



**More info about MacDiff**

**Welcome to MacDiff!**

Mac Diff is a programme for analysis and display of X-ray powder diffractogrammes on Apple Macintosh platforms. It is designed as a complement to the XRD applications distributed by Philips or Siemens and it is equipped with a GUI to facilitate user-friendly and interactive processing of XRD profiles. It offers conventional XRD profile-correction processes (e.g. outliers, smoothing, divergence, alpha2-stripping) and supports qualitative and quantitative phase analysis. Moreover, by its programmable peak analysis (recording of intensities, peak areas, half widths, etc.) it offers an automated analysis of entire series of diffractogrammes. By means of peak fits the contributions of coinciding lines can be calculated. The user has at his disposal the capability of continuous measurement checks and the possibility to perform corrections as well (e.g. by manual or computed background adaptations). For peak indication the user has the option to employ variable peak data sets. High resolution hardcopies of the diffractogrammes can be produced. The standard single-scan formats (Philips-ADP or some Siemens-RAW, ASCII) are identified automatically. Data and plots can be exported to most of the available table-processing or vector-graphics programmes.

The applications of MacDiff range from routine analysis in sedimentology, especially clay minerals, over analysis of X-ray diffractogrammes of all types of

rocks and minerals all the way to phase analysis of various crystalline substances.

**MacDiff is freeware and is available to everyone free of charge. It may be copied and distributed without restrictions for non-profit and non-commercial use. All rights reserved. Usage at your own risk.**

To use MacDiff successfully, please read the manual available in [English](#) or [German](#) language. If you want to look into changes since last versions read the [MacDiff Release Notes](#).

**MacDiff was continuously developed from 1991 to 2001. Since appearance of Mac OS X MacDiff's development was discontinued but it works in the Mac OS Classic mode. For all newer Leopard or Snow Leopard Macs as well as for Windows PCs MacDiff works in the [SheepShaver Virtual Machine](#).**

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**System requirements (2001)**

MacDiff runs on a PowerMacintosh with 8 MB RAM minimum. However, 16 MB with colour monitor is recommended. RAM requirements are 3.5 MB minimum.

Hard disk requirements are between 2 and 8 MB memory.

All Mac OS-systems older than 8.0 require the extension 'appearance extension' as well as the console 'appearance CDEV', which is available for downloading (name: 'Appearance Lib').

Minimum system:

Power Macintosh or first generation PPC-PowerBook (PPC 601) with 14" colour monitor (minimum 256 colours), system 7.1.2

Optimal system (required in particular for profile fit):

Power Macintosh or latest generation PPC-PowerBook (604c or G3) with 32 MB RAM minimum, 17 to 21" colour monitor (16 mio. colors), system 8.x

### **Developement** (discontinued 2000)

The software was developed in the Visual Interactive Programming BASIC-environment of [Mainstay](#). The code was converted to ANSI-C and compiled by [CodeWarrior](#) (today: Freescale).

### **Input - Output**

You can read the following diffractogram files:

- Philips ".RD" - APD- VMS-Format
- Philips ".RD" - APD- MSDOS-Format
- Philips APD - ASCII-MSDOS-Format (APD-"View Scan")
- Philips APD - APD-UDF-ASCII-MSDOS-Format
- Siemens ".RAW" - RAW2-MSDOS-Format
- Siemens ".RAW" - New RAW1 format
- Siemens ".RAW" - Old RAW format
- ".MDI" ASCII Text Format
- ".OUT" ASCII Text Format
- Sietronic ".CPI" ASCII Text Format
- Lauterjung ASCII Text format
- SCINTAG 2000 ASCII Format

File must be a single-scan.

No more than 16768 single counts in one file.

Count limit: 1.000.000 (Counts higher than 1.000.000 will decreased to 10%).

