http://mineral.gcdkit.org

Introducing *GCDkit.Mineral*: a package for interpretation of in-situ mineral analyses

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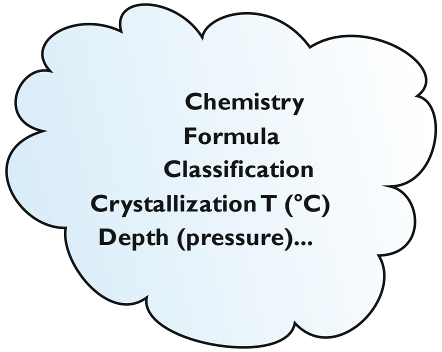
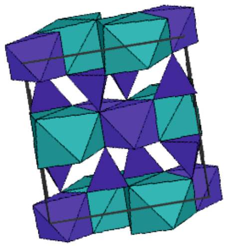
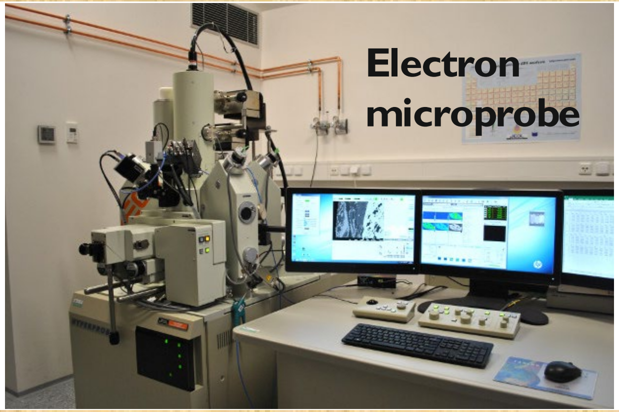
Problem: recalculation of *in-situ* mineral chemical data







Recalculation, statistical evaluation and plotting of mineral analyses

- Mineral analyses (wt. % oxides) need to be recast to atoms per formula unit (apfu):
  - to be employed for mineral classification according to the IMA rules
  - allow deeper insight into mineral crystal chemistry (e.g., nature and extent of substitutions at each of the crystallographic sites)
  - form a basis for most of the conventional geobarometers and geothermometers
  - facilitate a direct linkage with whole-rock geochemical parameters (e.g. millications-based ones) that are useful for nomenclature and petrogenetic considerations (De La Roche et al. 1980; Debon and Le Fort 1983, 1988; Bonin et al. 2020).

Software for mineral chemistry recalculation

Current tools:

- Restricted functionality
- Hard to modify
- Often just a single mineral species
- Poor graphical output
- Typically a single OS (Windows)

Mineral group	Program name	Reference	Programming environment
Amphiboles	PROBE-AMPH	(Tindle & Webb 1994)	MS Excel spreadsheet
	AMPH-CLASS	(Esawi 2004)	MS Excel spreadsheet
	WinAmphcal	(Yavuz 2007)	Visual Basic
	AMPH2012	(Locock 2014)	MS Excel spreadsheet
	WinAmptab	(Yavuz & Döner 2017)	Visual Basic
	AMFORM	(Ridolfi et al. 2018)	MS Excel spreadsheet
Garnets	'Support. Inform. A'	(Locock 2008)	MS Excel spreadsheet
	garnet.R	(Arai 2010)	R language script
	'Appendix 4'	(Grew et al. 2013)	MS Excel spreadsheet
	WinGrt	(Yavuz & Yildirim 2020)	Visual Basic
Pyroxenes	PYROX	(Yavuz 2001)	Visual Basic
	PX-NOM	(Sturm 2002)	MS Excel spreadsheet
	WinPyrox	(Yavuz 2013)	Visual Basic
	WinPLtb	(Yavuz & Yildirim 2018b)	Visual Basic
Spinels	WinSpingc	(Yavuz & Yavuz 2023)	Visual Basic
Tourmalines	WinClastour	(Yavuz et al. 2006)	Visual Basic
	WinTcac	(Yavuz et al. 2014)	Visual Basic
Feldspars	WinFeldth	(Yavuz & Yavuz 2022)	Visual Basic
Epidotes	WinEpclas	(Yavuz & Yildirim 2018a)	Visual Basic
Micas	Mica+	(Yavuz 2003a; 2003b)	Visual Basic
Chlorites	WinCcac	(Yavuz et al. 2015)	Visual Basic

Universal software for mineral chemistry recalculation

Program name	Reference	Programming environment
CALCMIN	(Brandelik 2009)	Visual Basic/Excel
MINCALC	(Bernhardt 2010)	Windows, ?
PET: Petrological Elementary Tools	(Dachs 1998, 2004)	Mathematica
MINERAL	(Angelis & Neill 2012)	MATLAB
MinPlot	(Walters 2022)	MATLAB
XMapTools	(Lanari et al. 2014, 2019)	MATLAB (runtime)

Ideal mineralogical software:

- Universal (numerous minerals)
- Modifiable, expandable
- Platform-independent
- Many I/O file formats
- Publication quality graphics
- (Advanced) statistical functions
- Free, including programming language

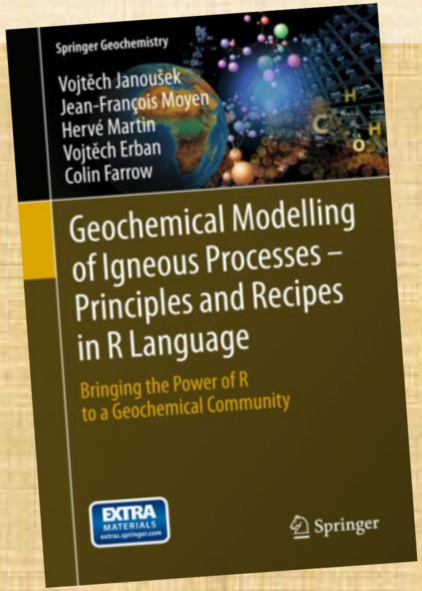
Scientific programming languages:

- Designed esp. for numerically demanding scientific computations
- Working with matrices/multidimensional data arrays
- Direct vs. batch mode (scripting)
- Free are *R, Python, Julia, Octave*

