R_application_01

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1 R applications – Part I Some useful graphs

- 1.1 Log-log binary plots
- 1.2 Harker plots and closure effect
- 1.3 Spiderplots
- 1.4 Ternary plots

1.1 Log-log binary plots

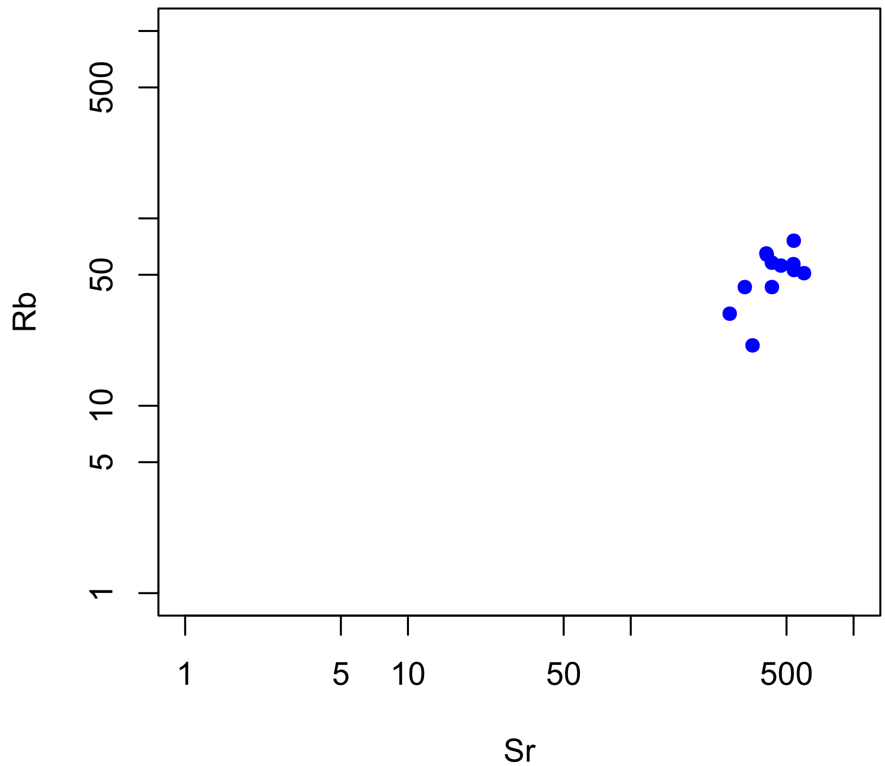
Plotting a binary plot in logarithmic coordinates enables examining both the elemental concentrations and their ratios. In this projection the fan of lines passing through the origin corresponding to analyses of constant ratio in a standard binary plot is transformed into a series of parallel lines of identical slope in logarithmic coordinates. In R, log–log diagrams are plotted using the function `plot`, specifying `log = "xy"`.

Plot binary diagrams of Sr vs. Rb for the `sazava` dataset in two versions, linear and log-log.

[1]:
```
options(repr.plot.width=5, repr.plot.height=5,repr.plot.res = 300) # image␣
 ↪resolution in dpi
options(jupyter.plot_mimetypes = "image/png") # Change mimetype to PNG

# Using image/svg+xml
# May not work in some browsers (but is optimal for Chrome, Firefox...)
options(repr.plot.width=5, repr.plot.height=5)
options(jupyter.plot_mimetypes = "image/svg+xml")
```

[2]:
```
sazava<- read.table("data/sazava.data",sep="\t")
plot(sazava[,"Sr"],sazava[,"Rb"],xlim=c(1,1000),ylim=c(1,1000),
     xlab="Sr",ylab="Rb",pch=16,col="blue",log="xy")
```

