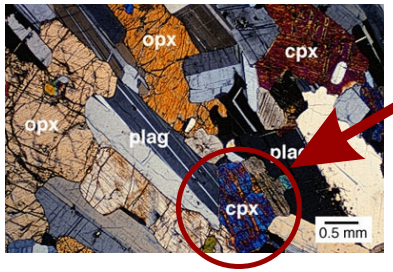
A rock (troctolite)



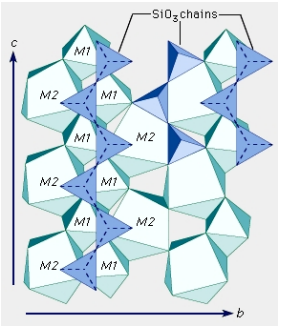
A mineral (pyroxene)

?

Chemical composition?
Genesis?
Crystallization temperature?
Depth of origin?
...

Clinopy-01	
SiO_2	51.41
TiO_2	0.93
Al_2O_3	2.55
Cr_2O_3	0.22
FeO	8.06
MnO	0.25
MgO	15.09
CaO	20.92
Na_2O	0.32
Sum	99.75

Structural formula (pyroxene)

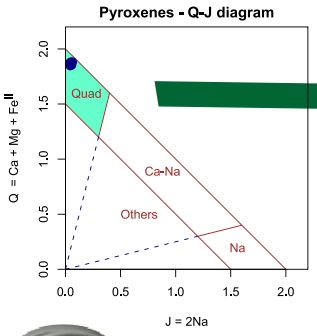


$M2.M1.T_2O_6$

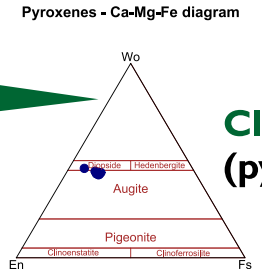
- **T** (tetrahedra): Si Al Fe^{3+}
- **M1** (small octahedron): Al Fe^{3+} Ti^{4+} Cr V Ti^{3+} Zr Sc Zn Mg Fe^{2+} Mn
- **M2** (larger cation site): Mg Fe^{2+} Mn Li Ca Na

Atoms per formula unit

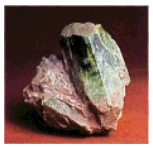
$[Fe^{II}_{0.137}\ Mn_{0.008}\ Ca_{0.832}\ Na_{0.023}]_1\ [Al_{0.02}\ Fe^{III}_{0.03}\ Ti_{0.026}\ Cr_{0.006}\ Mg_{0.835}\ Fe^{II}_{0.076}]_1\ [Si_{1.908}\ Al_{0.092}]_2$



...further classification applicable to "Quad"



Classification (pyroxene)



+GCDkit.Mineral

- Tools for data import/export *(RODBC)*, plotting and plot editing
- Each mineral = S4 class
- Methods for recalculations to **mineral formulae** (IMA)
- **Classifications:** functions for spatial data analysis (package *sp*) applied to polygons defined on a pre-defined sequence of binary or ternary plots