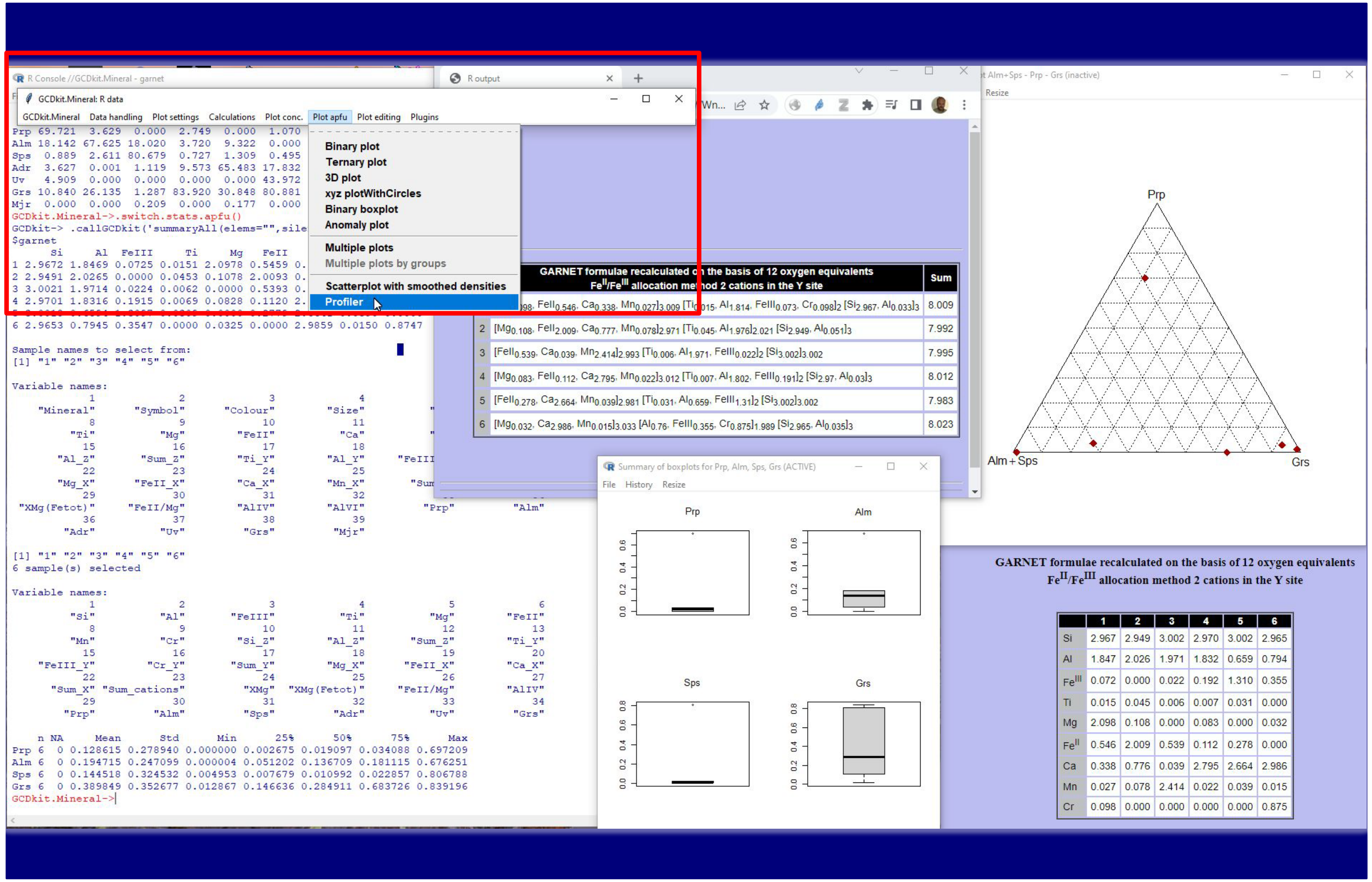
A revolution? The R language!

- Originally designed by Ihaka and Gentleman (1996)
- Version 1.0 published on 29 Feb 2000
- Based on syntax of the S language (Becker et al. 1988) which was developed at AT&T Bell Laboratories by John Chambers and colleagues
- The commercial version, S-PLUS, is still being distributed

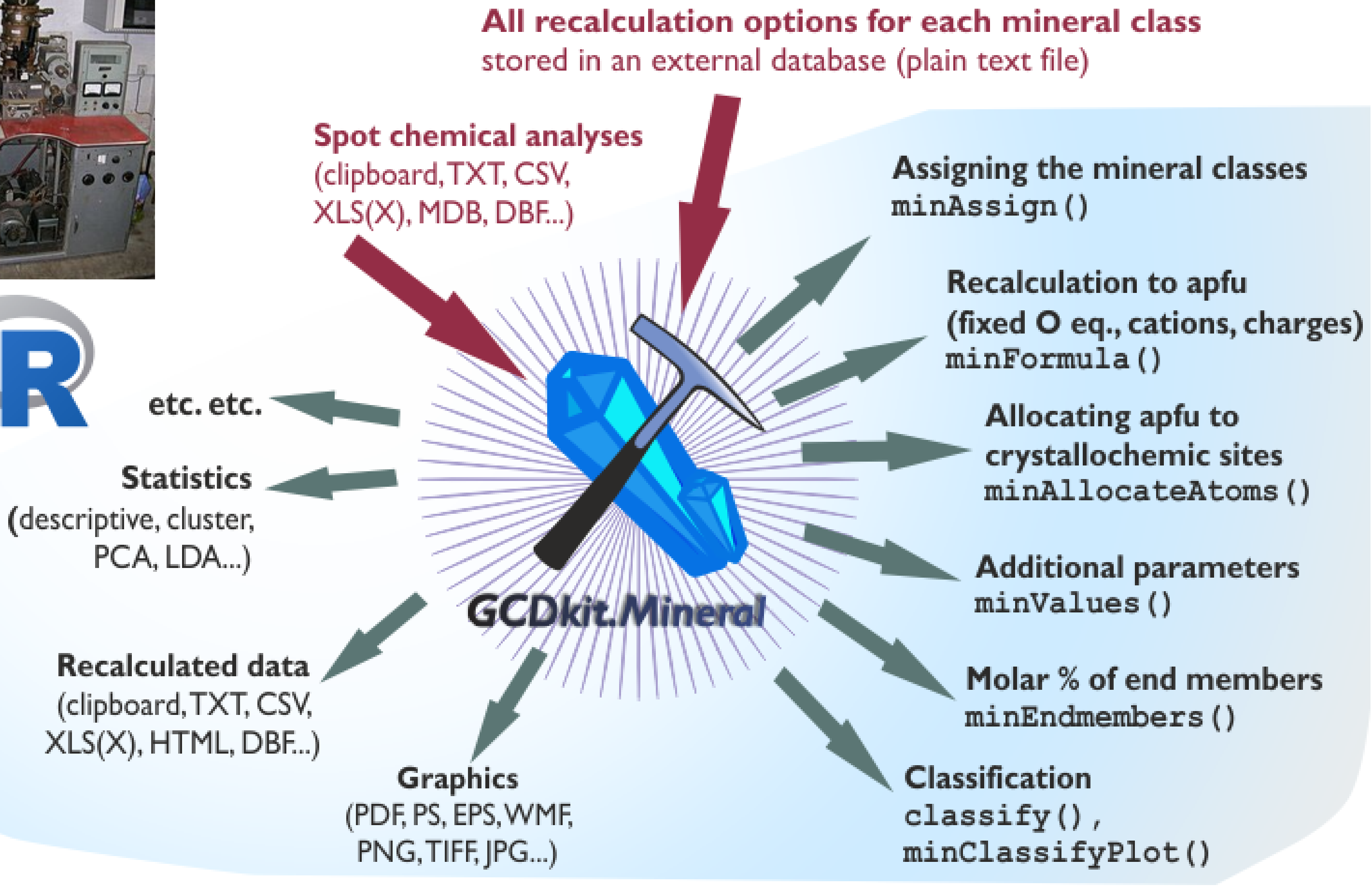
- Since 1997 the development of the R project is overseen by an open group of experts, the R Development Core Team (http://www.r-project.org)
- R is Free Software available for all main OS (incl. Linux, Windows and MacOS)
- > 20 years of development of software for igneous & metamorphic geochemistry *(gcdkit.org)*