You can read and write:

- Philips APD - APD-UDF-ASCII-MSDOS-Format
- ".MDI" ASCII Text Format
- Sietronic ".CPI" ASCII Text Format
- MacXFit of H.Stanjek, Freising, TU Munich

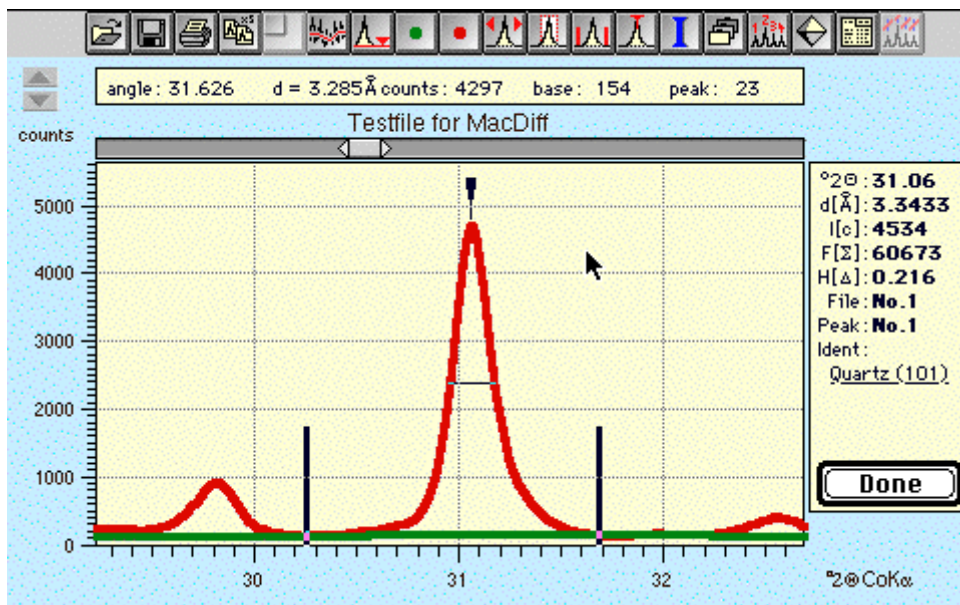
- Text-ASCII (angle, count [, base] - several delimiters possible)
- In MacDiff's native compact and fastest DIFF format (Version 2/3 or 4)

### **List of some features:**

- Up to ten colored diffractograms in independent windows.
- Up to seven multiple diffraction profiles showing in one diagram.
- Max. 16.383 single data and max. 1.000.000 counts per step in one diagram.
- Changable diffractogram size.
- Changable line color, size and type.
- Changable axis types (normal, inverted, square root, logarithmical, d-spacings).
- Button bar for 20 frequently used program functions.
- Base line removing.
- Optimized fast drawing and screen redraw.
- Mouse-sensitive zooming and scrolling.
- Cursor sensitive angle-, d-value and count display.
- High quality print, colored (if desired), optional logo.
- Prints and saves lists of counts and of all measuring data.
- Import of "good-old" analog diffractogram plots via scanner or by digitizing table.
- Import of scans of Debye-Scherrer- or Guinier camera photos
- Export vector graphics via clipboard or by PICT-files, also in 5 x resolution
- Editable counts and base values.
- Optional Debye-Scherrer like film image.
- single or multi peak correction
- Outlier and divergence filter, smoothing counts, alpha-2 stripping.
- Simple math manipulations.
- Changing K-Alpha-type on the fly.
- Recalculation to other wavelengths/K-Alpha type and step size.
- Determination of mean diffractograms from several profiles.
- Diffractogram subtraction.
- Base line determination (automatically or by drawability by user).
- Base line can be saved (MacDiff file format).
- Peak analysis by double click: d-value, counts, area, and FWHM as standard.
- Peak Fitting (Gauss, div. Lorentz, Pearson VII, and Pseudo Voigt) - single fit or multi fit of up to 7 peaks.
- Peak search routine.
- Labels of single peaks.
- About 30 optional peak parameter (i.e. half areas, integral widths).
- Implemented JCPDS (PDF)-like database interface.
- PDF-data can be imported.
- Generates artificial (synthetical) diffractograms from database.
- Comes with databases holding about 22.000 peaks of more than 500 rock-forming minerals.
- Links a given peak to a peak database index for identifying.
- Peak identify routine, also linkable to a peak database.
- User defined analysis program to evaluate data of up to 32 peaks.