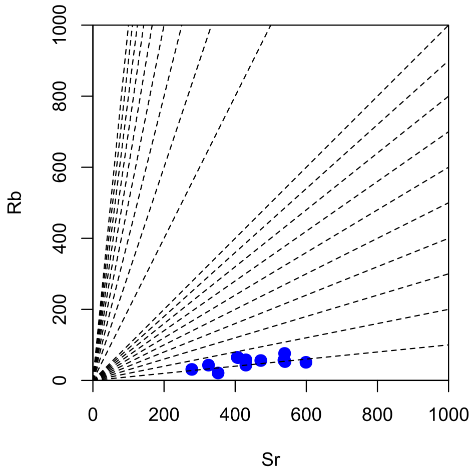


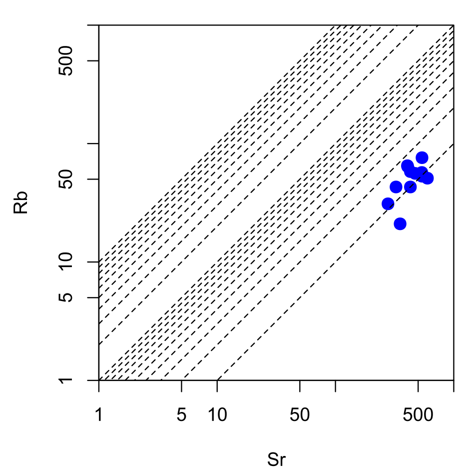
[3]:
```
options(repr.plot.width=10, repr.plot.height=5,repr.plot.res = 300) # image␣
 ↪resolution in dpi
#windows(width=10,height=5,pointsize=12) # empty window of correct size
```

[4]:
```
par(mfrow=c(1,2))                    # split screen for two graphs
#par(mar=c(4,4,1,1))                 # outer margins for each of the graphs
par(pty = "s")                       # forces the individual plots to be square

# Plot 1
plot(sazava[,"Sr"],sazava[,"Rb"],xlim=c(0,1000),ylim=c(0,1000),xlab="Sr",
     ylab="Rb",pch=16,col="blue",cex=1.5,xaxs="i",yaxs="i",log="")
ee <- sapply(c(seq(0.1,1,0.1),2:10),function(i)abline(0,i,lty="dashed"))

# Plot 2
plot(sazava[,"Sr"],sazava[,"Rb"],xlim=c(1,1000),ylim=c(1,1000),xlab="Sr",
     ylab="Rb",pch=16,col="blue",cex=1.5,xaxs="i",yaxs="i",log="xy")
ee <- sapply(c(seq(0.1,1,0.1),2:10),function(i)abline(log10(i),1,lty="dashed"))
```





1.2 Harker plots and closure effect

One of the most useful, most commonly employed and at the same time most questioned graphs in igneous geochemistry are the Harker plots, i.e. binary plots of silica versus major-element oxides (Harker 1909). These are simply binary diagrams of SiO2 (showing the progressive evolution of the given magmatic suite, i.e. serving as a differentiation index) vs. oxides of other major elements.

Warning: geochemical jargon ahead!

Numerous workers have argued that much of correlation observed in binary plots involving silica is spurious, due to the constant sum effect (e.g., Chayes 1960; Skala 1979; Rock 1988; Rollinson 1992, 1993). This effect arises from the fact that major elements sum up to 100 % and thus, if one oxide increases in abundance, all others must decrease. Therefore, everything must be anti-correlated with silica. In any binary diagram (especially using SiO2 which is the most abundant component), this results in formation of a “Forbidden zone”, into which no analyses could plot.

One solution to this problem has been proposed by Bonin (1986) who introduced the SiO2 vs. oxide* plots, where oxide* represents the proportion of the relevant oxide in the non-silica portion of the rock (in wt. %)