GCDkit.Mineral: Graphical User Interface (GUI)



GCDkit.Mineral: Program scheme



Data input

- *In-situ* chemical analyses (typically, EPMA) given as oxides: SiO_2, TiO_2, MgO…
- Plain ASCII text (*data), CSV, MS Excel XLS(X), MS Access (MDB), or DBF files
- Pasting data from clipboard
- Sample data sets (Deer, Howie & Zussman: Introduction to Rock-Forming Minerals)
- Individual analyses stored in rows, variables in columns, essentially random order
- May include textual meta-information (on mineral species, locality, etc.) = labels
- Missing values, b.d.l. etc. possible
- Plotting properties (Symbol, Colour and/or Size)
- Mineral (to identify a mineral species for the given analysis)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Sample	Symbol	Colour	Mineral	SiO2	TiO2	Al2O3	Cr2O3	FeO	MnO	MgO	CaO	Na2O	K2O	BaO
2	Har-01	1	red	Grt	38.83	0.34	19.43		6.50	1.15	0.22	32.91	0.01		
3	Har-02	1	red	Grt	38.89	0.18	20.33		4.92	0.66	0.24	33.88	0.01		
4	Har-03	1	red	Grt	38.24	0.38	17.97		8.39	1.02	0.18	32.73	b.d.l.		
5	Egypt-01	4	black	Fsp	65.90		20.23		0.36			1.15	7.33	5.27	b.d.l.
6	Egypt-02	4	black	Fsp	60.69		24.38		0.24			5.85	7.42	1.40	0.17
7	Egypt-03	4	black	Fsp	66.18		19.01		0.50			0.22	6.29	7.23	b.d.l.
8	Clino-01	15	darkgreen	Cpx	51.41	0.93	2.55	0.22	8.06	0.25	15.09	20.92	0.32	b.d.l.	
9	Clino-02	15	darkgreen	Cpx	51.08	1.10	2.46	0.11	8.84	0.21	14.91	20.72	0.34	b.d.l.	
10	Clino-03	15	darkgreen	Cpx	51.18	1.20	2.66	0.09	9.08	0	14.45	20.5	0.43	b.d.l.	

Sample

Připraven 100 %

Mineral species recognition

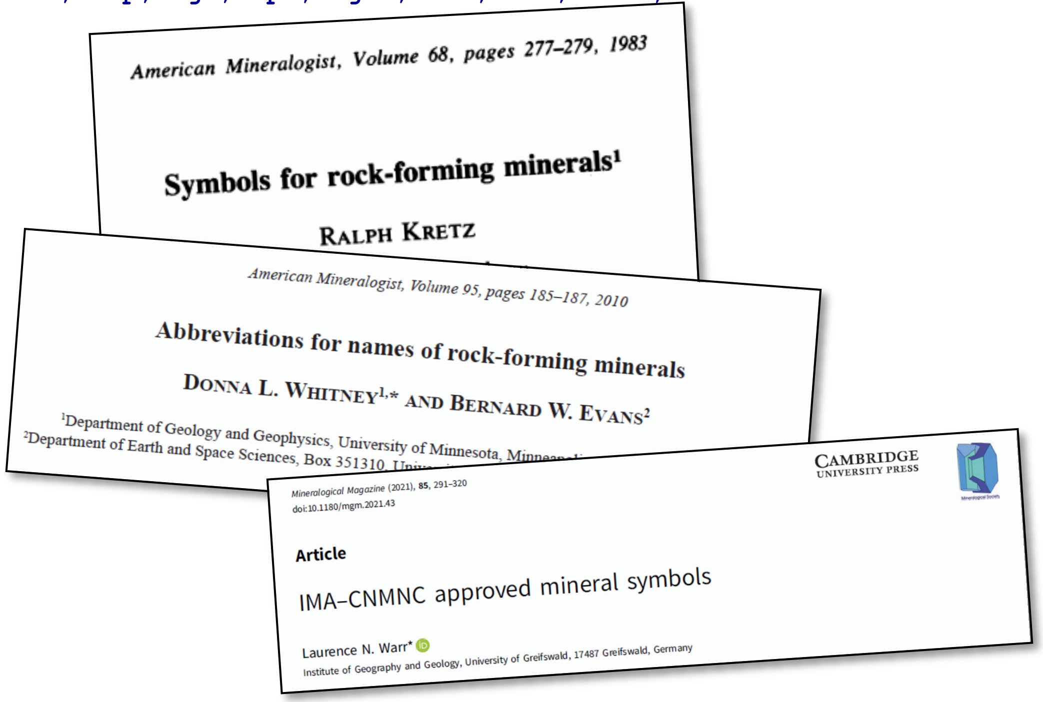
`minAssign()`

Column `'Mineral'` in the original file:

- Contains any of the pre-defined full or abbreviated names
- Abbreviations:
  - Kretz (1983), Whitney & Evans (2010), Warr (2021)
  - other software packages, e.g. MinPet (Richard 1995), Thermocalc (Holland & Powell 1998) or PET (Dachs 1998, 2004)
- Full names = various formal or informal names occurring in the given mineral group

```
Full name(s):
clinopyroxene, Ca clinopyroxene, aegirine, augite,
burnettite, clinoenstatite, clinoferrosilite,
colomeraite, davisite, diopside, esseneite,
grossmanite, hedenbergite, jadeite, jervisite,
johannsenite, kanoite, kosmochlor, kushiroite,
namansilite, natalyite, omphacite, petedunnite,
pigeonite, ryabchikovite, spodumene, tissintite

Abbreviation(s):
Px, Cpx, Aeg, Ae, Aug, Cen, Cfs, Di, Hd, Jd, Jh,
Jhnt, Omp, Pgt, Spd, mgts, hed, acm, cats, PYR
```


American Mineralogist, Volume 68, pages 277–279, 1983

Symbols for rock-forming minerals[1]

RALPH KRETZ

American Mineralogist, Volume 95, pages 185–187, 2010

Abbreviations for names of rock-forming minerals

DONNA L. WHITNEY[1,*] AND BERNARD W. EVANS[2]

[1]Department of Geology and Geophysics, University of Minnesota, Minneapol...

[2]Department of Earth and Space Sciences, Box 351310, Univ...