- Semi-automatic processing by file sessions (batches of up to 255 profiles).
- Reports of all peak data, exporting as TEXT-files.
- Automatic FWHM calibration of five different peaks.

### Example screenshots:



Analysis of Quartz (101) peak

**Peak Database: Minerals**

Record No. 176 of 240      locked !      File: Minerals

Quartz (Alpha Quartz)      Lake Toxaway, Pattern at 25°C      **Get Other Database...**

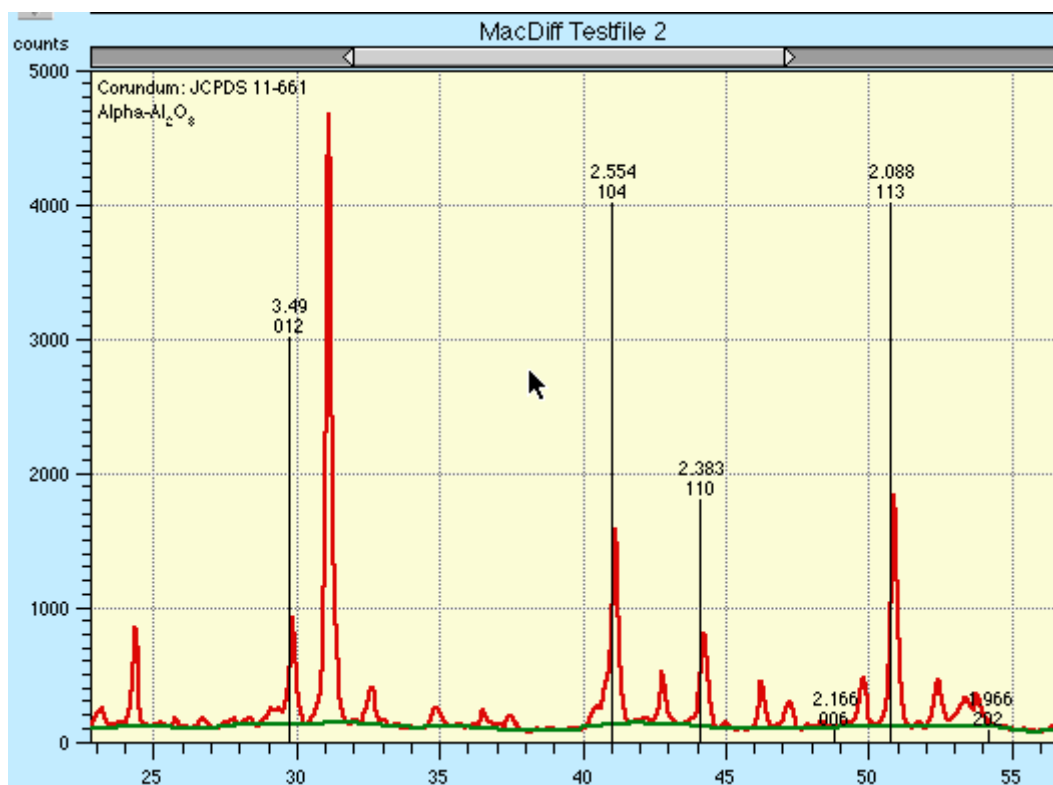
#Ref.No: JCPDS 5-0490      Comment:      **Hexagonal**