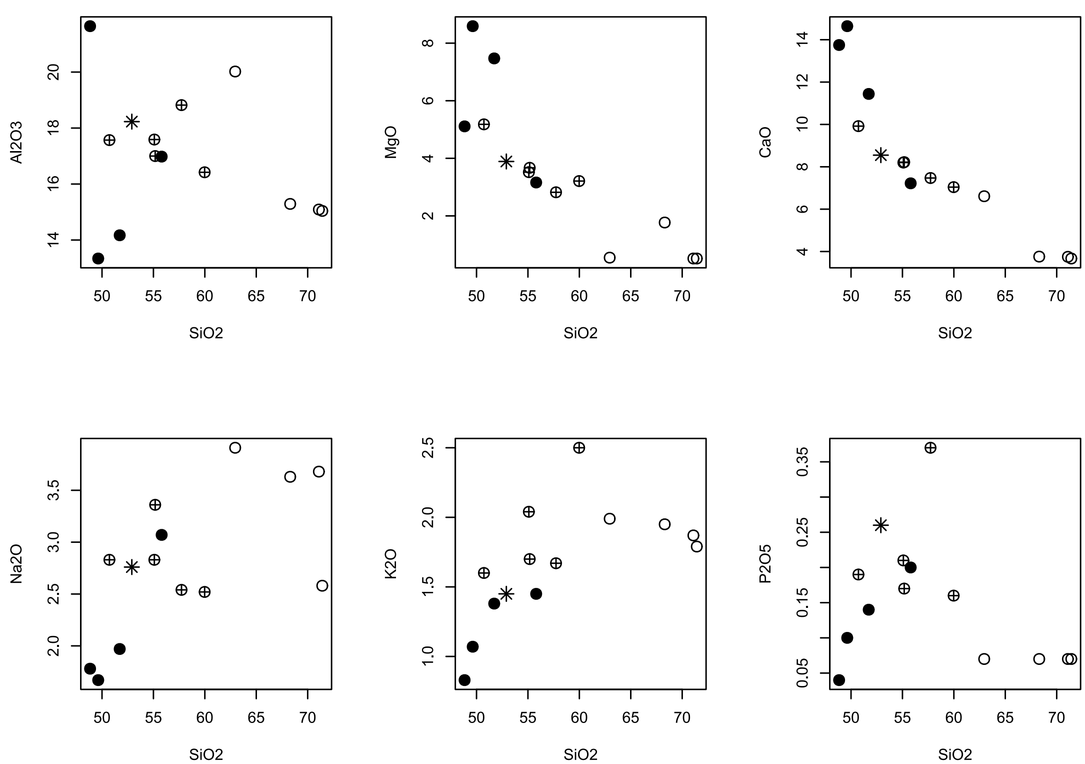
*Derivation of an oxide** diagram for the Sázava dataset. **a** Alumina plotted in wt. %. Note the “Forbidden zone”, approached by the trend as differentiation progresses, meaning that Al2O3 becomes an increasingly important part of the “non-silica” portion of the rock. This is underlined by the sharp increase in Al2O3 (**b**).

Another classic numerical remedy to the constant-sum problem are log-ratio transformations (Aitchison 1986). See Reimann et al. (2008) for details.

Using a loop and function `par(mfrow)`, write a short program that would plot six binary plots of SiO2 vs. major-element oxides of your choice.

[5]:
```
options(repr.plot.width=8, repr.plot.height=6,repr.plot.res = 300)
#windows(width=8,height=6,pointsize=12)
```

[6]:
```
sazava <- read.table("data/sazava.data",sep="\t")
par(mfrow=c(2,3))          # Split screen for 6 graphs
ee <- c("Al2O3","MgO","CaO","Na2O","K2O","P2O5")
for(f in ee){
    par(pty = "s")
    plot(sazava[,"SiO2"],sazava[,f],xlab="SiO2",ylab=f,
         pch=sazava[,"Symbol"],cex=1.5)
}
```