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Article

IMA–CNMNC approved mineral symbols

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Formula calculation (oxides to apfu)

minFormula()

- Formula calculation is based on:
  - Σ of O equivalents
  - Σ atoms
    (entire formula unit, selected ones)
  - Fixed charge
- Methods to assess Fe^{II}/Fe^{III}:
  - Σ of cations in entire formula
    (Droop 1987)
  - Σ of cations in selected crystal site
    (iterative)
  - Specific methods for amphiboles
    (Leake et al. 2003) and pyroxenes
    (Papike et al. 1974).

```
##################################################
CLINOPYROXENE formulae recalculated on basis of
6 oxygen equivalents
FeII/FeIII allocation method 4 cations per formula
unit (Droop 1987)
##################################################

Number of O:
6

Number of cations:
4

Iron recalculation:
Droop

Atom names:
Si, Al, FeIII, FeII, Ti, Cr, V, Zr, Sc, Zn, Ni,
Co, Mg, Mn, Li, Ca, Na, K
```

Atoms allocation to crystallographic sites

`minAllocateAtoms()`

- Computed apfu are allocated to crystallographic sites of the given mineral(s)
- Individual sites are filled by each of the atoms in the order specified, from left to right
- If some of the atoms may be present in two sites, the `site.sums` must give the required sum for the first of them
- When the first site is filled (`site.sums` value is reached), any excess of the given element is passed to the next available position

```
####################################################
FELDSPAR formulae recalculated on the basis of 8
oxygen equivalents
####################################################

Number of O:
8

Atom names:
Si, Al, FeIII, Ti, Na, K, Ca, Sr, Ba, Rb, Li, Cs,
Pb, Eu, Mg, Mn, P

Site allocation:
$`Si = 2`
[1] "Si"

$`T = 2`
[1] "P, Si, Al, FeIII, Ti"

$`A = sum not fixed`
[1] "Na, K, Ca, FeIII, Mg, Mn, Sr, Ba, Rb, Li, Cs,
Pb, Eu"
```

```
sites = list(Z = c("Si", "Al"),
X = c("Mg","Fe"), Y = c("Ti", "Al")),
site.sums = c(6, NA, NA)
```

Additional values, end members

`minValues()`

- Extra values, such as Fe#
- Specified by simple formulae or in external R script
- Formulae can refer to valid atom names, and/or the names of the atoms allocated to the crystallographic sites

`minEndmembers()`

- Molar percentages of end members for minerals forming solid solutions
- Formulae may again refer to valid atom names, names of the atoms allocated to the individual crystallographic sites and/or special parameters computed at the previous step

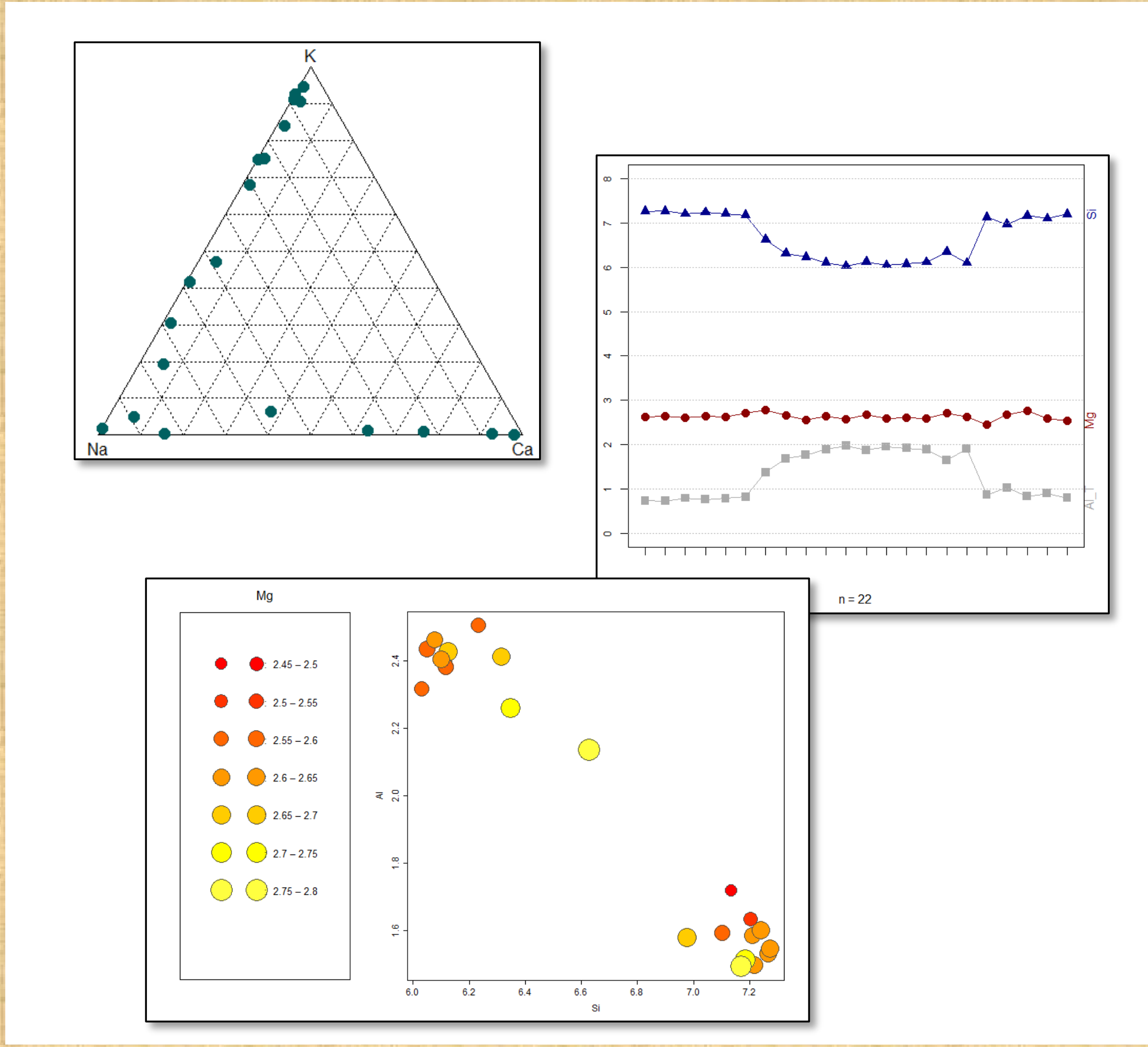
```
values.formulae = c("Ca/(Ca+Mg+FeII+Mn)", "FeII/Mg",
"Al_Z/Al_Y"),
values.names = c("XCa", "Fe2+/Mg", "AlIV/AlVI")
```

```
####################################################
FELDSPAR formulae recalculated on the basis of 8
oxygen equivalents
####################################################

Atom names:
Si, Al, FeIII, Ti, Na, K, Ca, Sr, Ba, Rb, Li, Cs,
Pb, Eu, Mg, Mn, P

End members:
Ab = Na/(Na+Ca+K+Ba+Sr), An = Ca/(Na+Ca+K+Ba+Sr), Or
= K/(Na+Ca+K+Ba+Sr), Cln = Ba/(Na+Ca+K+Ba+Sr), Sl =
Sr/(Na+Ca+K+Ba+Sr)
```

```
values.formulae = c("FeII/(Ca+Mg+FeII+Mn)",
 "Mg/(Ca+Mg+FeII+Mn)", "Mn/(Ca+Mg+FeII+Mn)"),
values.names = c("XFe", "XMg", "XMn"),
end.member.formulae = c("XMg","XFe","XMn","FeIII/2"),
end.member.names = c("Prp", "Alm", "Sps", "Adr")
```