Formula: SiO2

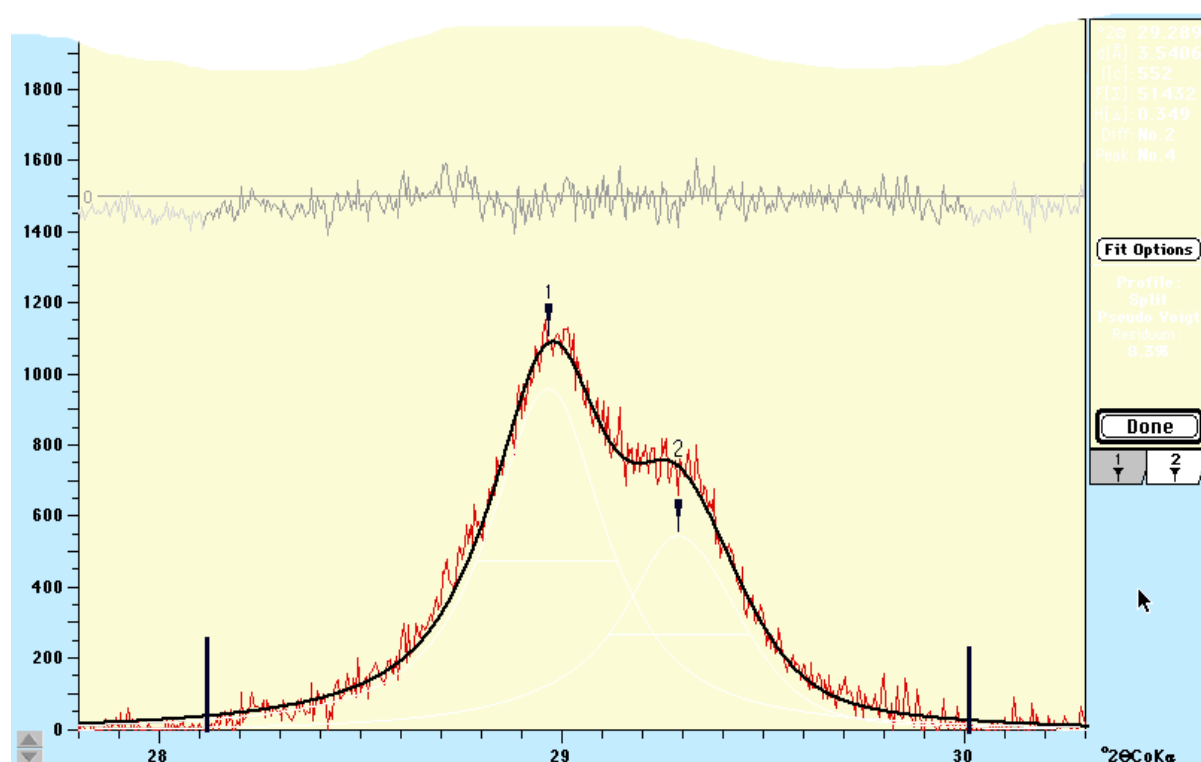
No.	d Å	I/100	hkl	No.	d Å	I/100	hkl	No.	d Å	I/100	hkl
1	4.26	35	100	9	1.801	1	003	17	1.375	11	203
2	3.343	100	101	10	1.672	7	202	18	1.372	9	301
3	2.458	12	110	11	1.659	3	103	19	1.288	3	104
4	2.282	12	102	12	1.608	1	210	20	1.256	4	302
5	2.237	6	111	13	1.541	15	211	21	1.228	2	220
6	2.128	9	200	14	1.453	3	113	22	1.1997	5	213
7	1.98	6	201	15	1.418	1	300	23	1.1973	2	221
8	1.817	17	112	16	1.382	7	212	24	1.1838	4	114

☐ Kill on Update      ☒ Lock this Record      **Print...**      **Goto...**      **Update...**      **Draw**  
☐ Show 2°Thetas      **Create New Record**      **Copy**      **List...**      **Append...**      **Done**  
☐ Auto Update

Peak database dialog (shown here: Alpha Quartz)



Comparison of the measured profile with line graphs showing reflections as available in a peak database. Here: Detection of corundum.



