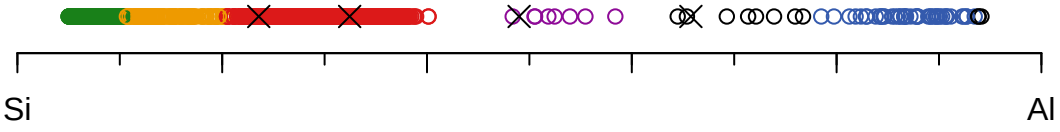
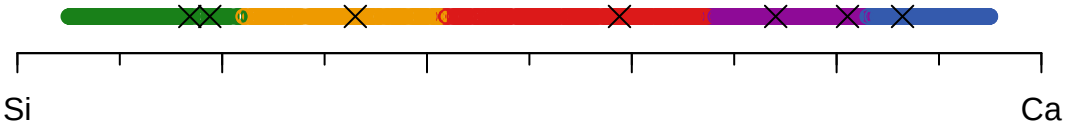
Code for subclasses

× reference concentration
○ subclass 0 (unknown)
○ subclass 1
○ subclass 2
○ subclass 3
○ subclass 4
○ subclass 5
○ subclass 6
○ subclass 7
○ subclass 8
○ subclass 9
○ subclass 10
○ subclass 11
○ subclass 12
○ subclass 13
○ subclass 14

Si, Al

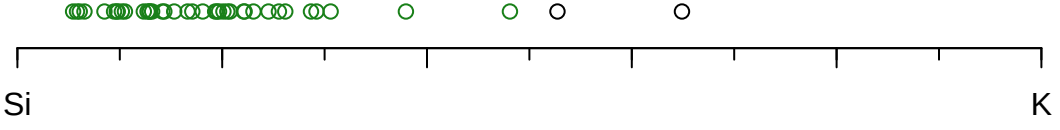


Si, Ca



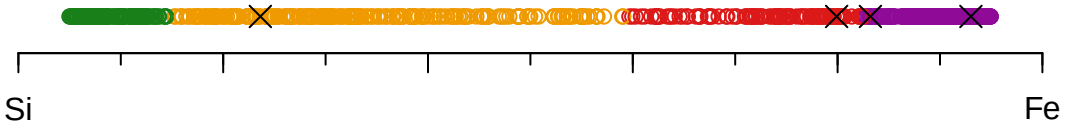
Si, Mg

Si, K



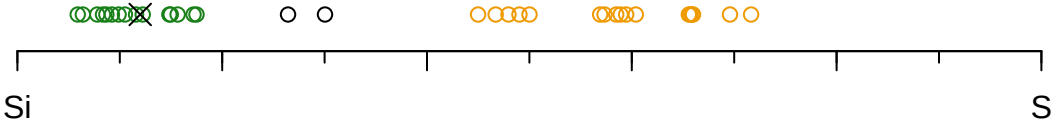
Si, Ti

Si, Fe

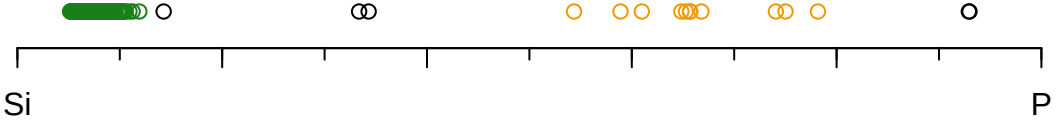


Si, Cl

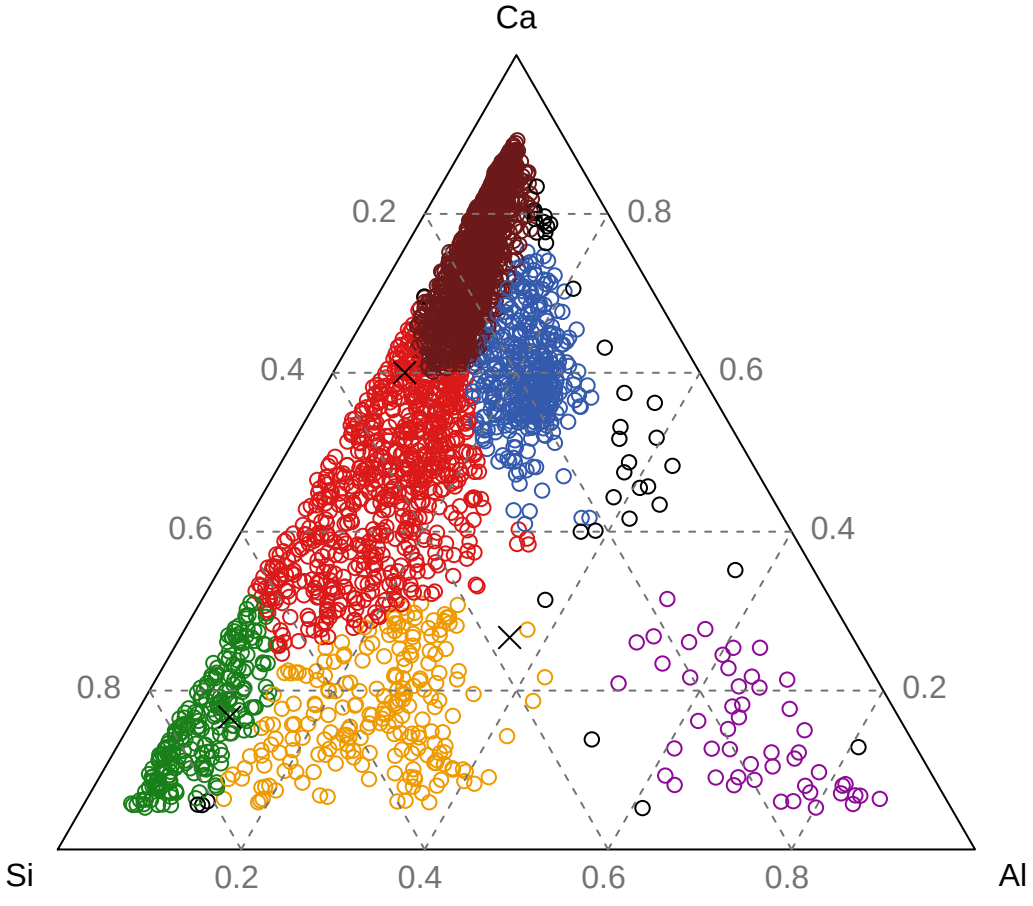
Si, S



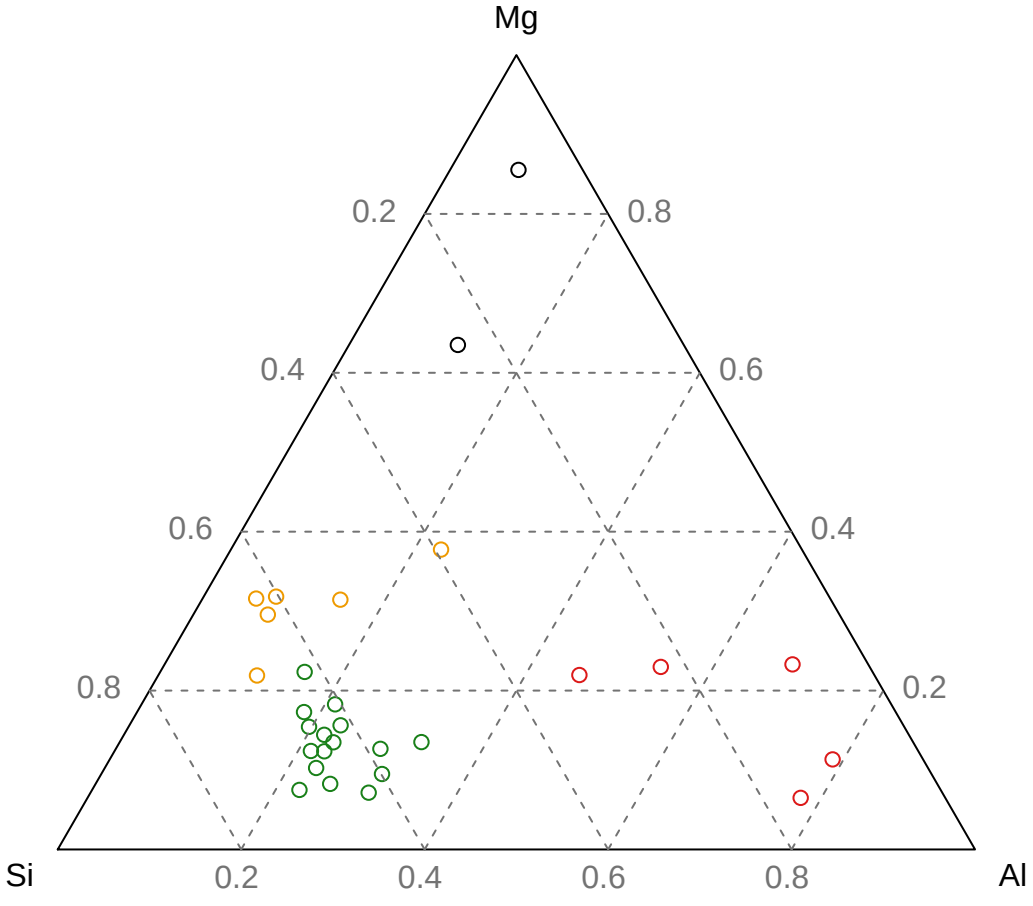
Si, P



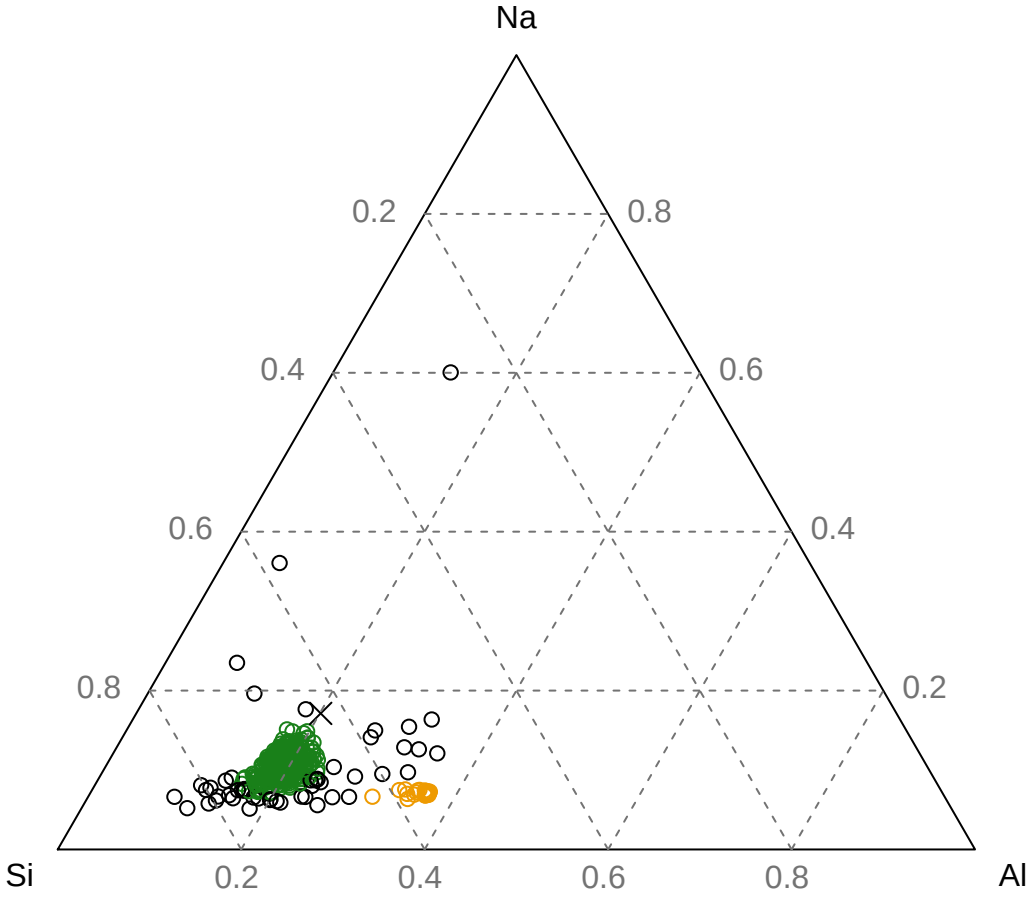
Si, Al, Ca



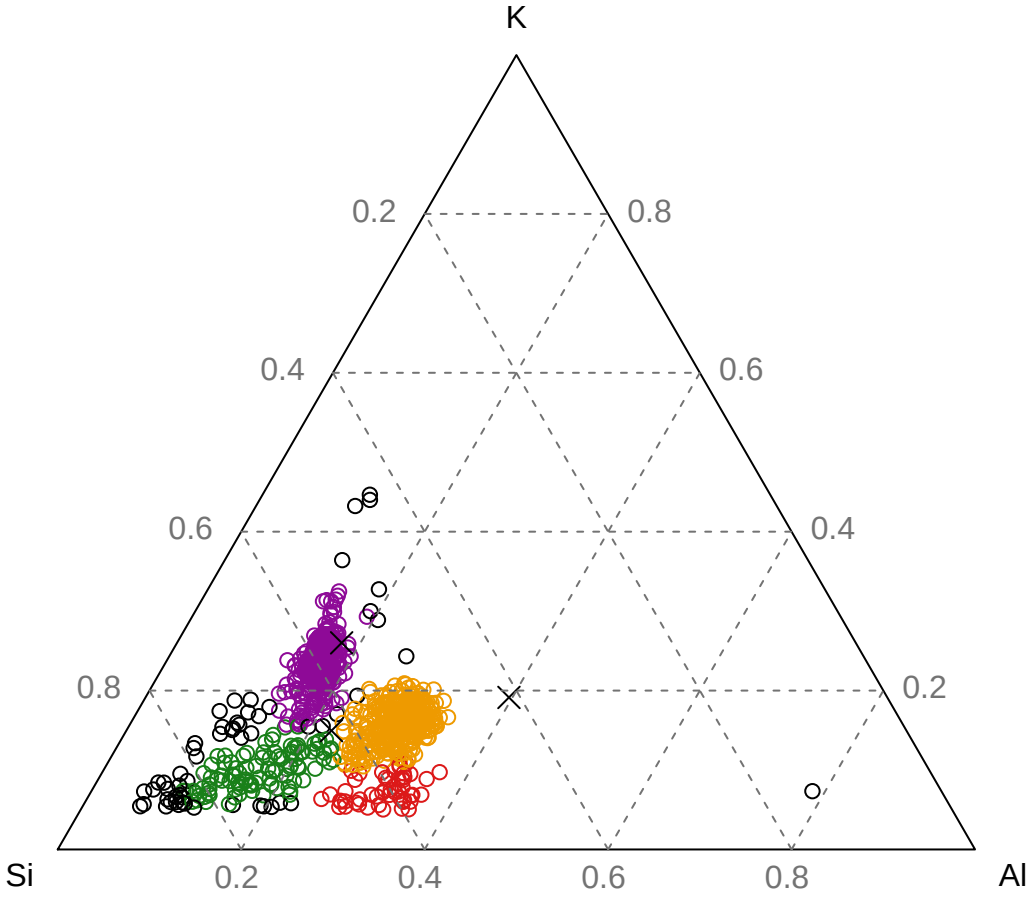
Si, Al, Mg



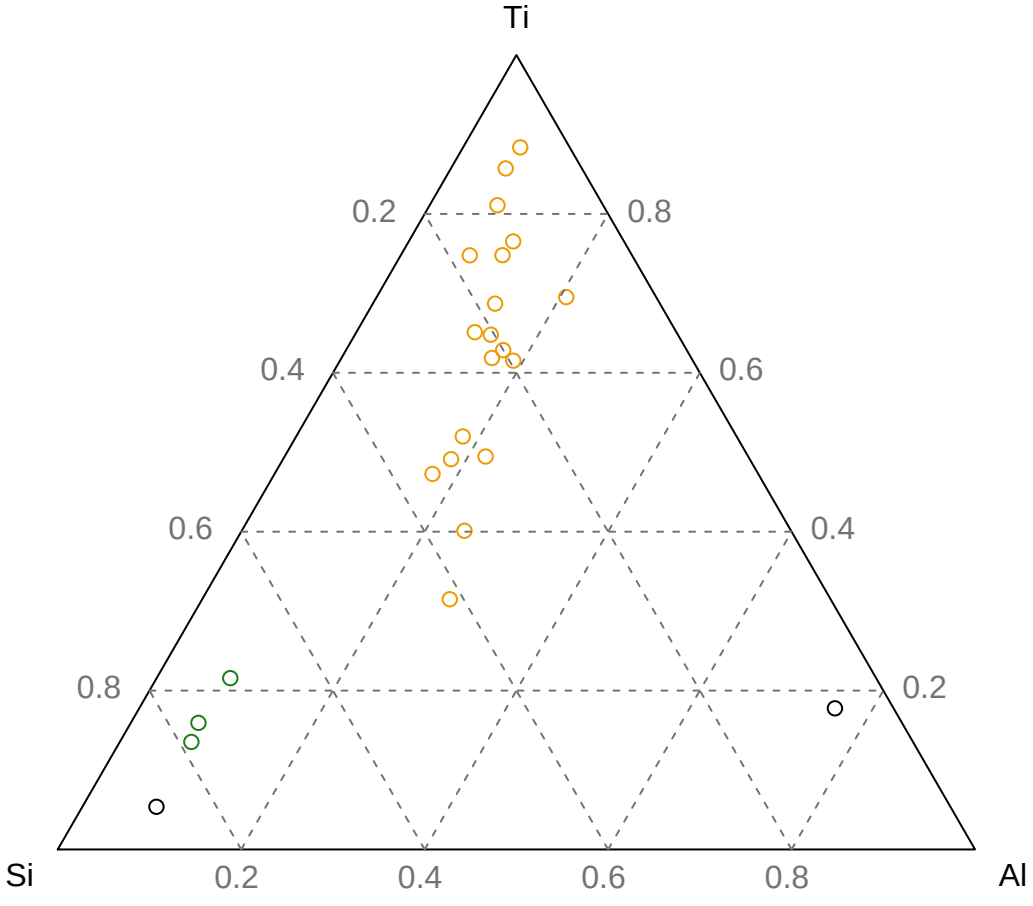
Si, Al, Na



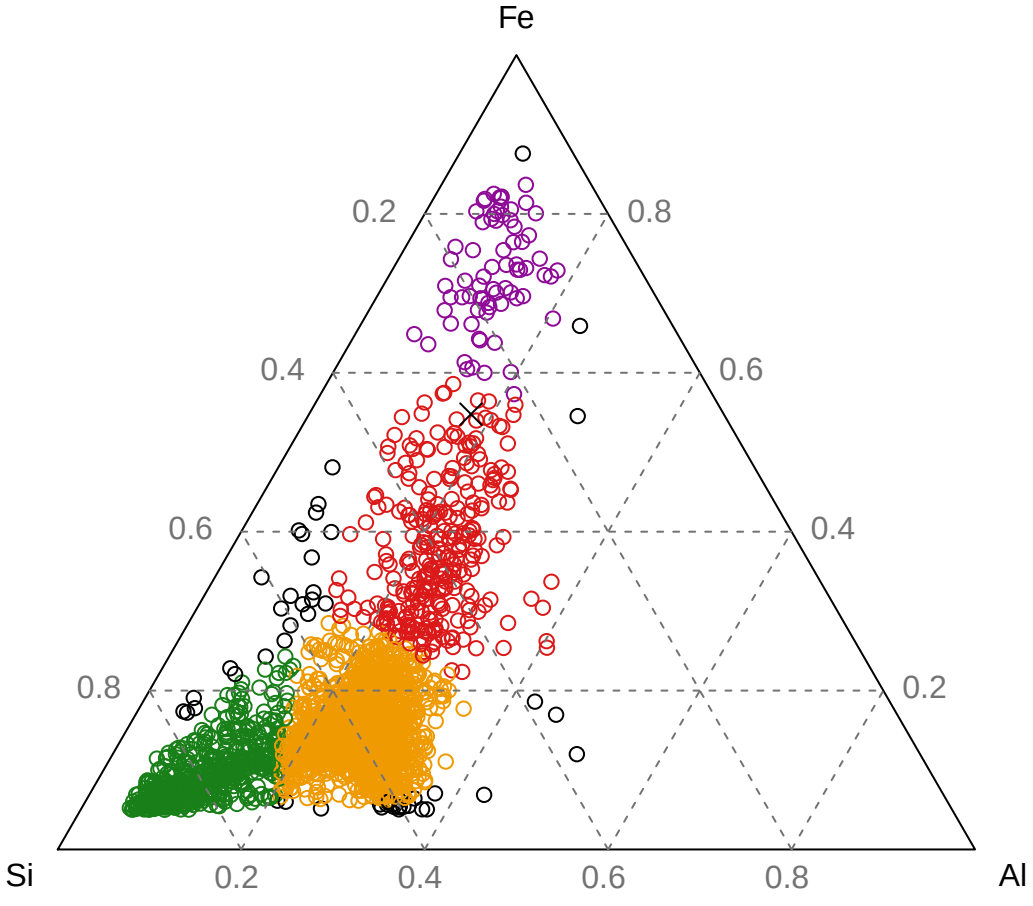
Si, Al, K



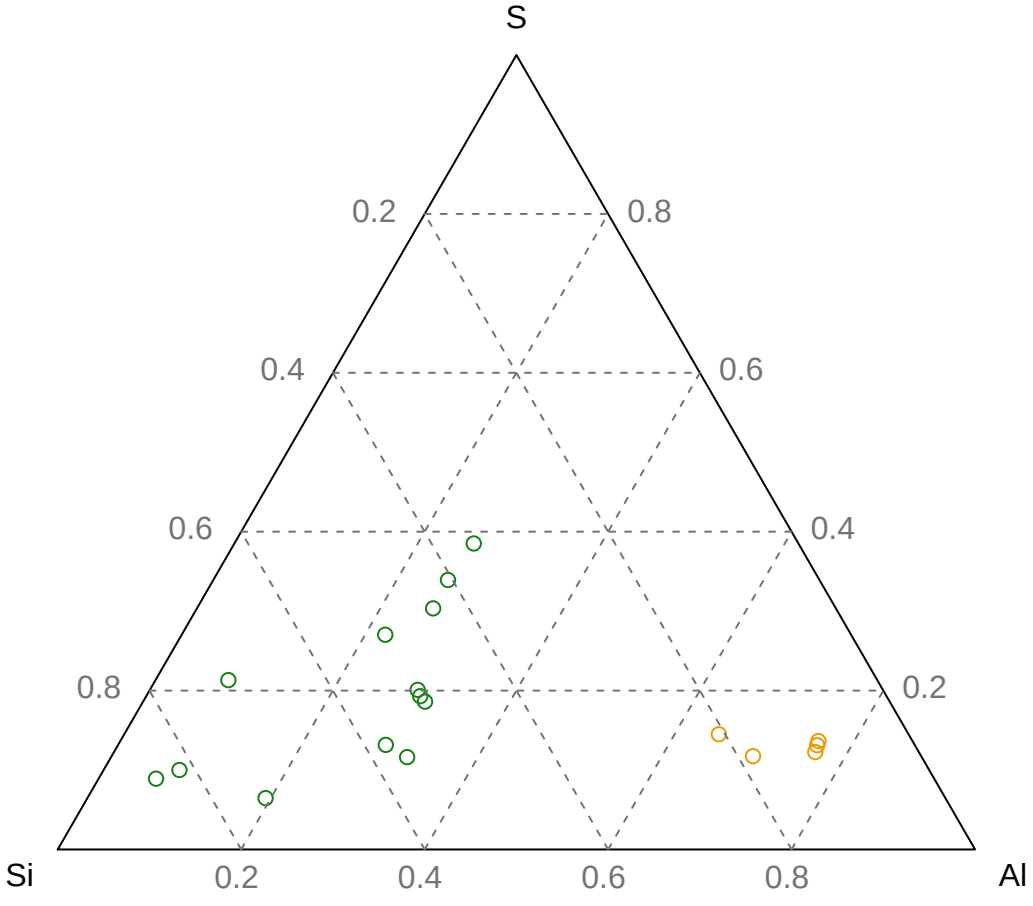
Si, Al, Ti



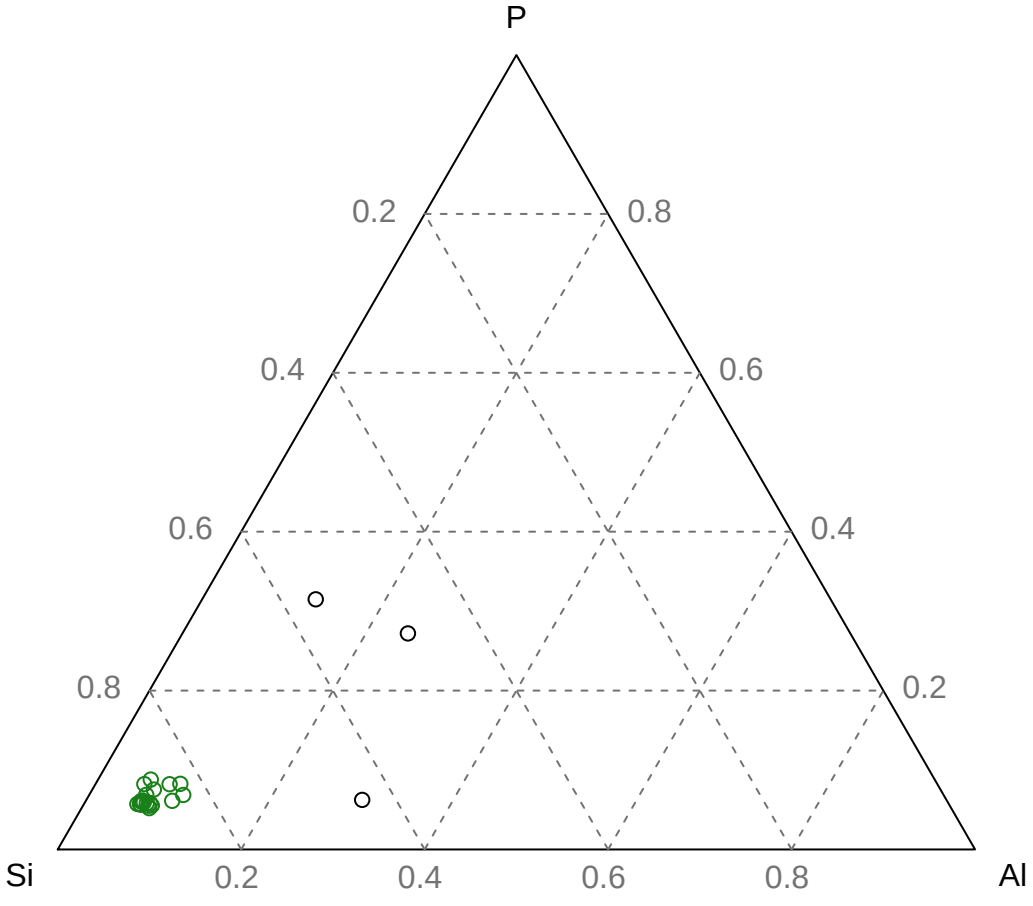
Si, Al, Fe

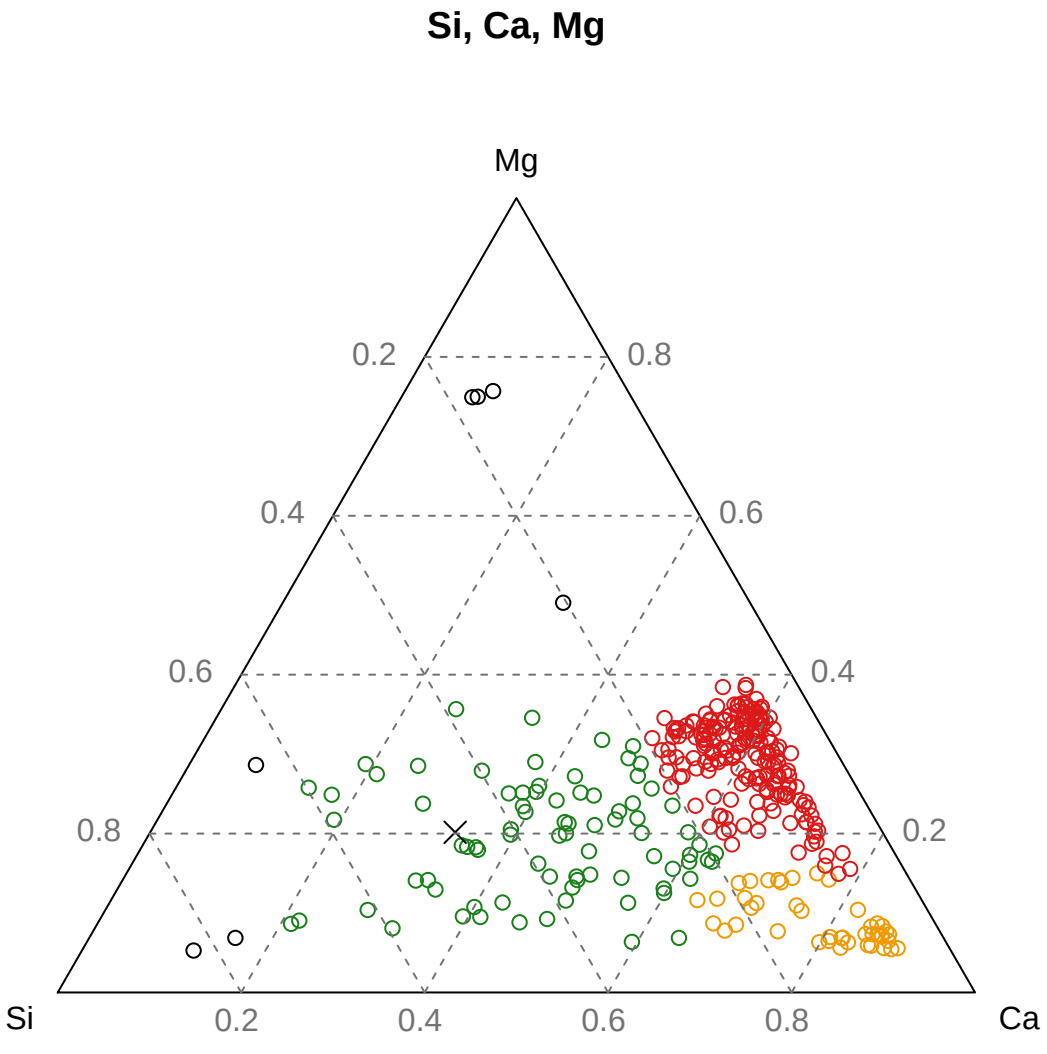


Si, Al, S



Si, Al, P




Si, Ca, Mg
Mg
Si
Ca
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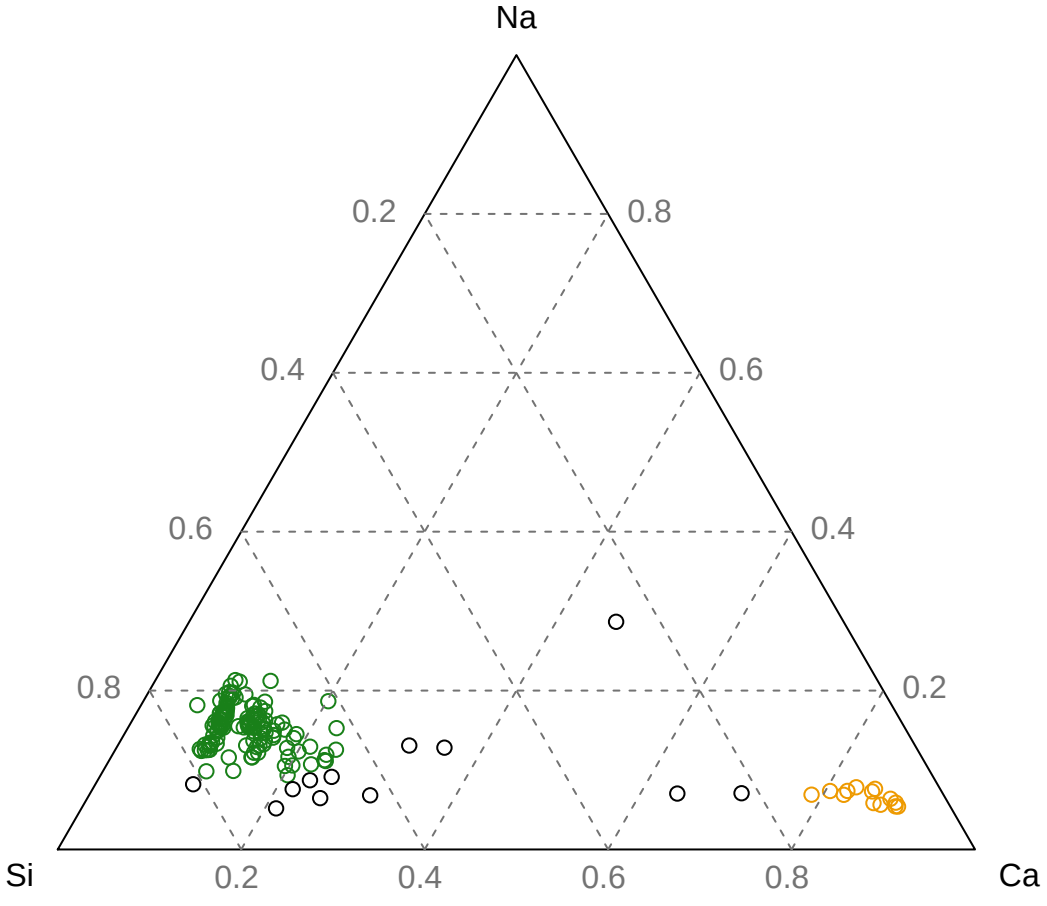
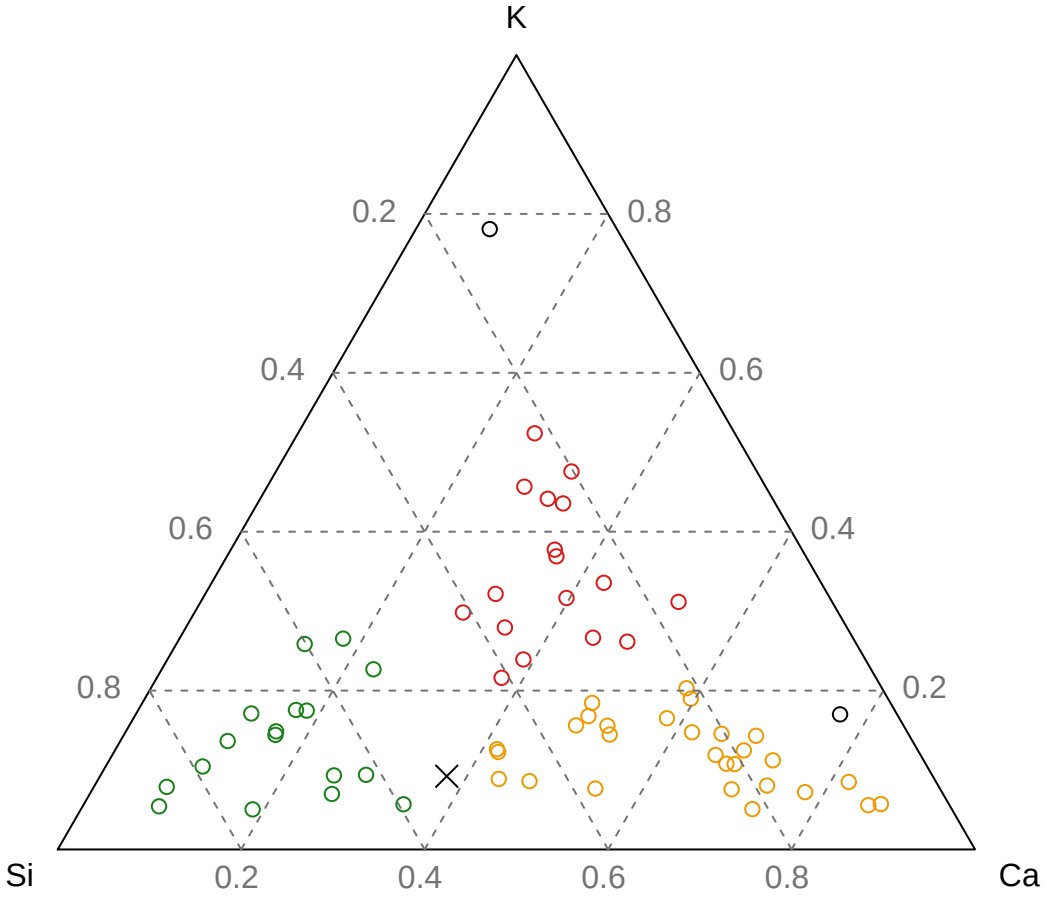
0.6
0.8
0.8
0.6
0.4
0.2
0.2
0.4
0.6
0.8

