This bug has been fixed
- On export of CIF files, the space group is now correctly given using the CIF command '_symmetry_space_group_name_H-M'
- "Replace Scan Data" now also supports FullPROF and GSAS type measurement data

- User-defined names for indexing ranges have not been saved to PRO files. This bug has been fixed
- "Export to INP File" exported only one indexing range, additional ranges were ignored. This bug has been fixed.

5.3 Most important new features

5.3.1 General

- Completely new graphical user interface with Windows XP look & feel
- A customizable Essential Help window can be displayed
- Variable Counting Time (VCT)
- Charge Flipping method for structure determination
    - Works with powder or single crystal data
    - Tangent formula can be used in each Charge Flipping iteration
    - For powder data the A matrix from a Pawley refinement can be used to attribute intensities to E-values each Charge Flipping iteration
    - A new electron density atom picking routine that is both fast and independent of atom size
    - Can operate in any space group and not just P1
    - Space group symmetry restraints can be applied to the electron density each Charge Flipping iteration
    - Further options include histogram matching, low density elimination and the random omitting and insertion of atoms
    - Real time 3D display of electron density with atom picking in the "Structure Viewer" window
    - Computer algebra control for up to 30 Charge Flipping parameters
- 3D display of electron densities
    - Works with powder or single crystal data
    - Observed, calculated, and difference electron density maps
    - Can simultaneously display electron densities, structures and picked atoms
    - Allows for enlargement of the Ewald sphere with Fobs set to Fcalc
    - Inserts missing reflections within the Ewald sphere with Fobs set to Fcalc
    - Comprises a computer algebra equation that can be a function of Fobs, Fcalc and D_spacing
- The Cloud - an atomic position averaging technique that allows for the visual display of atomic movements. High density positions in the cloud can be searched and atomic positions extracted. Good for locating heavy elements or tracking atomic movements in general.

- The Structure Viewer window has been combined with the Rigid Body Editor; it can load and overlay rigid bodies, structures, clouds and INP files
- Fundamental parameters for linear position sensitive detectors and capillaries
- Beam overflow correction
- Output of plot data. The new option “Save if displayed Yobs, Ycalc, Diff, Phases, Bkg” allows to save observed, calculated, difference, background and individual phase intensity data in a comma separated text file for plot generation using 3rd party software. Data is saved according to the y-axis scaling and the x-axis is changed to the selected 2θ, d, Q.
- Support of scattering factors of atoms / ions with Z>92:
    - Np, Np+3, Np+4, Np+6, Pu, Pu+3, Pu+4, Pu+6, Am, Cm, Bk, Cf
- Support of user-defined scattering factors
- The inclusion of torsion angle penalties to complement distance and angle restraints
- Double precision for absolutely everything achieving greater stability for refinements with many parameters or high correlations.
- The bootstrap method of error determination has been implemented; it can be used to determine esds and in particular errors can be estimated for very large problems where matrix inversion is impractical.
- Bootstrap errors for fractional coordinates that are a function of a rigid body.
- A completely rewritten version of the BFGS method for approximating the Hessian matrix. This Quasi-Newton method has been modified to dampen changes in the system in early iterations of a refinement. It converges better in cases where the minimum is far off. It's convergence in general on smaller structure refinement problems is comparable in time to that of the fully calculated Hessian matrix. Together with a reworking of the automatic parameter removal scheme structure solution can now progress at a rapid pace. Version 4 solves structures that version 3 could not.
- The BFGS method together with aggressive memory conservation techniques now allow for refinements comprising tens of thousands of parameters. Refinements of this sort were not possible with version 3.
- Memory usage is further reduced when the “conserve_memory” switch is used.
- INP files are more rigorously validated, for example, parameter input such as 1/3 are now disallowed; instead an equation such as =1/3; is necessary. In addition parameters that cannot be a function of multivalued parameters are now checked. For example, an x coordinate written in terms of H, K, L etc... will throw an exception. Validation is also performed regarding the type of multivalued parameters used in equations. For example, the fourier_map_formula can only be a function of its multivalued parameters of Fobs, Fcalc and D_spacing.
- New single crystal refinement features
    - Implementation of the Flack parameter
    - Output of more single crystal details with phase symmetry considered

- New indexing features
    - Peaks phase – creating indexing range: If peaks / wavelengths are present then they are placed into the indexing range
    - The weighting in indexing can now be turned ON/OFF without changing the weightings
    - LP-Search now works with neutron data
    - Improved sorting of indexing results

5.3.2 Graphical user interface

5.3.2.1 General

- Docking of the Structure Viewer window is now possible
- Customizable color schemes
- Customizable toolbar
- The Window Left/Right Button has been removed from all plot windows. Left/Right scrolling of plots is now achieved with the mouse wheel.