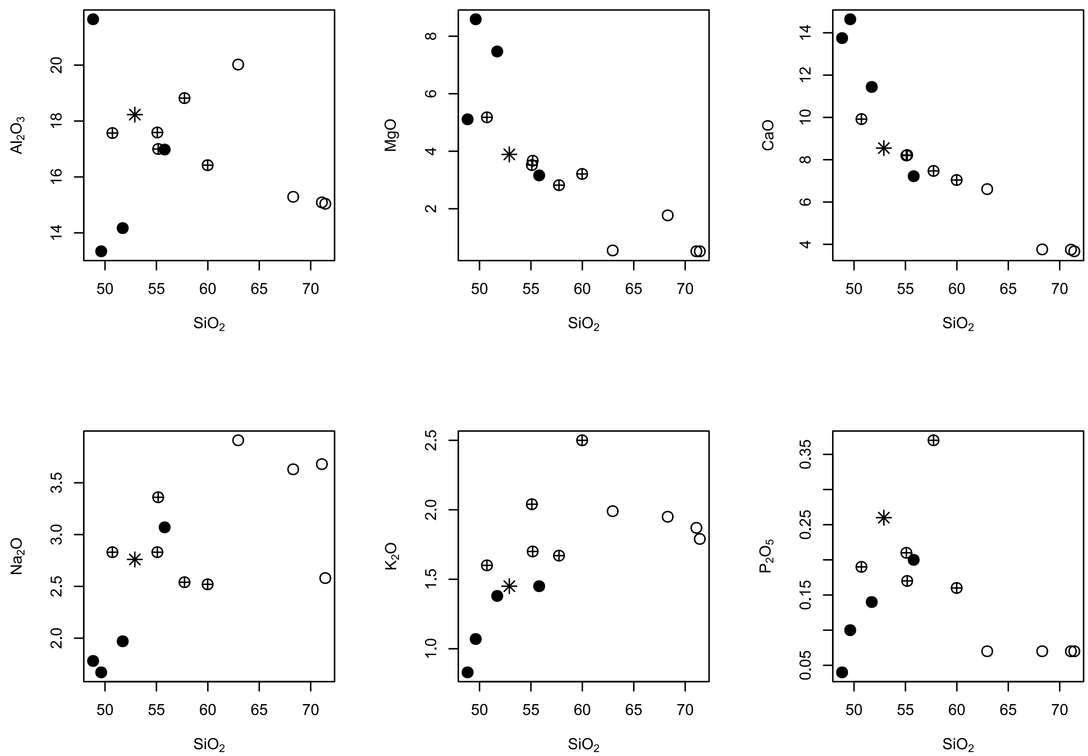


[7]:
```
options(repr.plot.width=8, repr.plot.height=6,repr.plot.res = 300)
#windows(width=10,height=6,pointsize=12)
```

[8]:
```
# Fancier version
sazava <- read.table("data/sazava.data",sep="\t")

par(mfrow=c(2,3))          # Split screen for 6 graphs
ee <- c("Al2O3","MgO","CaO","Na2O","K2O","P2O5")
lab <- c("Al[2]*O[3]","MgO","CaO","Na[2]*O","K[2]*O","P[2]*O[5]")
```

```
for(f in 1:length(ee)){
    par(pty = "s")
    plot(sazava[,"SiO2"],sazava[,ee[f]],xlab=expression(SiO[2]),
         ylab=parse(text=as.expression(lab[f])),
         pch=sazava[,"Symbol"],cex=1.5)
}
```



1.3 Spiderplots

Geochemists often like to express the compositional differences between the studied sample and given geochemical reservoir in the form of the so-called spiderplots (also known as spiderdiagrams/spidergrams or (better) multi-element diagrams). Spiderplots allow representing much of the sample's composition on a single graph. Technically these are logarithmic plots of elemental concentrations (allowing comparison of several orders of magnitude different concentrations) in the sample divided (normalized) by those in the selected standard. The most common spiderdiagrams are chondrite-normalized REE plots.

The added value of spiderplots consists in elimination of the Oddo-Harkins effect: in the Solar System, the abundances of even-numbered elements are greater than those of neighbouring odd-numbered ones. Moreover, abundances generally decrease with increasing atomic number. Non-normalized data thus show zigzag, slightly sloped patterns. Normalized patterns (spiderplots) smooth out such differences. *Illustration of the Oddo-Harkins effect. Non-normalized patterns (ppm) for average chondrite meteorites (Boynton 1984) and the Požáry trondhjemite Po-1 from the Sázava dataset (**a**–**b**). **c** – Normalization to a common reference (chondrites in this case) compensates for this effect and allows focusing on differences between individual terrestrial rocks.*

We shall write a function that will normalize REE concentrations in the sample by chondritic contents according to Boynton (1984). The normalizing data are stored in a comma-delimited file `boynton.data`. Then we will use it to calculate the normalized REE concentrations for analyses of the Sázava suite and display — using the functions `plot`, `axis`, `points` and `lines` – spiderdiagrams for trondhjemites Po-1 and Po-4.

[9]:
```
options(repr.plot.width=5, repr.plot.height=4.5, repr.plot.res = 300)
```

[10]:
```
sazava <- read.table("data/sazava.data",sep="\t")

x <- read.table("data/boynton.data",sep=",")
chondrite <- as.numeric(x)          # conversion to numeric vector
names(chondrite) <- names(x)
print(chondrite)
```

```
    La     Ce     Pr     Nd     Sm     Eu     Gd     Tb     Dy     Ho     Er
0.3100 0.8080 0.1220 0.6000 0.1950 0.0735 0.2590 0.0474 0.3220 0.0718 0.2100
    Tm     Yb     Lu
0.0324 0.2090 0.0322
```