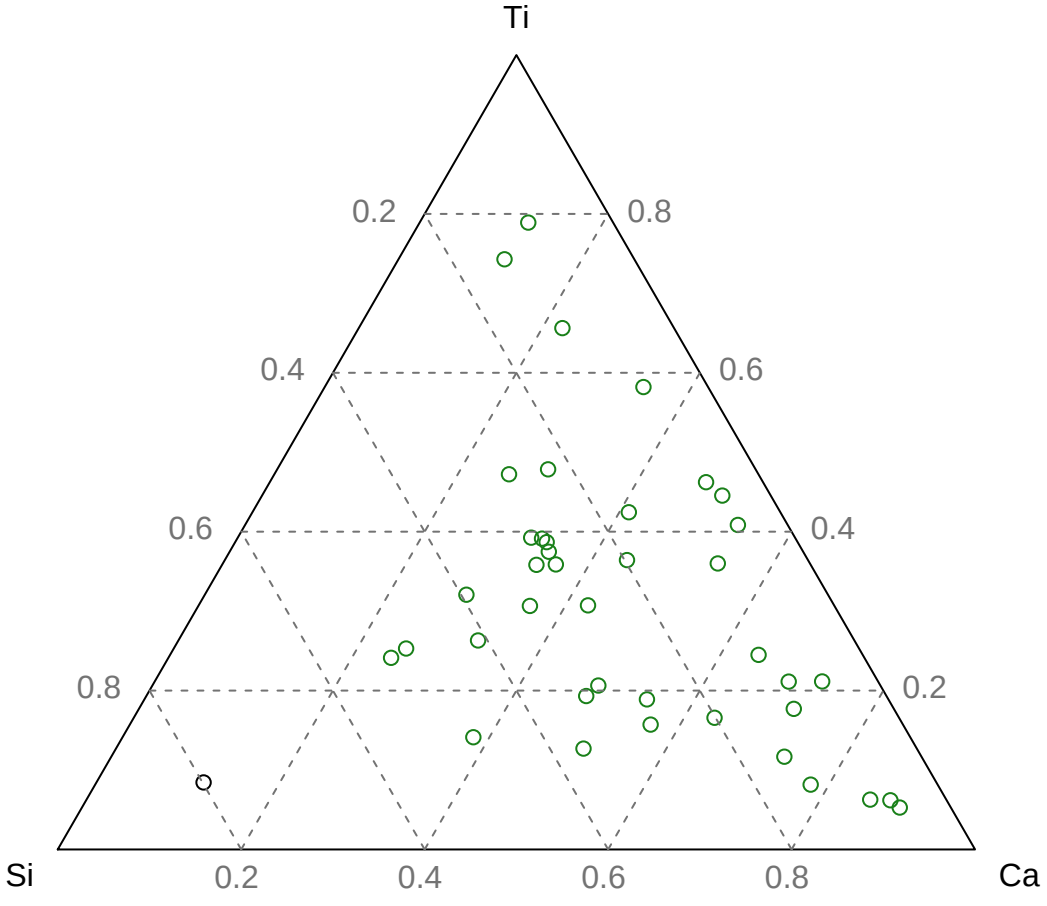
Si, Ca, Na



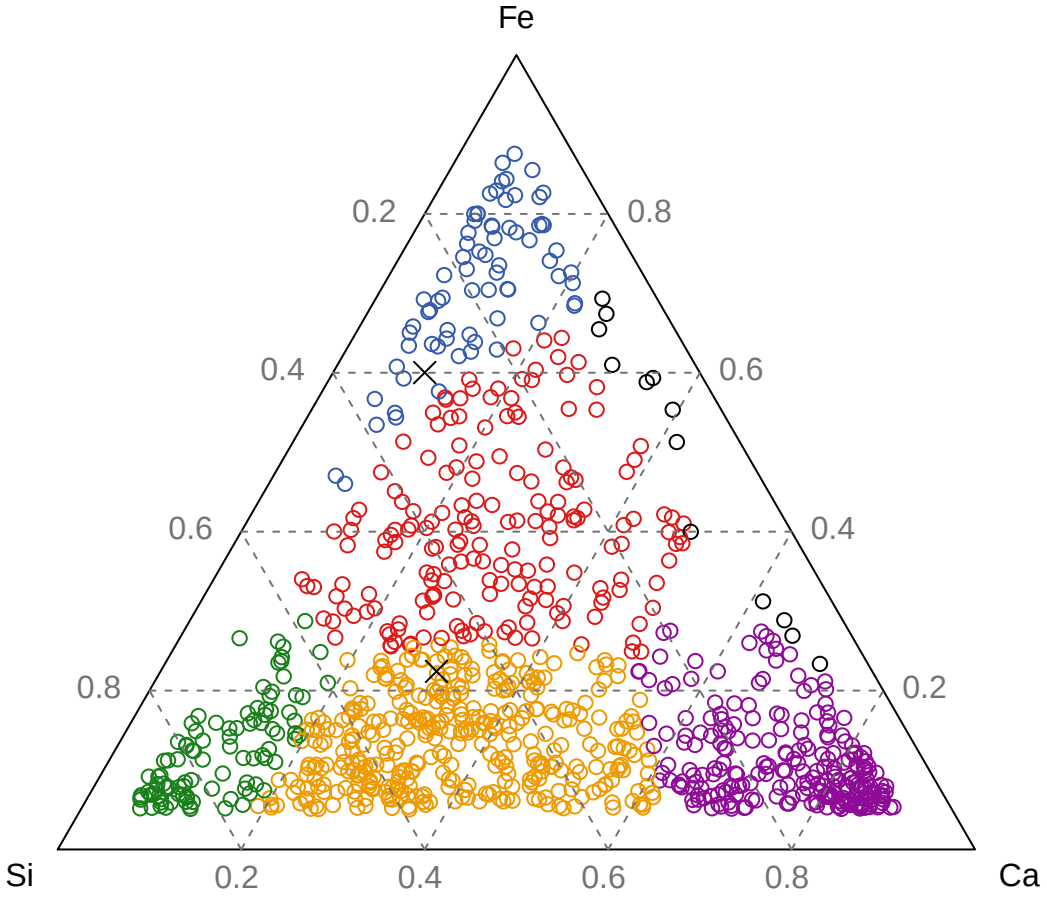
Si, Ca, K



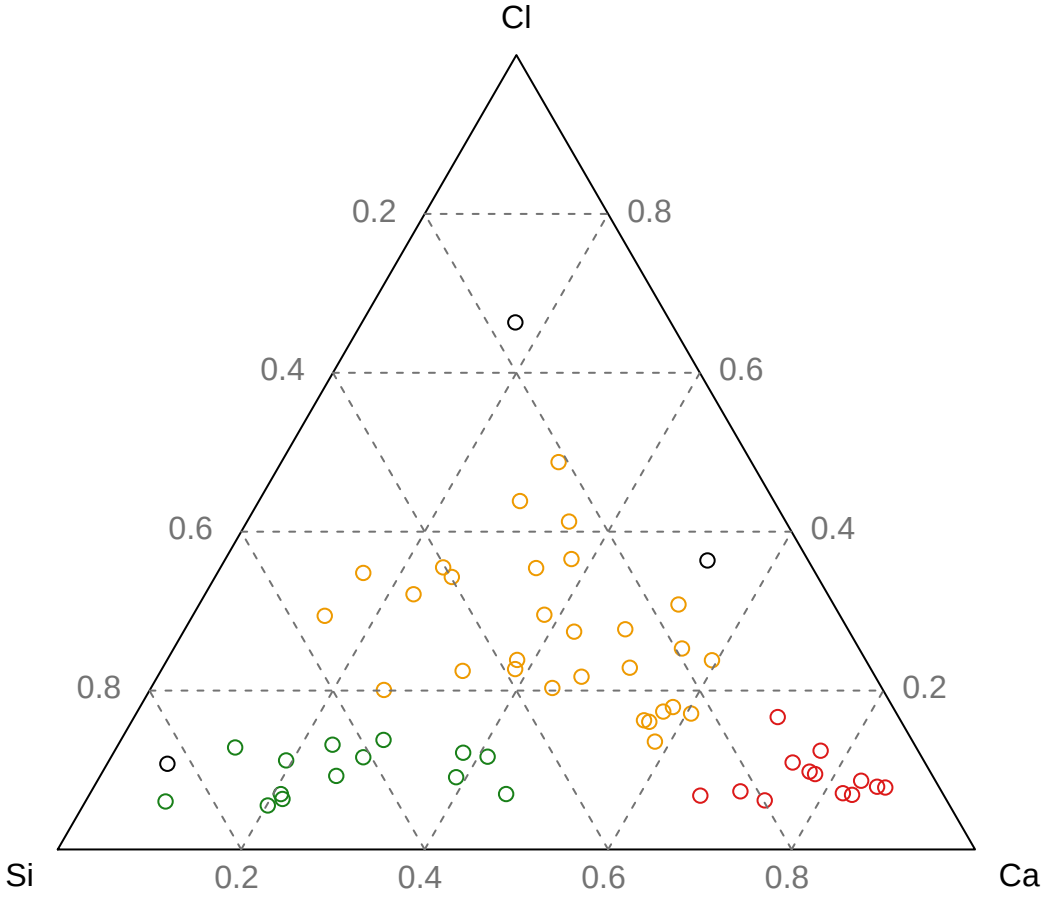
Si, Ca, Ti



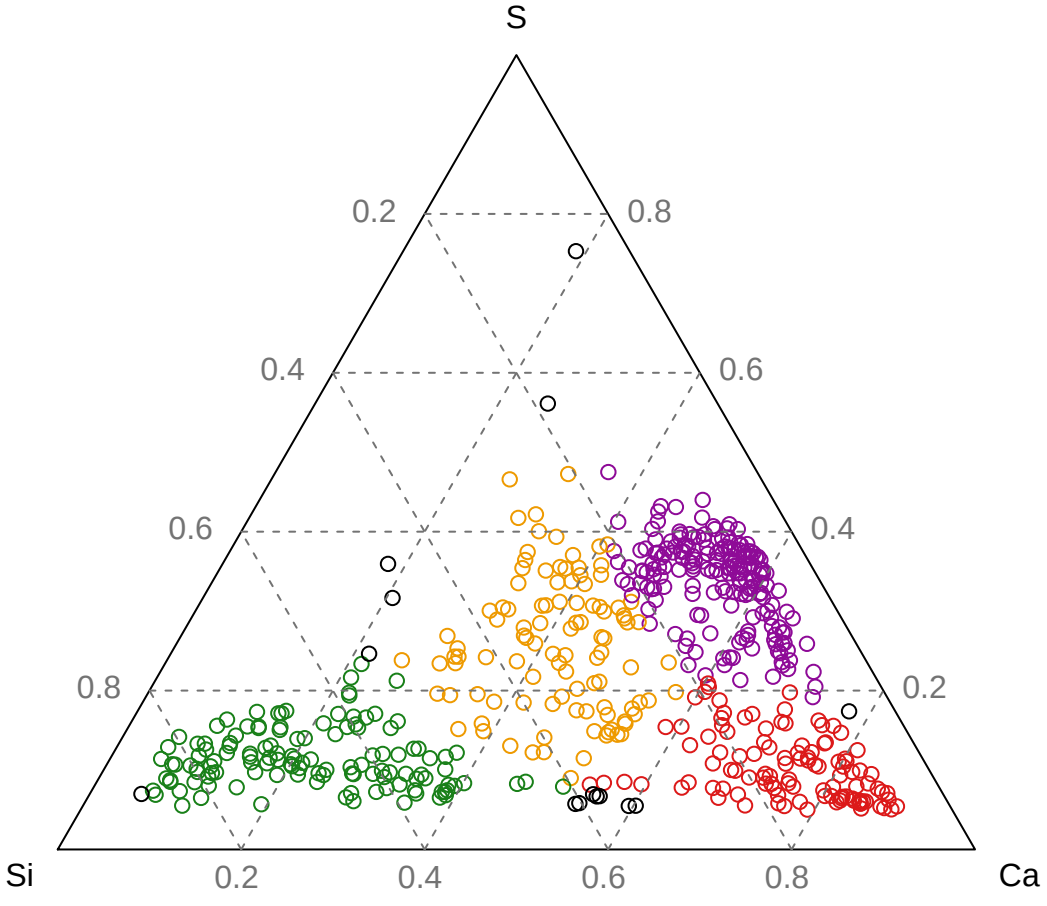
Si, Ca, Fe



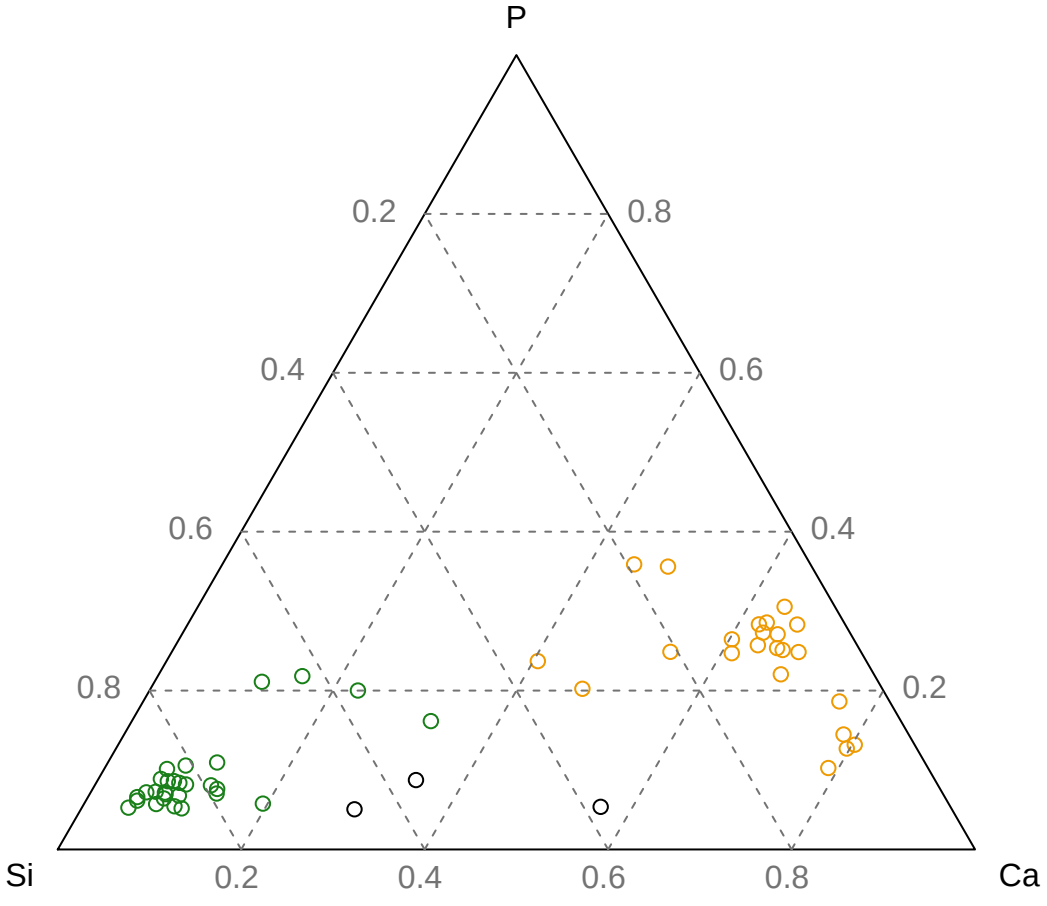
Si, Ca, Cl



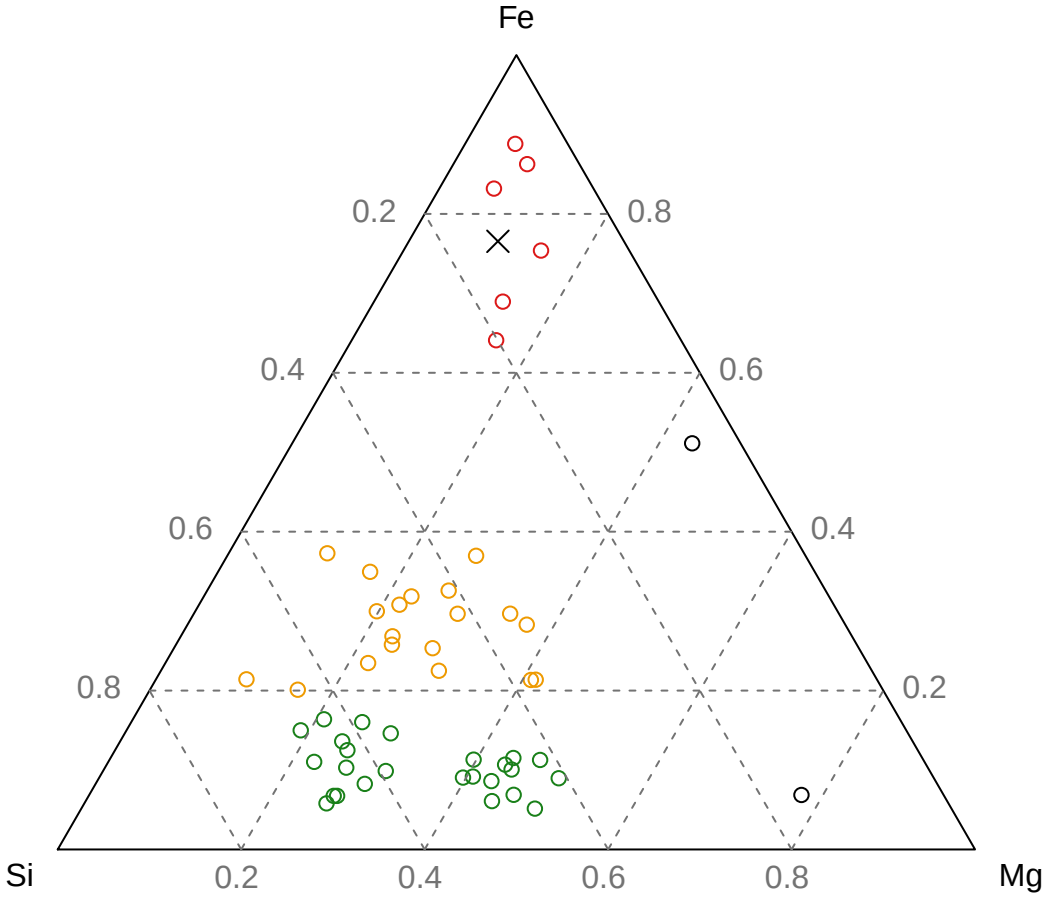
Si, Ca, S



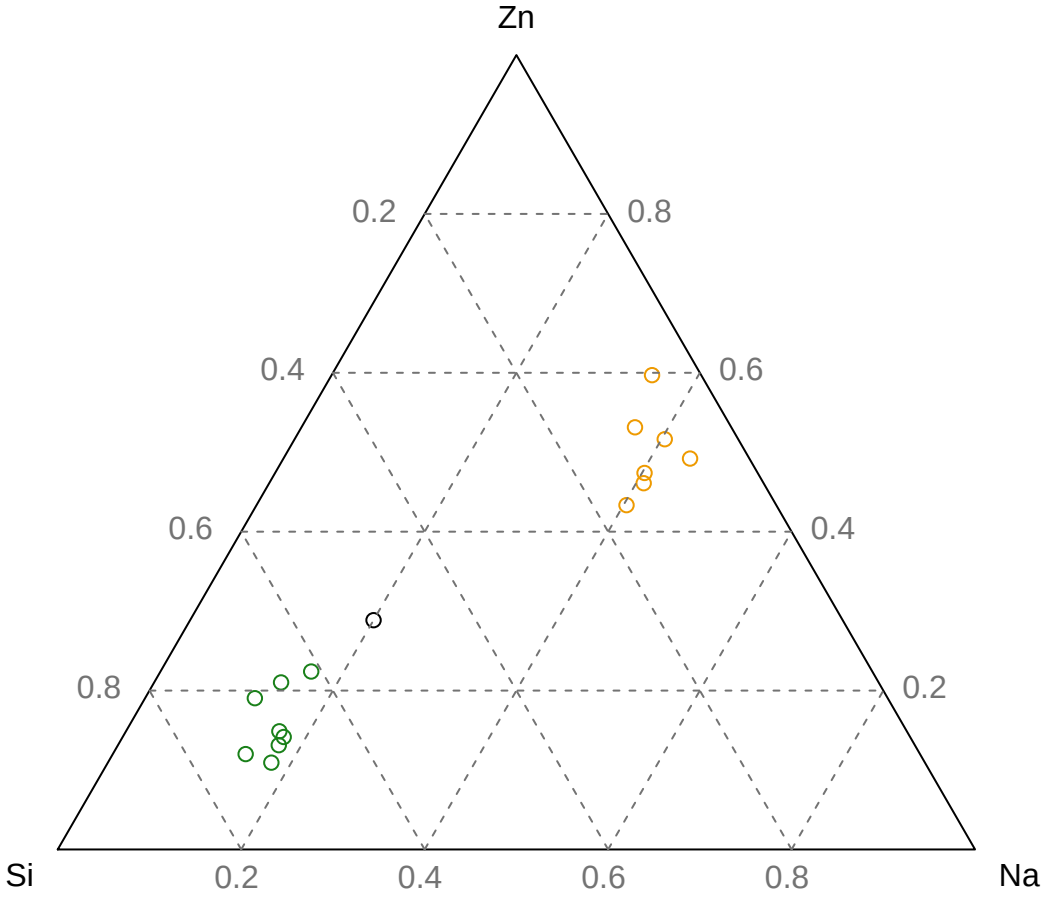
Si, Ca, P

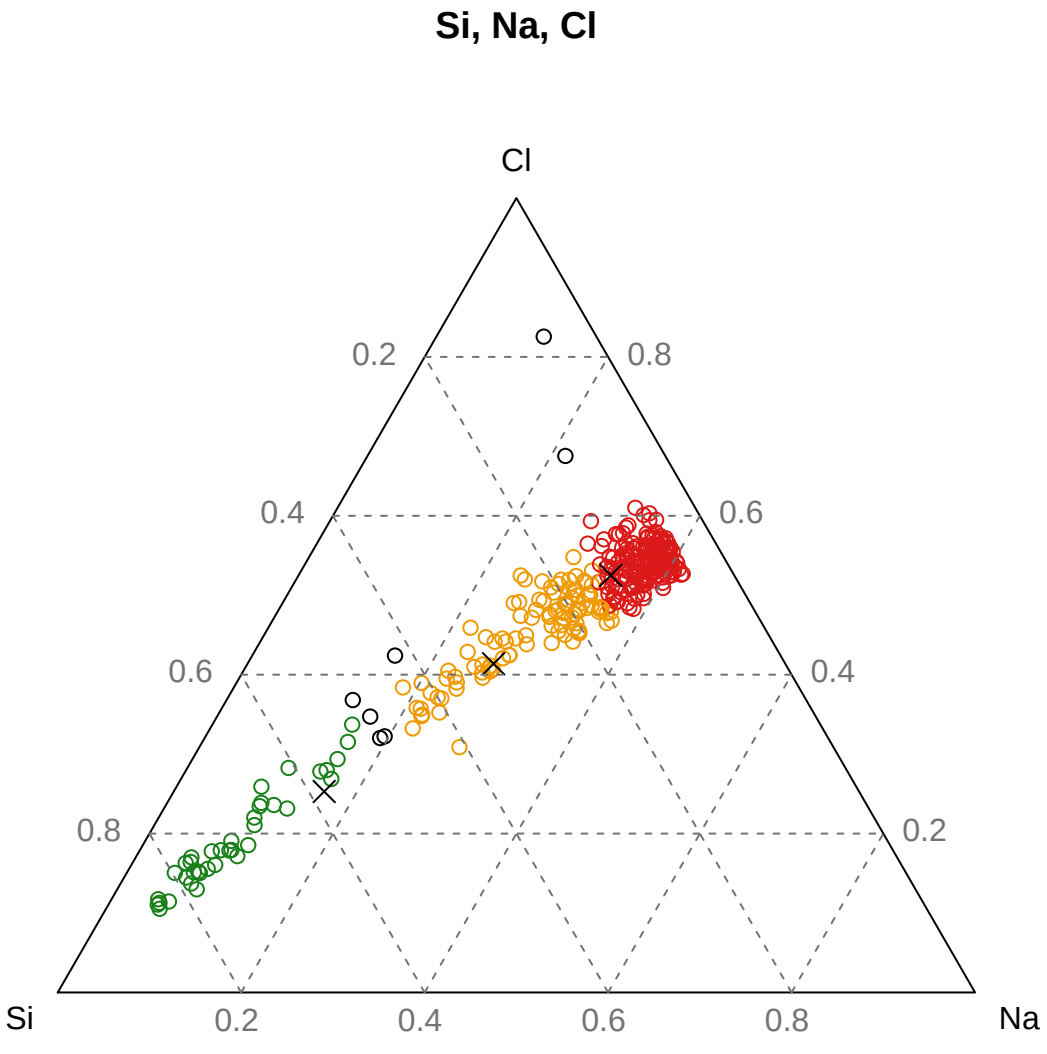


Si, Mg, Fe

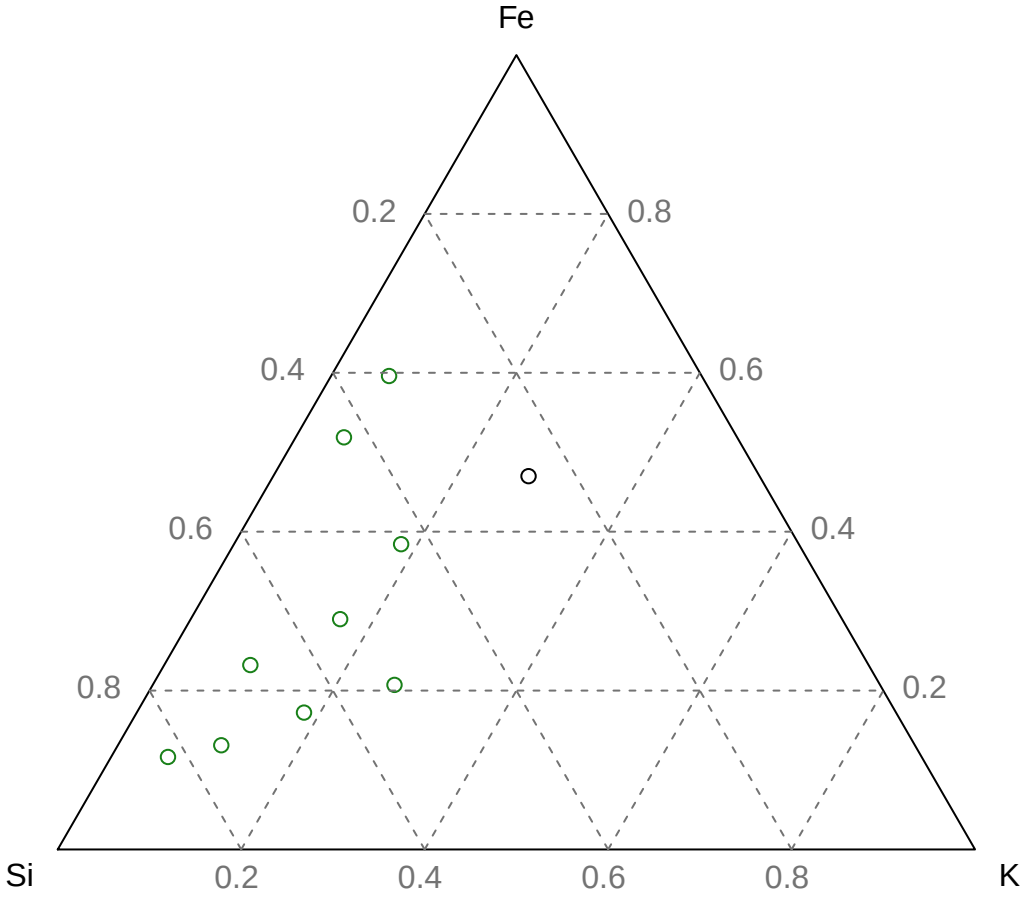


Si, Na, Zn

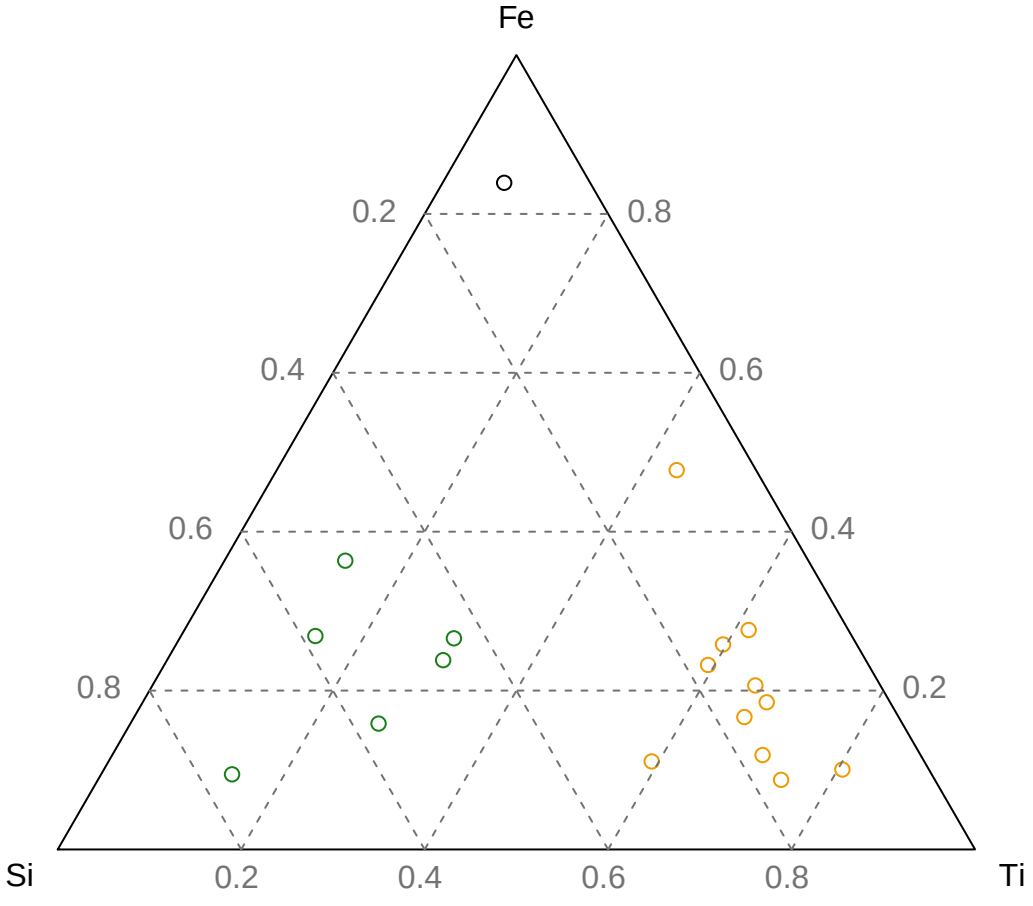



Si, Na, Cl
Cl
Si
Na
0.2
0.4
0.6
0.8
0.2
0.4
0.6
0.8
0.8
0.6
0.4
0.2

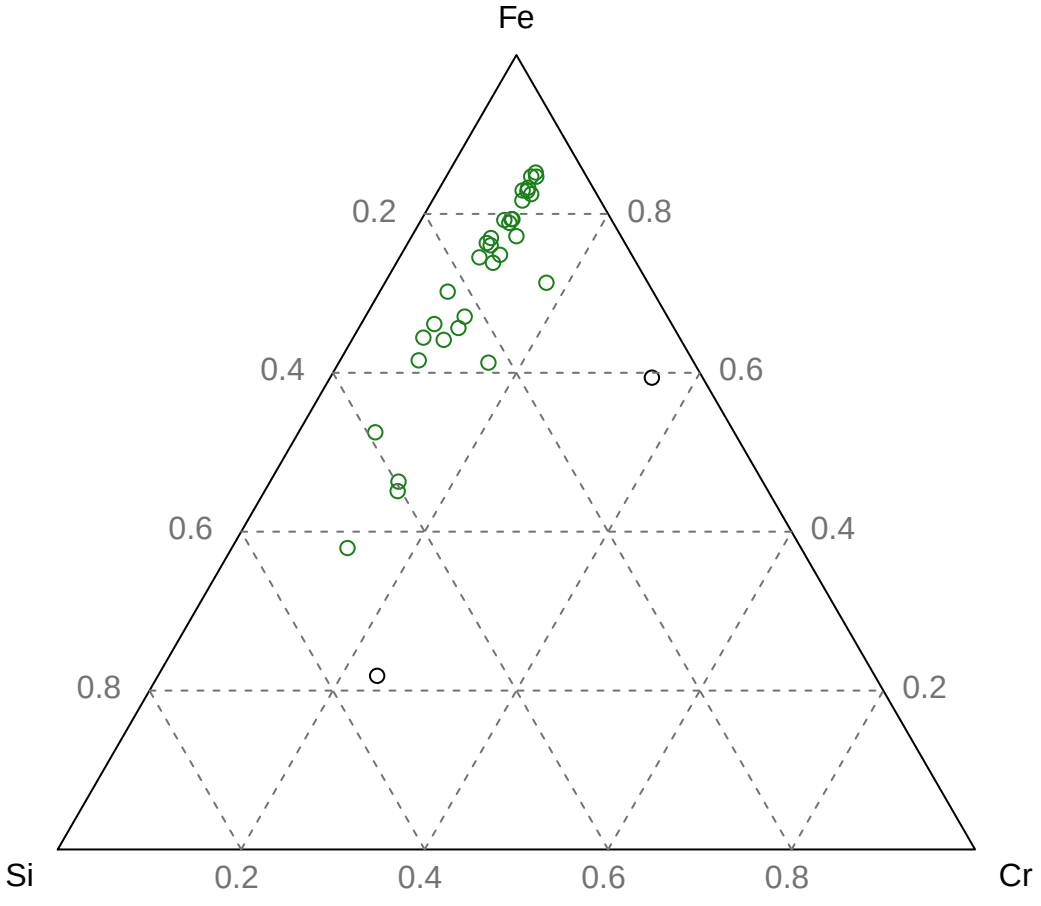
Si, K, Fe



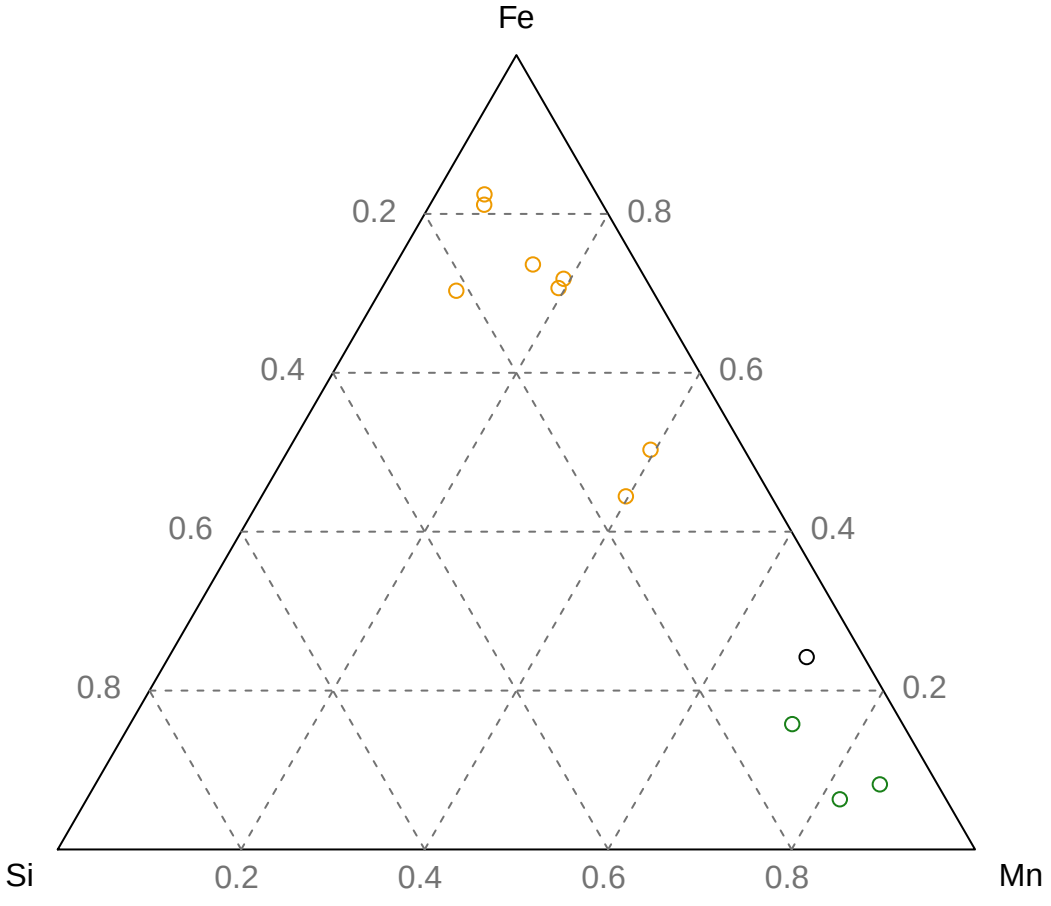
Si, Ti, Fe



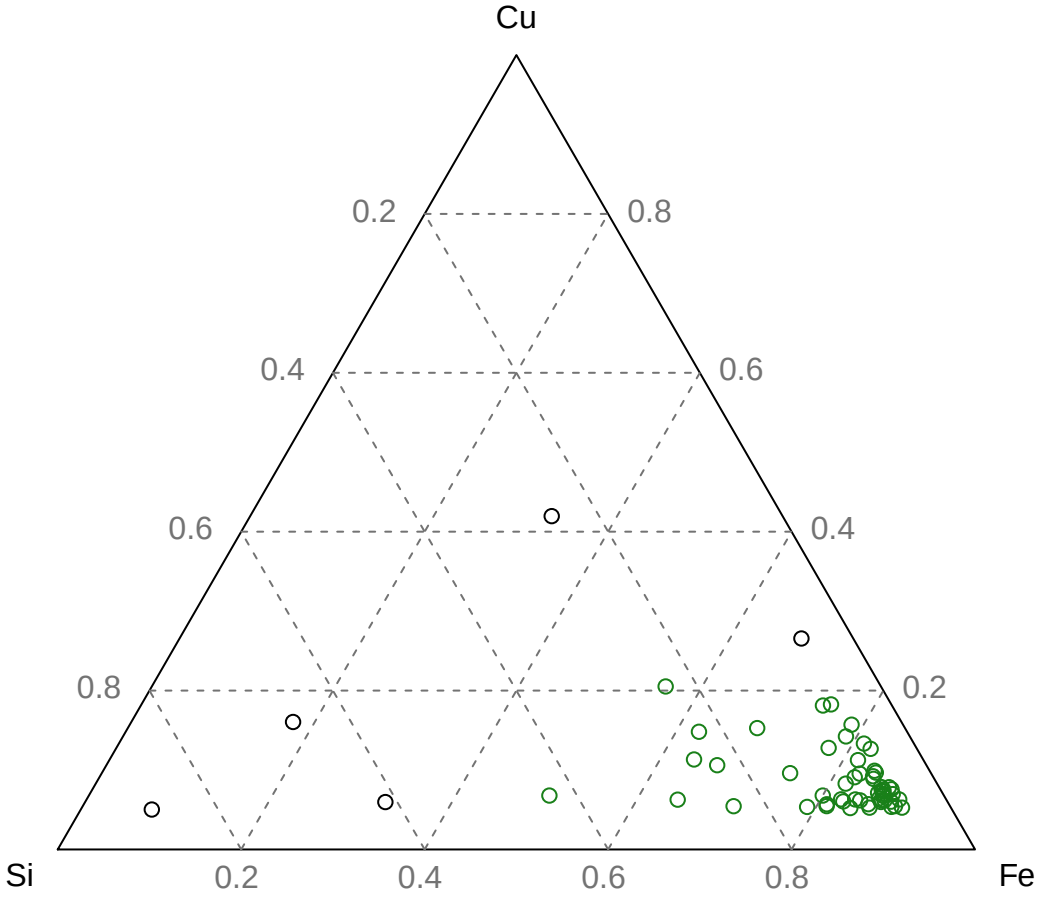
Si, Cr, Fe



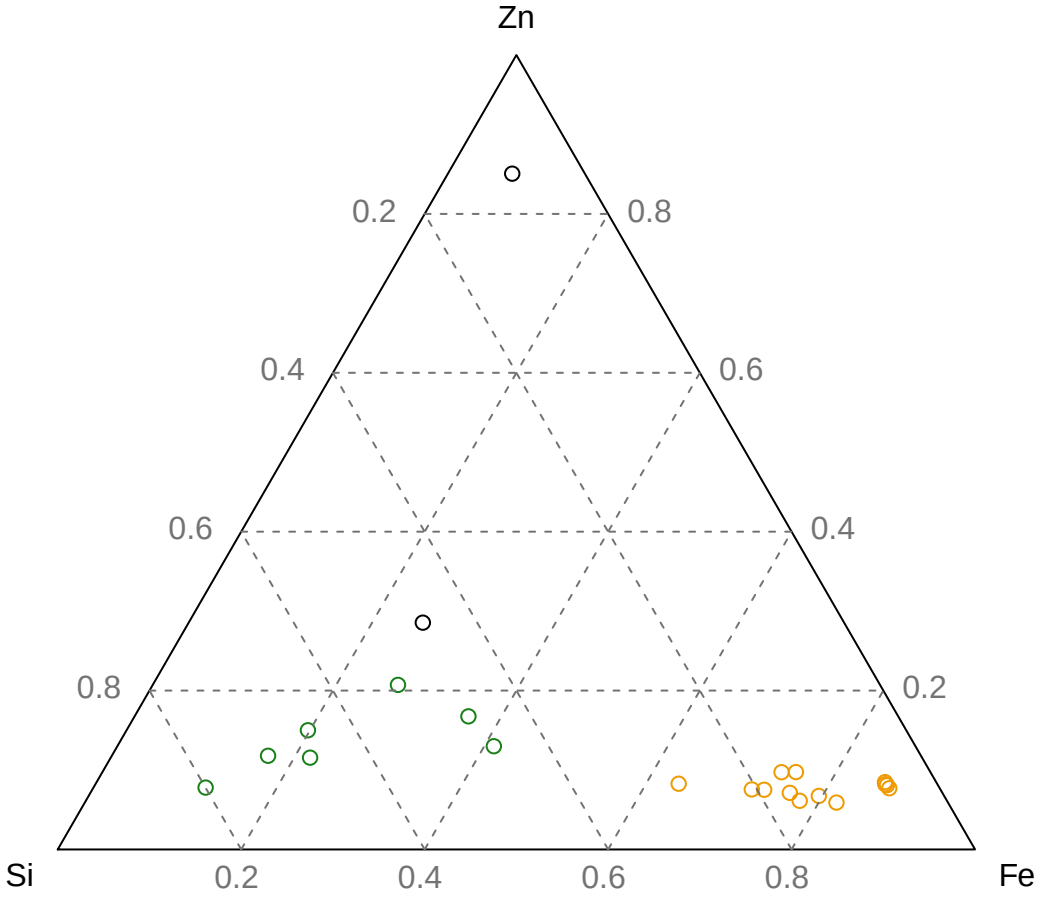
Si, Mn, Fe



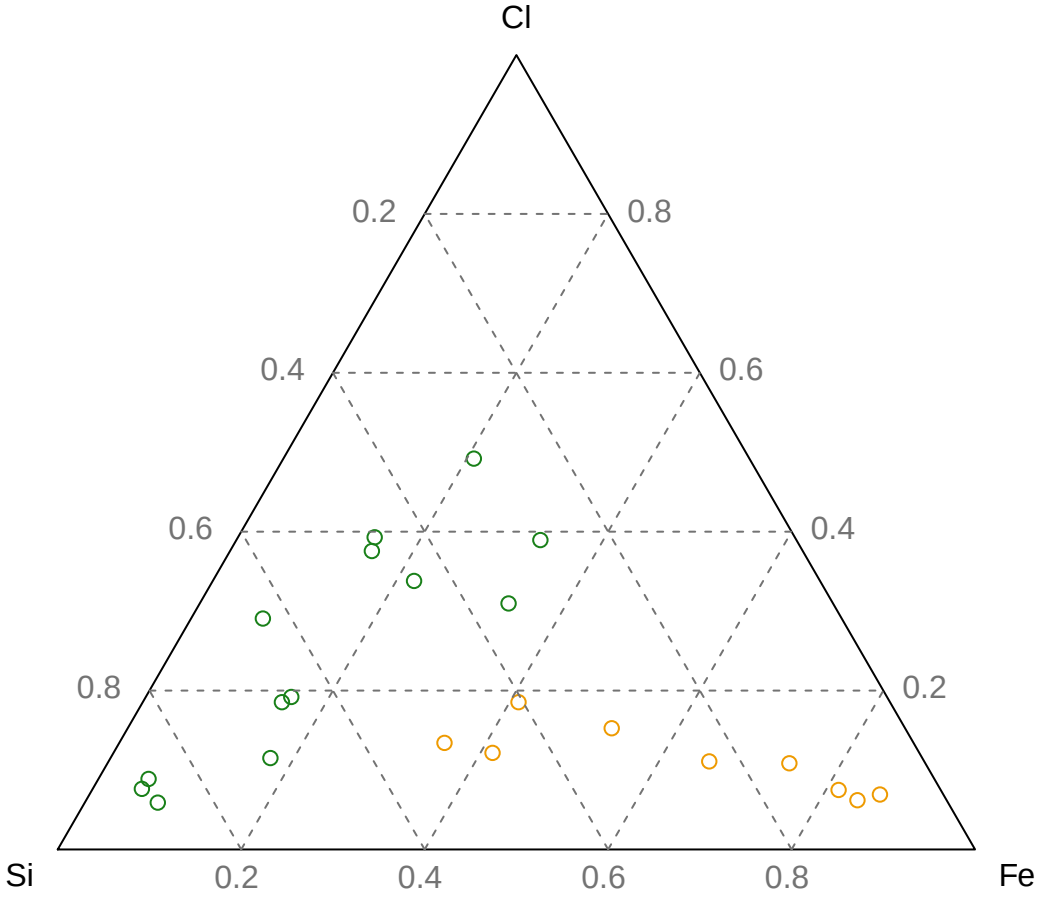
Si, Fe, Cu



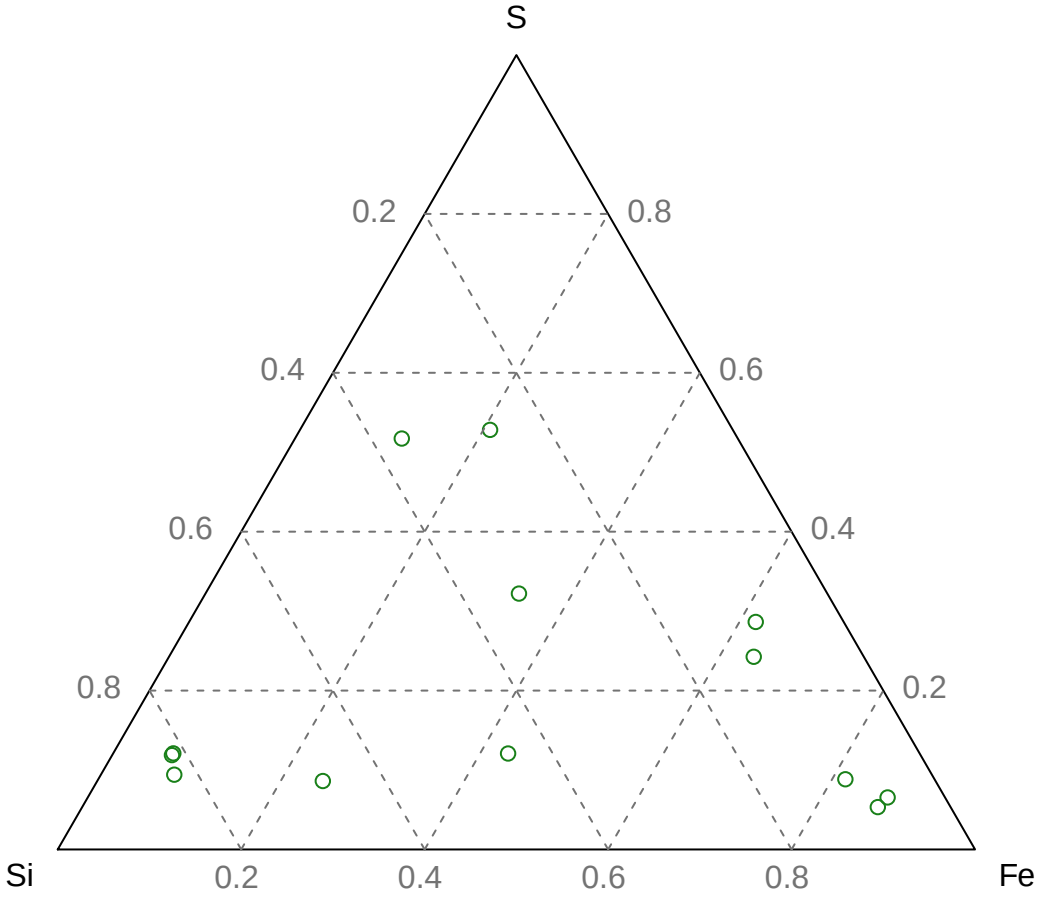
Si, Fe, Zn



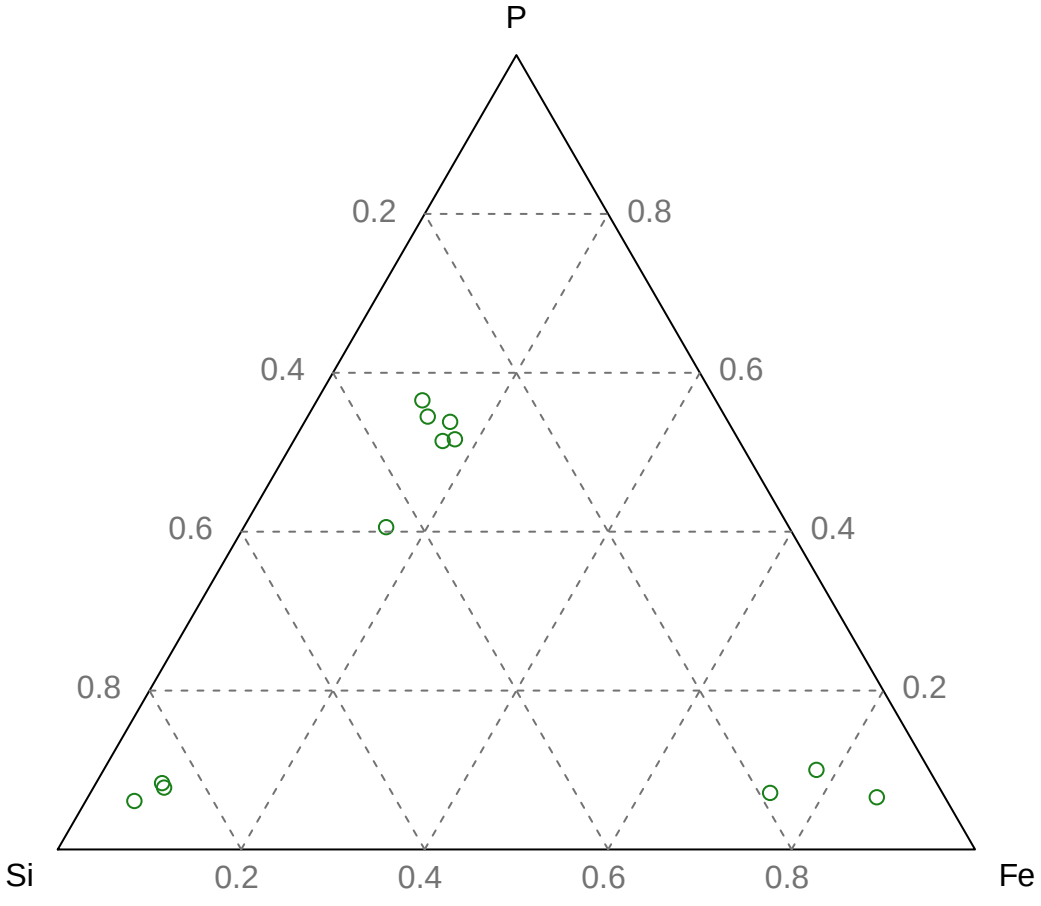
Si, Fe, Cl