Peak fit analysis of kaolinite (1) and chlorite (2) (3.58 and 3.54Å). Profile function (blue): Pseudo Voigt (split). Black: curve in common (envelope), grey: residuum curve, red: original data. Background removed. The peak data display shows the data of the 2nd peak (chlorite)

[More about Peak fit analysis...](#)



### Peak Identify

'Complete': 22282 peaks Other...

Filter: showing all peaks Options...

☐ List 2-Thetas Show All

Open Record... Draw Report...

- 3.3490 Å: 21 Kalinite
- 3.3480 Å: 100 Phlogopite-1M
- 3.3480 Å: 2 Gmelinite
- 3.3470 Å: 100 Cassiterite, syn
- 3.3460 Å: 33 Fibroferrite
- 3.3460 Å: 12 Ramsdellite
- 3.3460 Å: 45 Gormanite
- 3.3460 Å: 40 Calcioferrite
- 3.3450 Å: 74 Akaganeite-M
- 3.3450 Å: 8 Quenstedtite
- 3.3450 Å: 57 Anilite
- 3.3440 Å: 12 Pickeringite
- 3.3440 Å: 100 Augelite
- 3.3433 Å: ● last peak ●
- 3.3430 Å: 5 Halotrichite
- 3.3430 Å: 2 Vivianite, syn
- 3.3420 Å: 15 Apatite Strontium-apat
- 3.3420 Å: 100 Quartz, syn
- 3.3410 Å: 2 Arsenic Oxide
- 3.3400 Å: 60 Sepiolite, ferrian
- 3.3400 Å: 100 Illite-2M1
- 3.3400 Å: 10 Corrensite
- 3.3400 Å: 10 Montmorillonite-14A
- 3.3400 Å: 25 Rhodonite
- 3.3400 Å: 5 Sapphirine-2M
- 3.3400 Å: 25 Muscovite-2M1

### MacDiff Report

Delete Kill Page Print Page...

Diff 2: Daten von Karroo-Staub X Luft

Phase	d(Å)	Int.	Area	FwHM
1	10.235 Å	10.235: not measured.		
2	3.343 Å	3.343 4524	59980.2	0.216
3	2.551 Å	2.551 1446	26441	0.256
4	2.087 Å	2.087 1709	24691	0.256
5	Smektit (001)	16.061 30	1060	0.477
6	Illit (001)	9.934 280	5311	0.25
7	6.15 Å	6.15: not measured.		
8	Illit (002)	4.973 137	2906	0.304
9	Illit (010)	4.471 147	3000	0.336
10	Quarz (100)	4.253 733	8981	0.197
11	Feldsp (110)	3.193 281	5036	0.285
12	Amphibol	8.451 26	260	0.211
13	9.37 Å	9.37: not measured.		
14	Calzit	3.048 2	69	0.211
15	Goethit	4.189 23	120	0.079
16	Gibbsit	4.821 46	1228	0.555

### MacDiff Peak Info

Remove Print... Save...