Plotting

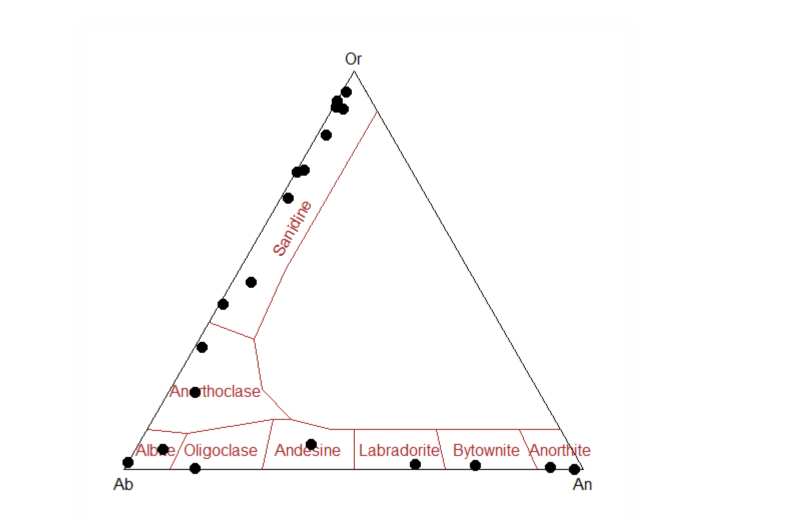
- Original analyses in wt. % or calculated parameters
  (apfu, end-member mol. %, ...)
- Binary, ternary plots, profiles
- Most diagrams defined as objects
  (= Figaro templates), whose properties can be modified subsequently, and which can be combined into plates
  Changing range of axes, adding legend, changing plotting attributes (symbols, colour, size), interactive identification of samples…
- Fields defined as closed polygons – basis for classification
- Export into various file formats:
  - Vector (PDF, PS, EPS, WMF)
  - Bitmap (PNG, TIFF, JPG...)

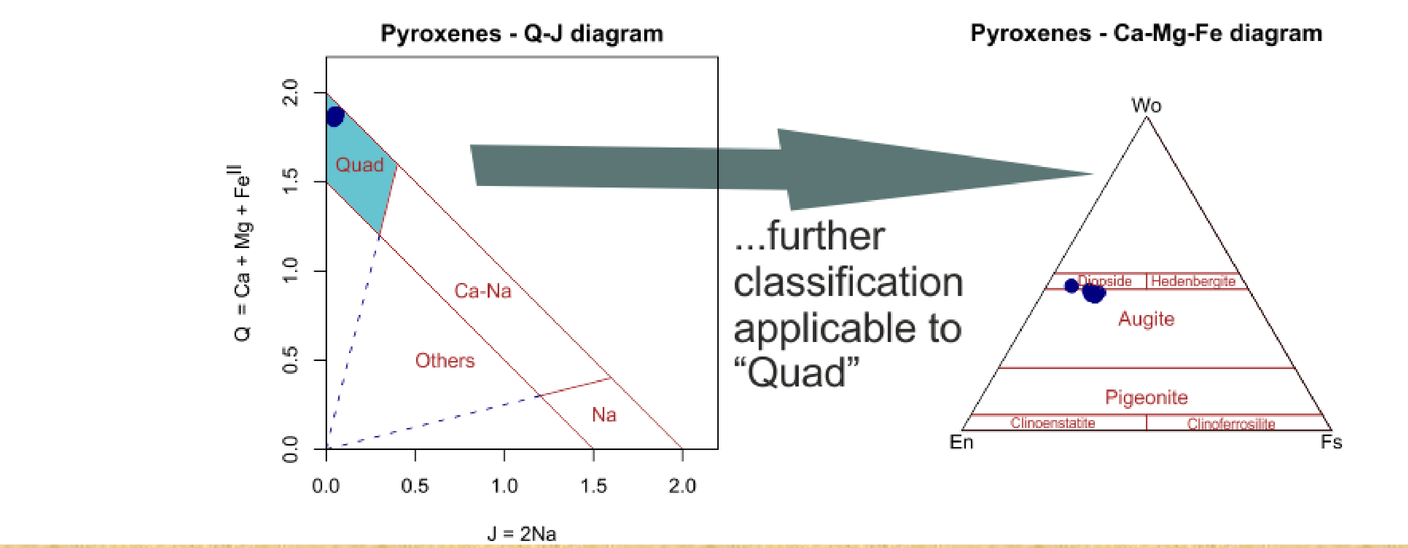


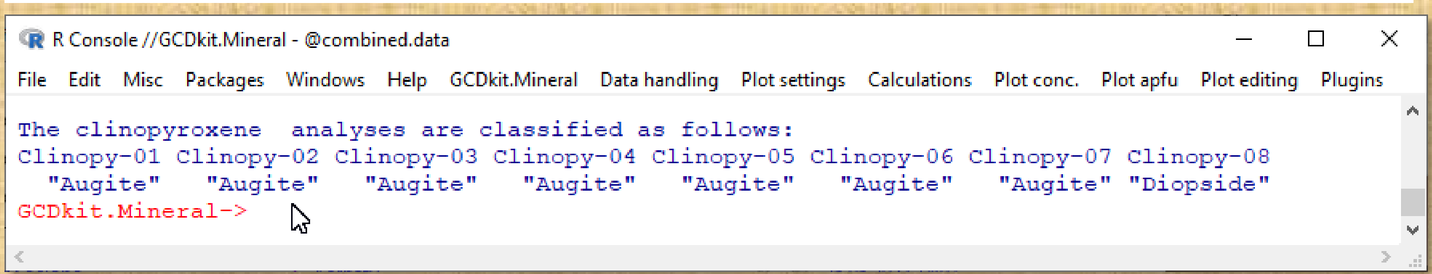
Classification

`classify()`, `minClassifyPlot()`

- Hierarchical classification schemes (decision trees)
- Based on a sequence of binary or ternary plots,
- Can be supplemented by simple R scripts







Data output

- Recalculated data can be pasted to clipboard, or saved to TXT, CSV, XLS, DBF formats
- Formatted HTML (Web page) output
- Export structural formulae to HTML

	PYROXENE formulae recalculated on the basis of 6 oxygen equivalents FeII/FeIII allocated assuming 4 cations per formula unit (Droop 1987)	Sum
Clinopy-01	$[FeII_{0.137}, Mn_{0.008}, Ca_{0.832}, Na_{0.023}]_1$ $[Al_{0.02}, FeIII_{0.037}, Ti_{0.026}, Cr_{0.006}, Mg_{0.835}, FeII_{0.076}]_1$ $[Si_{1.908}, Al_{0.092}]_2$	4
Clinopy-02	$[FeII_{0.143}, Mn_{0.007}, Ca_{0.826}, Na_{0.025}]_1$ $[Al_{0.008}, FeIII_{0.052}, Ti_{0.031}, Cr_{0.003}, Mg_{0.827}, FeII_{0.08}]_1$ $[Si_{1.9}, Al_{0.1}]_2$	4
Clinopy-03	$[FeII_{0.149}, Ca_{0.819}, Na_{0.031}]_1$ $[Al_{0.026}, FeIII_{0.025}, Ti_{0.034}, Cr_{0.003}, Mg_{0.804}, FeII_{0.108}]_1$ $[Si_{1.909}, Al_{0.091}]_2$	4
Clinopy-04	$[FeII_{0.123}, Mn_{0.006}, Ca_{0.843}, Na_{0.028}]_1$ $[Al_{0.02}, FeIII_{0.062}, Ti_{0.03}, Mg_{0.79}, FeII_{0.098}]_1$ $[Si_{1.885}, Al_{0.115}]_2$	4
Clinopy-05	$[FeII_{0.121}, Mn_{0.007}, Ca_{0.849}, Na_{0.024}]_1$ $[Al_{0.027}, FeIII_{0.043}, Ti_{0.028}, Cr_{0.016}, Mg_{0.824}, FeII_{0.062}]_1$ $[Si_{1.882}, Al_{0.118}]_2$	4
Clinopy-06	$[FeII_{0.131}, Mn_{0.008}, Ca_{0.839}, Na_{0.022}]_1$ $[Al_{0.039}, FeIII_{0.031}, Ti_{0.029}, Cr_{0.005}, Mg_{0.809}, FeII_{0.087}]_1$ $[Si_{1.888}, Al_{0.112}]_2$	4
Clinopy-07	$[FeII_{0.121}, Mn_{0.008}, Ca_{0.848}, Na_{0.024}]_1$ $[Al_{0.028}, FeIII_{0.035}, Ti_{0.024}, Cr_{0.015}, Mg_{0.827}, FeII_{0.072}]_1$ $[Si_{1.898}, Al_{0.102}]_2$	4
Clinopy-08	$[Mg_{0.026}, FeII_{0.076}, Mn_{0.002}, Ca_{0.874}, Na_{0.022}]_1$ $[Al_{0.027}, FeIII_{0.049}, Ti_{0.016}, Cr_{0.036}, Mg_{0.872}]_1$ $[Si_{1.877}, Al_{0.123}]_2$	4