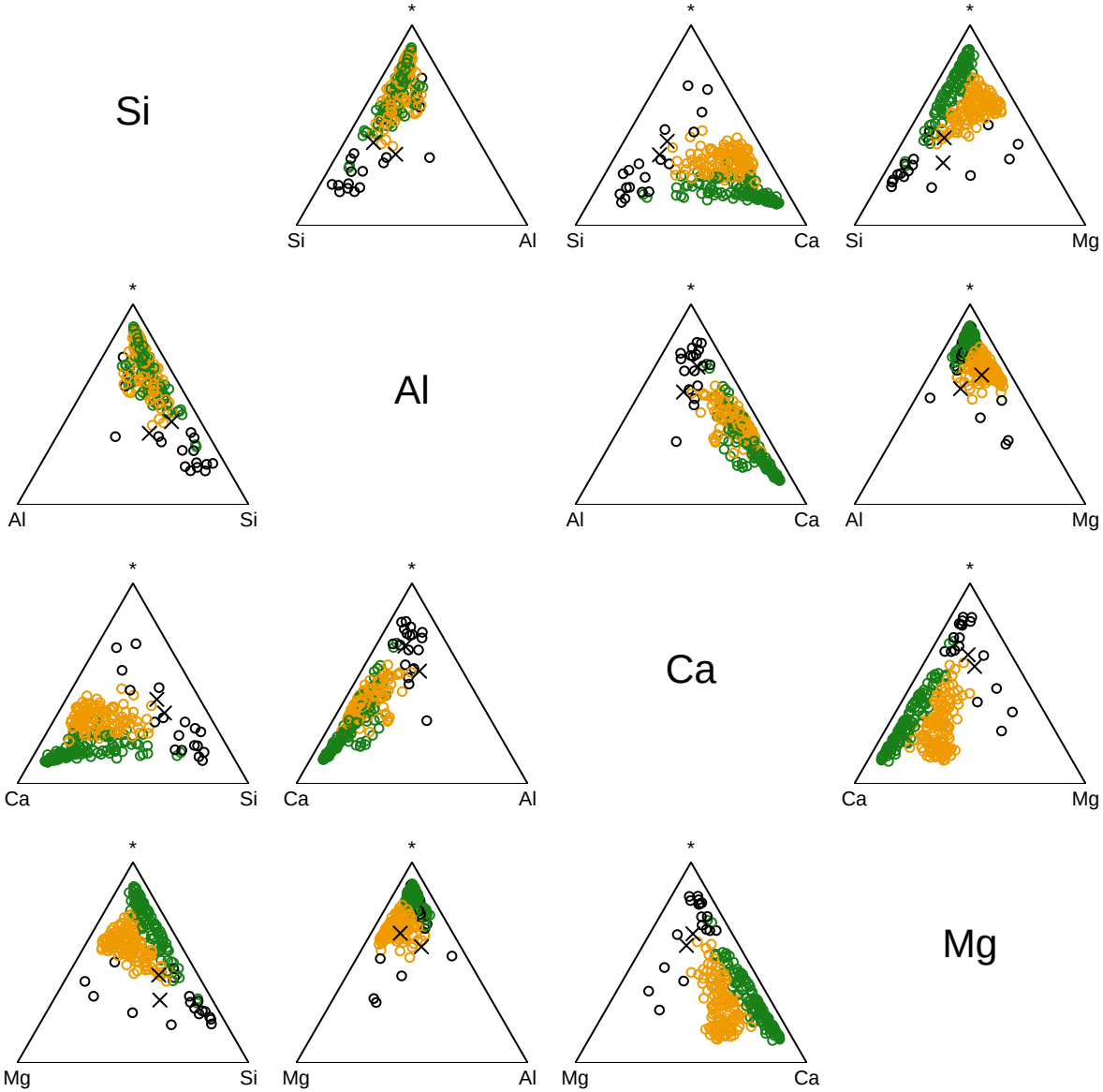
Si, Fe, S



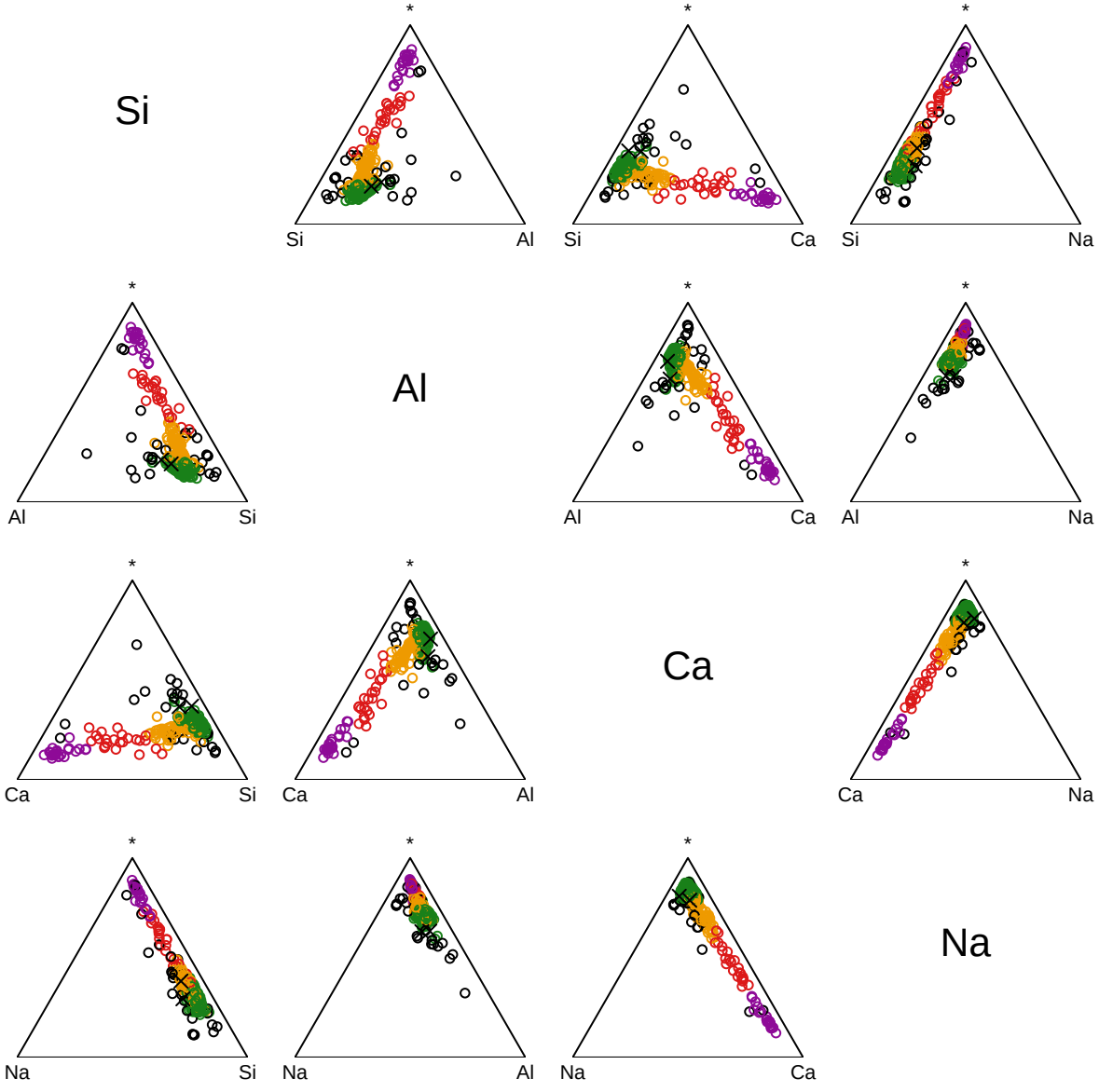
Si, Fe, P



Si, Al, Ca, Mg



Si, Al, Ca, Na


Si
Al
Ca
Na
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Al
Si
Ca
Si
Na
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Ca
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Na
Ca
Si
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Ca
Na
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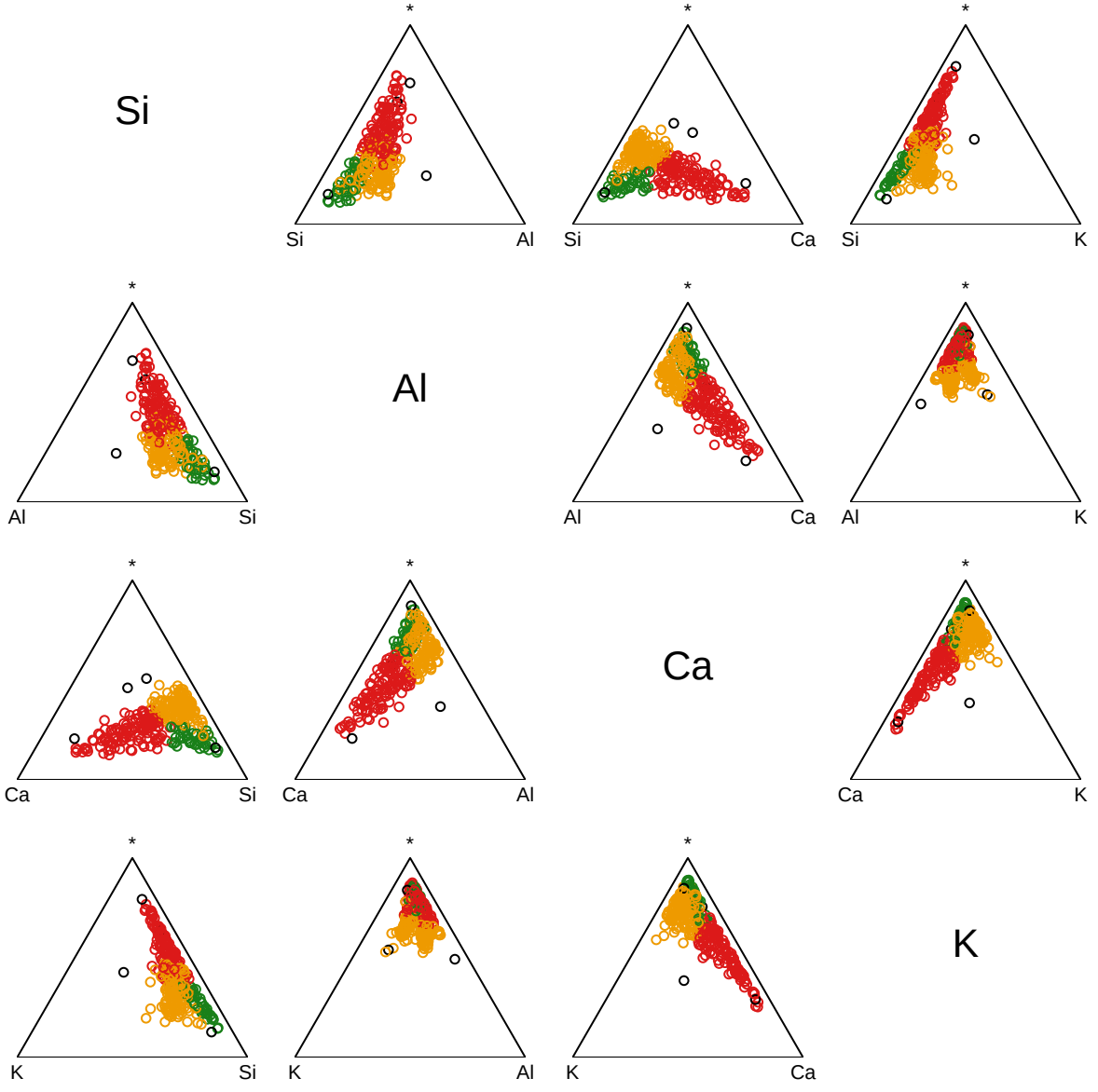
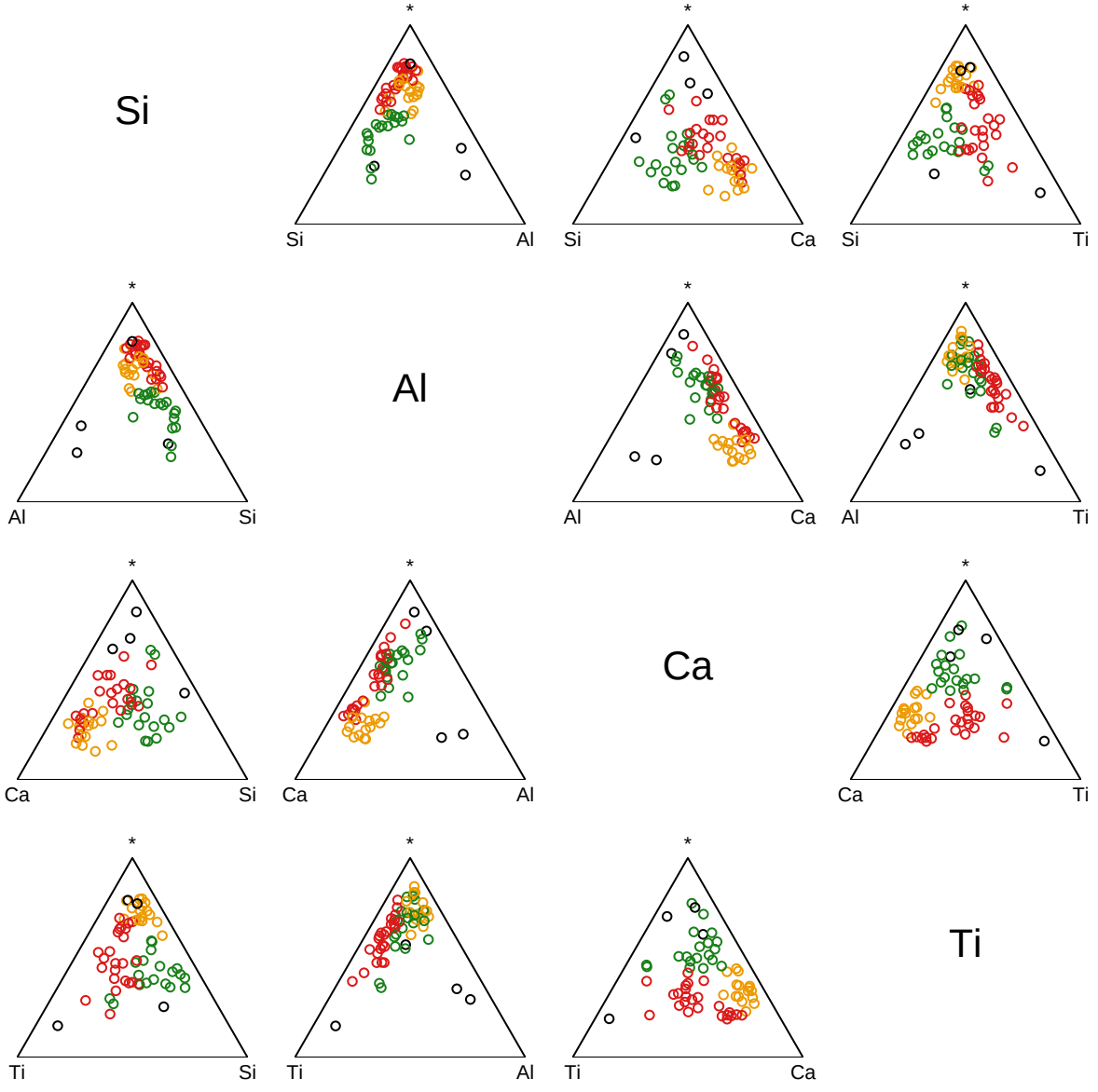
Si
Na
Al
Na
Ca

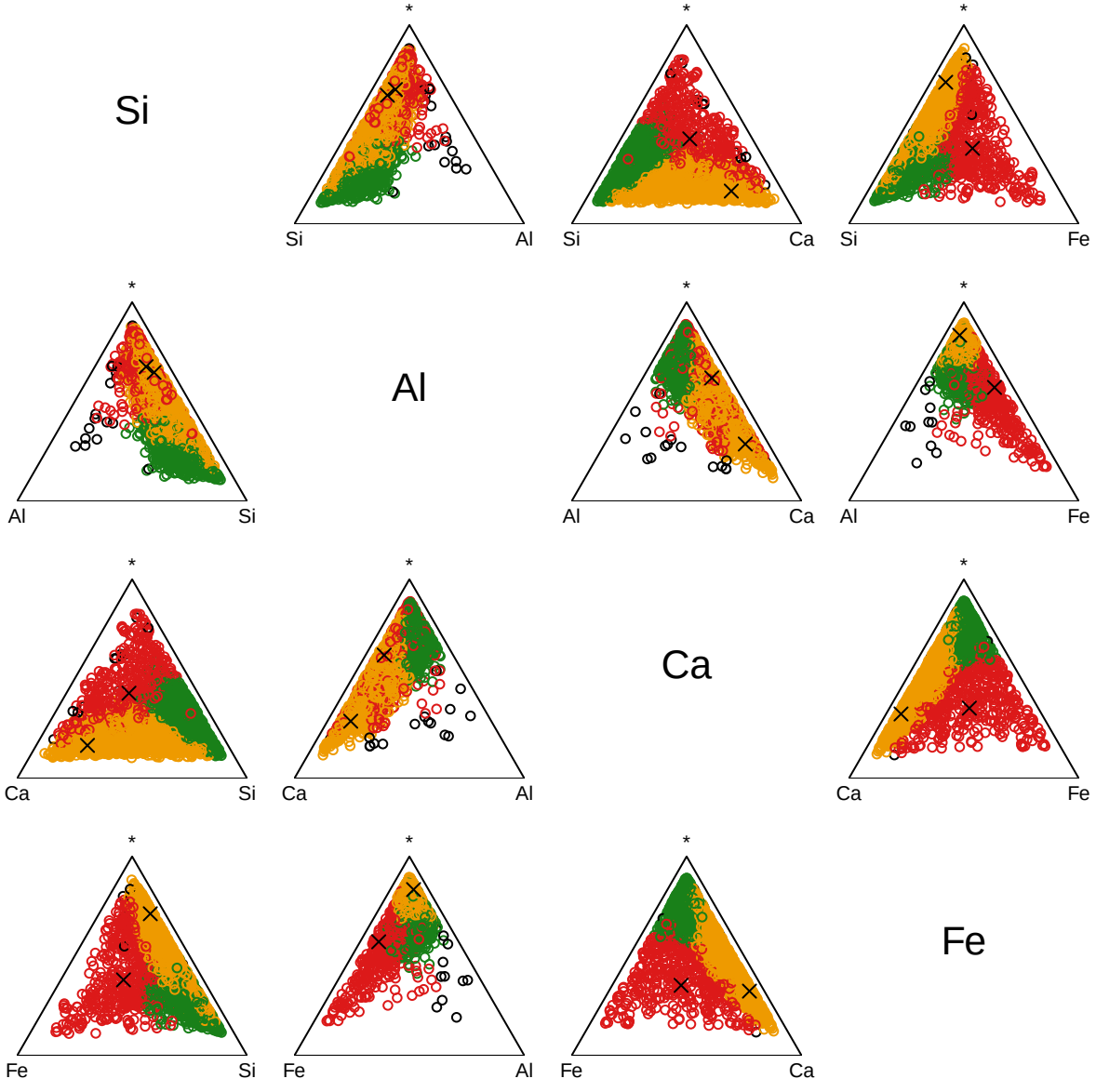
Si, Al, Ca, K



Si, Al, Ca, Ti



Si, Al, Ca, Fe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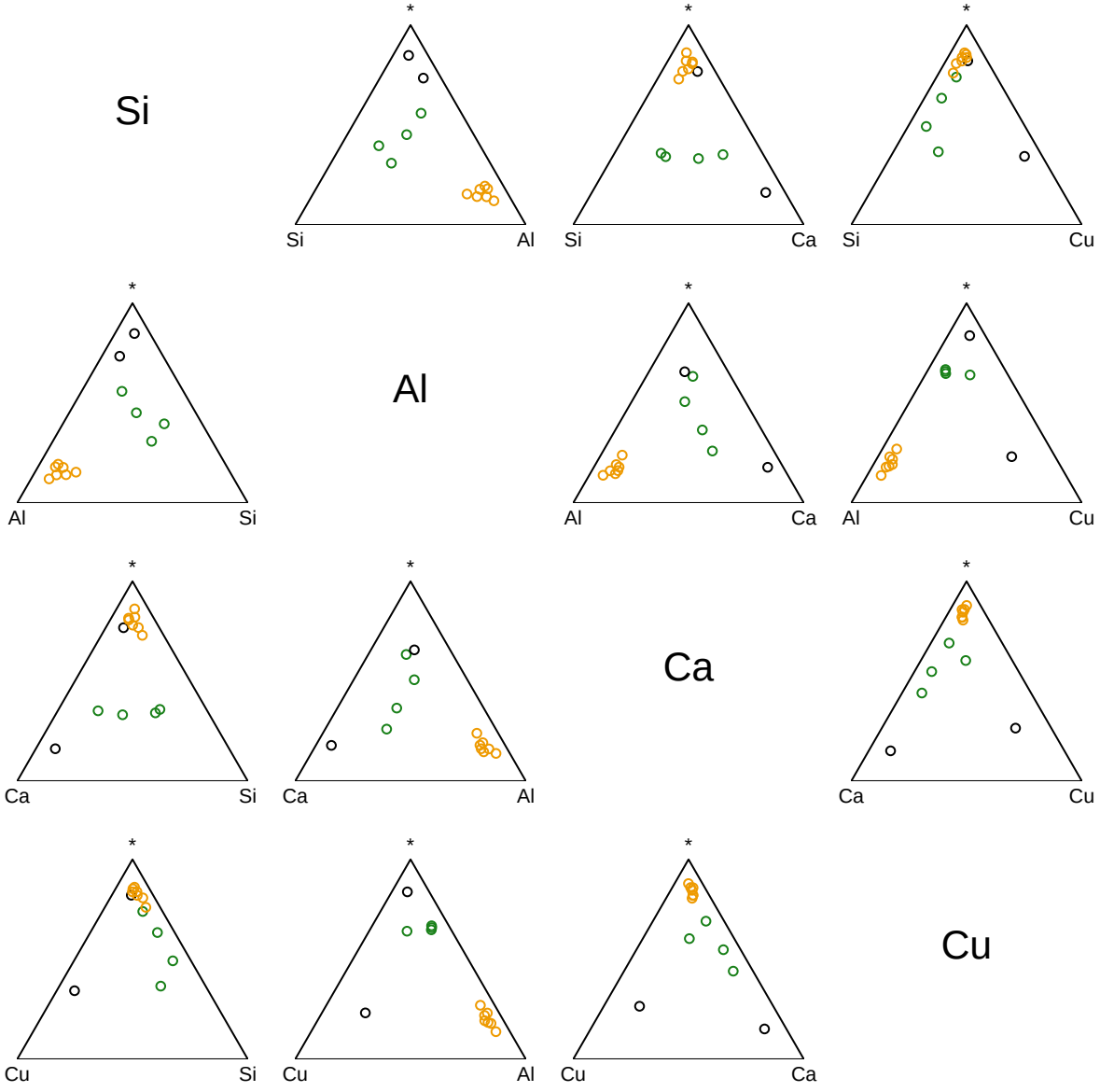
Al
Ca
Fe
Si Al
Si Ca
Si Fe
Al Si
Al Ca
Al Fe
Ca Si
Ca Al
Ca Fe
Fe Si
Fe Al
Fe Ca

Si, Al, Ca, Cu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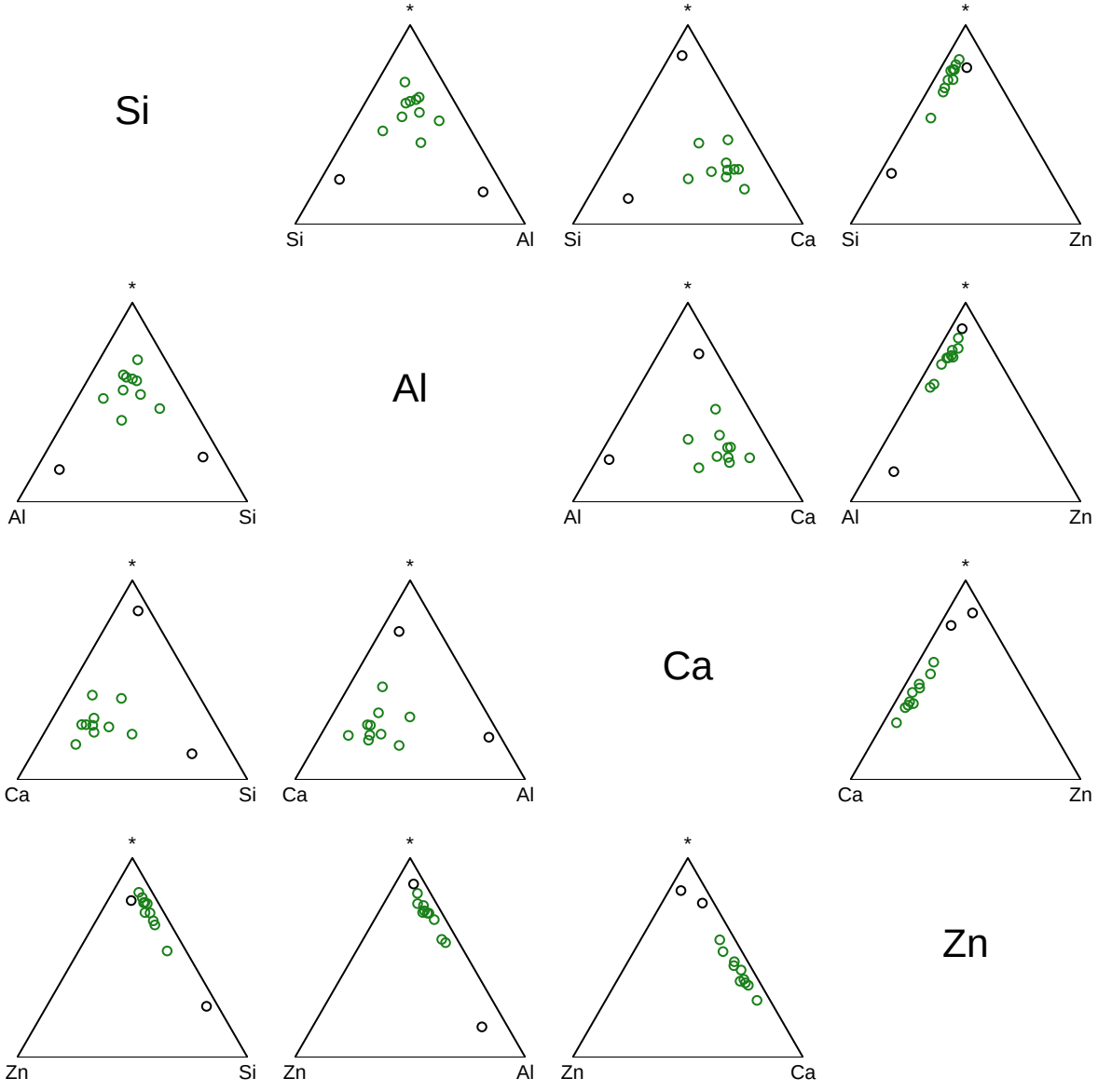
Al
Ca
Cu
Si Al
Si Ca
Si Cu
Al Si
Al Ca
Al Cu
Ca Si
Ca Al
Ca Cu
Cu Si
Cu Al
Cu Ca