Daten von Karroo-Staub X Luft

Diff. No. 2 Peak-No. 2

Phase: Quartz

Bragg Angle (°2θ):	31.06
d-value (Å):	3.343
Intensity (counts):	4524
Peak Area (counts):	59980.2
FwHM (Δ°2θ)/calibr.:	0.216/-
<hr/>	
<input type="checkbox"/> Low Angle Area:	28506
<input type="checkbox"/> High Angle Area:	31474.1
<input type="checkbox"/> 2x Low Angle Area:	57012
<input type="checkbox"/> 2x High Angle Area:	62948.3
<input type="checkbox"/> Area - 2xLow Area:	2968.1
<input type="checkbox"/> Area Asymmetry:	0.906
<hr/>	
<input type="checkbox"/> FwHM (linear):	0.216
<input type="checkbox"/> Low angle WHM:	0.105
<input type="checkbox"/> High angle WHM:	0.11
<input type="checkbox"/> 2x Low angle FwHM:	0.211
<input type="checkbox"/> 2x High angle FwHM:	0.221
<input type="checkbox"/> FwHM Asymmetry:	0.954
<input type="checkbox"/> Fw at 1/4 maximum:	0.333
<input type="checkbox"/> Fw at 3/4 maximum:	0.132
<input type="checkbox"/> Peak basis width:	1.34
<input type="checkbox"/> Integral width:	0.265
<hr/>	
<input type="checkbox"/> Intensity / FwHM:	20969
<input type="checkbox"/> Intensity * FwHM:	976.03
<input type="checkbox"/> Base at peak:	161
<input type="checkbox"/> Valley/Peak (Low):	1
<input type="checkbox"/> Valley/Peak (High):	1.004

Three self updating windows for displaying and handling peak identify, report data and advanced peak info listings. They can be opened constantly.

### Acknowledgements:

For all their critical remarks and for their help to improve MacDiff, many thanks to ...

H. Bartl (Frankfurt, Germany)  
H. Barwood (Bloomington, Indiana, U.S.A.)  
M. Beck (Golden, Colorado, U.S.A.)  
B. Bookhagen (Potsdam, Germany)  
G. Bormann (Kiel, Germany)  
J. Brugger (Basel, Switzerland)  
F. Butt (Oslo, Norway)  
B. Diekmann (Potsdam, Germany)  
P. Covert (Seattle, U.S.A.)  
H. Cynn (Livermore, California, U.S.A.)  
W. Ehrmann (Halle, Germany)  
R. Ferrell (Oslo, Norway / Zürich, Switzerland / Batton Rouge, U.S.A.)  
R. Ferreira Mählmann (Basel, Switzerland)  
F. Gingele (Warnemünde, Germany)  
F. Girod (Lausanne, Switzerland)  
H. Gorter (Eindhoven, The Netherlands)  
H. Grobe (Bremerhaven, Germany)  
U. Gronemann (BEB, Germany)  
E. Hagen (Norway)  
B. Haskell (Minneapolis, Minnesota, U.S.A.)  
M. Herzog (Kronberg, Germany)  
A. Kern (Frankfurt, Germany)  
H. Kollmann (Frankfurt, Germany)  
H. Krumm (Frankfurt, Germany)  
S. Krumm (Erlangen, Germany)  
G. Kuhn (Bremerhaven, Germany)  
V. Kuhnert (Giessen, Germany)  
H. LaViers (acpub.duke.edu)  
Chao R. Li (U.S.A.)  
B. Luckie (Mainstay, U.S.A.)  
A. Menegatti (Zürich, Switzerland)  
L. Morse (Pocatello, Idaho, U.S.A.)  
J. Nakken (Oslo, Norway)  
R. Oberhänsli (Potsdam, Germany)  
H. Ortner (Innsbruck, Austria)  
T. Pletsch (Hanover, Germany)  
J. Rössler (Frankfurt, Germany)  
Thanks for your 'peak fit' help and for your manual translation, Jochen!  
M. Schrier (Berkeley, U.S.A.)  
M. Schmith (Wilmington, North Carolina, U.S.A.)  
H. Stanjek (Munich, Germany)  
I. Steyer (Frankfurt, Germany)  
M. Sturzenegger (Switzerland)  
P. Talbot (Queensland, Australia)



M. Underwood (Columbia, Missouri, U.S.A.)  
C. Vogt (Bremen, Germany)  
L. Warr (Heidelberg, Germany)  
J. Warren (Mitcham, Australia)  
... and to all other users of MacDiff!

Rainer Petschick

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