feldspar

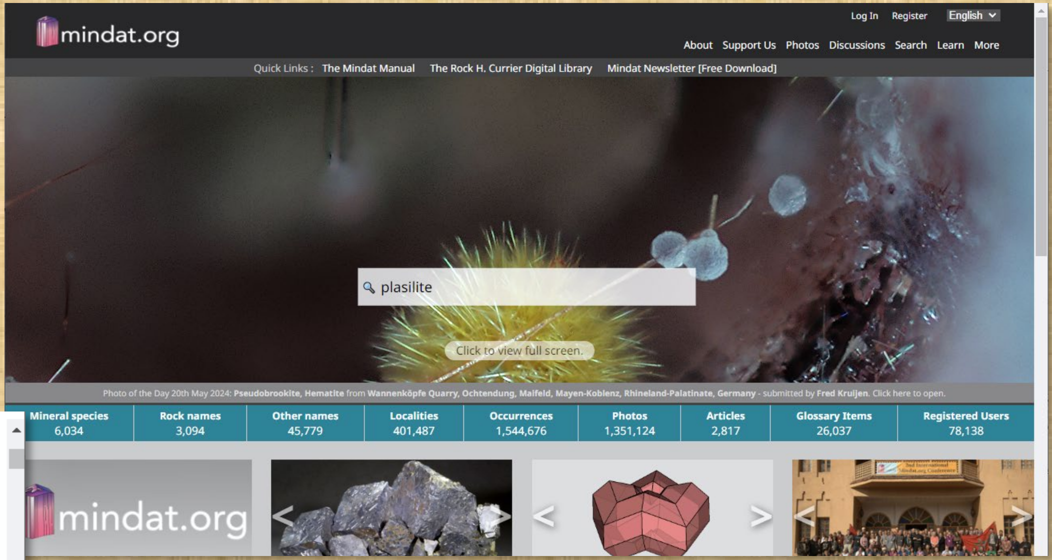
FELDSPAR formulae recalculated on the basis of 8 oxygen equivalents

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Mineral	orthoclase	orthoclase	orthoclase	orthoclase	microcline	microcline	microcline	sanidine	sanidine	anothoclase	adularia	orthoclase	albite	albite	oligoclase	andesine	labradorite	bytownite	anorthite	anorthite
Si_Si	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
Σ_Si	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
Si_T	0.930	0.938	0.949	0.940	0.958	0.931	0.985	1.008	0.947	0.983	0.963	1.003	0.991	0.940	0.816	0.602	0.386	0.248	0.059	0.032
Al_T	1.062	1.067	1.060	1.063	1.037	1.062	1.012	0.967	1.044	0.984	1.042	0.912	1.021	1.061	1.173	1.396	1.593	1.735	1.920	1.974
Fe^{III}_T	0.006	0.000	0.000	0.000	0.005	0.007	0.003	0.025	0.010	0.029	0.000	0.085	0.000	0.000	0.011	0.002	0.017	0.009	0.021	0.000
Ti_T	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000
Σ_T	2.001	2.005	2.009	2.003	2.000	2.000	2.000	2.000	2.000	1.998	2.006	2.000	2.012	2.001	2.000	2.000	2.000	1.992	2.000	2.006
Na_A	0.729	0.487	0.302	0.072	0.232	0.139	0.044	0.559	0.239	0.680	0.082	0.071	0.946	0.889	0.842	0.563	0.354	0.228	0.071	0.020
K_A	0.187	0.470	0.682	0.919	0.750	0.834	0.949	0.402	0.714	0.306	0.900	0.904	0.016	0.050	0.003	0.063	0.012	0.010	0.003	0.000
Ca_A	0.057	0.041	0.017	0.025	0.017	0.020	0.008	0.007	0.002	0.017	0.005	0.002	0.000	0.059	0.153	0.376	0.617	0.755	0.930	0.961
Fe^{III}_A	0.000	0.003	0.003	0.004	0.009	0.012	0.002	0.006	0.007	0.000	0.003	0.004	0.002	0.000	0.000	0.005	0.000	0.000	0.002	0.003
Mg_A	0.007	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.004	0.000	0.007	0.003	0.003	0.000	0.016	0.002	0.005	0.014	0.000	0.000
Ba_A	0.011	0.000	0.000	0.000	0.000	0.006	0.000	0.000	0.028	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Σ_A	0.990	1.001	1.004	1.019	1.008	1.015	1.003	0.974	0.994	1.004	0.999	0.984	0.967	0.998	1.015	1.009	0.989	1.007	1.007	0.983
Σ_cations	4.991	5.006	5.012	5.022	5.008	5.015	5.003	4.974	4.997	5.002	5.005	4.984	4.979	4.999	5.015	5.009	4.988	4.999	5.007	4.989

Generated on: *Mon May 20 12:10:58 2024* - **GCDkit.Mineral via R2HTML**

Helper functions (tools)

- Ideal mineral compositions (based on database from Le Maitre 1982: *Numerical Petrology*)
- Search minerals by chemistry (via *webmineral.com*)
- Mineral data at *mindat.org*



Click Here for Mineral Species Sorted By %Mg

Mineral Name	Chemical Formula	Mg	MW
Actinolite	Ca2(Mg,Fe++)5Si8O22(OH)2	9.71% Mg	853.16
Adelite	CaMg(AsO4)(OH)	11.03% Mg	220.31
Admontite	MgB6O10•7(H2O)	6.48% Mg	375.27
Aegirine-augite *	(Ca,Na)(Mg,Fe++,Fe+++)[Si2O6]	5.33% Mg	228.05
Aenigmatite	(Na,Ca)4(Fe++,Ti,Mg)12Si12O40	0.65% Mg	1,717.59
Aerinite	(Ca,Na)6FeAl(Fe++,Mg)2(Al,Mg)6[Si12O36(OH)12H][(H2O)12(CO3)]	1.25% Mg	1,944.10
Akatoreite	(Mn++,Fe++)9Al2Si8O24(OH)8	0.17% Mg	1,282.75
Akermanite	Ca2MgSi2O7	8.92% Mg	272.63
Akimotoite !	(Mg,Fe)SiO3		
Akrochordite	Mn4Mg(AsO4)2(OH)4•4(H2O)		
Aksaite	MgB6O7(OH)6•2(H2O)		