Si, Al, Ca, Zn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Al
Ca
Zn
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Si Zn
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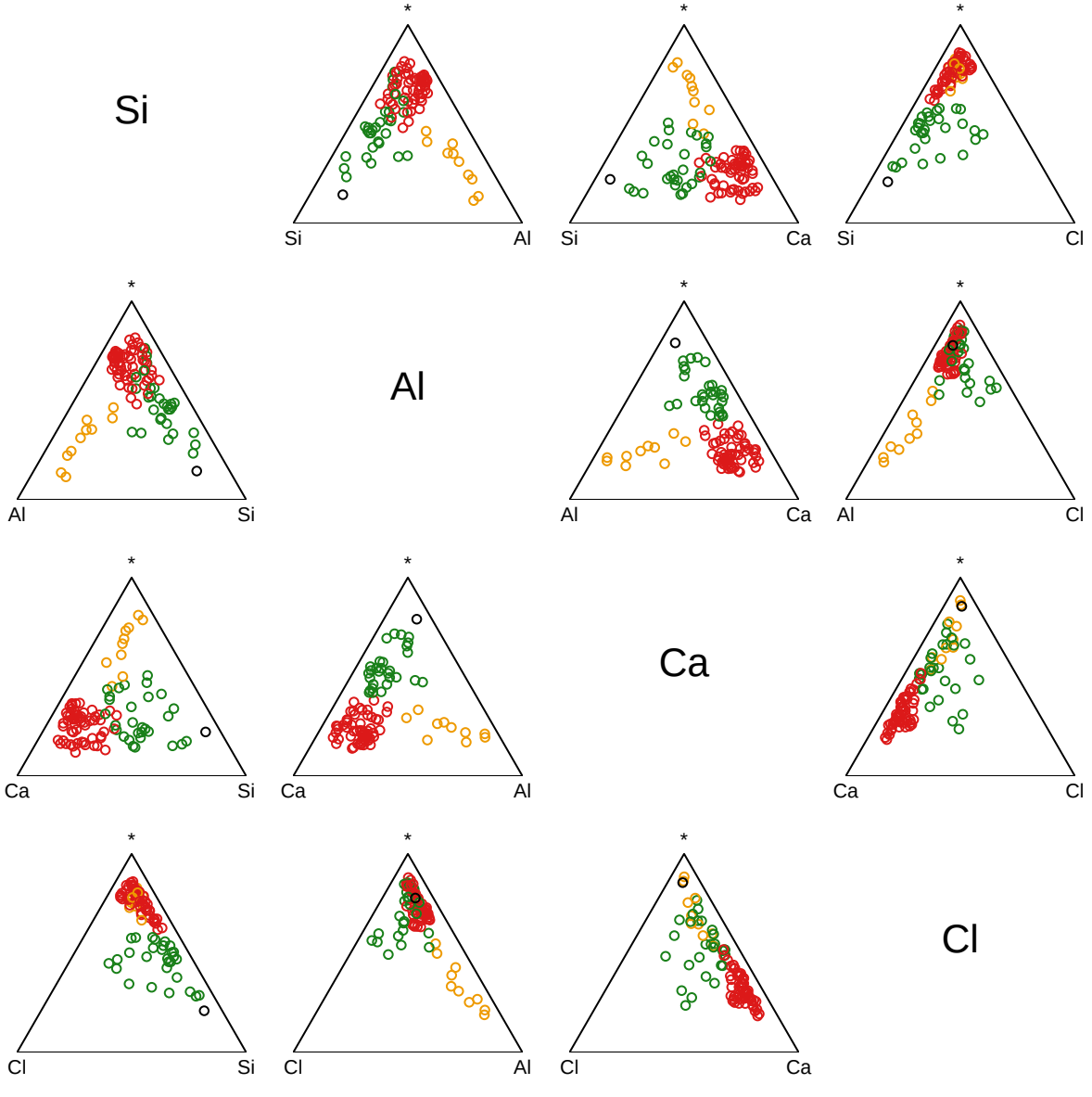
Ca Si
Ca Al
Ca Zn
Zn Si
Zn Al
Zn Ca

Si, Al, Ca, Cl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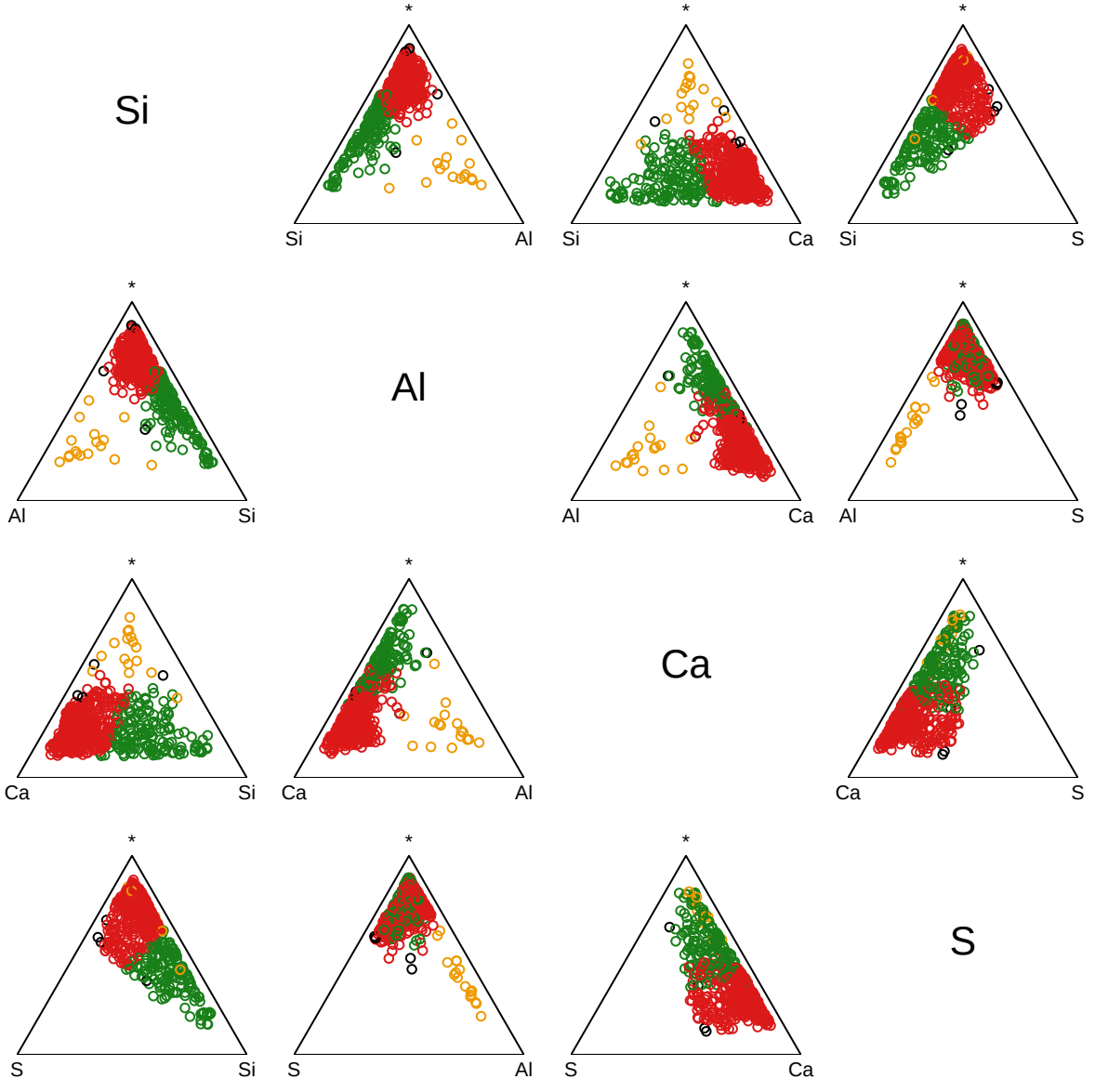
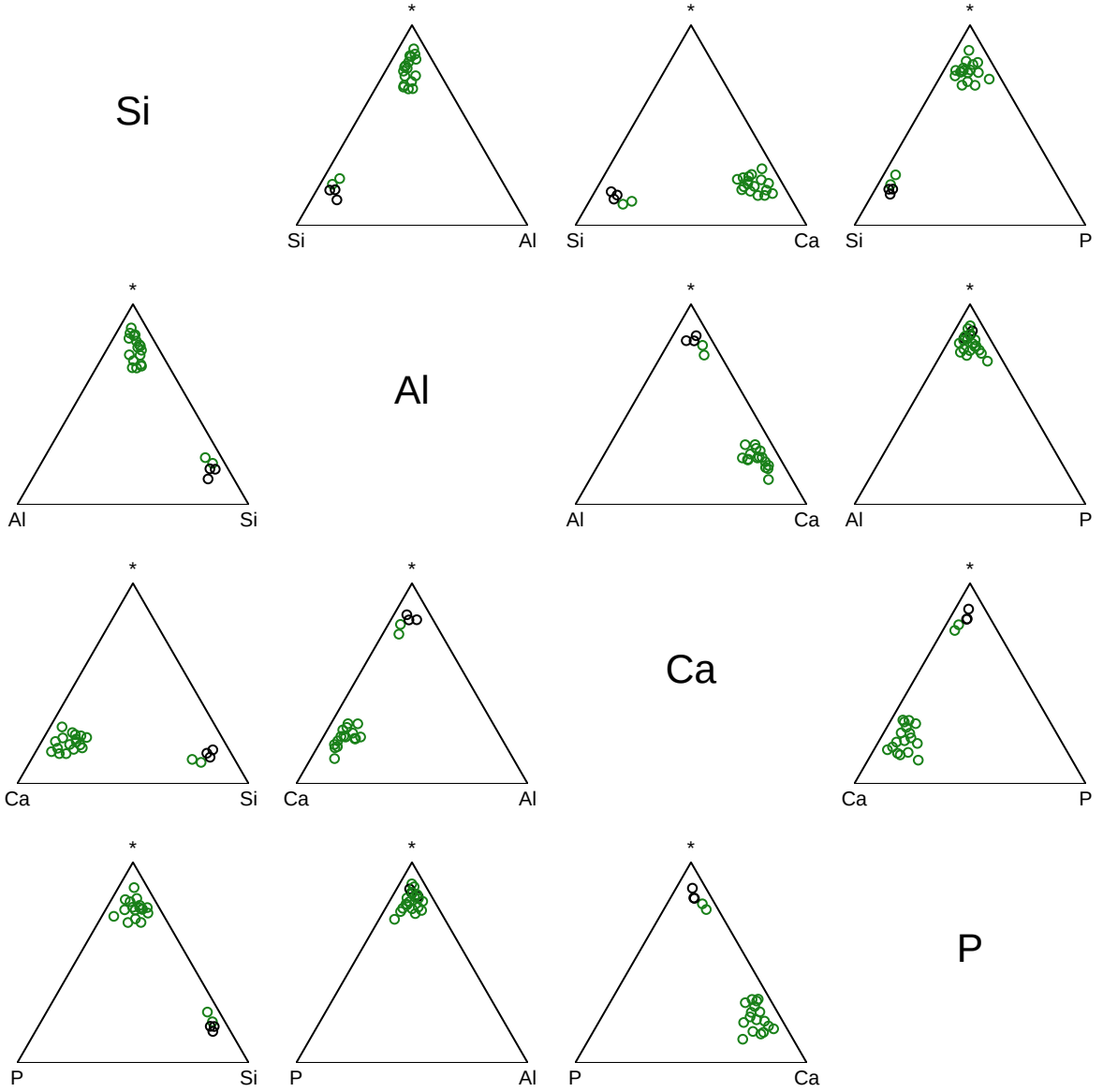
Cl
Ca

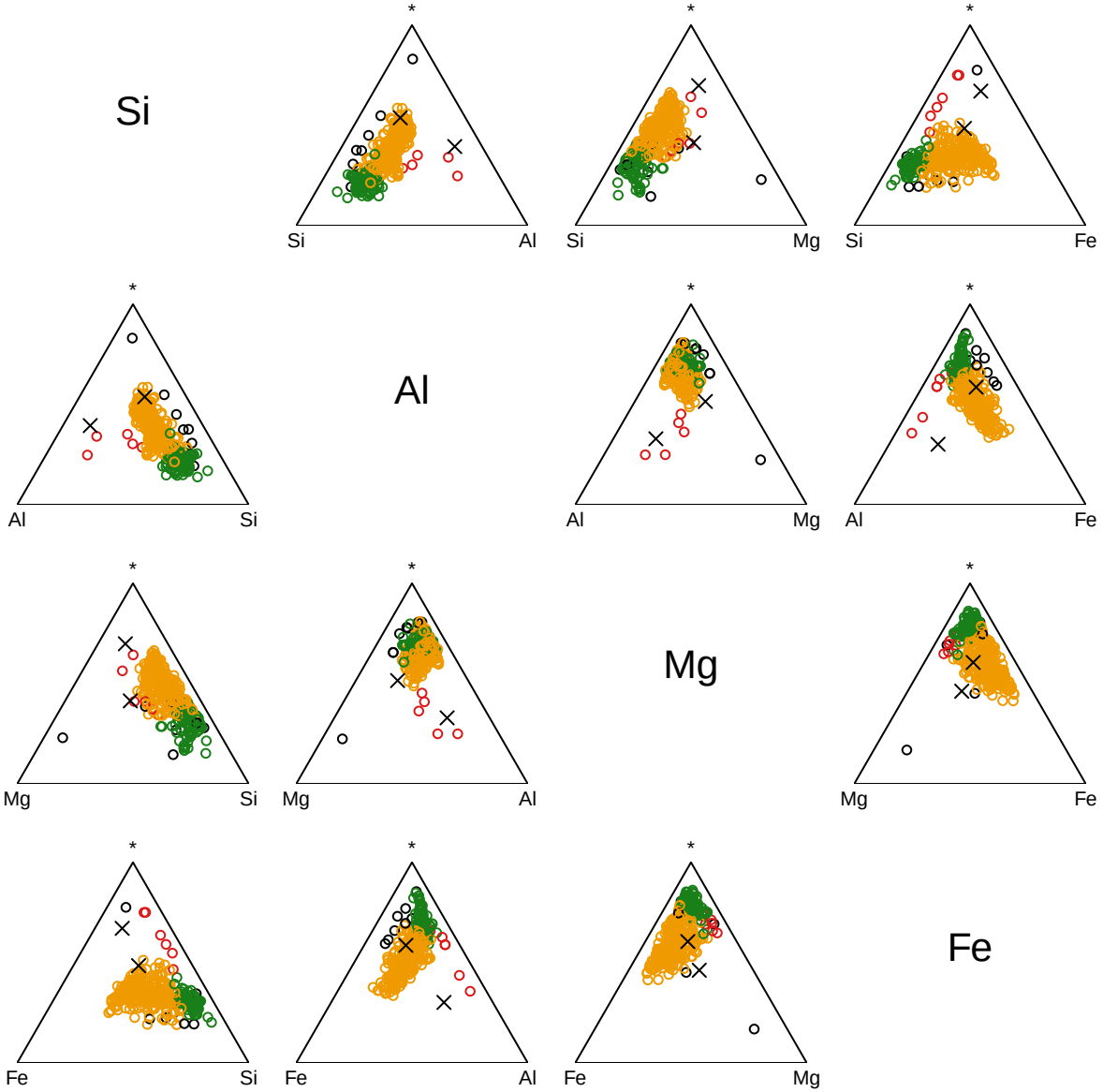
Si, Al, Ca, S



Si, Al, Ca, P



Si, Al, Mg, Fe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Fe
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Si Fe
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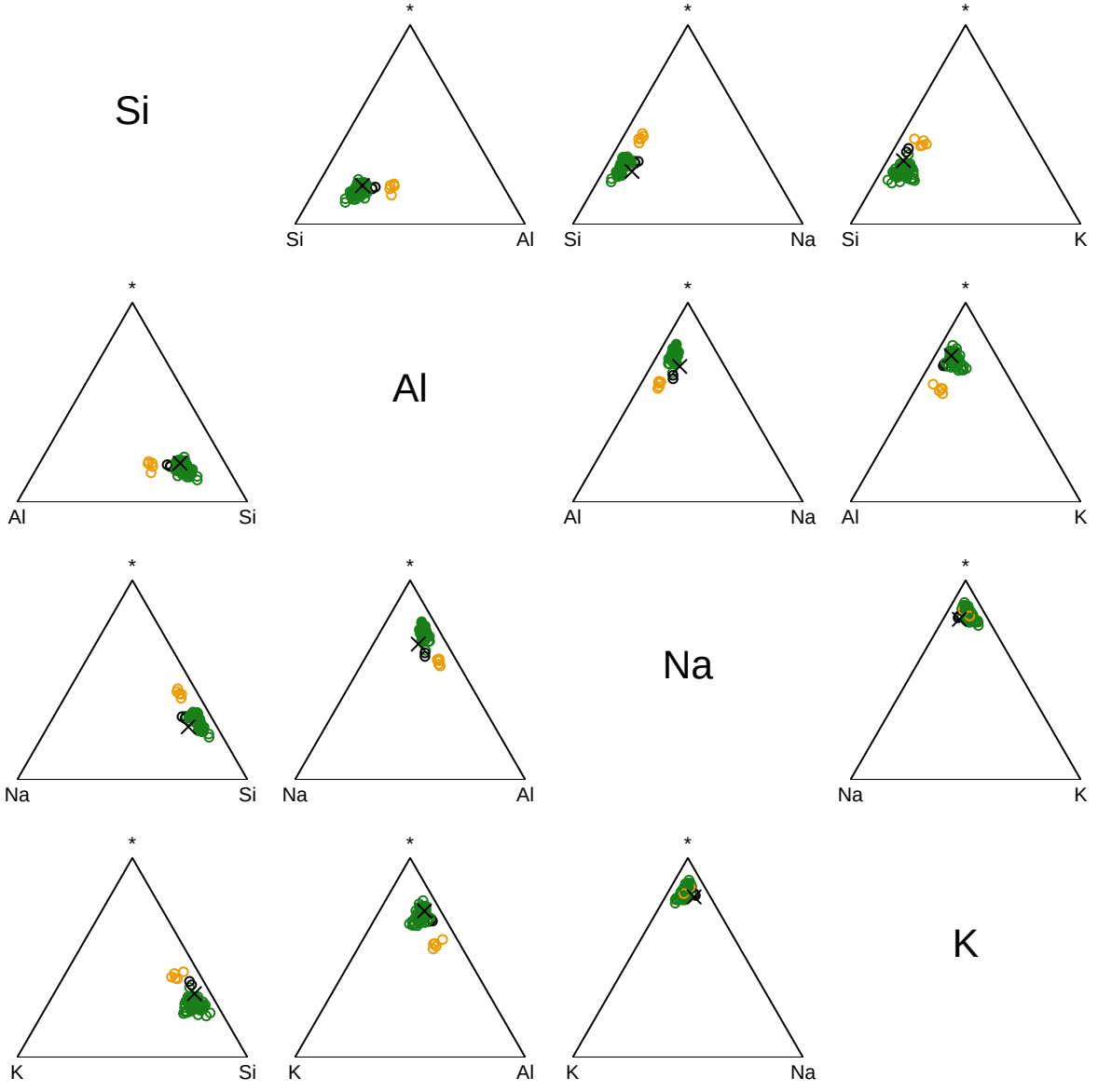
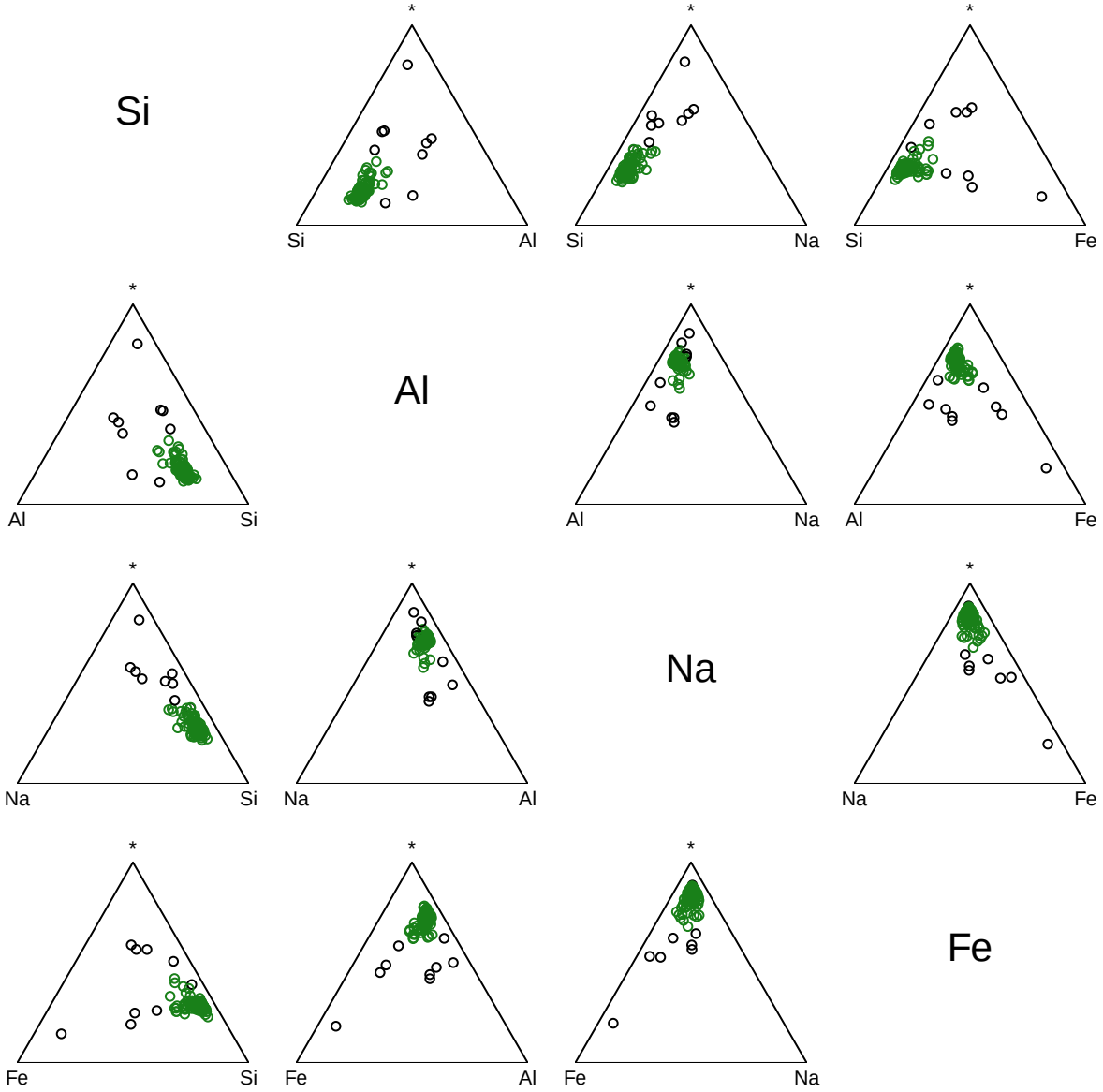
Mg Si
Mg Al
Mg Fe
Fe Si
Fe Al
Fe Mg

Si, Al, Na, K



Si, Al, Na, Fe


Si
Al
Na
Fe
Si Al
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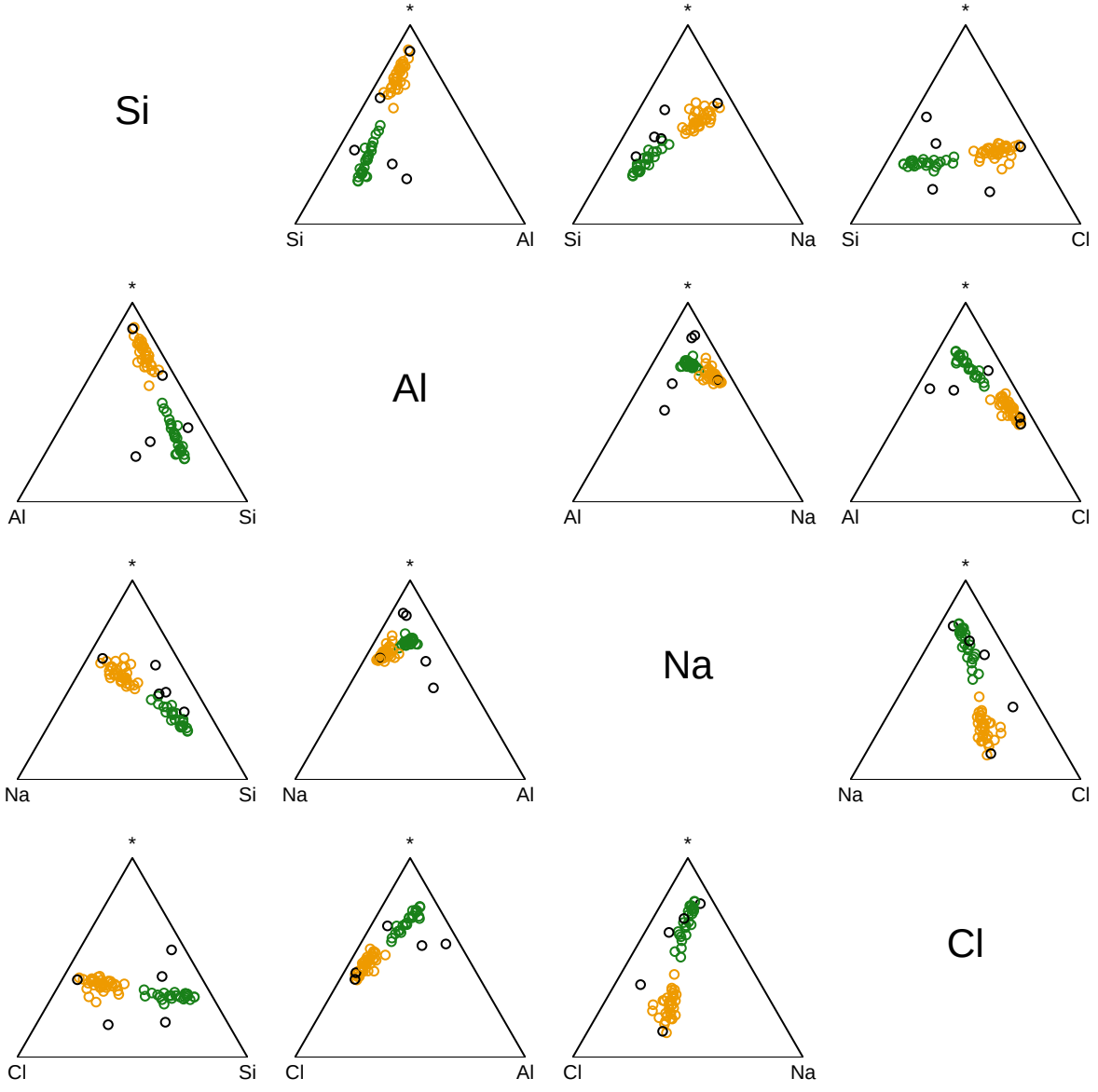
Si Fe
Al Si
Al Na
Al Fe
Na Si
Na Al
Na Fe
Fe Si
Fe Al
Fe Na

Si, Al, Na, Cl


Si
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Na
Cl
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Na
Si
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Cl
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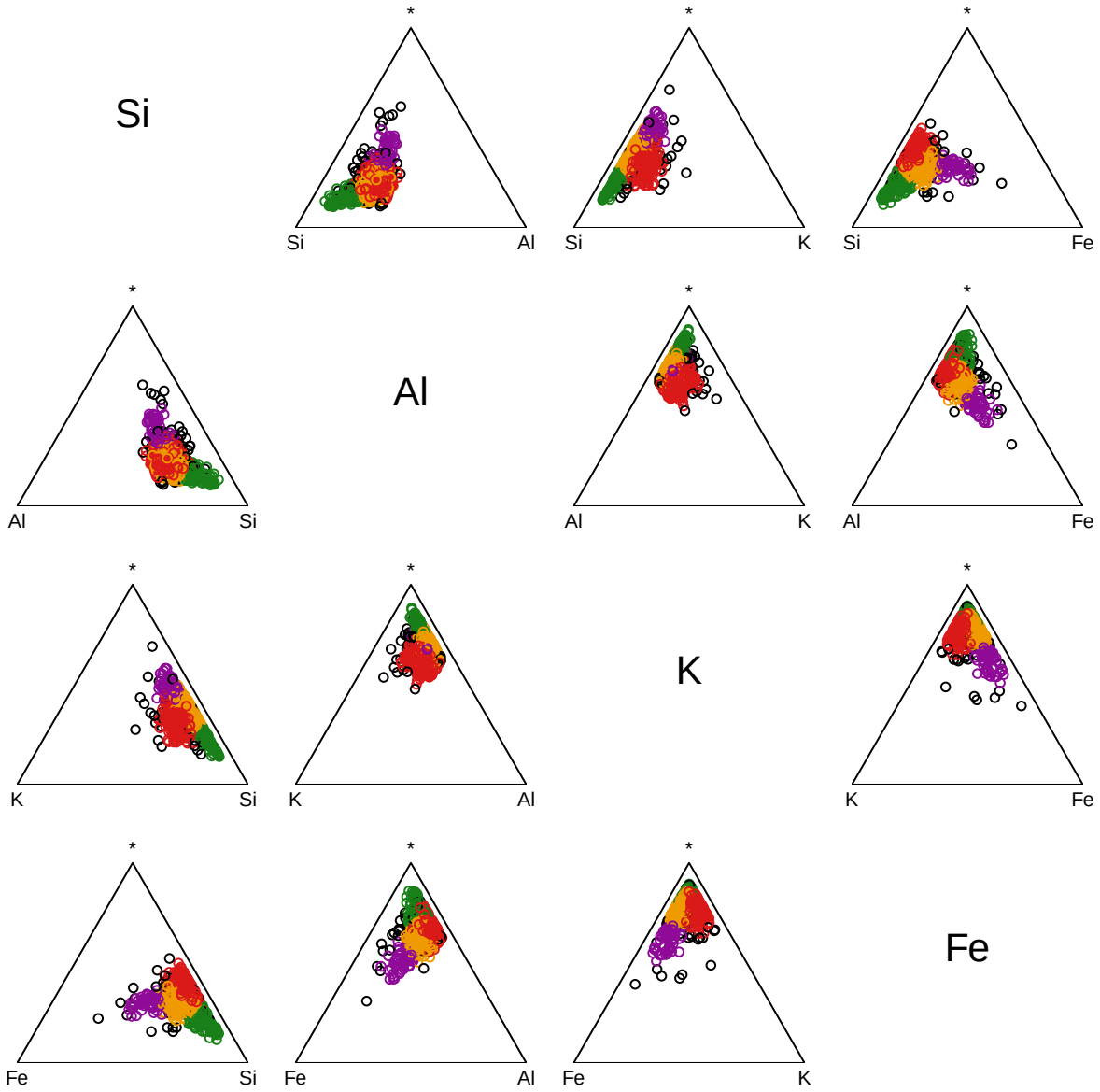
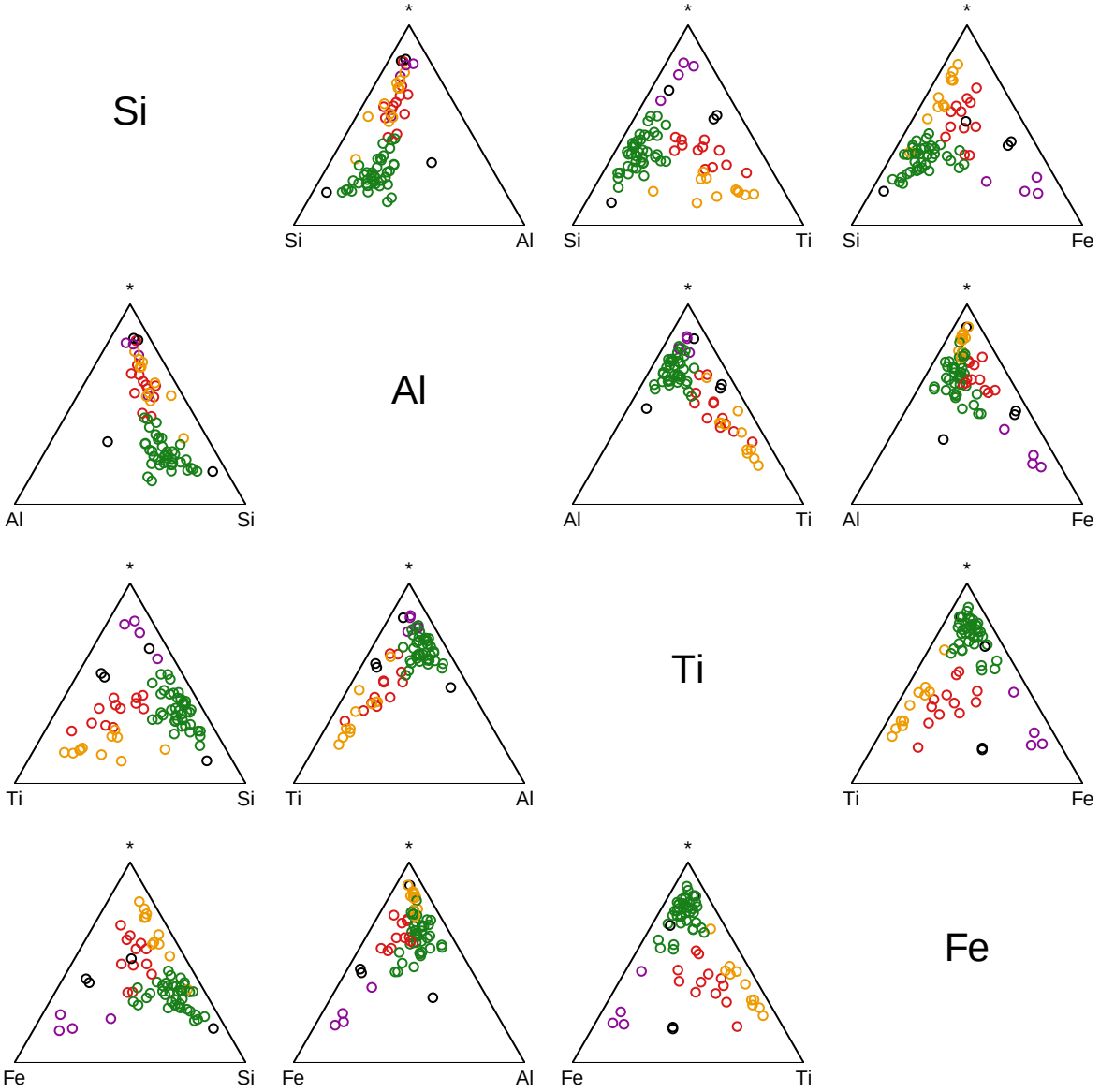
Al
Cl
Na

Si, Al, K, Fe



Si, Al, Ti, Fe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Ti
Fe
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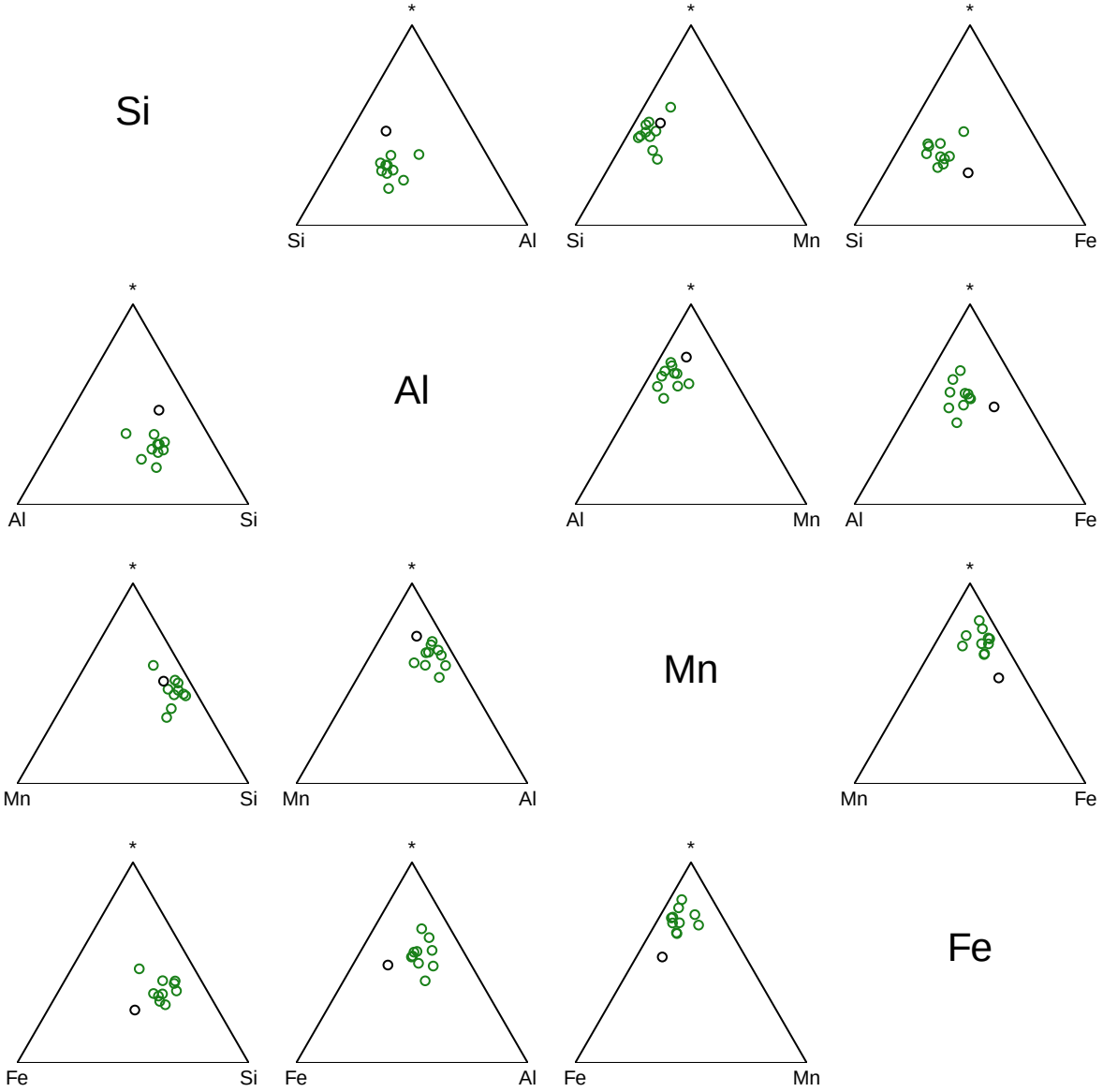
Al
Fe
Ti