[11]:
```
# Normalizing the values in x by some standard chon
# NB the transposition needed as the operations take place along columns in R
norm <- function(x,chon){           # normalizing function
    z <- t(x[,names(chon)])/chon
    return(z)
}

y <- norm(sazava,chondrite)         # normalized values
print(y)
```

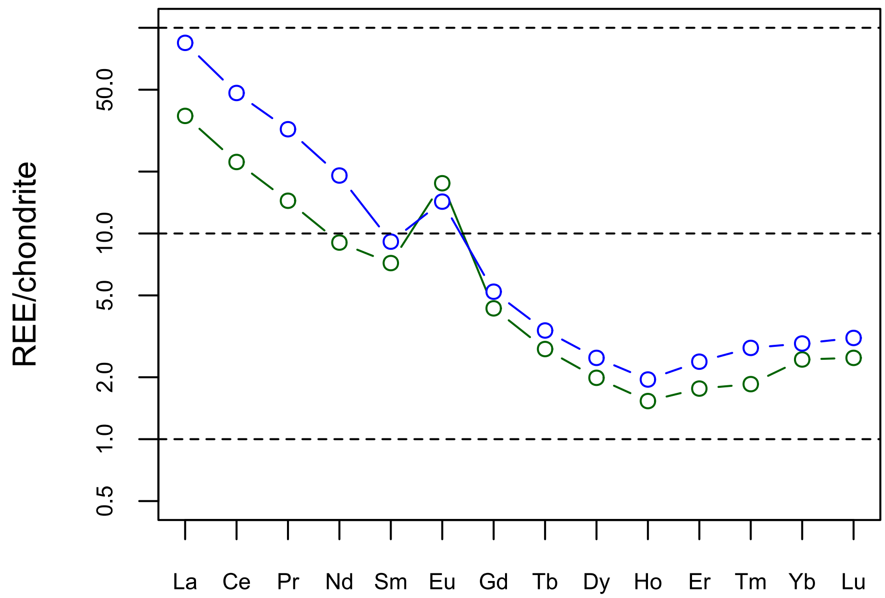
```
   Sa-1 Sa-2 Sa-3      Sa-4      Sa-7 SaD-1 Gbs-1 Gbs-20 Gbs-2 Gbs-3      Po-1
La   NA   NA   NA 69.90323 66.967742    NA    NA     NA    NA    NA 37.290323
Ce   NA   NA   NA 88.83663 52.004950    NA    NA     NA    NA    NA 22.264851
Pr   NA   NA   NA 56.88525 40.655738    NA    NA     NA    NA    NA 14.426230
Nd   NA   NA   NA 49.51667 29.066667    NA    NA     NA    NA    NA  9.033333
Sm   NA   NA   NA 32.00000 19.282051    NA    NA     NA    NA    NA  7.179487
Eu   NA   NA   NA 20.40816 24.081633    NA    NA     NA    NA    NA 17.551020
Gd   NA   NA   NA 23.51351 14.517375    NA    NA     NA    NA    NA  4.324324
Tb   NA   NA   NA 19.40928 11.814346    NA    NA     NA    NA    NA  2.742616
Dy   NA   NA   NA 18.01242  8.385093    NA    NA     NA    NA    NA  1.987578
Ho   NA   NA   NA 14.34540  7.799443    NA    NA     NA    NA    NA  1.532033
Er   NA   NA   NA 13.33333  7.809524    NA    NA     NA    NA    NA  1.761905
Tm   NA   NA   NA 13.27160  7.407407    NA    NA     NA    NA    NA  1.851852
```

```
Yb   NA   NA   NA 13.77990  7.272727    NA     NA      NA     NA     NA  2.440191
Lu   NA   NA   NA 13.35404  7.763975    NA     NA      NA     NA     NA  2.484472
   Po-3       Po-4 Po-5
La   NA 84.483871   NA
Ce   NA 48.205446   NA
Pr   NA 32.131148   NA
Nd   NA 19.133333   NA
Sm   NA  9.128205   NA
Eu   NA 14.285714   NA
Gd   NA  5.212355   NA
Tb   NA  3.375527   NA
Dy   NA  2.484472   NA
Ho   NA  1.949861   NA
Er   NA  2.380952   NA
Tm   NA  2.777778   NA
Yb   NA  2.918660   NA
Lu   NA  3.105590   NA
```