5.3.2.2 Parameters Dialog

- The "Bragg-Brentano" page has been renamed to "Divergent Beam" and has been redesigned to include the new linear position sensitive detector and capillary aberrations
- References to *axial_del* have been removed (Full Axial Model). The GUI and Kernel will still load the keyword but there's no effect on refinement.
- The "Cylindrical 2Th" and "Cylindrical Intensity" corrections have been moved on a new, separate page: "Cylindrical sample (Sabine)"
- The "Concatenate Ranges" feature has been removed as it caused too many and partly serious issues on how to deal with overlapping or missing data regions, or with data regions measured with different step time, step size, instruments, and so on.
- The "Export data as" feature has been removed and is replaced by the new option “Save if displayed Yobs, Ycalc, Diff, Phases, Bkg”
- The default value for Lorentz-Polarisation has been changed to 90, that is no monochromator present

5.3.2.3 Scan Window

- The Bouncing Ball feature for peak insertion
- The Range Combo Box and Peak Phase Combo Box have been removed. Peak insertion is now accomplished with the new Bouncing Ball feature

- Peak search now also works for *.xy and *.xye data. For data with $2\theta < 0°$ or $2\theta > 180°$ the "Remove K-Alpha 2 Peaks" check box is left unchecked in the Peak Search Dialog.
- Display of d next to 2θ in linear x-axis mode

5.3.2.4 Fit Dialog

- Refinement results can now be checked before accepting the refinement run

6 TOPAS V4.1

6.1 Bug fixes

- Adding sites/atoms in the Parameters Dialog now works correctly. Instead of adding sites/atoms to an "edited" site/atom (which didn't work) the new procedure adds sites/atoms to selected sites/atoms. This allows for more than one site/atom to be added at a time. The text describing the option has also changed to reflect the change, ie.
  - "Add Site(s) before selected site(s)"
  - "Add Atom at selected site(s)"
- Polygon selection whilst Charge Flipping is operating gave an integrity bug in some situations.
- Atom selection in the Structure Viewer / Rigid Body Editor did not work on some graphic cards. This problem has been fixed.
- A bug related to the phase_out keyword has been fixed, preventing the output of hkl and M(ultiplicity) information. As a result it was impossible to generate e.g. *.HKL files for structure determination.
- For a phase which had been flagged for no use in the Parameters Window after a refinement, the calculated pattern could still be displayed after subsequent refinements (although the phase had been removed from refinement). This bug has been fixed.
- A bug has been fixed, which prevented the use of elements with Z>92.
- A bug has been fixed where the C_matrix_normalized has been outputted more than once when already defined in an INP file. Now an existing C_matrix_normalized found in the INP file will be overwritten.
- A bug has been fixed, which prevented the import of CIF files when occupancy information was missing.
- A bug related to crystallite size calculations using the Scherrer equation has been fixed. This bug prevented profile fitting convergence.

6.2 Errata

The following errata have been corrected:

- Incorrect polarisation values for unpolarized and for synchrotron radiation have been given in the TOPAS V4 Technical Reference Manual, section 8.3.8, and the TOPAS V4 User's Manual, section 4.2.2.4.
- Incorrect instructions for automated TOPAS operation using user task files have been given in the TOPAS V4 Technical Reference manual, section 13.
- The *degree_of_crystallinity*, *crystalline_area* and *amorphous_area* keywords were not described in the TOPAS V4 Technical Reference manual.

7 TOPAS V4.2

7.1 Bug fixes

- The import of CIF files didn't work when installing TOPAS in a directory containing blank characters in the directory name, e.g. "c:\program files". This bug has been fixed.
- A bug related to the export of INP files has been fixed, where the (raw) data file extension had been mistakenly extended by the range number, e.g. *.RAW_1
- In rare cases, when doing a constrained refinement of both Soller slit angles (set to identical values), the angles refined to different values in the last iteration. This problem has been fixed.
- R-Bragg hasn't been updated correctly in the GUI when a new refinement has been started. This bug has been fixed.
- A bug has been fixed causing divergence of the zero-point error parameter in rare cases.
- Several spelling errors in the GUI have been fixed
- The help file couldn't be opened in V4.1, this problem has been fixed.
- The “reverse data and make x-axis positive” command didn't work correctly on data files that had negative 2theta values. This bug has been fixed.

7.2 Improvements:

- TOPAS has the ability to turn off animated fitting to significantly speed up calculations, this is very useful specifically for structure determination. However, when TOPAS reached convergence, the best fit / structure was not shown when animated fitting was turned off. This behaviour has been changed: The Animated Fitting button now displays the graphical output if turned ON while the "Refinement converged" dialog is displayed.
- hkl input for the March-Dollase preferred orientation correction is now rigorously validated to avoid ambiguities. Three values separated by blanks have to be provided to define hkl, otherwise an error will be thrown.