Si, Al, Mn, Fe


Si
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Mn
Fe
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Mn
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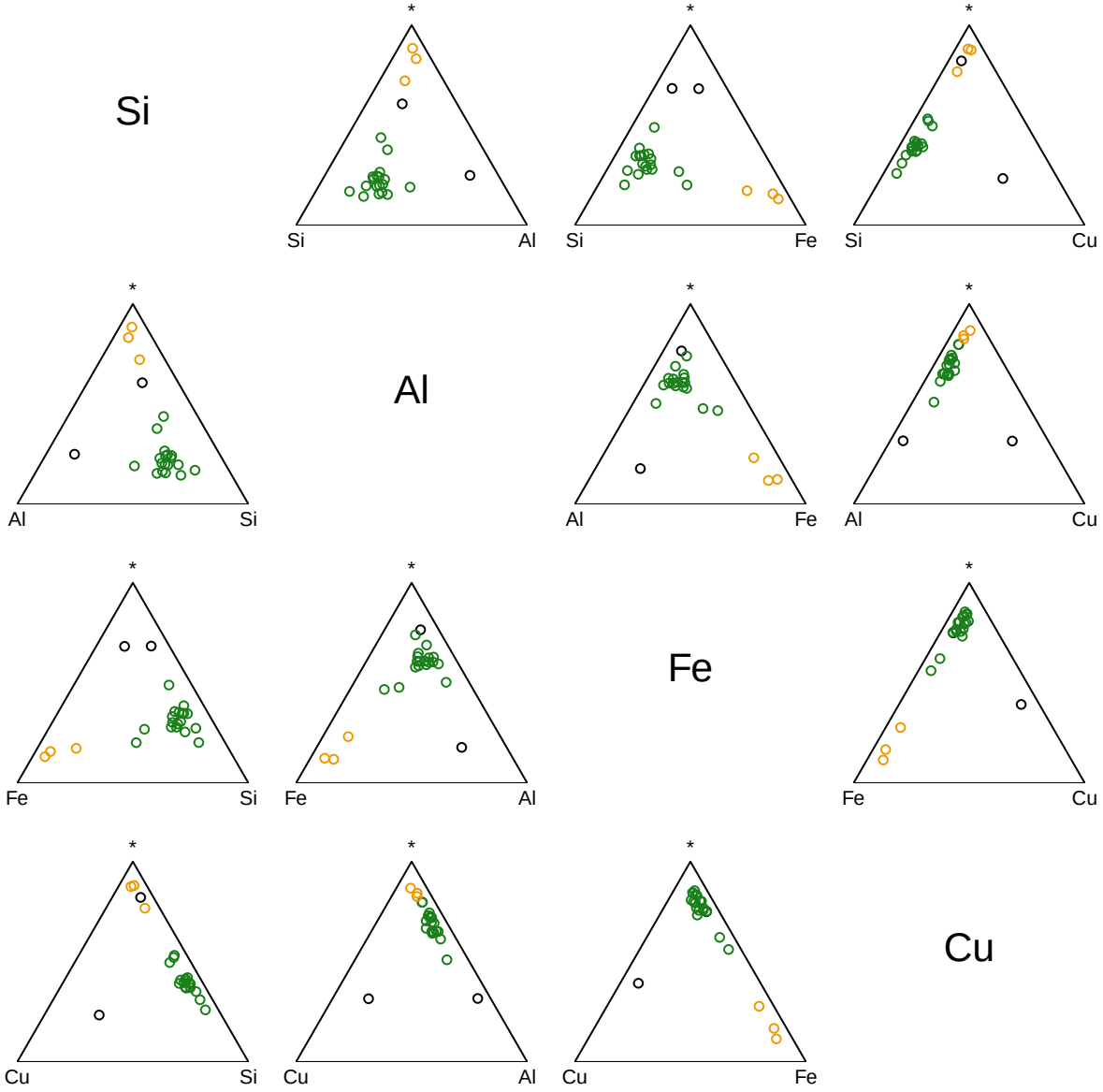
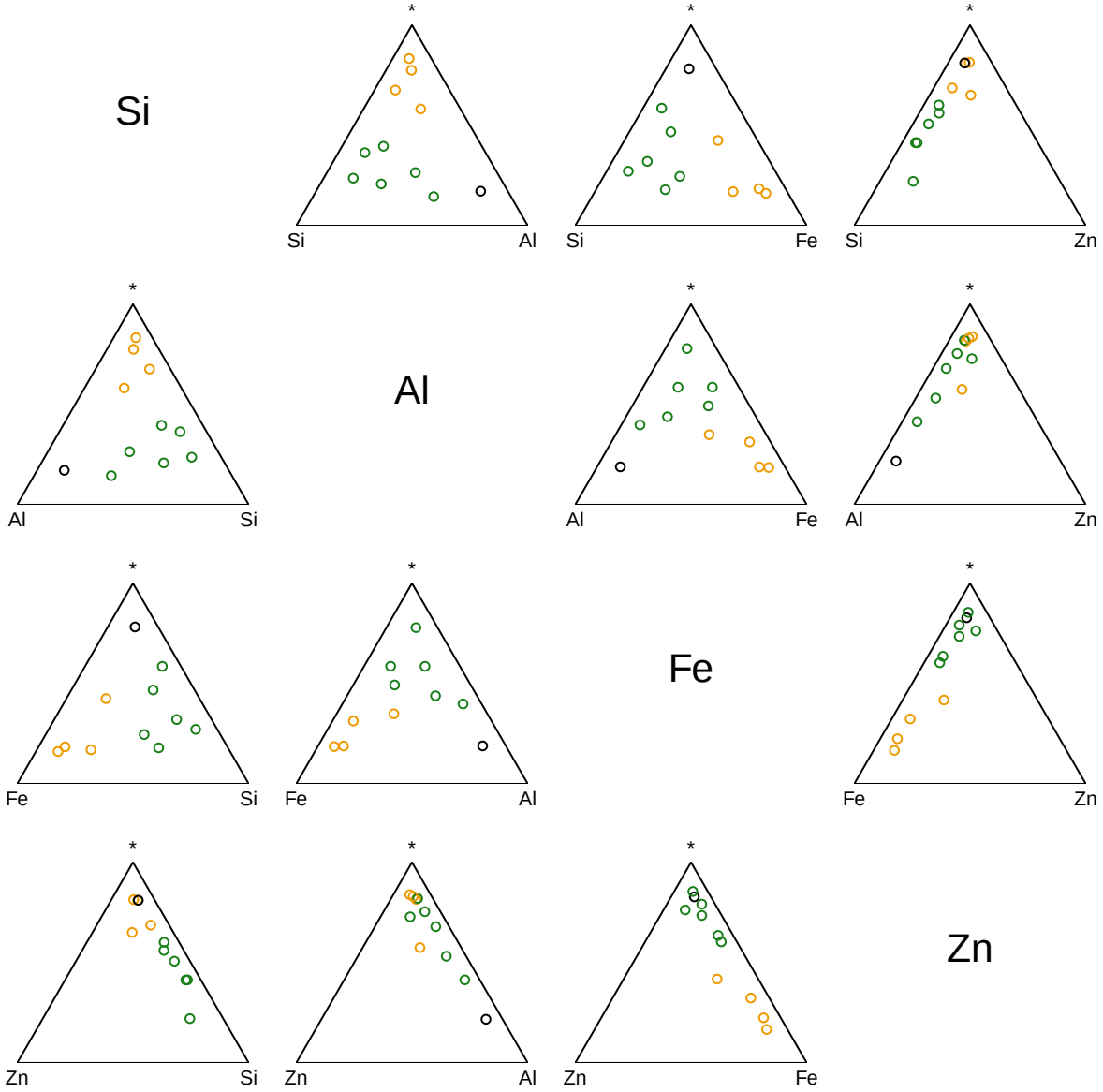
Si
Fe
Al
Fe
Mn

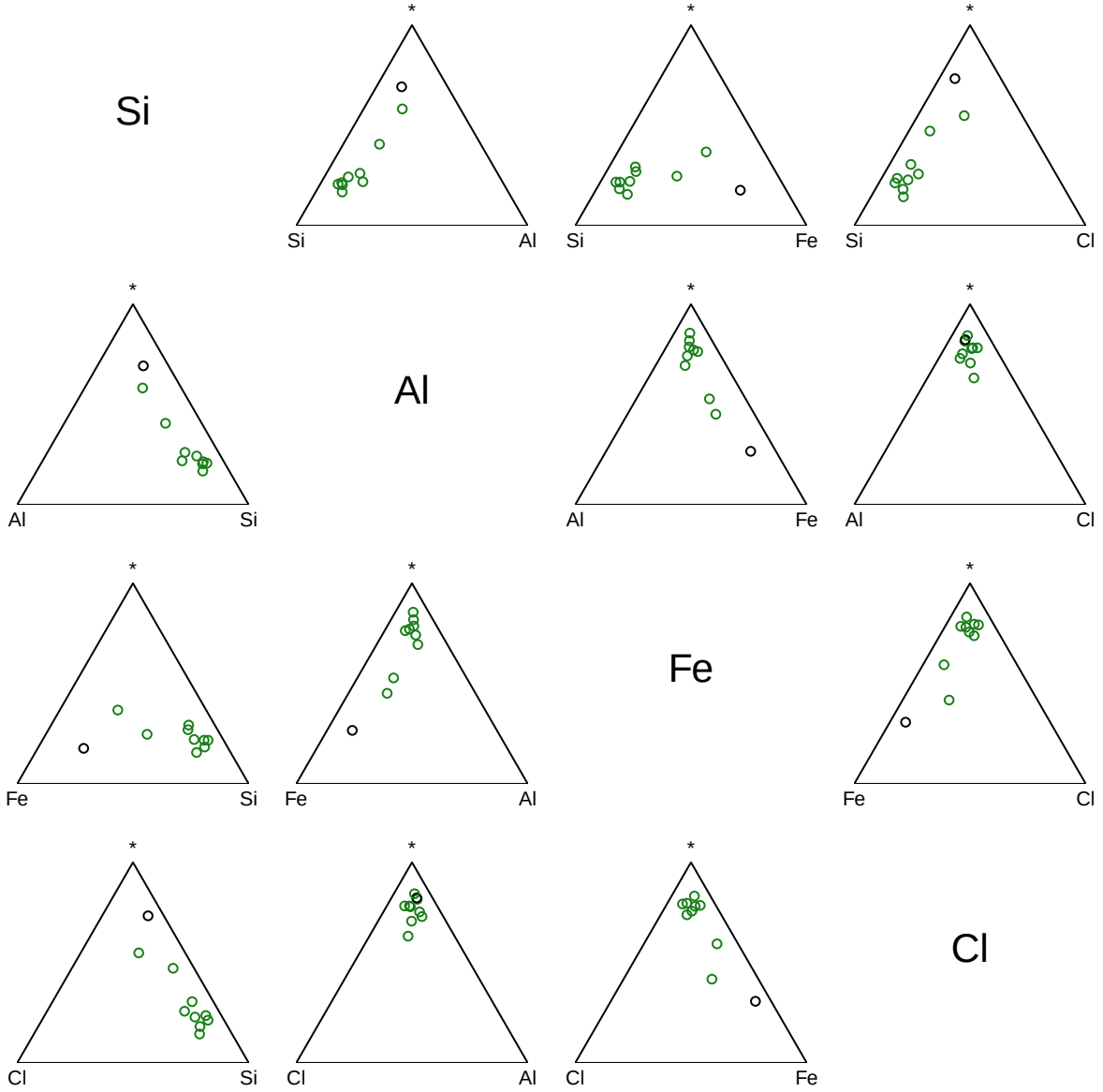
Si, Al, Fe, Cu


Si
Al
Fe
Cu
Si Al
Si Fe
Si Cu
Al Si
Al Fe
Al Cu
Fe Si
Fe Al
Fe Cu
Cu Si
Cu Al
Cu Fe

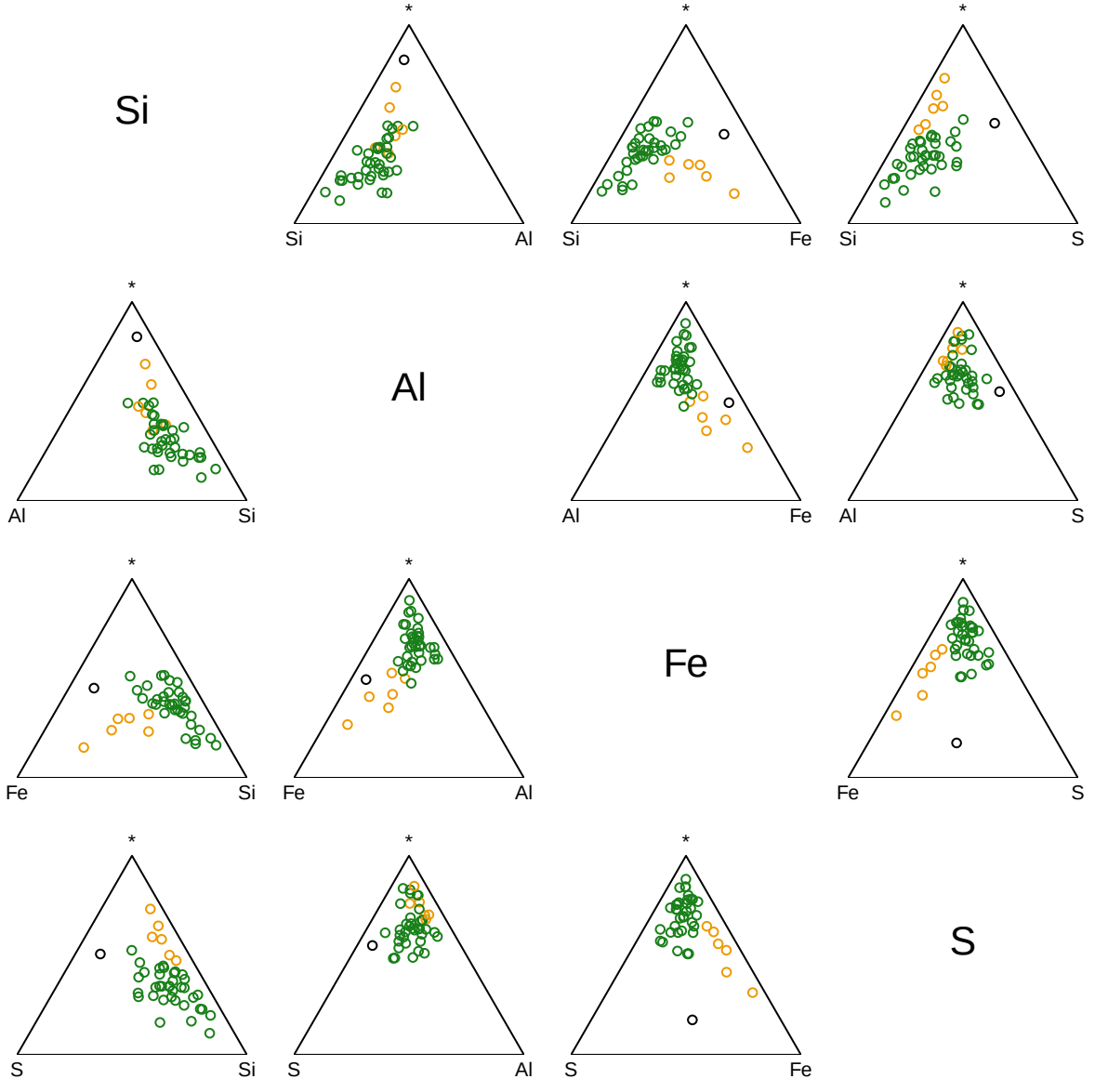
Si, Al, Fe, Zn



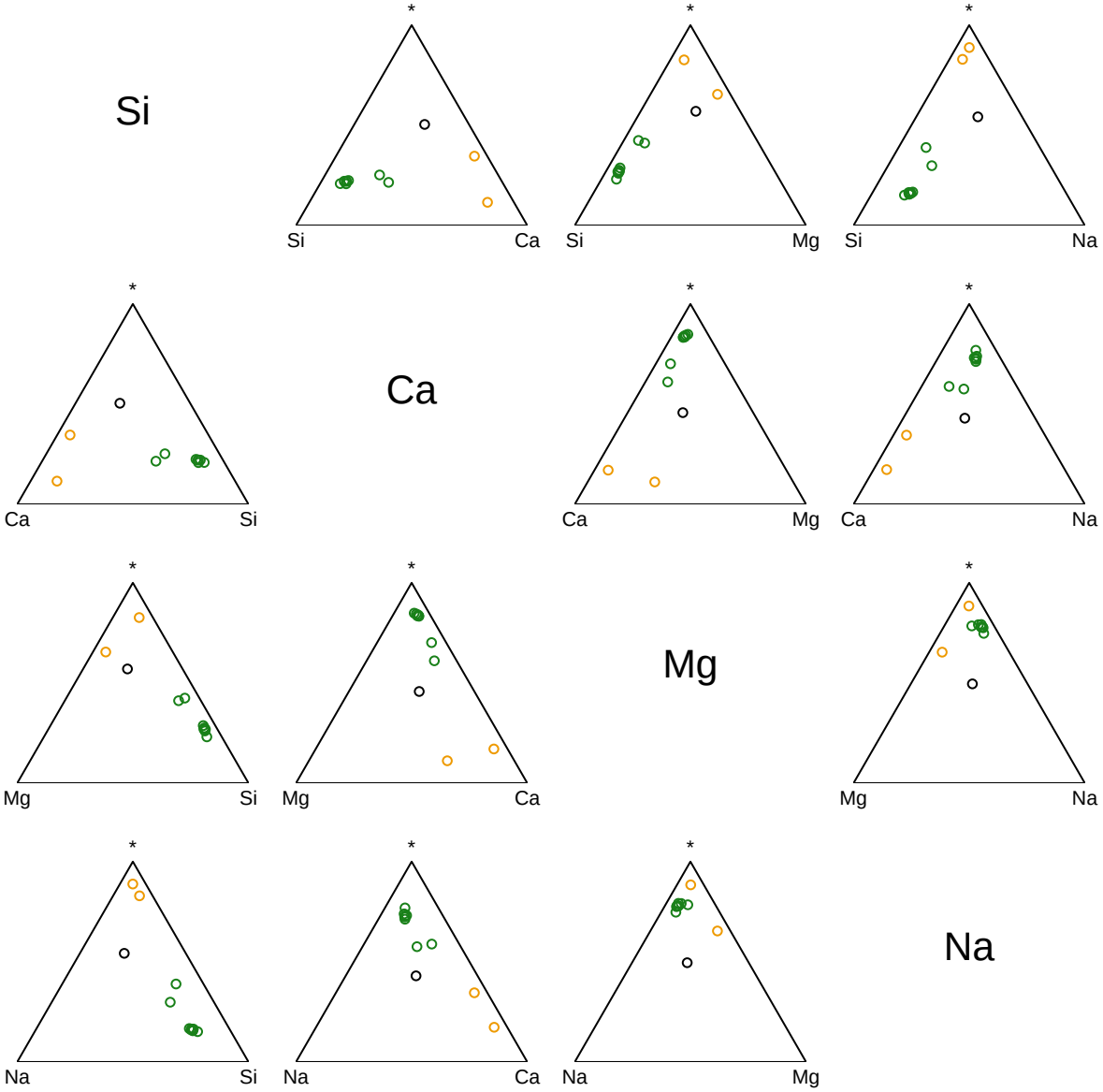
Si, Al, Fe, Cl



Si, Al, Fe, S



Si, Ca, Mg, Na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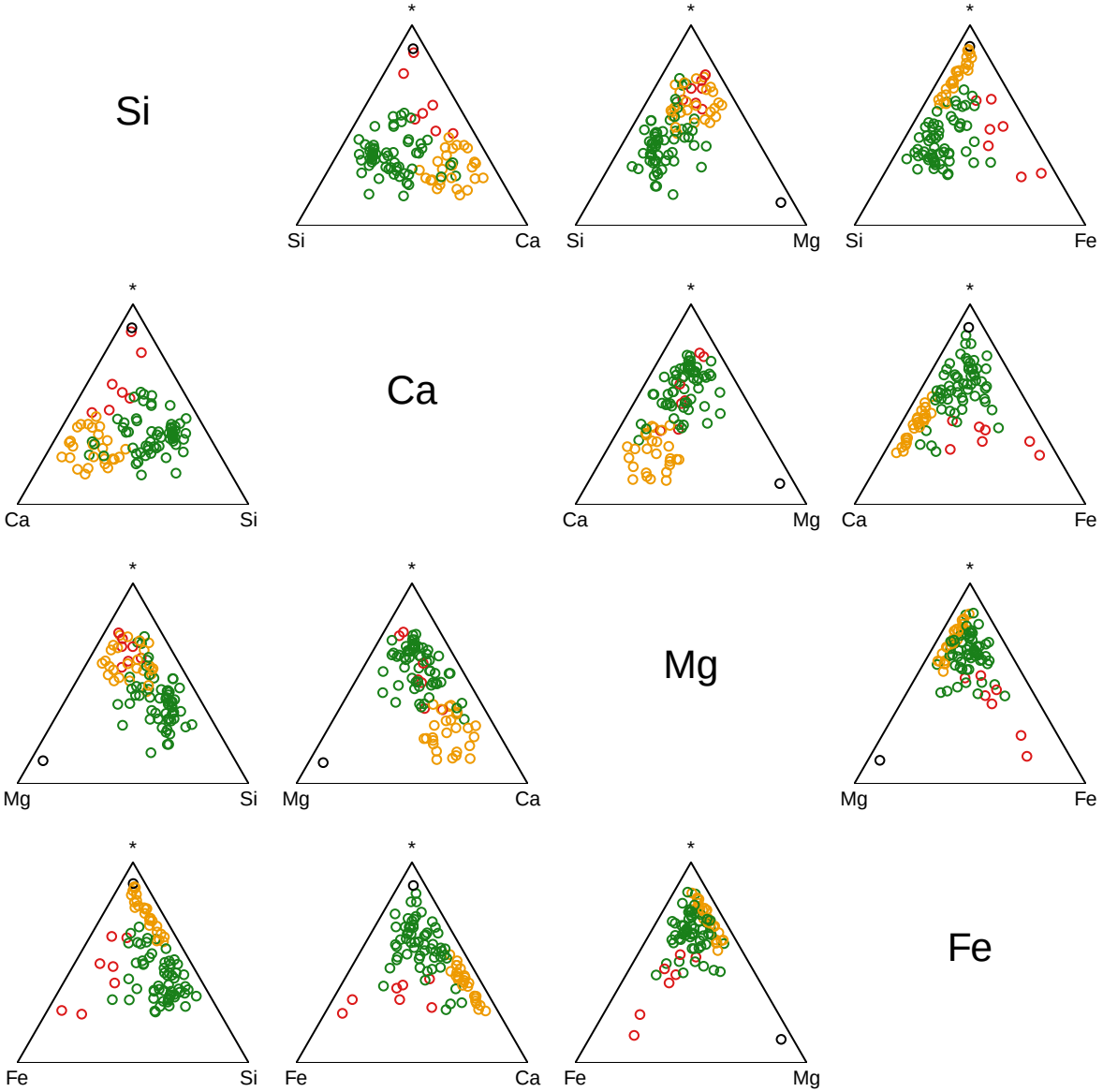
Na Mg

Si, Ca, Mg, Fe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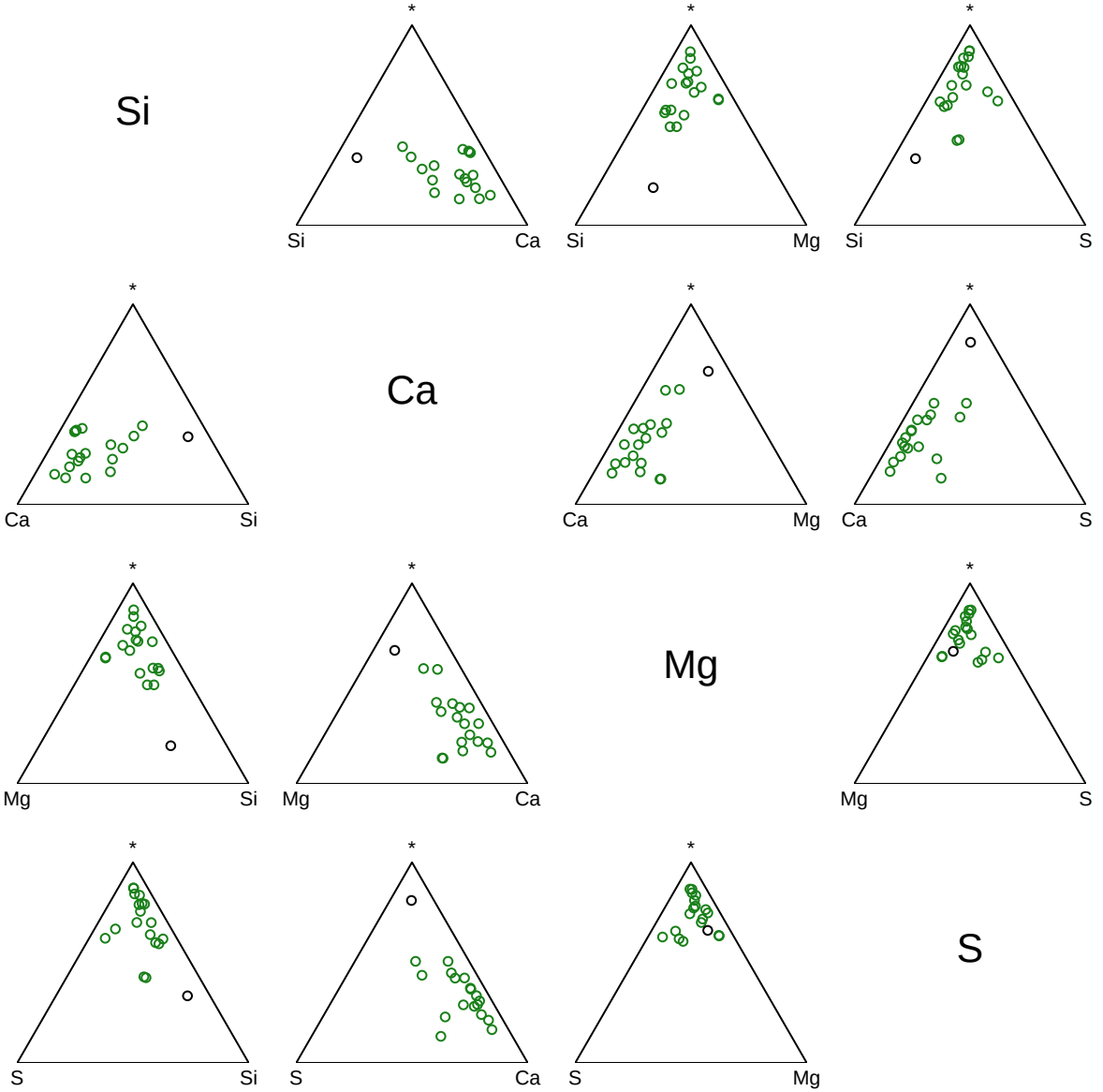
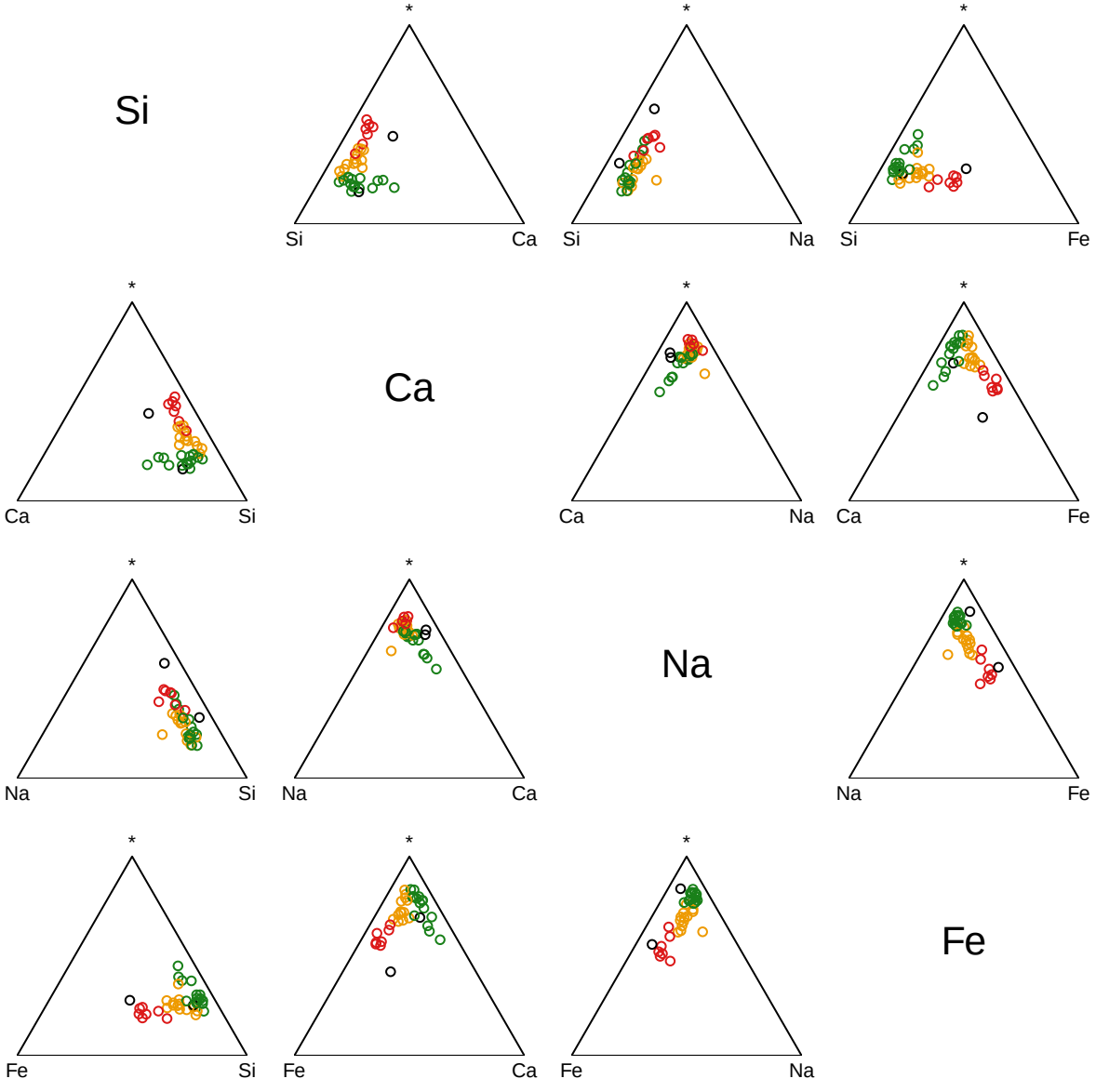
Si, Ca, Mg, S



Si, Ca, Na, Fe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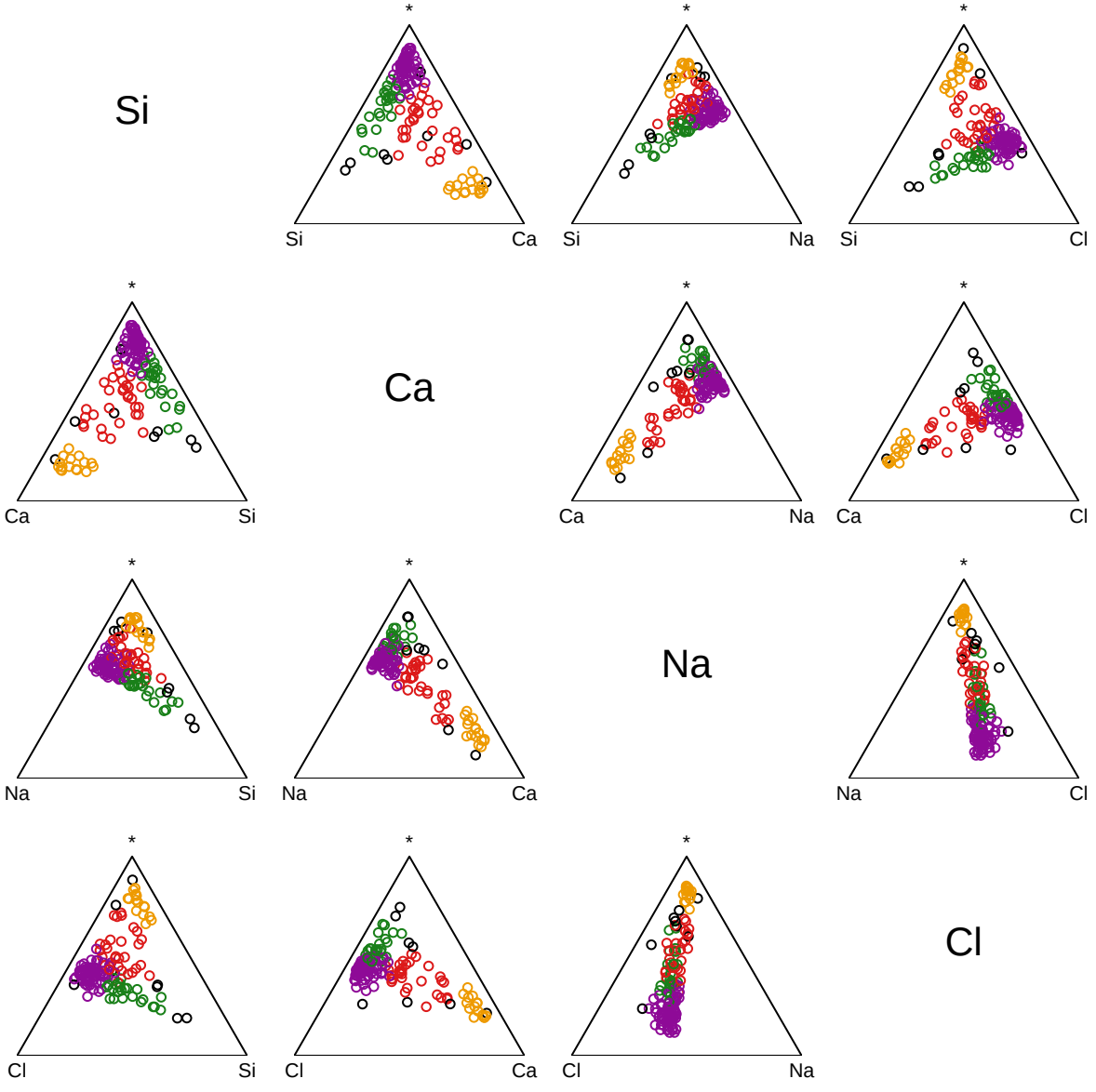
Si, Ca, Na, Cl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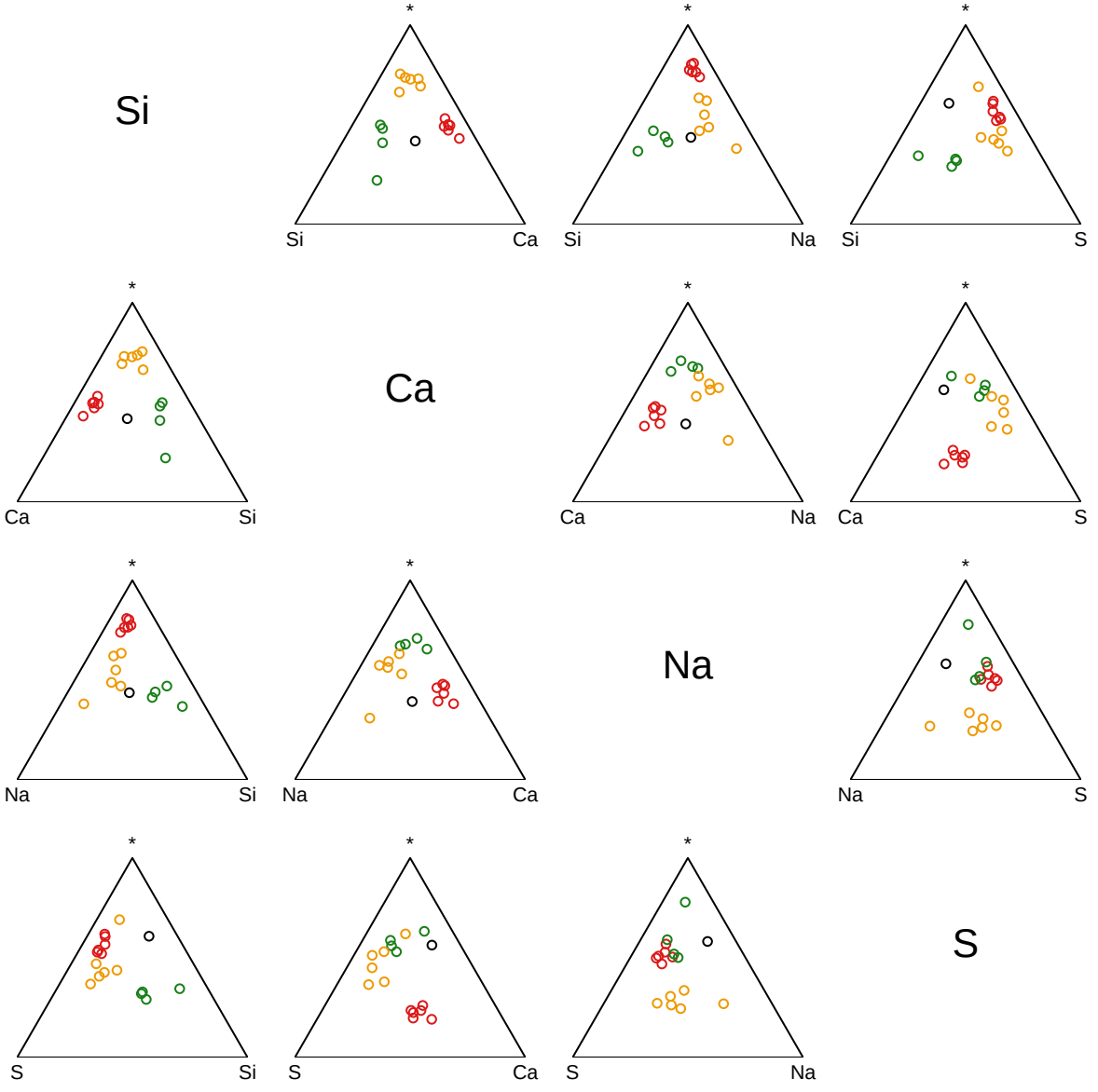
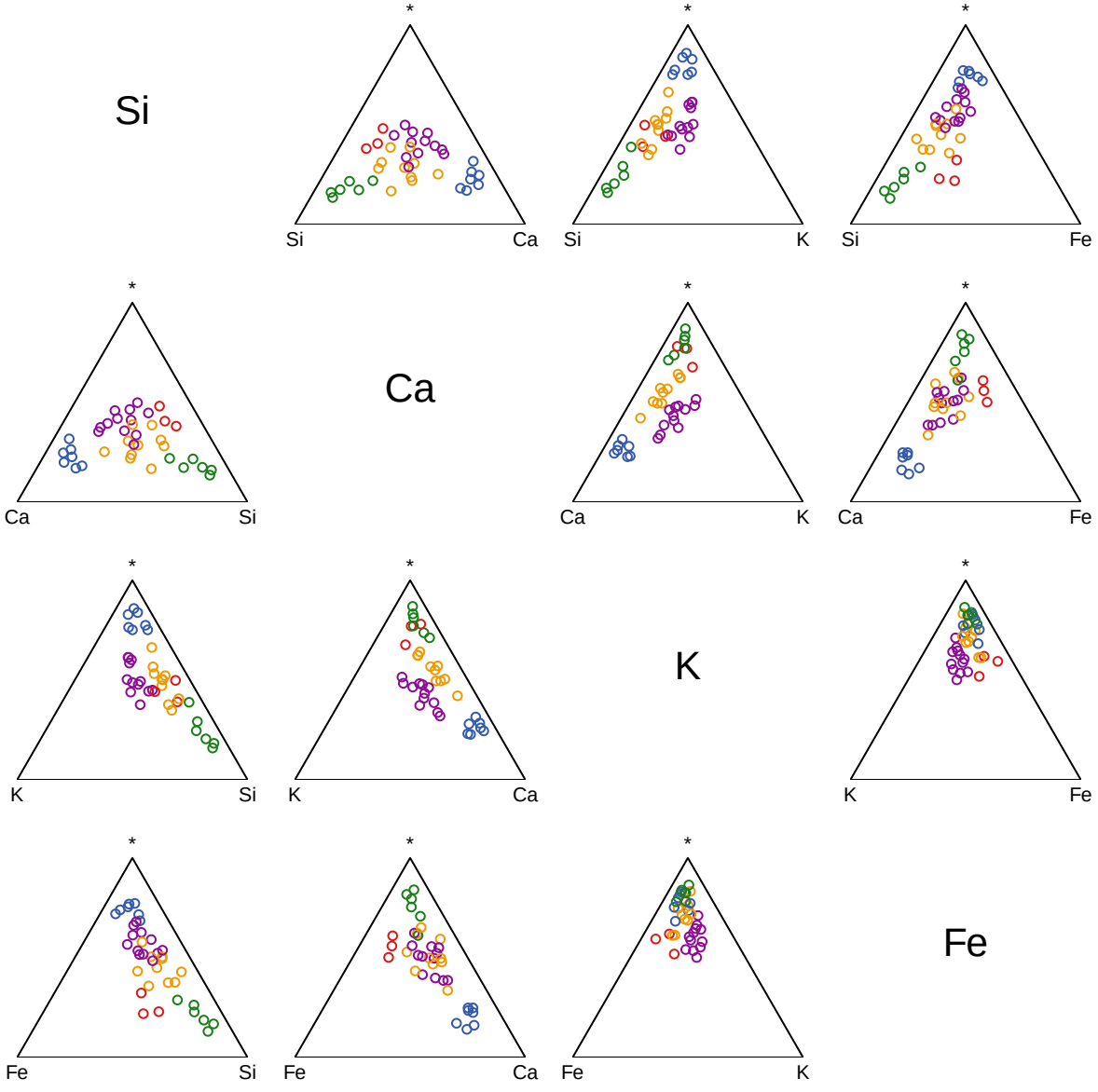
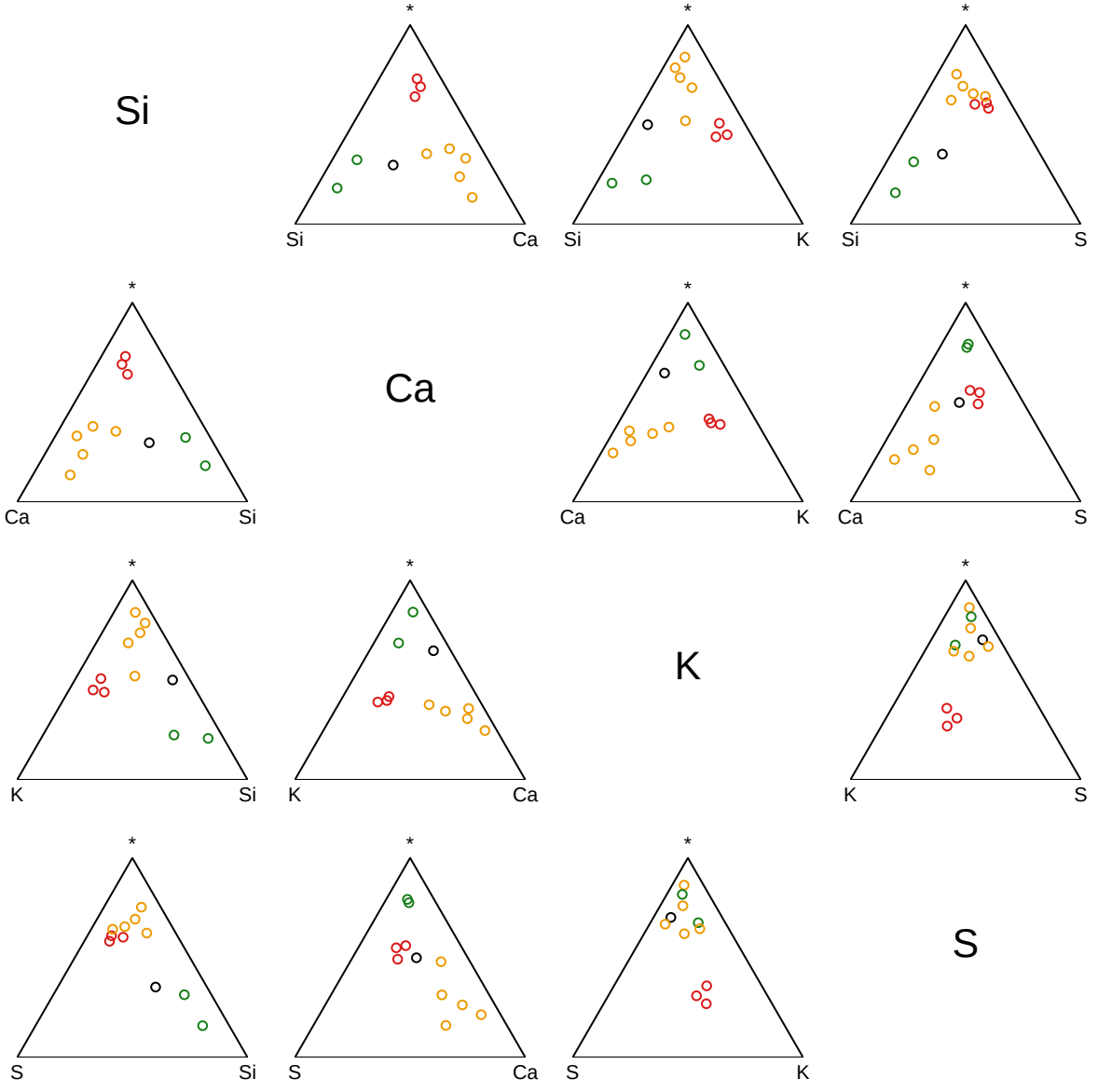
Si, Ca, Na, S