Dysprosium
Einsteinium
Erbium
Europium
Fermium
Fluorine
Francium
Gadolinium
Gallium
Germanium


```
              Abbreviation        MW                Formula
Albite                  Ab 262.22451             NaAlSi3O8
Hedenbergite            Hd  248.0954             CaFeSi2O6
Riebeckite             Rbk 935.90394 Na2Fe3FeIII2Si8O22(OH)2

                 SiO2 TiO2    Al2O3    Fe2O3      FeO Mn2O3 MnO MgO      CaO      Na2O K2O P2O5
Albite       68.73808    0 19.44307  0.00000  0.00000     0   0   0  0.00000 11.818851   0    0
Hedenbergite 48.43594    0  0.00000  0.00000 28.95893     0   0   0 22.60513  0.000000   0    0
Riebeckite   51.35903    0  0.00000 17.06294 23.02995     0   0   0  0.00000  6.623018   0    0
                  H2O CO2 B2O3 BaO SrO Li2O ZnO PbO Ce2O3 ZrO2 BeO Cr2O3 F Cl S F.eq Cl.eq
Albite       0.000000   0    0   0   0    0   0   0     0    0   0     0 0  0 0    0     0
Hedenbergite 0.000000   0    0   0   0    0   0   0     0    0   0     0 0  0 0    0     0
Riebeckite   1.925066   0    0   0   0    0   0   0     0    0   0     0 0  0 0    0     0
```

Recalculation parameters

- Each mineral (feldspar, pyroxene…) = a subclass of the class *mineral*
- Independent methods for recalculation, classification, plotting… for each subclass
- Recalculation options stored externally in a lucid plain-text file (aka standard database): `mineral_db.r`
- Can be also specified upon function call

```
##########################################################################
#                           CLINOPYROXENE                                #
#                         M2[1]M1[1]T[2]O[6]                             #
##########################################################################
setClass("clinopyroxene",representation(),contains="mineral",
    prototype(
        abbreviated=c("Px","Cpx","Aeg","Ae","Aug","Di","Hd","Jd"),
        full=c("clinopyroxene","Ca clinopyroxene","aegirine",
            "augite","clinoenstatite","clinoferrosilite",
            "diopside","hedenbergite","jadeite"),
        oxygens=6,
        cations=4,
        iron="Droop",
        atom.names=c("Si","Al","FeIII","FeII",
            "Ti","Cr","V","Zr","Zn","Ni","Co","Mg","Mn",
            "Li","Ca","Na","K"),
        sites=list(T=(c("Si","Al","FeIII")),
            M1=c("Al","FeIII","Ti","Cr","V","Zr","Ni","Co","Mg","FeII","Mn"),
            M2=c("Mg","FeII","Mn","Li","Ca","Na","K")),
        site.sums=c(2,1,NA),
        values.formulae="clinopyroxene.r",
        values.names=c("FeIII/Fetot","XMg","AlIV/AlVI","AlIV","AlVI","aDi"),
        end.member.formulae="clinopyroxene.end.r",
        end.member.names=c("Jd","CaTs","CaTi","CrCaTs","DiHd","EnFs")
    )
)
```

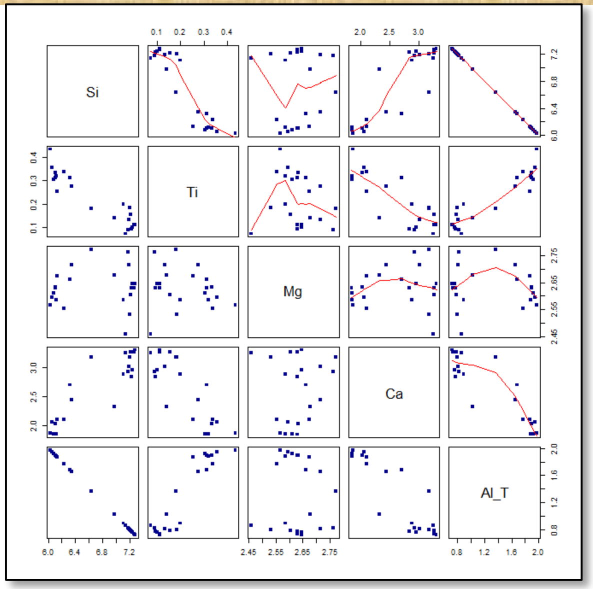
```
minMain("clinopyroxene",
  list(oxygens=6))
```

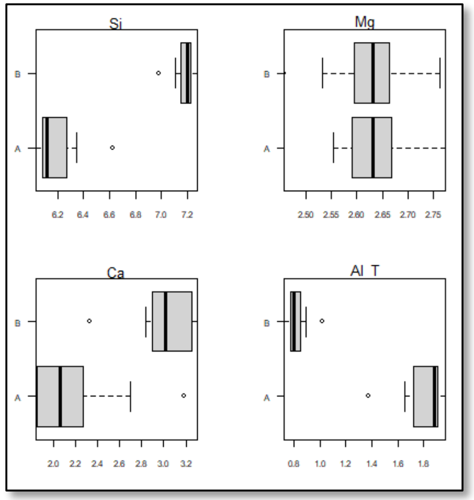
```
minMain("clinopyroxene",
  list(cations=4))
```

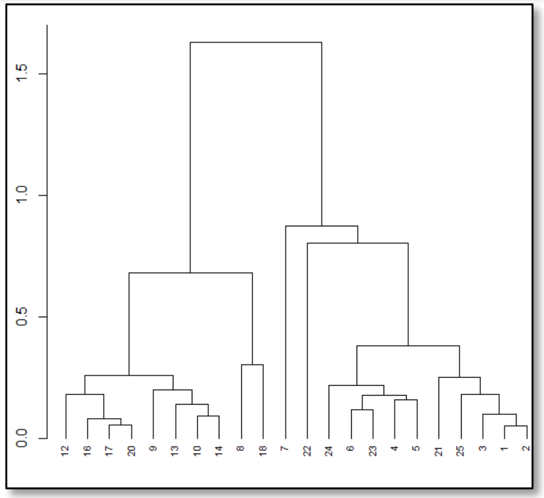
```
minMain("clinopyroxene",
  list(oxygens=6, cations=4, iron="Droop"))
```