[12]:

```
plot(y[,"Po-1"],type="b",log="y",axes=FALSE,xlab="",ylab="REE/chondrite",
     ylim=c(0.5,100),col="darkgreen")
axis(1,1:length(chondrite),labels=names(chondrite),cex.axis=0.7)
axis(2,cex.axis=0.7)

points(y[,"Po-4"],col="blue",type="b")
abline(h=(10^(-1:2)),lty="dashed")   # grid
box()                                # bounding box
```



1.4 Ternary plots

Ternary plots rank among important and widely used geochemical tools. Setting the sides of the triangle to equating a unity, its vertices (bottom-left, top, and bottom-right) have `[x,y]` coordinates of `A[0,0]`, `B[0.5,sqrt(3)/2]` and `C[1,0]`.

The ternary coordinates `[a,b,c]` of a data point `X` can be transformed to binary ones `[x,y]` as follows:

$x = 1 - a - \frac{b}{2}$ and $y = \frac{\sqrt{3}}{2}b$.

We can now use standard R functions for binary plot; the trick is that (binary) axes are not shown and triangle outline is drawn using `lines`.

First, we design a function plotting ternary diagrams and then will employ it to display a Ba–Rb–Sr ternary plot for the Sázava suite.

[13]:
```
options(repr.plot.width=5,repr.plot.height=5, repr.plot.res = 300)
```

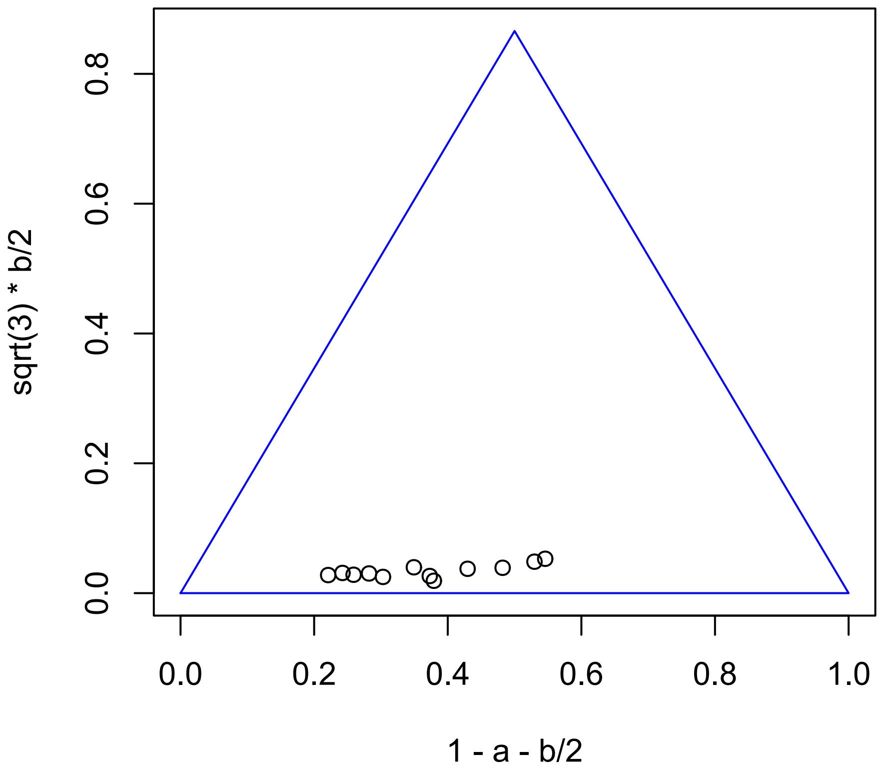
[14]:
```
# Let's read the data and renormalize the Ba, Rb and Sr columns to 1
sazava <- read.table("data/sazava.data",sep="\t")
sums <- apply(sazava[,c("Ba","Rb","Sr")],1,sum)
```

```
a <- sazava[,"Ba"]/sums
b <- sazava[,"Rb"]/sums
c <- 1-a-b
print(cbind(a,b,c))
```

```
               a          b         c
Sa-1   0.6277240 0.04600484 0.3262712
Sa-2   0.4953191 0.04510638 0.4595745
Sa-3          NA         NA        NA
Sa-4   0.4235808 0.06113537 0.5152838
Sa-7   0.5486322 0.04331307 0.4080547
SaD-1  0.6825503 0.02885906 0.2885906
Gbs-1  0.6098326 0.02196653 0.3682008
Gbs-20        NA         NA        NA
Gbs-2  0.4422383 0.05595668 0.5018051
Gbs-3  0.7003257 0.03501629 0.2646580
Po-1   0.6117085 0.03046595 0.3578256
Po-3   0.7396352 0.03593145 0.2244334
Po-4   0.7246050 0.03273138 0.2426637
Po-5   0.7629332 0.03214465 0.2049221
```