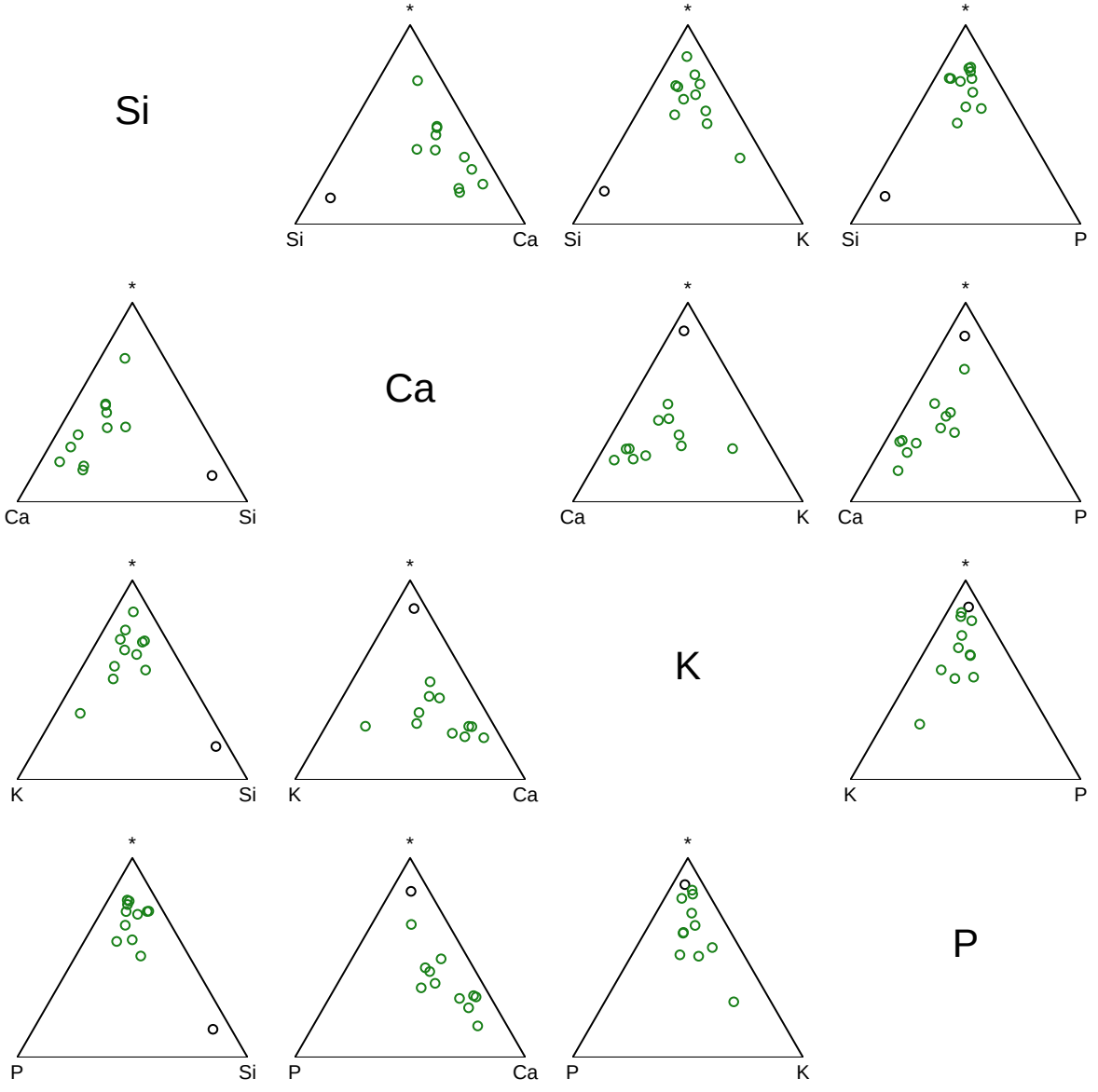
Si, Ca, K, Fe



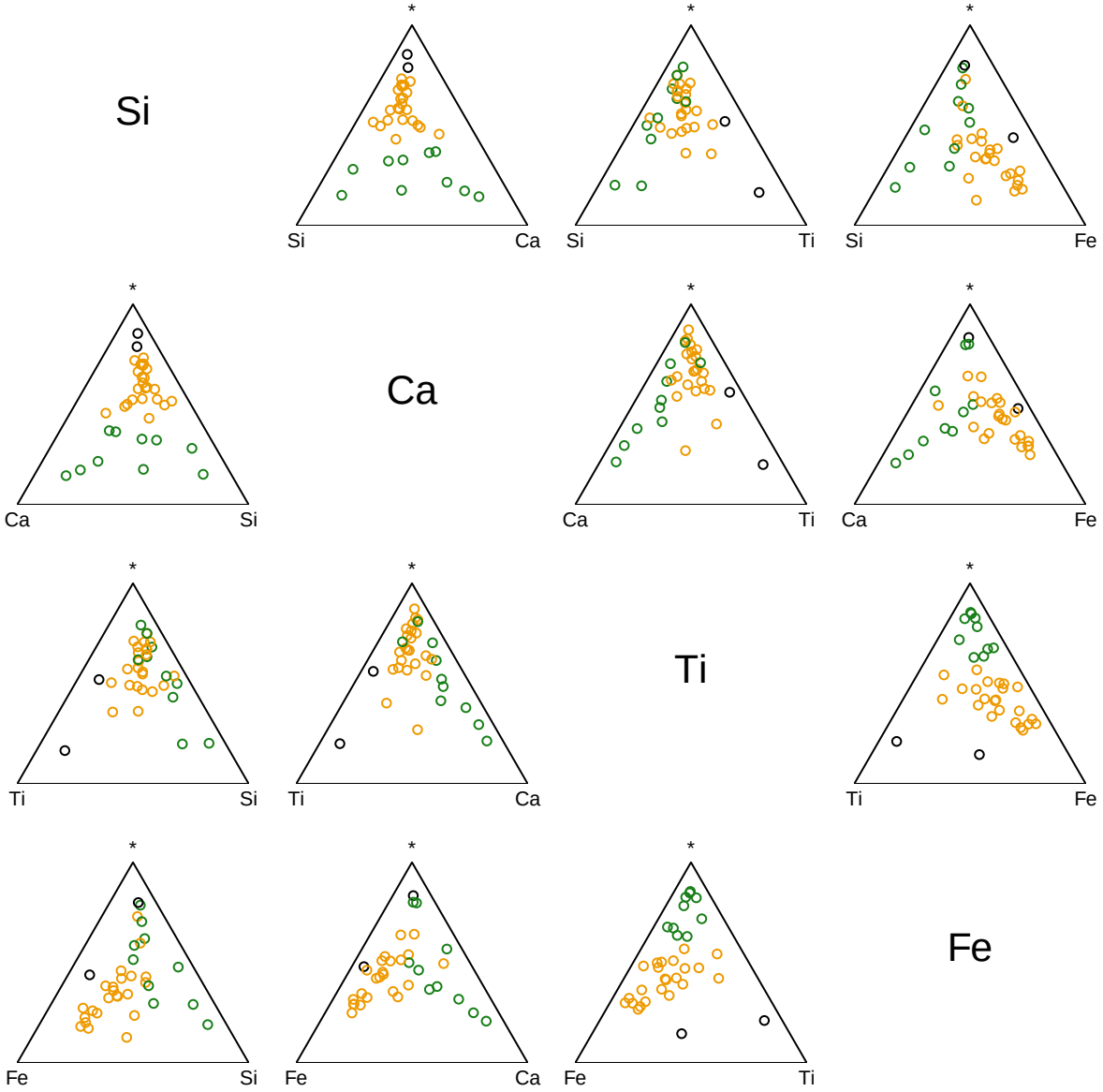
Si, Ca, K, S



Si, Ca, K, P



Si, Ca, Ti, Fe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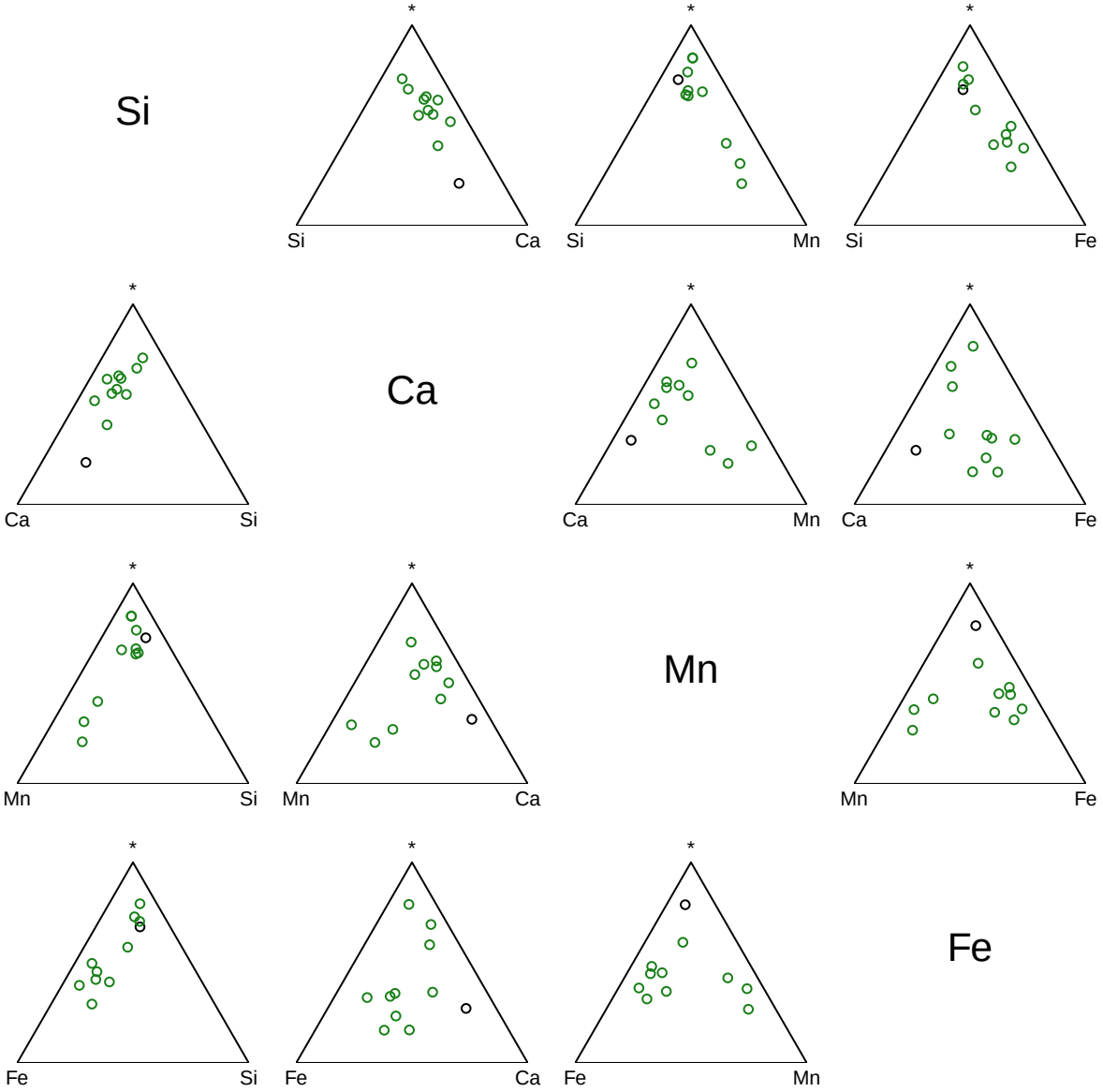
Si, Ca, Mn, Fe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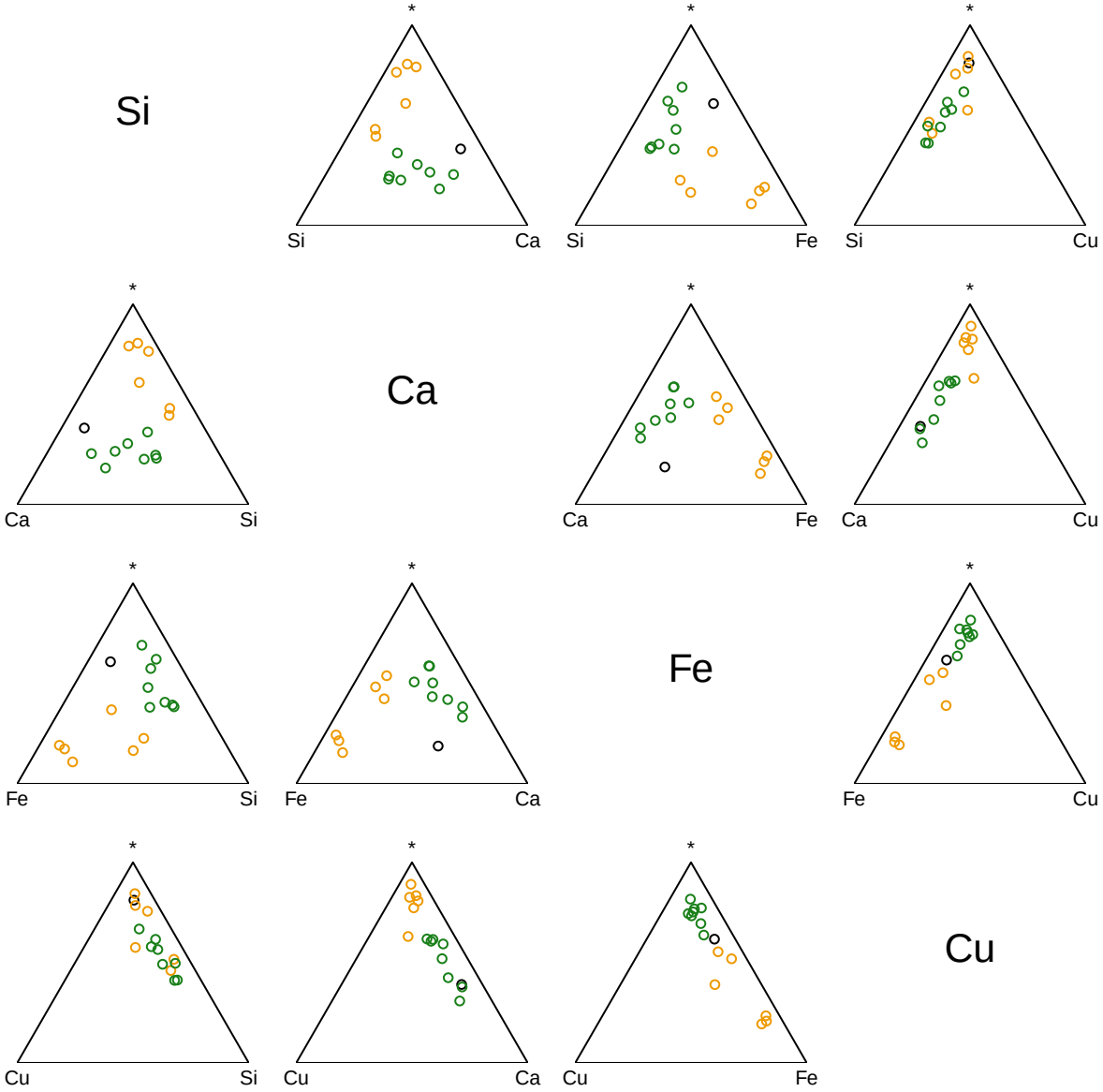
Si, Ca, Fe, Cu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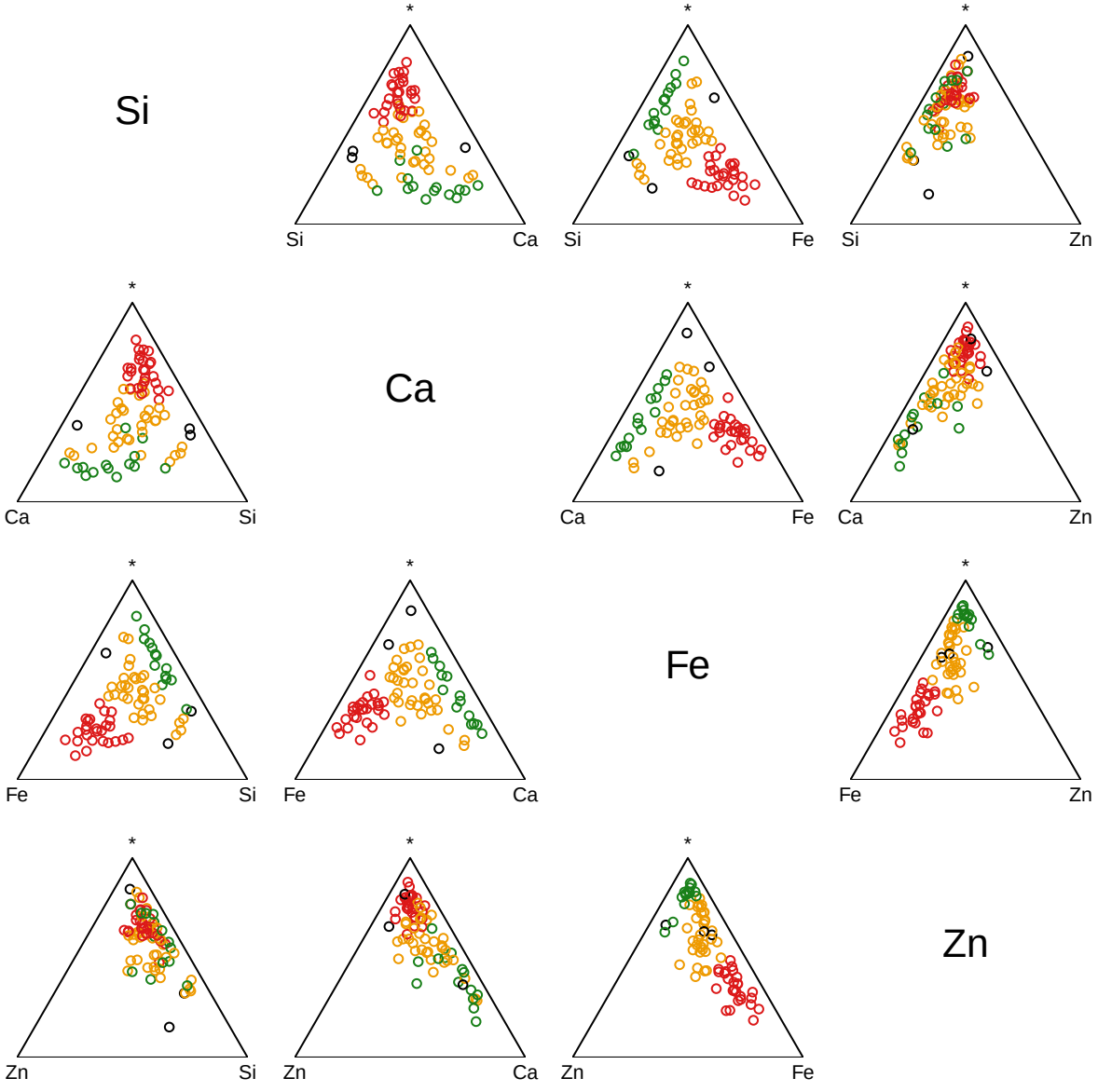
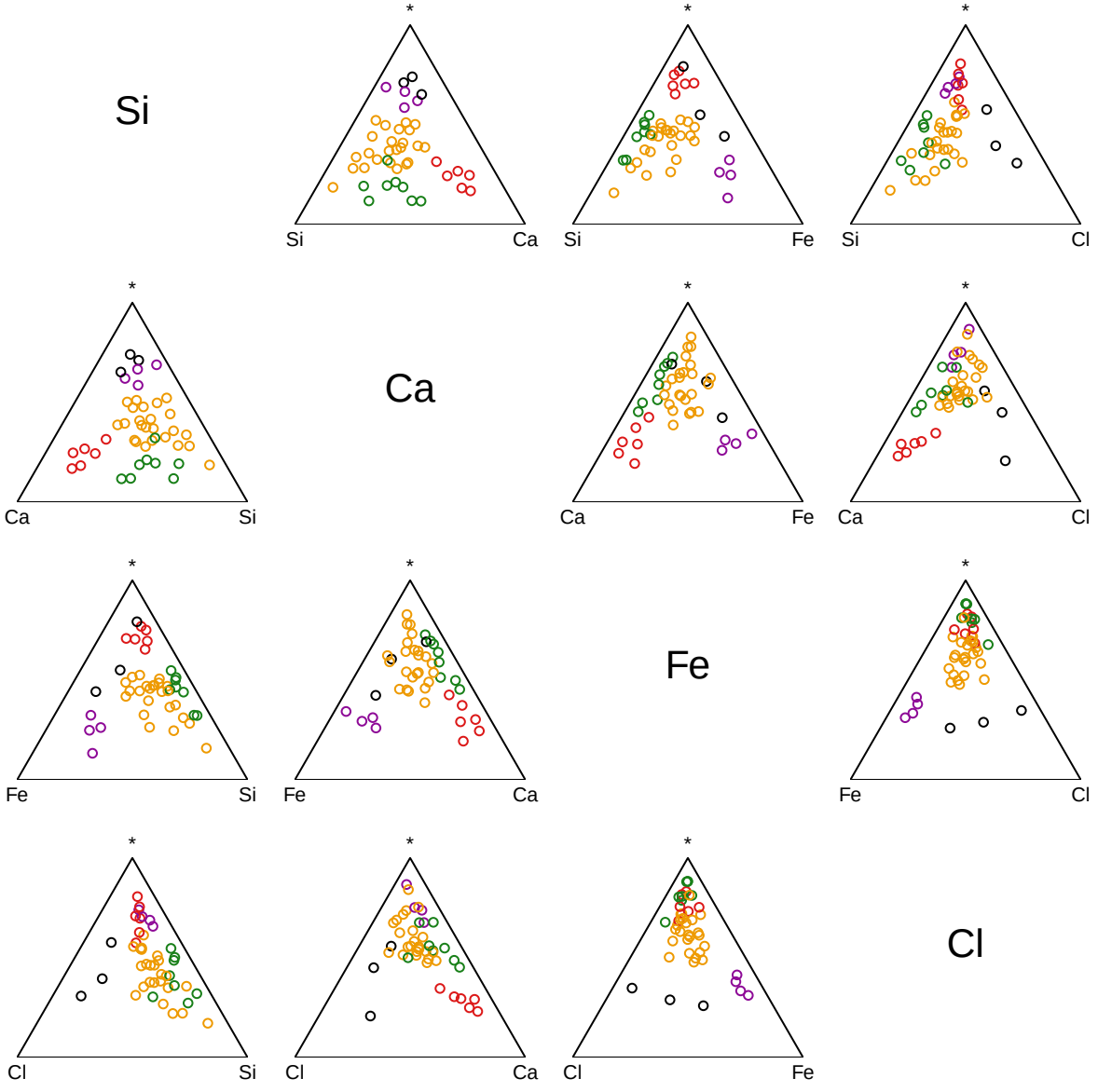
Fe

Si, Ca, Fe, Zn



Si, Ca, Fe, Cl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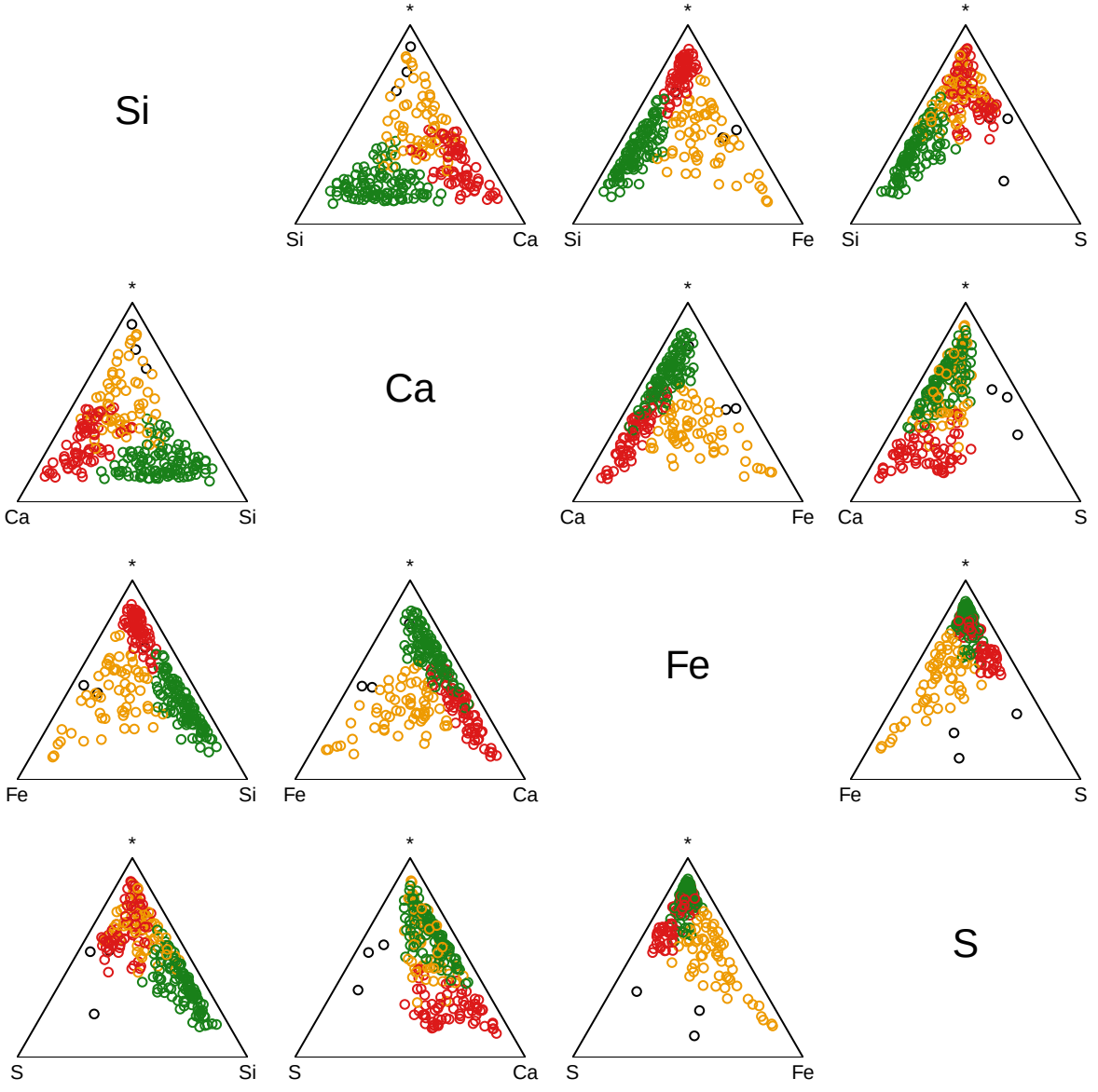
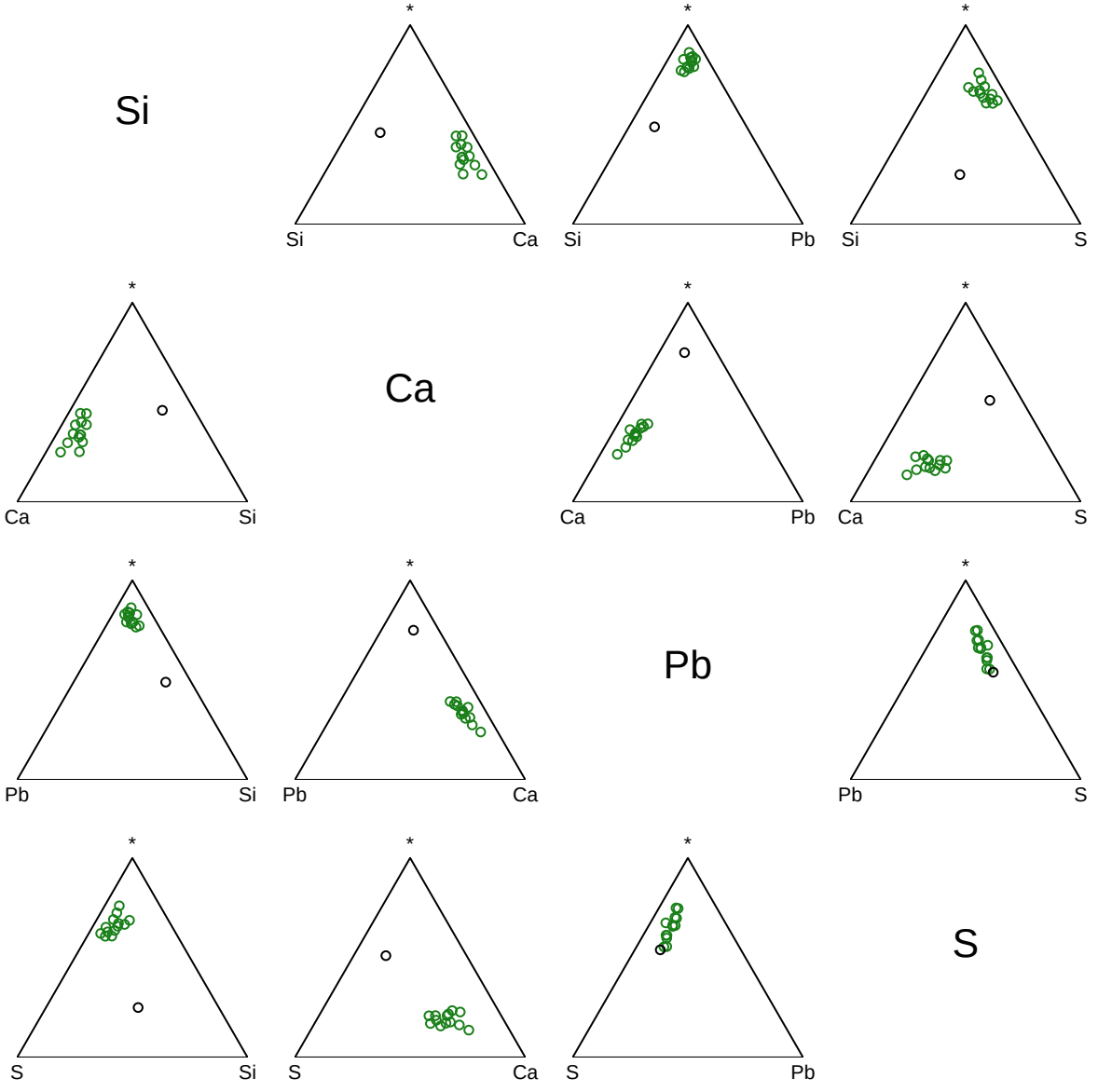
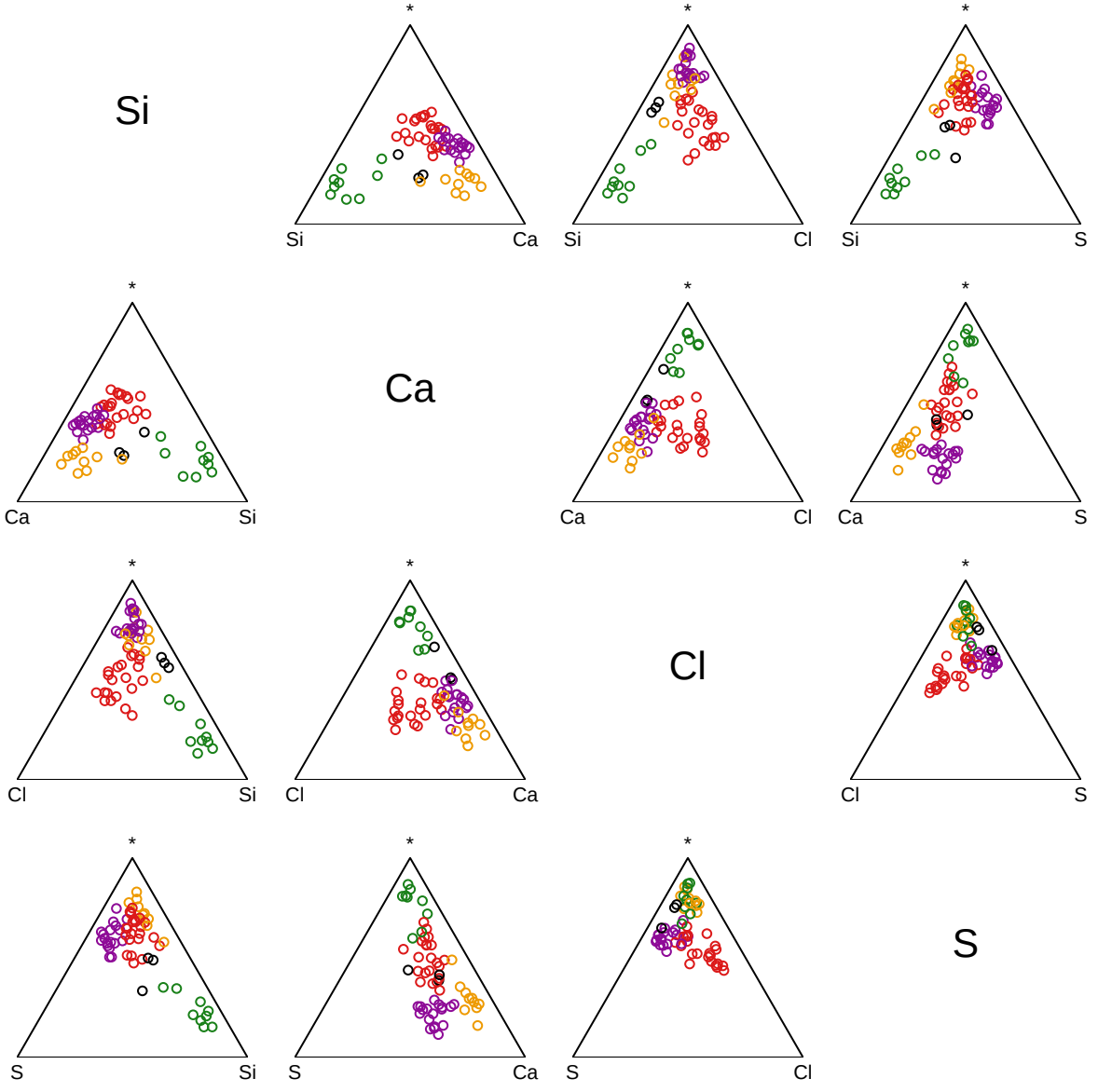
Si, Ca, Fe, S