Statistics

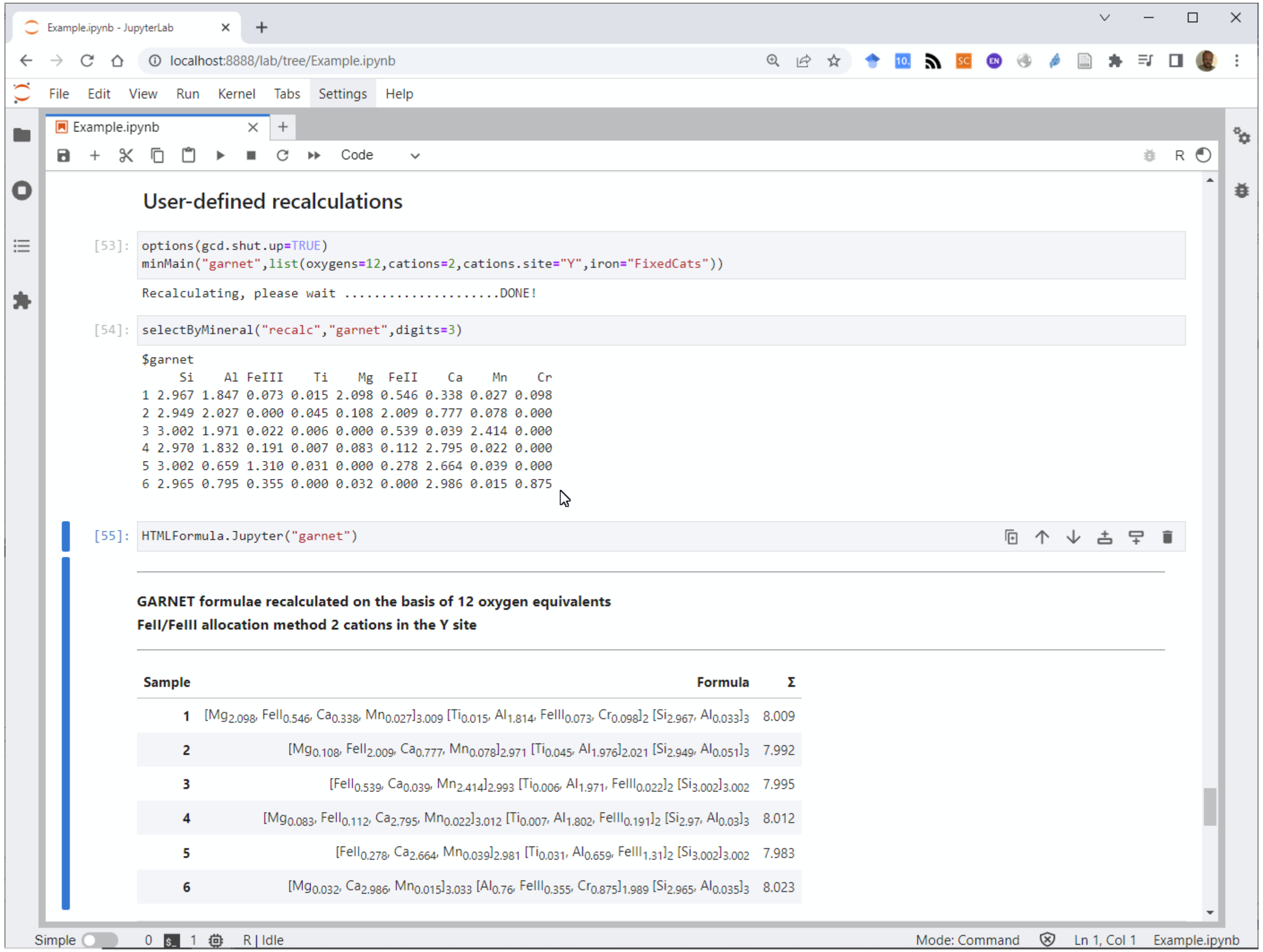
- Original analyses in wt. % or calculated parameters (apfu, end-member mol. %, ...)
- **Subsetting =** simple database functionality
- **Grouping =** coherent groups defined based on various criteria
- **Descriptive statistics**
- Boxplots, histograms, correlation plots,...
- **Multivariate statistical methods** (e.g., cluster analysis, PCA – principal components a., LDA – linear discrimination a.)
- Plethora of statistical tools in R and user-contributed packages







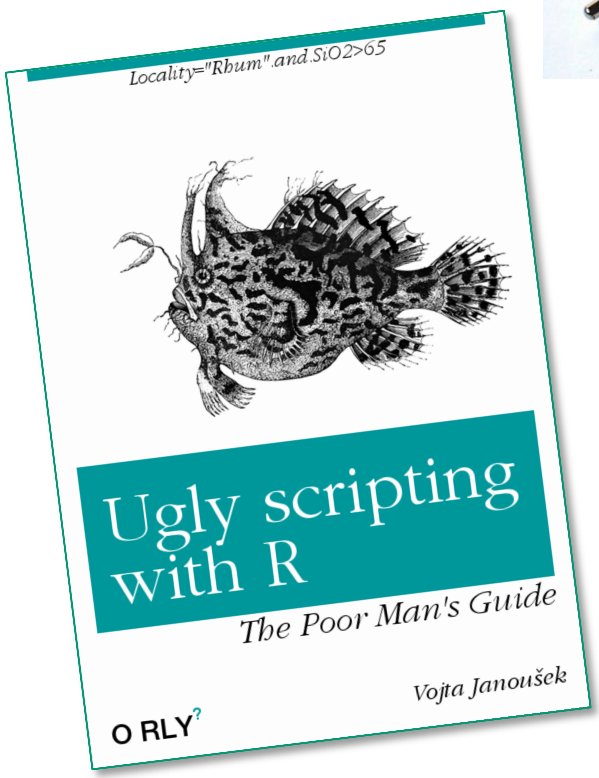
Scripting



- Python-driven Jupyter notebooks: http://jupyter.org
- Editing code in the WWW browser
- Kernel runs R on the background
- Results shown directly in the notebook (incl. graphics)
- Reproducibility, teaching tool

Plugins

- R scripts stored in *Plugin* subdirectory
- All run whenever a new dataset is loaded
- Additional functions, added from newly appended menus
- Standard plugins, e.g. for multivariate statistics
- Code designed for special purposes (e.g. a certain mineral)
- Amp and Px thermobarometry (under development)
- Platform to develop user-defined extensions/enhancements of the system



Conclusions

GCDkit.Mineral = platform-independent freeware:

- Workbench for daily ordinary recalculations and plotting in petrology and mineralogy
- Predefined default recalculation schemes for common minerals
- Advanced graphical and statistical capabilities
- Graphical user interface (GUI), direct or batch mode (scripting)
- Open environment, effortlessly customizable and expandable
- Flexible platform for community-driven development of new tools

Known limitations

- Cannot deal with elements with multiple valencies (apart from Fe^{II}/Fe^{III})
- Extra H_2O determinations are not taken into account
- Limited choice of IMA classification schemes (only Fsp, Amp, Cpx, Opx)
- Missing templates to diagrams used for individual mineral groups
- Dataset switching and overplotting of multiple datasets onto the same diagram N/A
- Future version shall import trace-element determinations, obtained e.g. by LA ICP-MS or ion probe, and will contain means for their interpretation (e.g. spiderplots)

http://mineral.gcdkit.org

Janoušek, V., Farrow, C. M., & Erban, V.
GCDkit.Mineral – a customizable, platform-independent R-language environment for recalculation, plotting and classification of electron-probe micro-analyses of common rock-forming minerals.
Am Min 109 (9): 1598–1607

American Mineralogist

MINERALOGIST
noun (mineralogist)
Someone who solves a problem you didn't know you had in a way you don't understand.

see also:
handsome, exceptional, legend

Thank you for your attention!

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