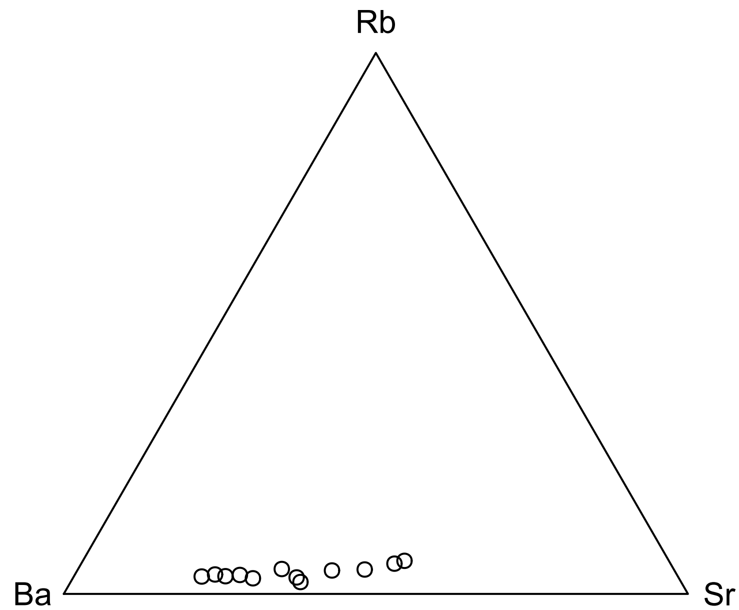
[15]:

```
# Plot the first, rough version within the x-y coordinates
plot(1-a-b/2,sqrt(3)*b/2,xlim=c(0,1),ylim=c(0,sqrt(3)/2))
x1 <- c(0,1,.5,0)
y1 <- c(0,0,sqrt(3)/2,0)
lines(x1,y1,col="blue")
```



[16]:
```
# Wrapping the final product as a user-defined function
# x = matrix with the data
# alab, ylab, clab = names of variables to be plotted
tri <- function(x,alab,blab,clab){
    sums <- apply(x[,c(alab,blab,clab)],1,sum)
    a <- x[,alab]/sums
    b <- x[,blab]/sums
    plot(1-a-b/2,sqrt(3)*b/2,xlab="",ylab="",
         xlim=c(0,1),ylim=c(0,0.9),axes=FALSE,asp=1)
    # axes=FALSE: no plotting of axes; asp: aspect ratio
    x1 <- c(0,1,.5,0)
    y1 <- c(0,0,sqrt(3)/2,0)
    lines(x1,y1)
    text(-0.05,0,alab)
    text(0.5,sqrt(3)/2+0.05,blab)
    text(1.05,0,clab)
}
```

```
tri(sazava,"Ba","Rb","Sr")
```



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Bonin B (1986) Ring Complexes and Anorogenic Magmatism. Elsevier, Amsterdam

Boynton WV (1984) Cosmochemistry of the rare earth elements: meteorite studies. In: Henderson P (eds) Rare Earth Element Geochemistry. Elsevier, Amsterdam, pp 63–114

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Harker A (1909) The natural history of igneous rocks. Methuen & Co., London

Reimann C, Filzmoser P, Garrett R, Dutter R (2008) Statistical Data Analysis Explained: Applied Environmental Statistics with R. John Wiley & Sons, Chichester

Rock NMS (1988) Numerical geology. A source guide, glossary and selective bibliography to geological uses of computers and statistics. Lecture Notes in Earth Sciences, vol 18. Springer, Berlin

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Skala W (1979) Some effects of the constant-sum problem in geochemistry. Chem Geol 27:1–9