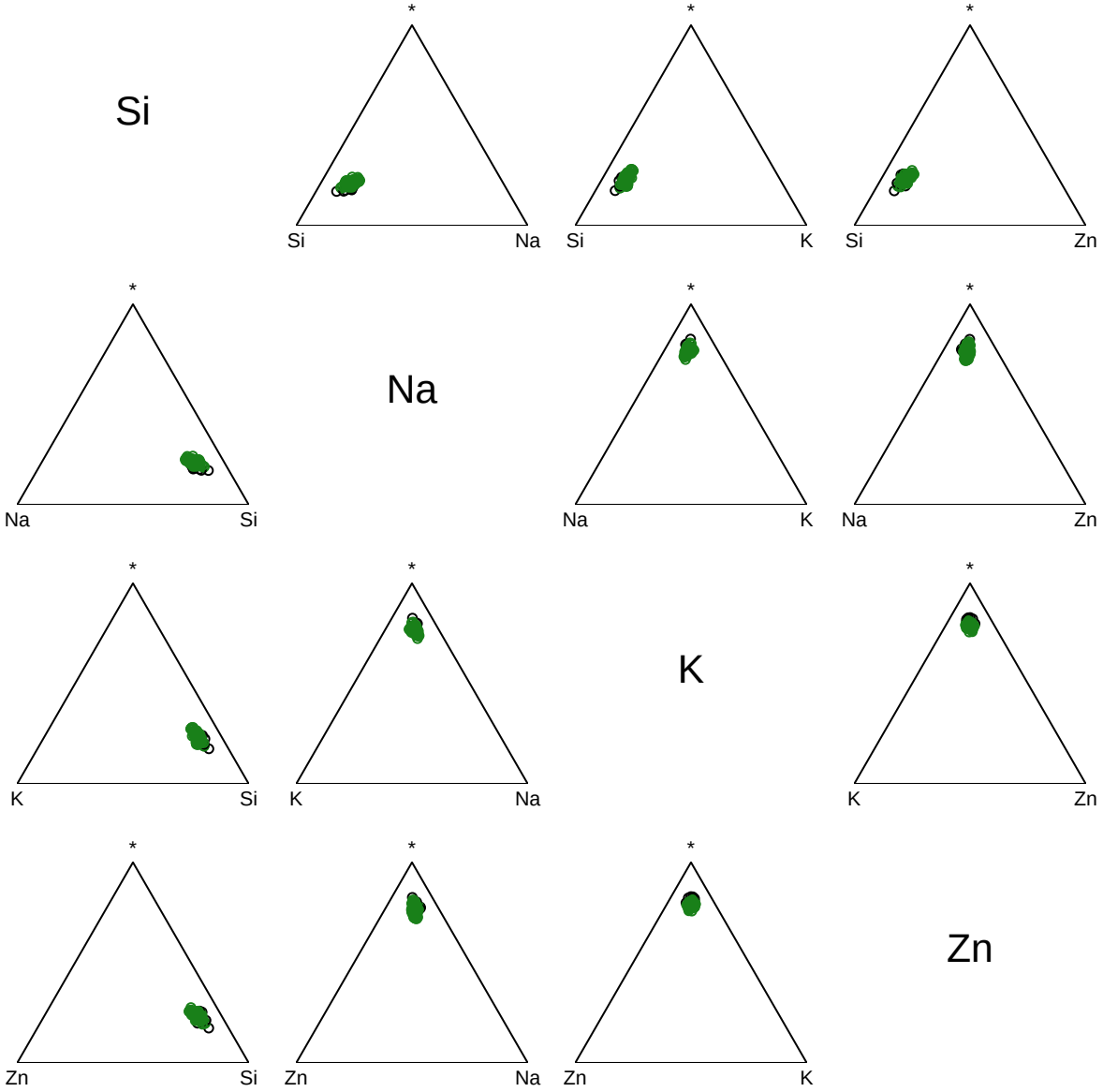
Si, Ca, Pb, S



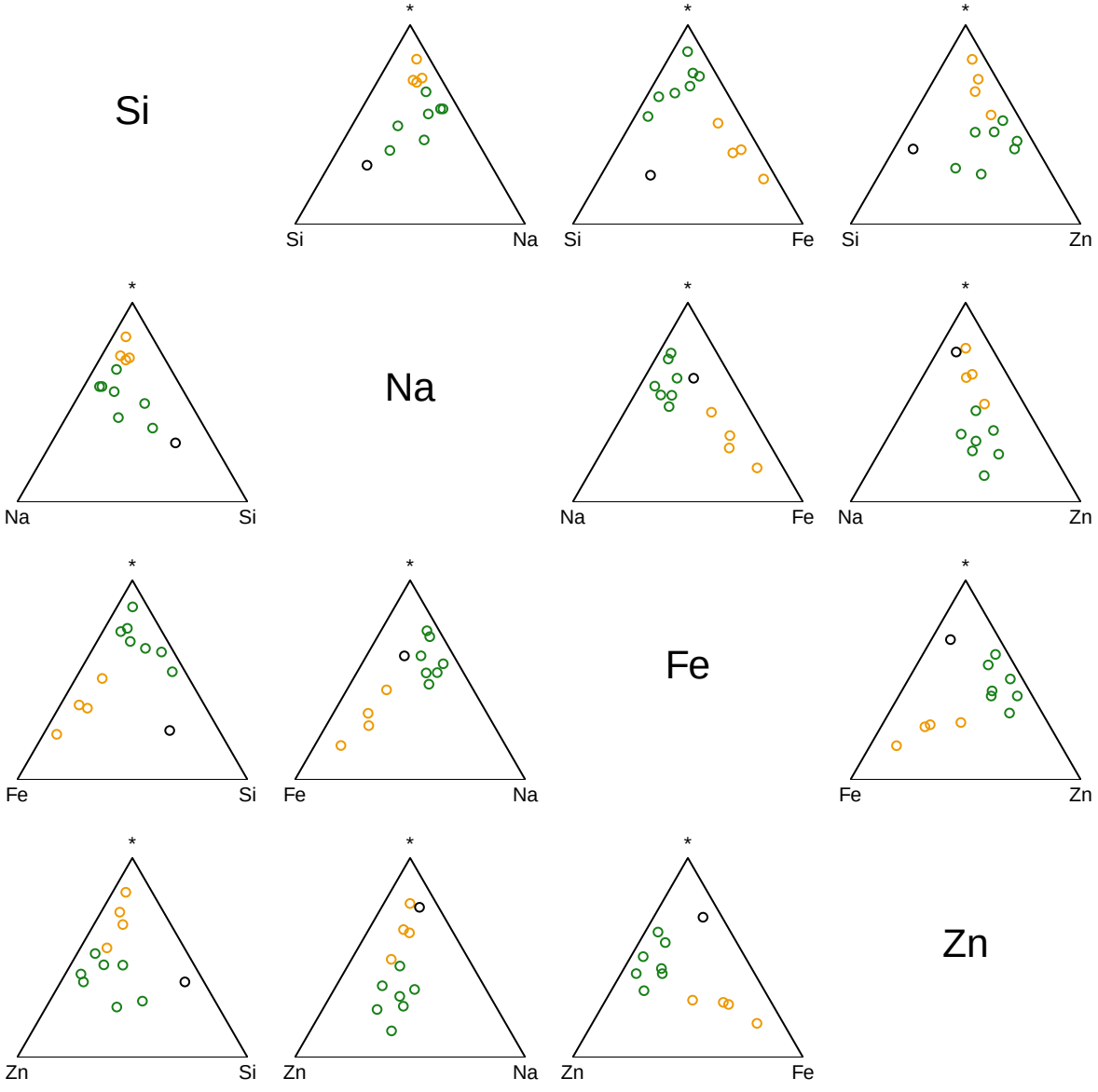
Si, Ca, Cl, S



Si, Na, K, Zn



Si, Na, Fe, Zn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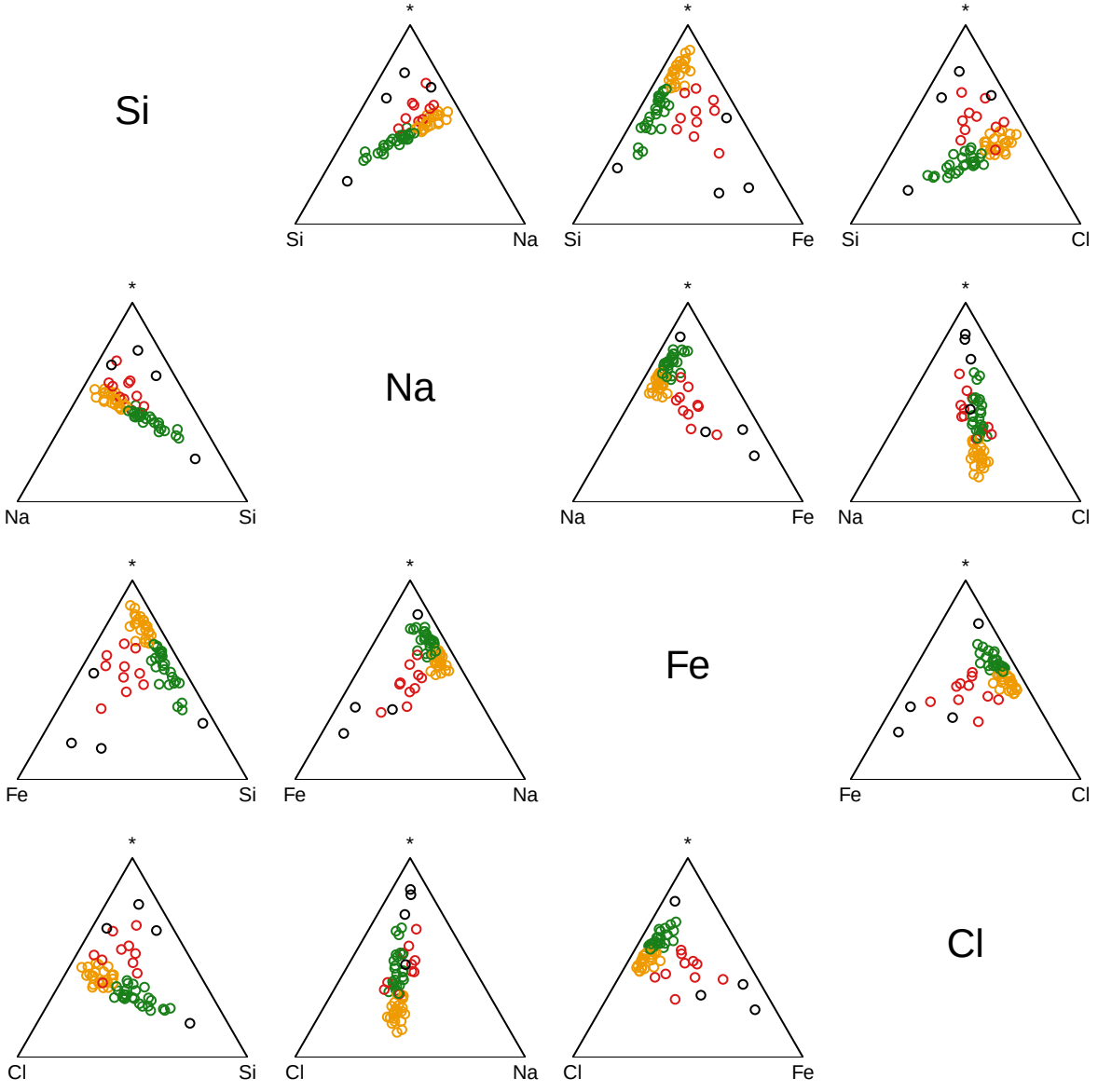
Si, Na, Fe, Cl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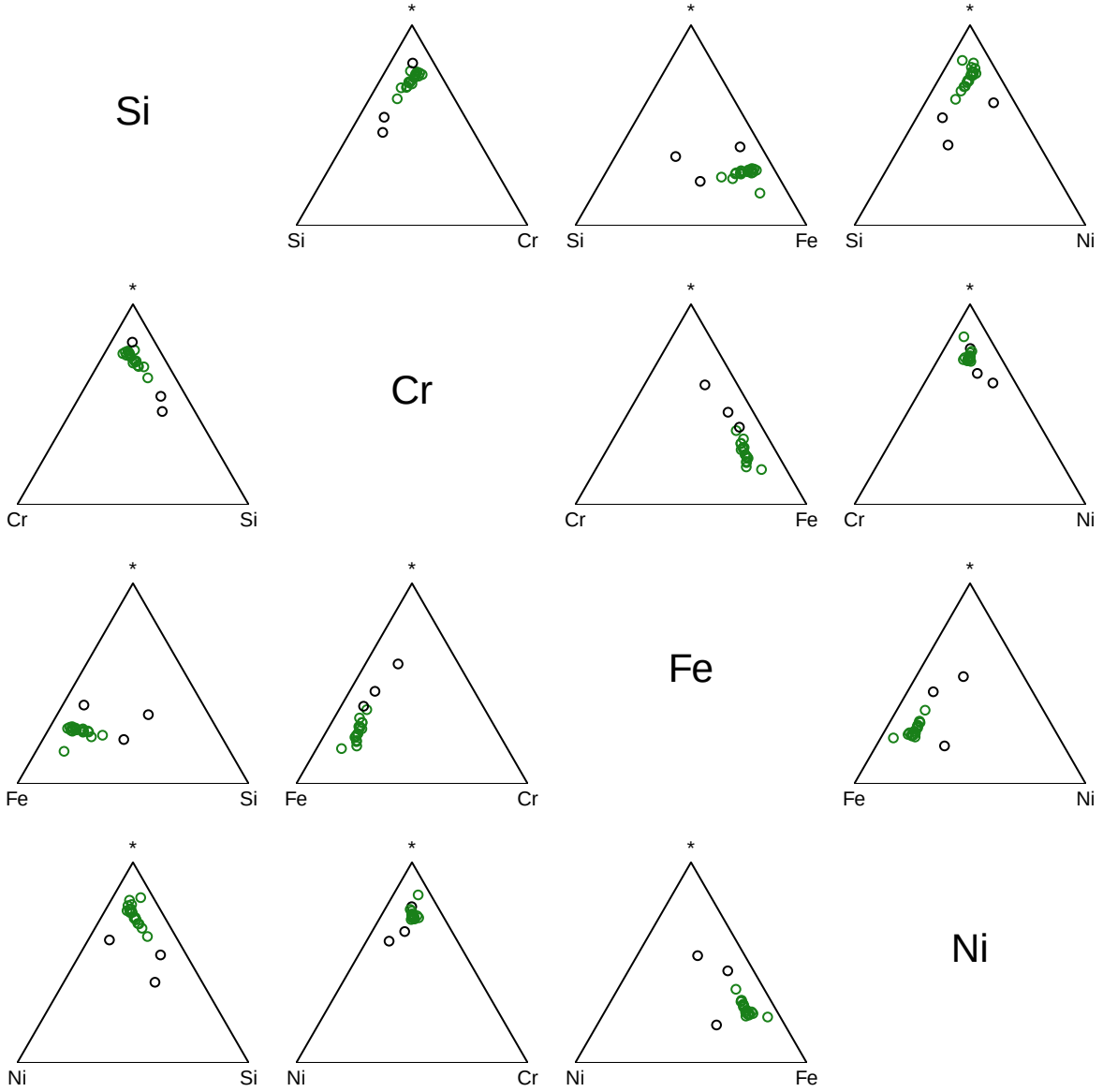
Si, Cr, Fe, Ni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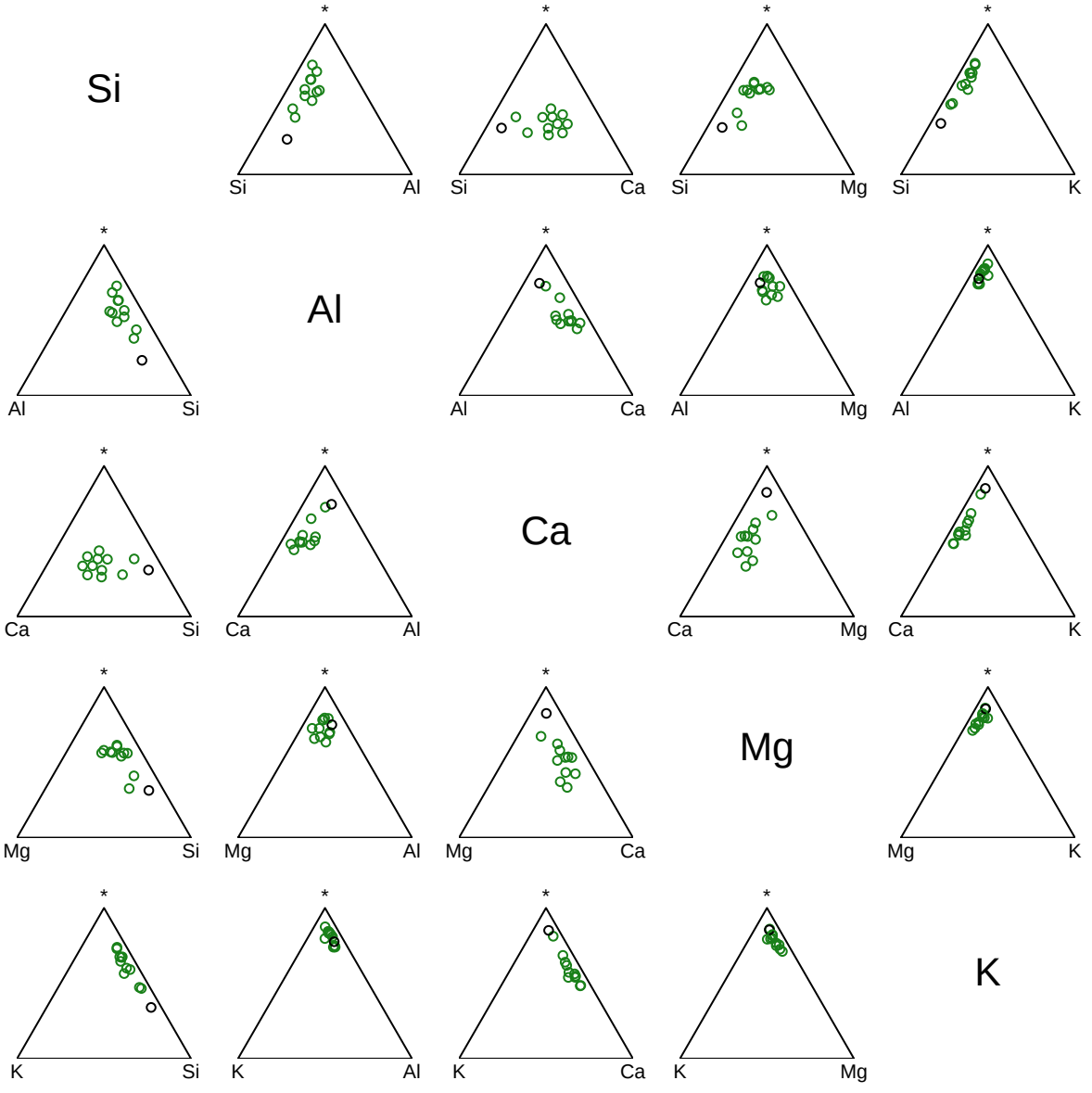
Si, Al, Ca, Mg, K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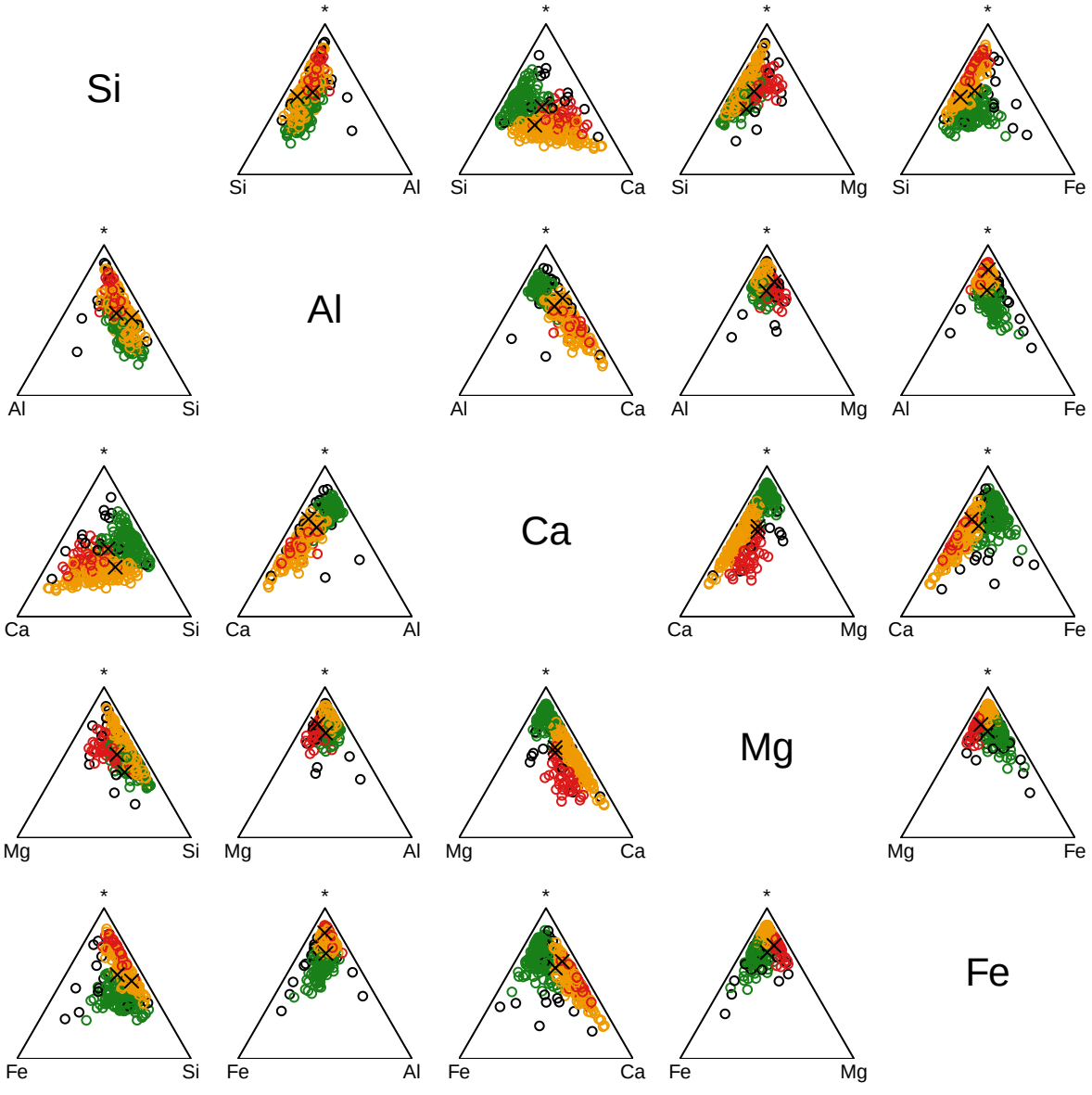
Si, Al, Ca, Mg, Fe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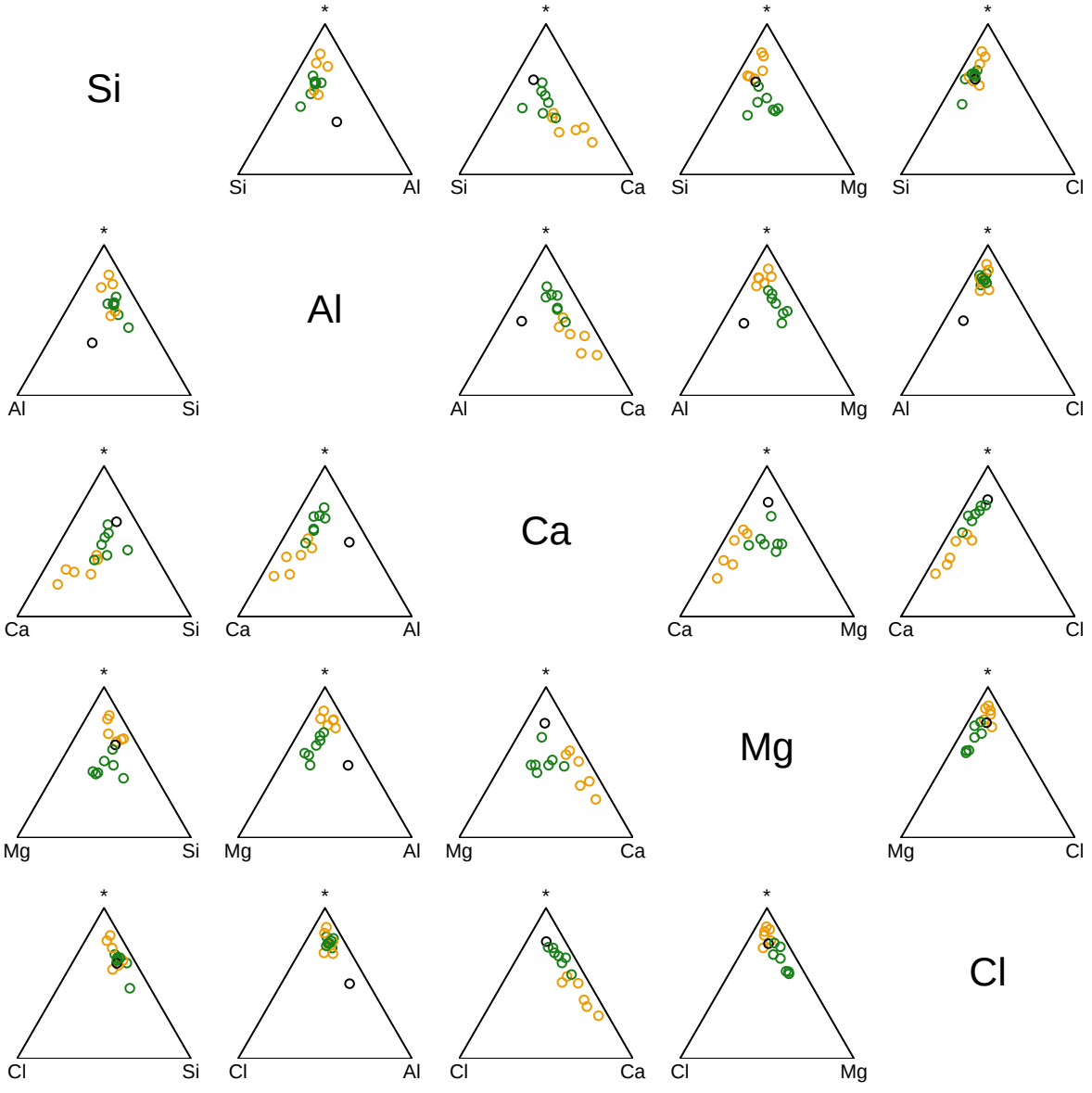
Si, Al, Ca, Mg, Cl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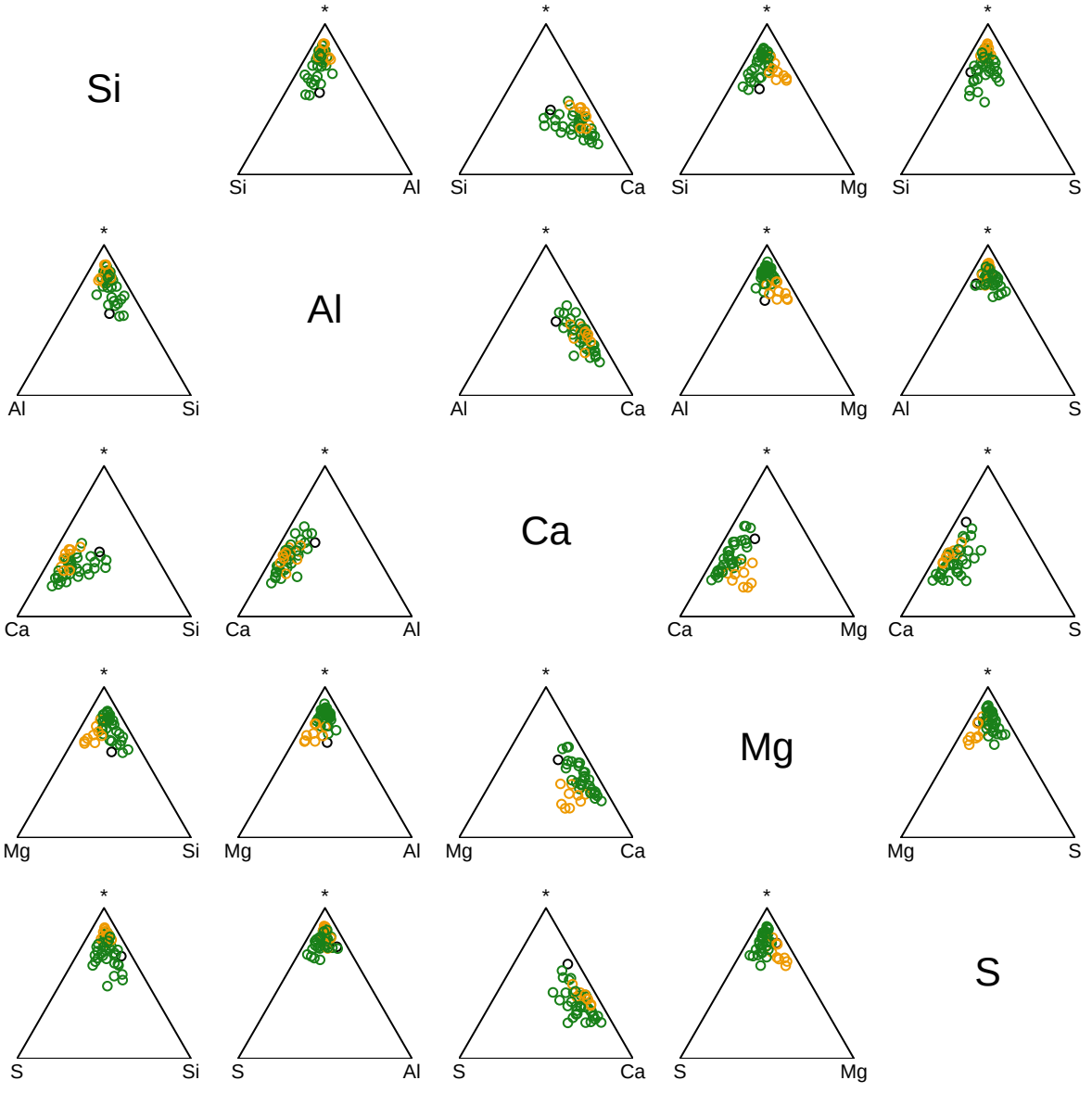
Si, Al, Ca, Mg, S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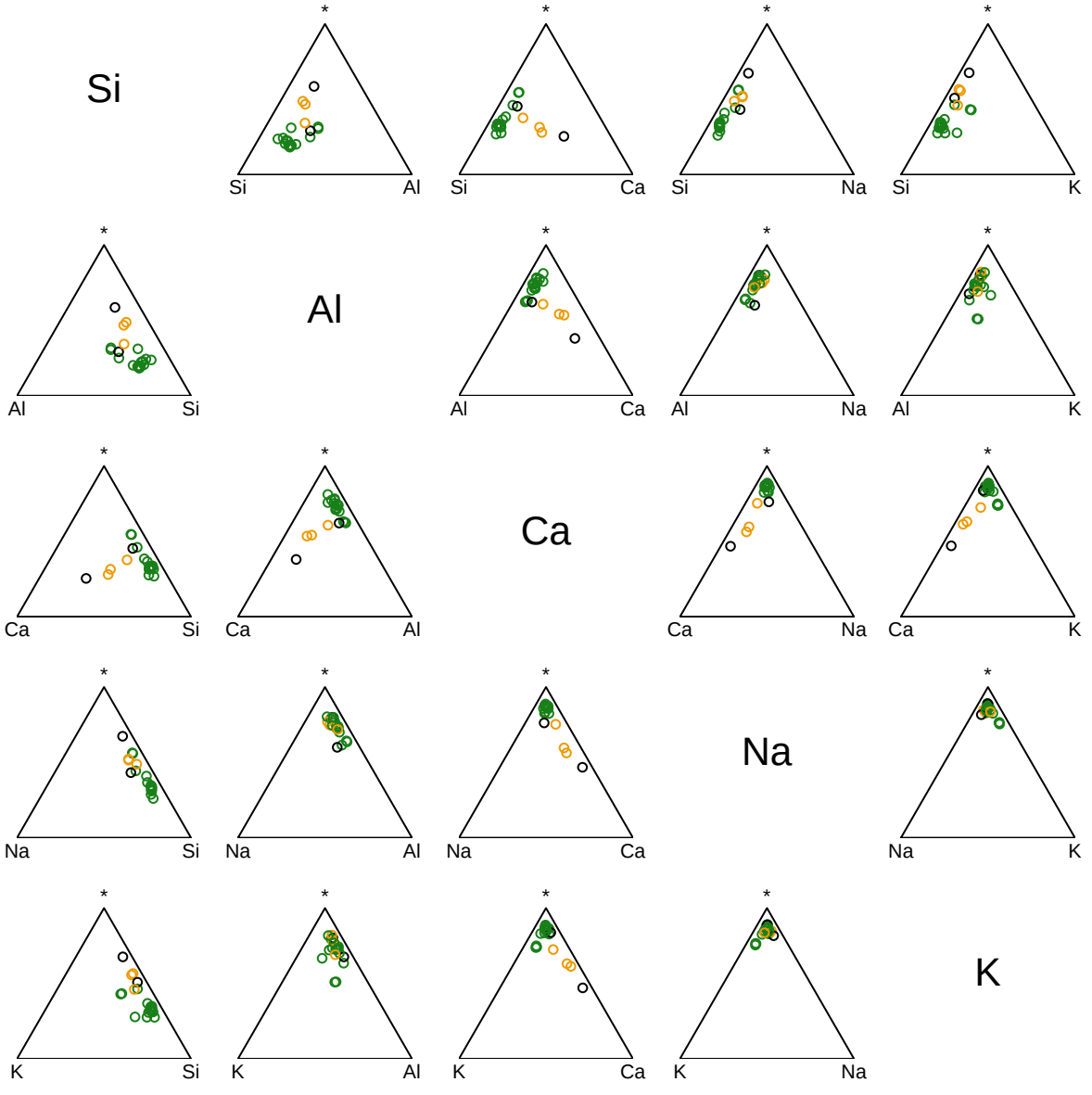
Si, Al, Ca, Na, K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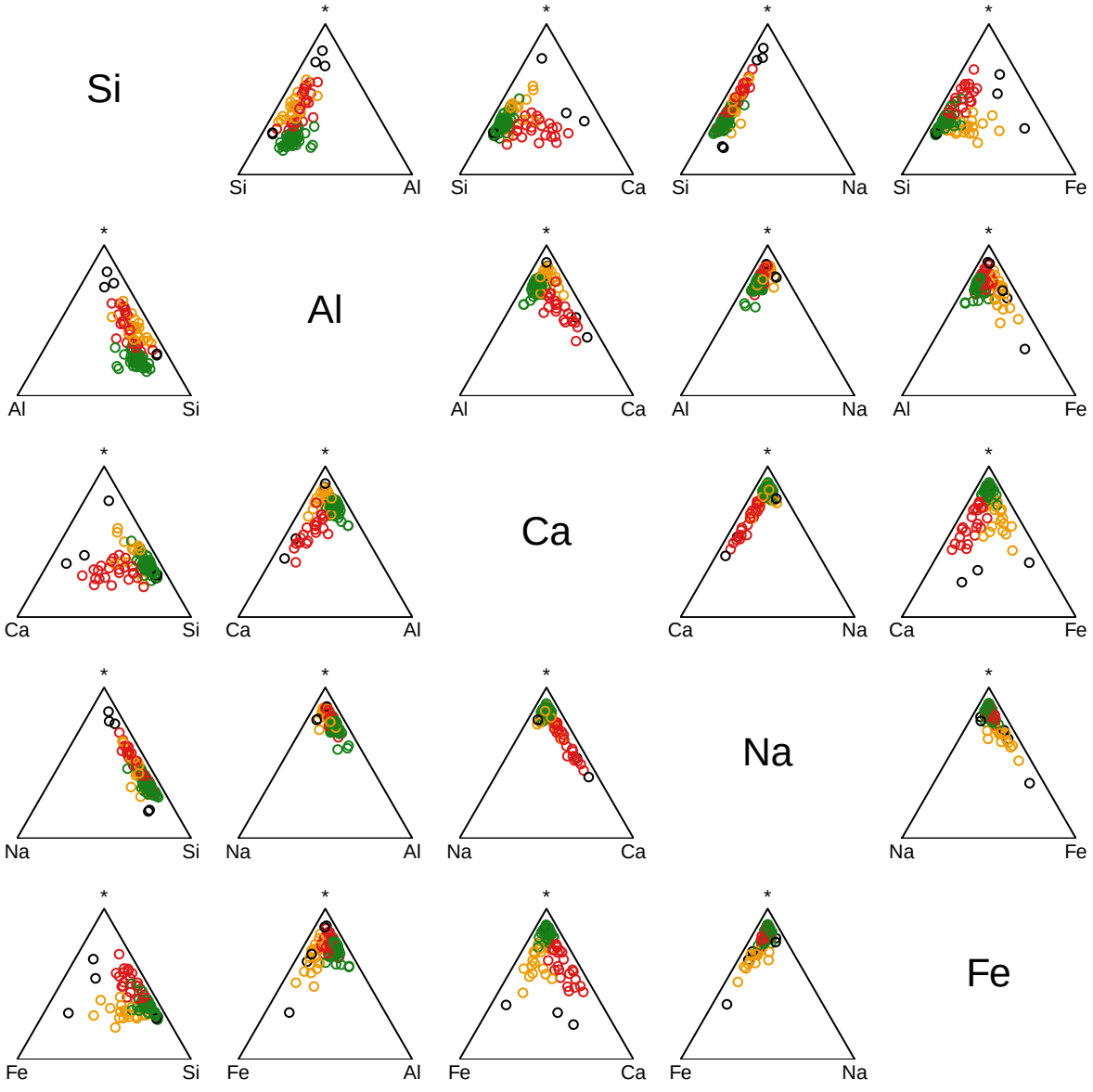
Si, Al, Ca, Na, Fe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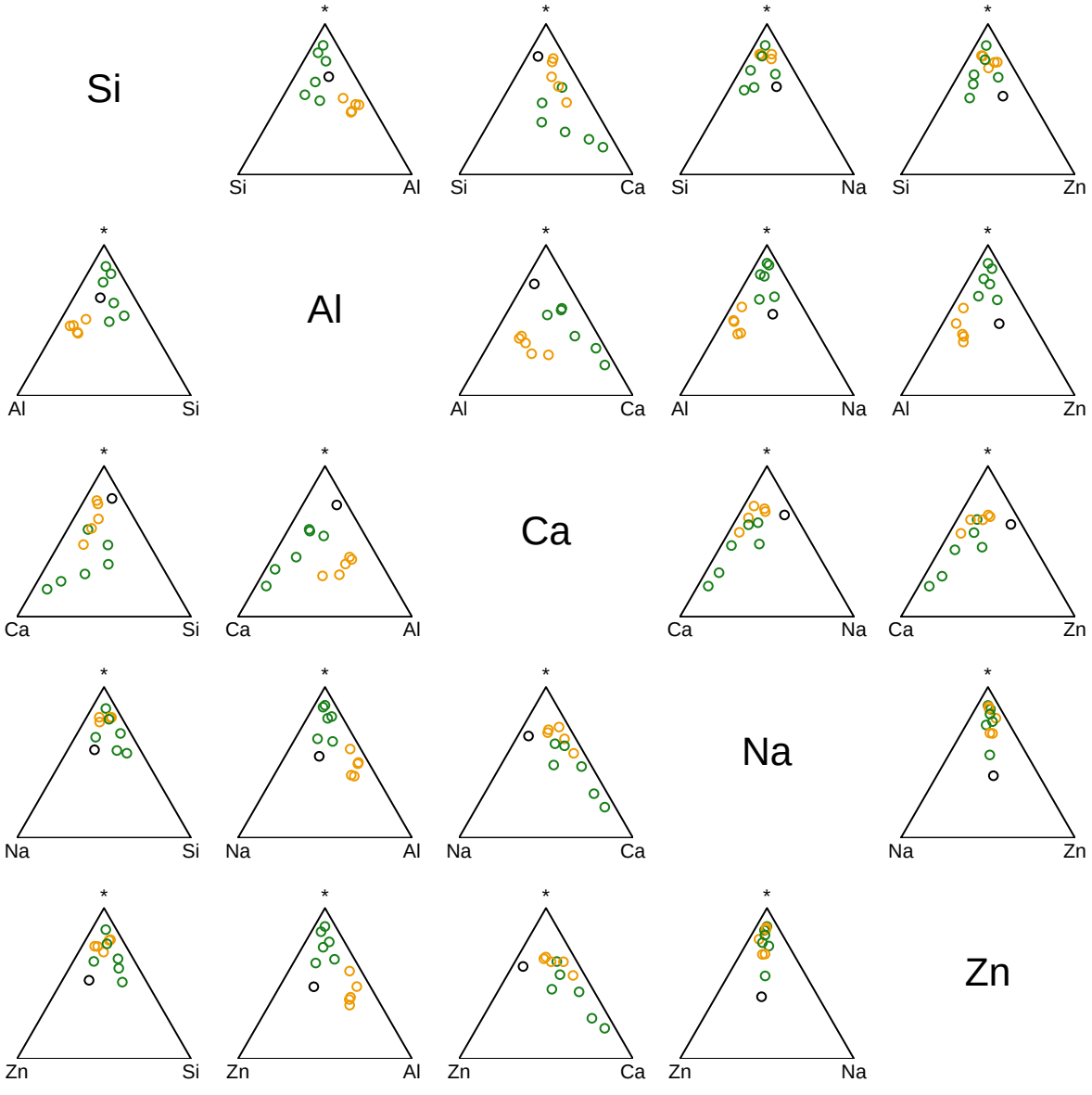
Si, Al, Ca, Na, Zn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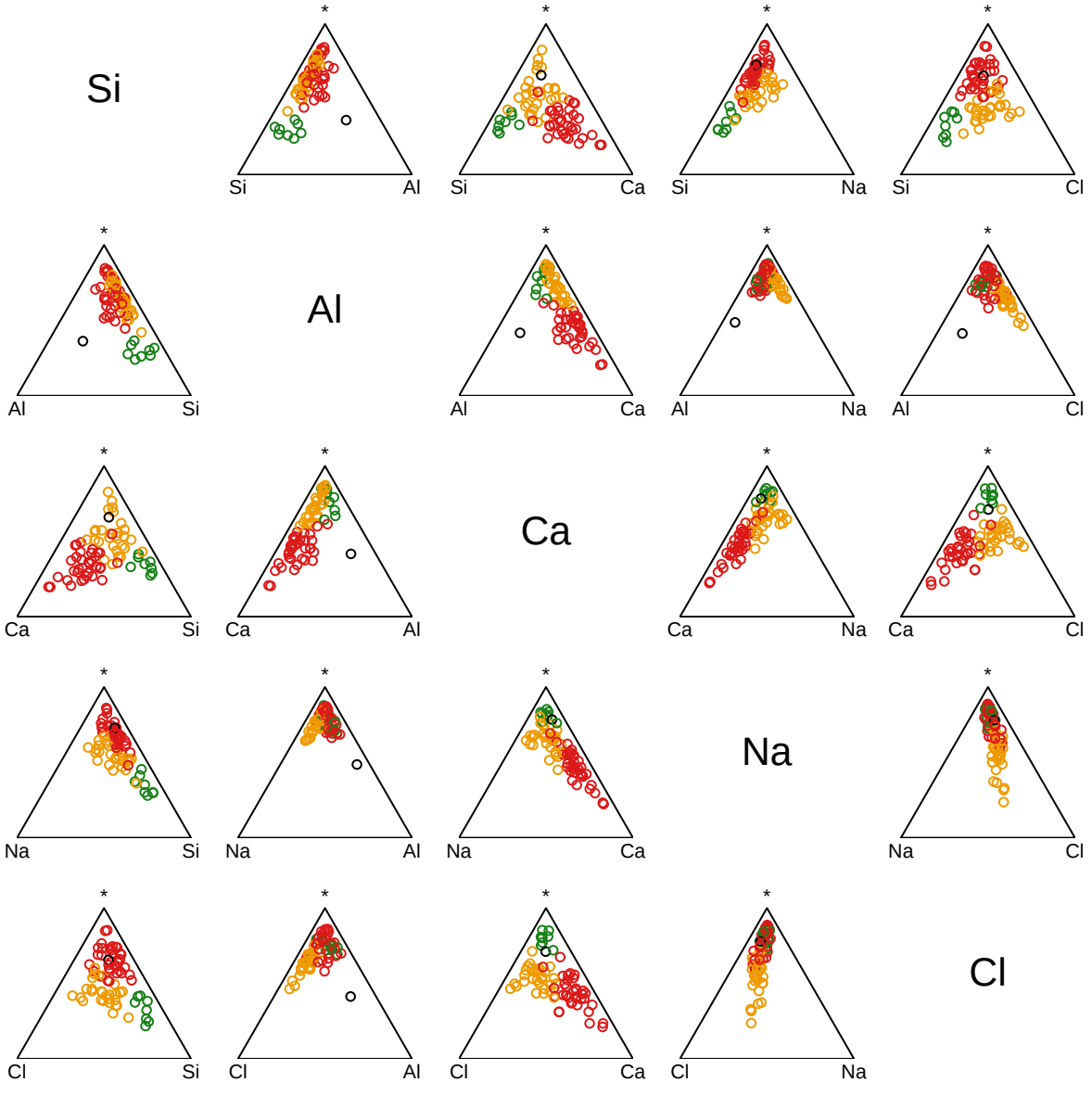
Si, Al, Ca, Na, Cl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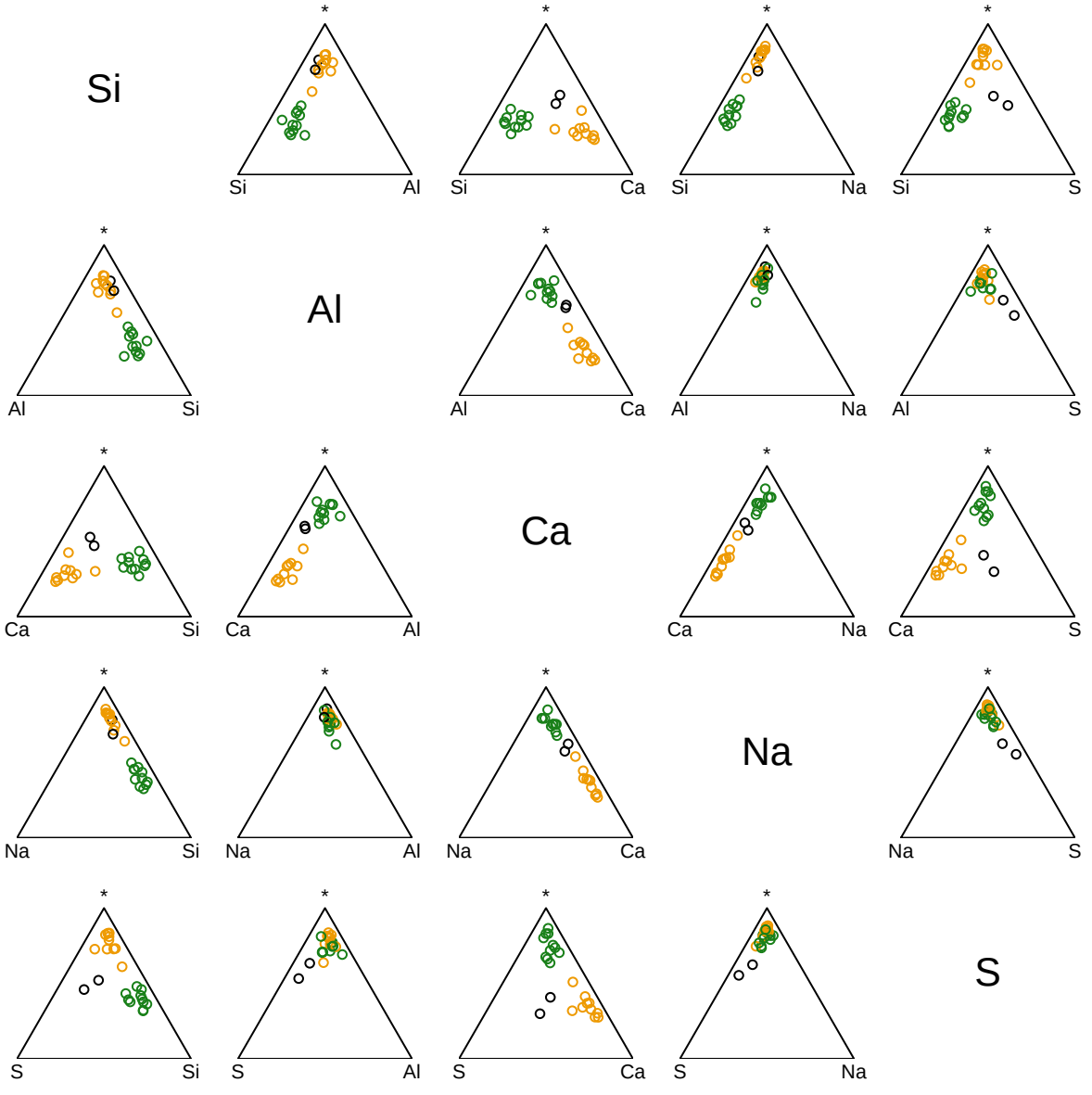
Si, Al, Ca, Na, S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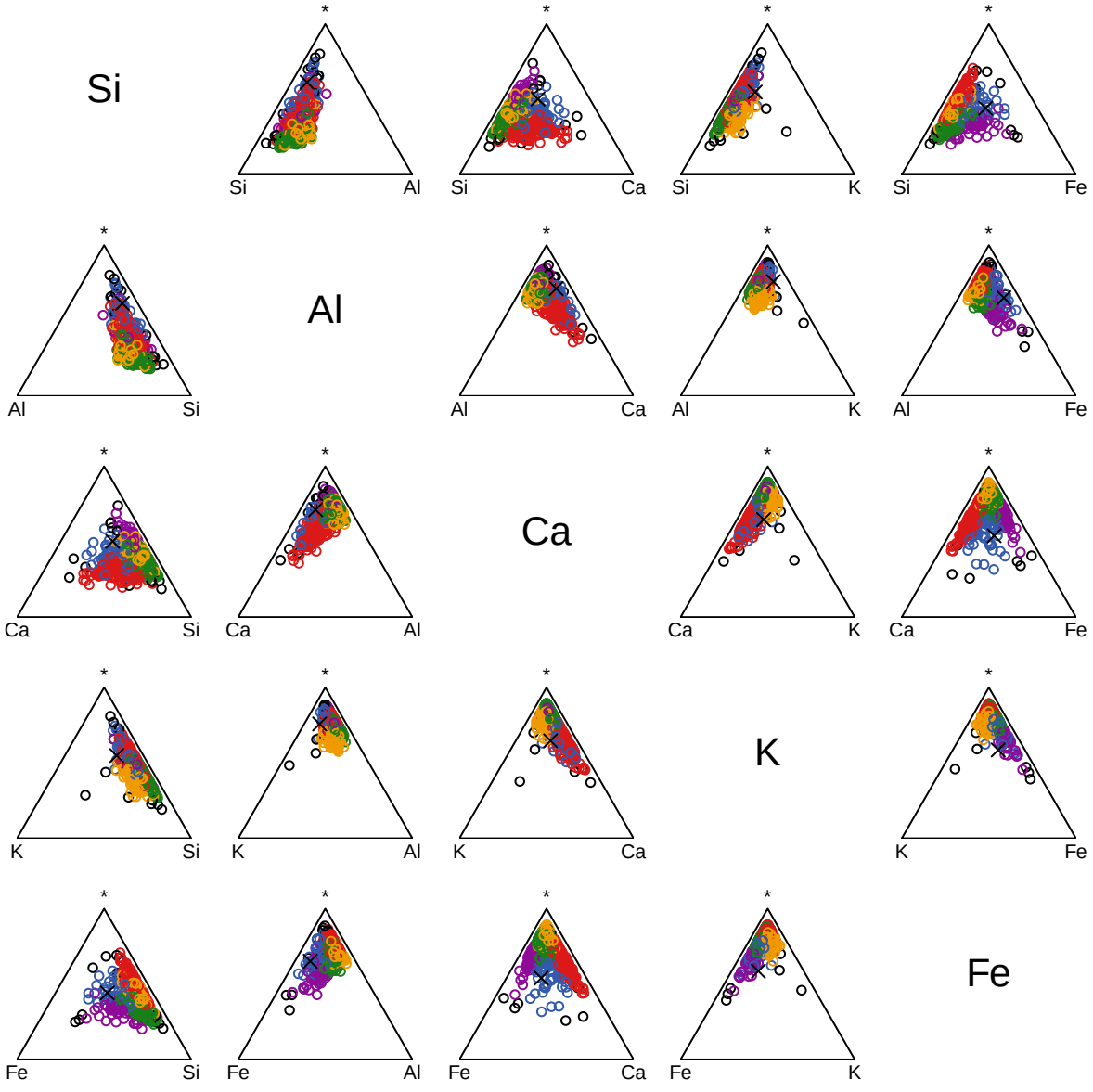
Si, Al, Ca, K, Fe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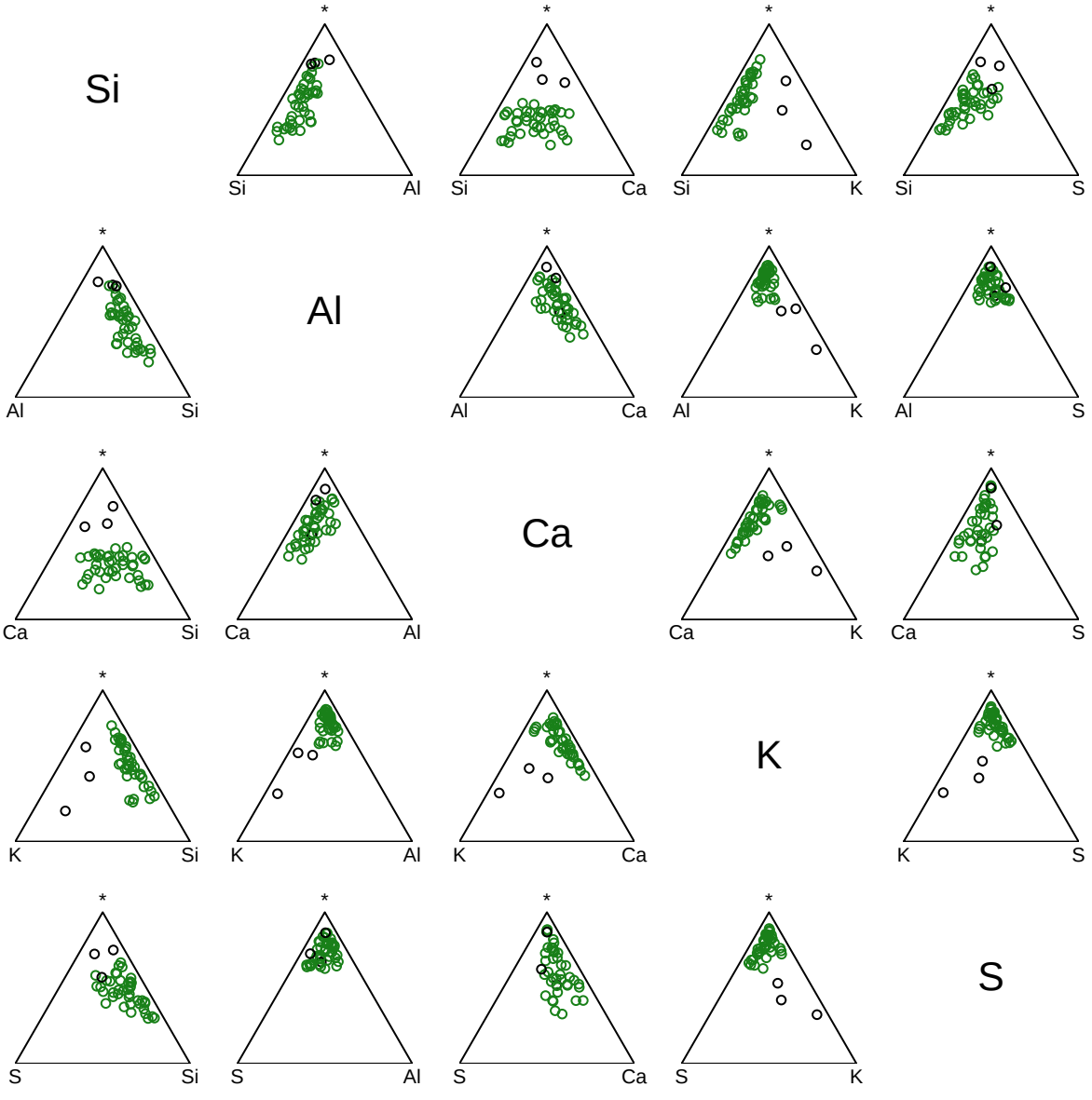
Si, Al, Ca, K, S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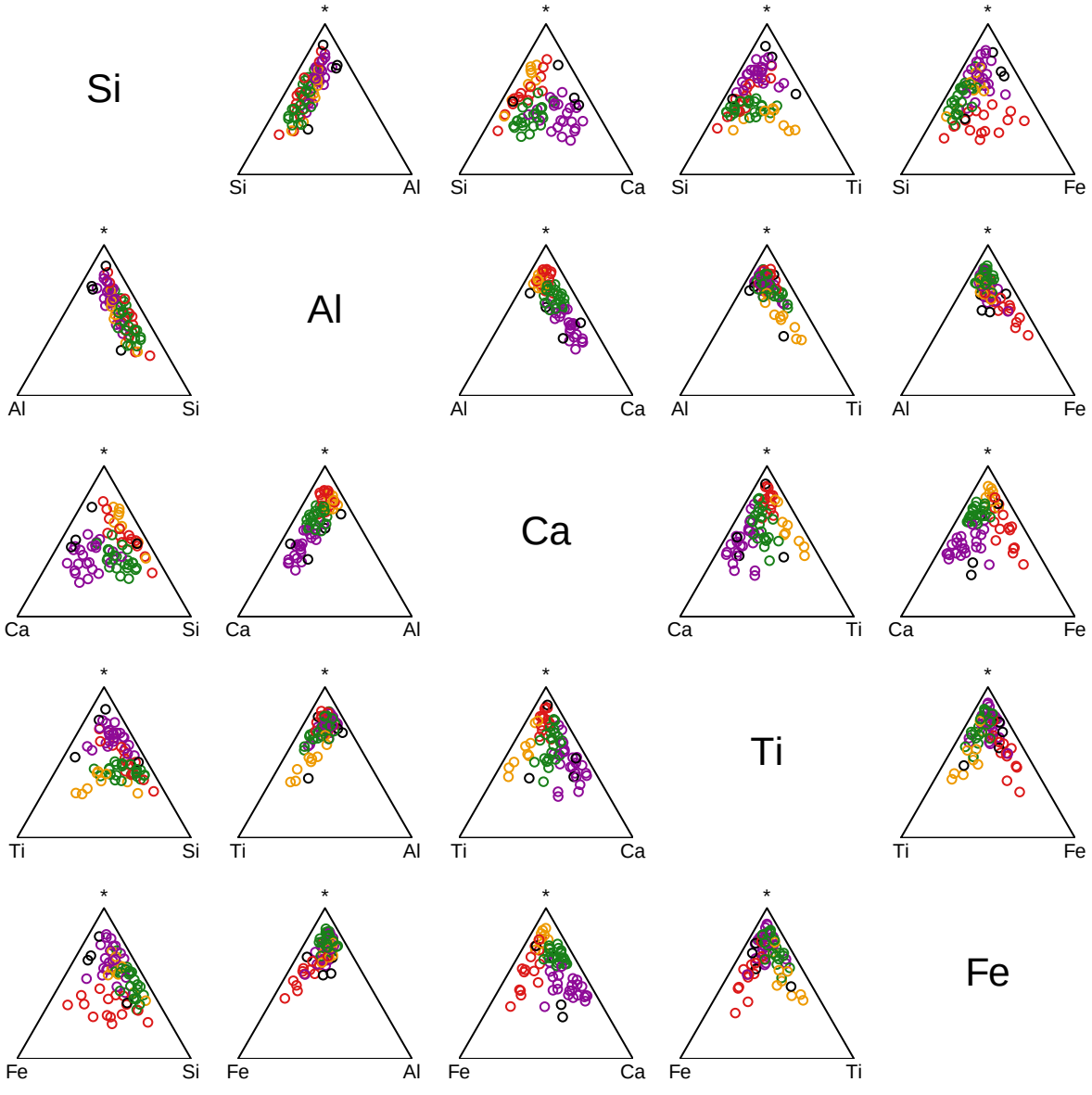
Si, Al, Ca, Ti, Fe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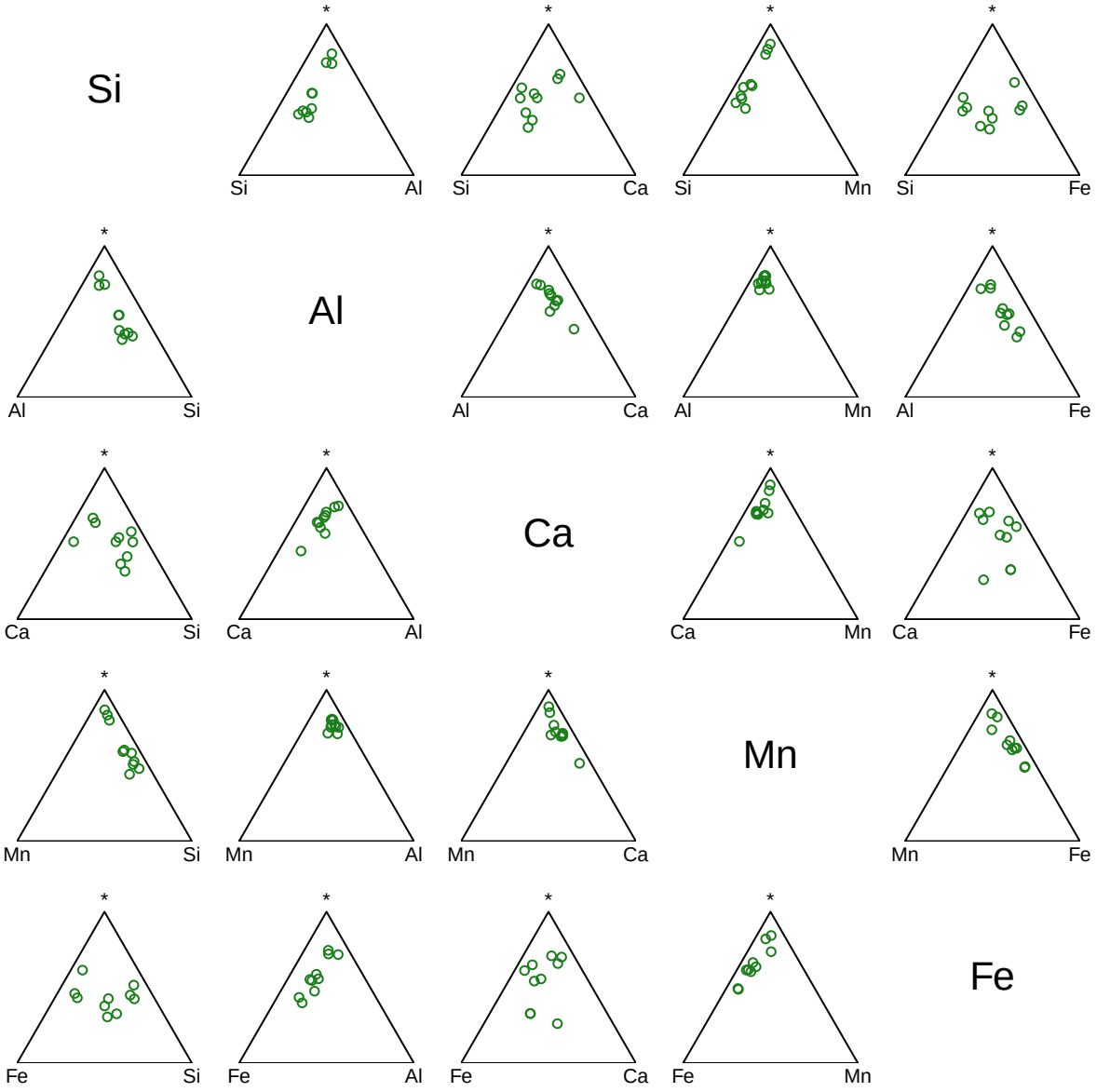
Si, Al, Ca, Mn, Fe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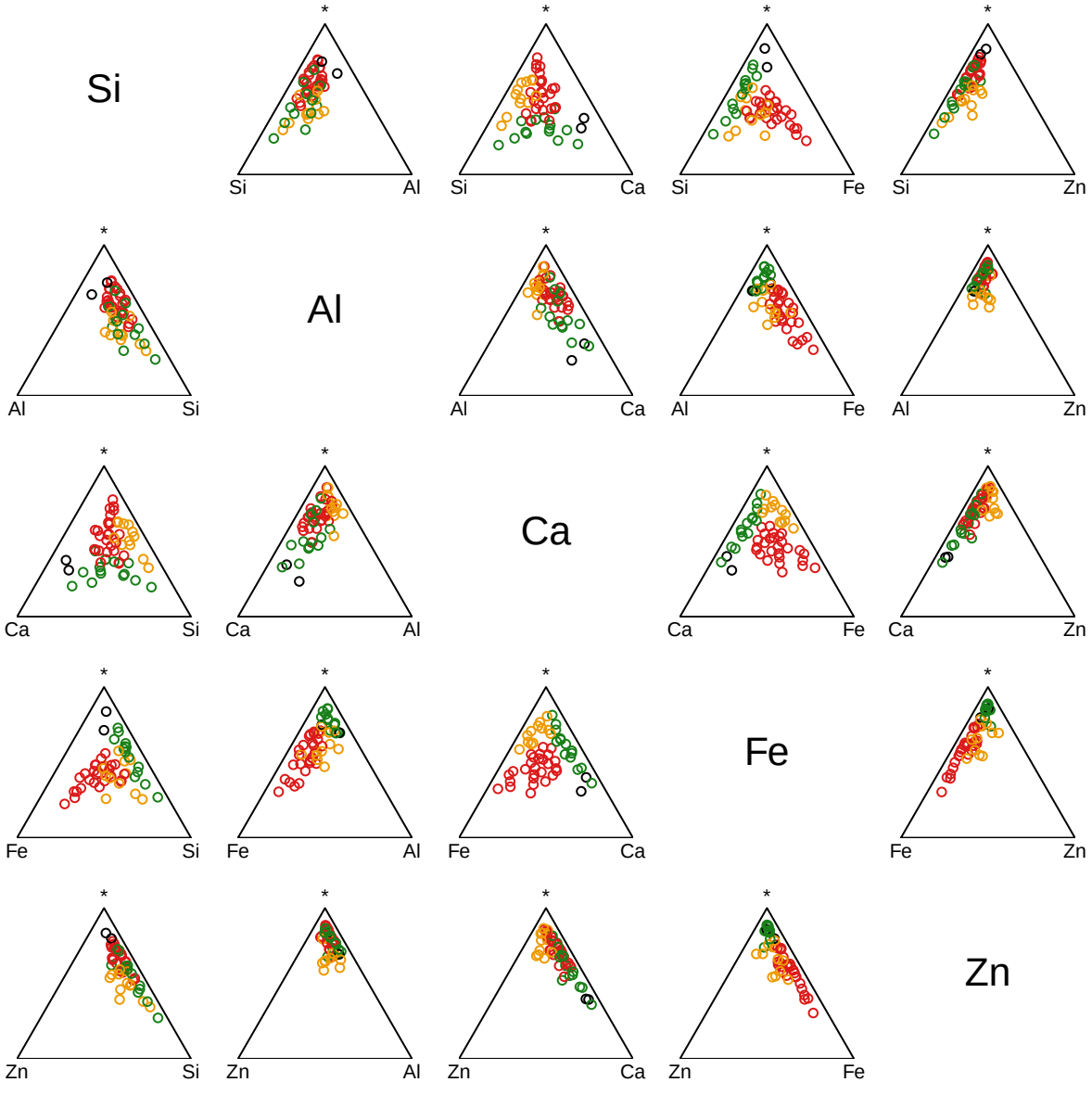
Si, Al, Ca, Fe, Zn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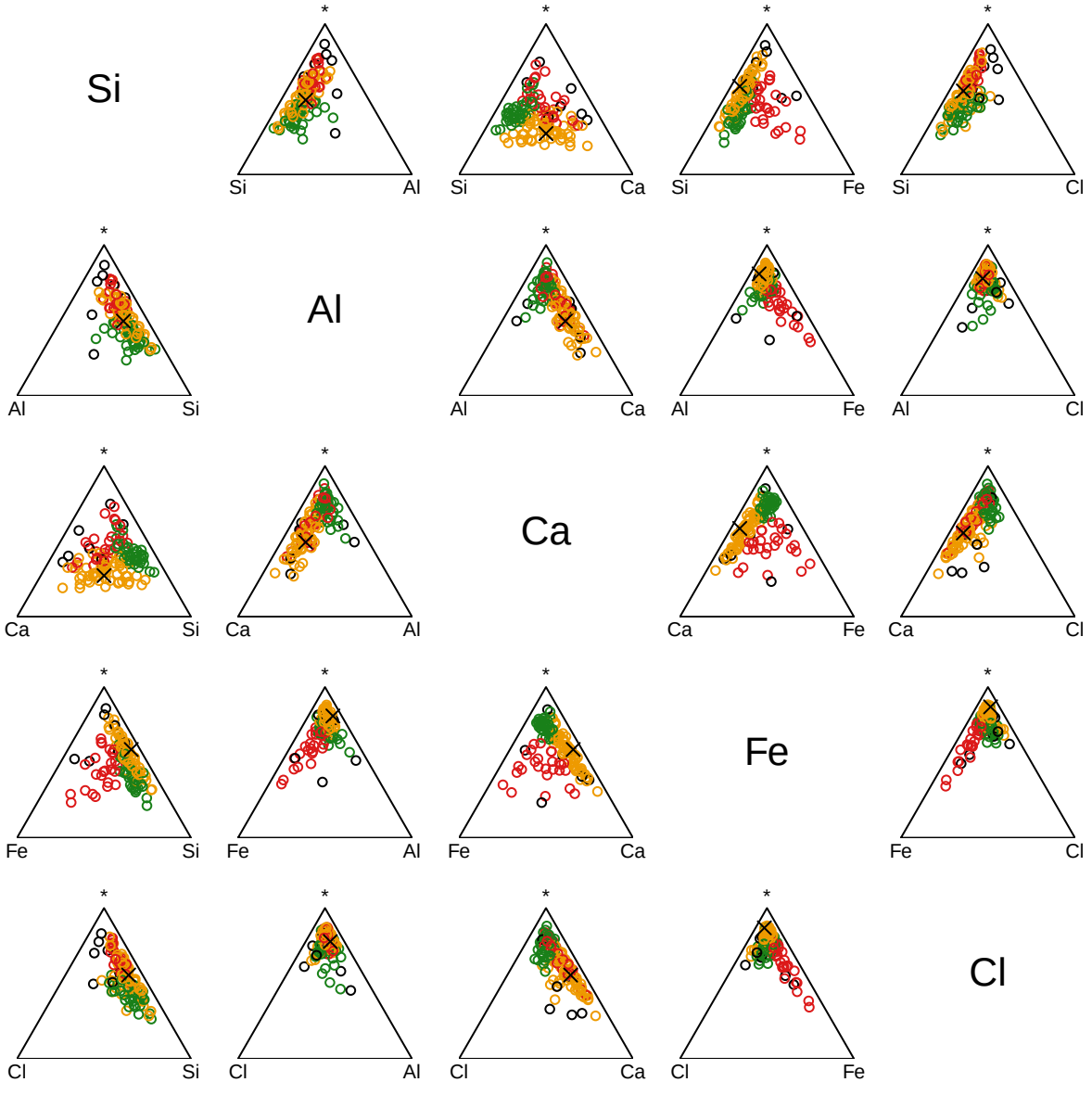
Si, Al, Ca, Fe, Cl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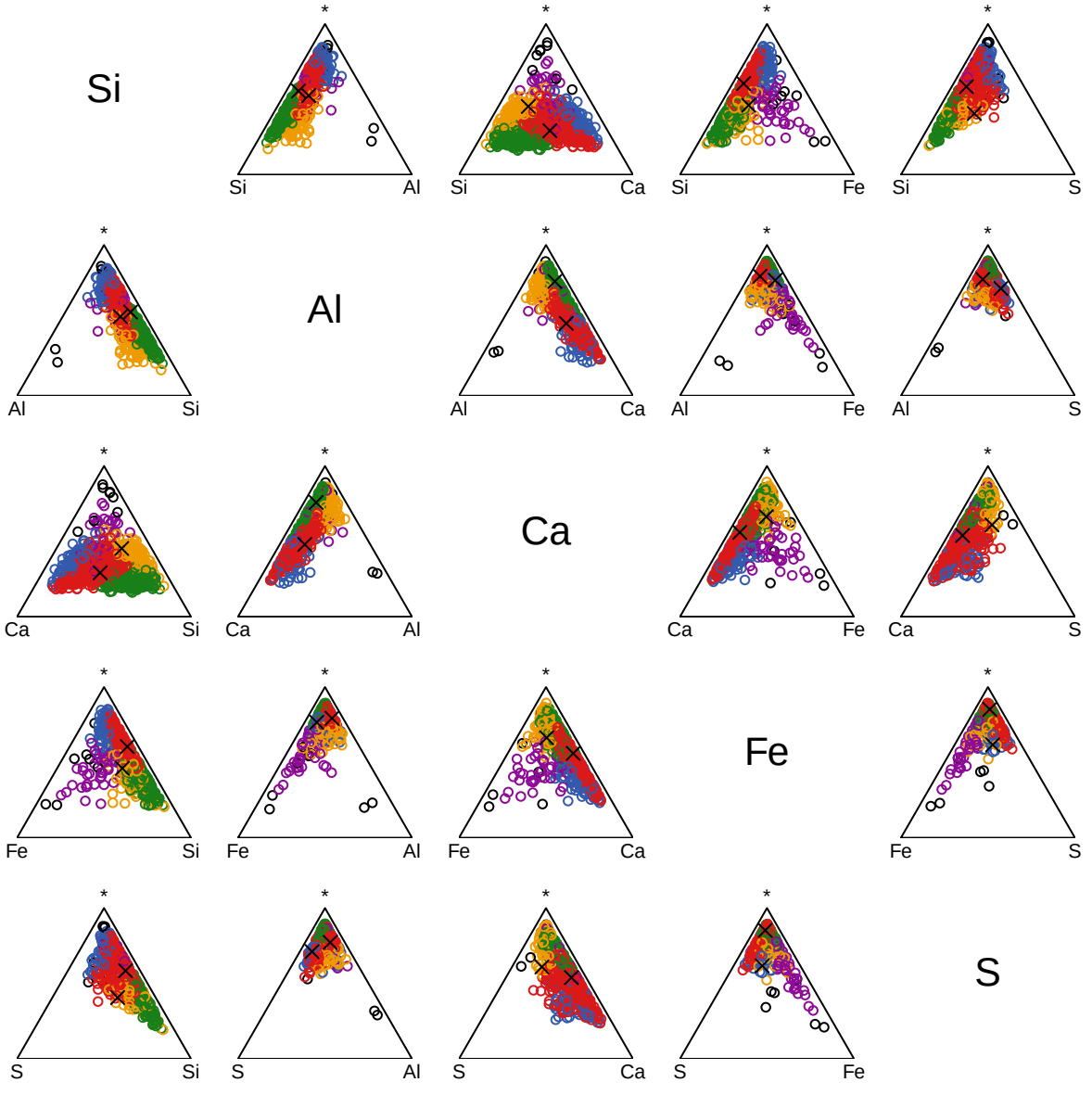
Si, Al, Ca, Fe, S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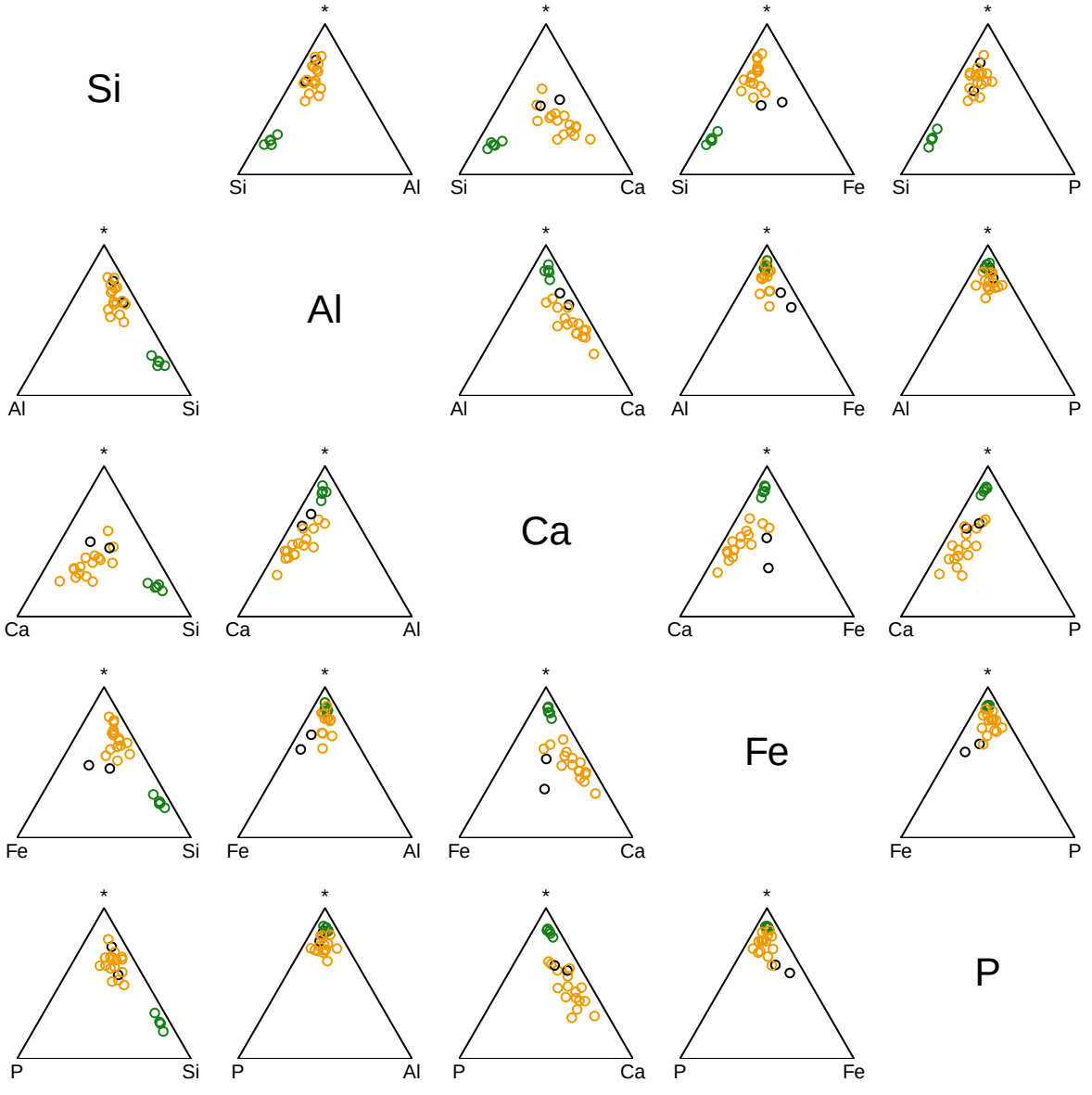
Si, Al, Ca, Fe, P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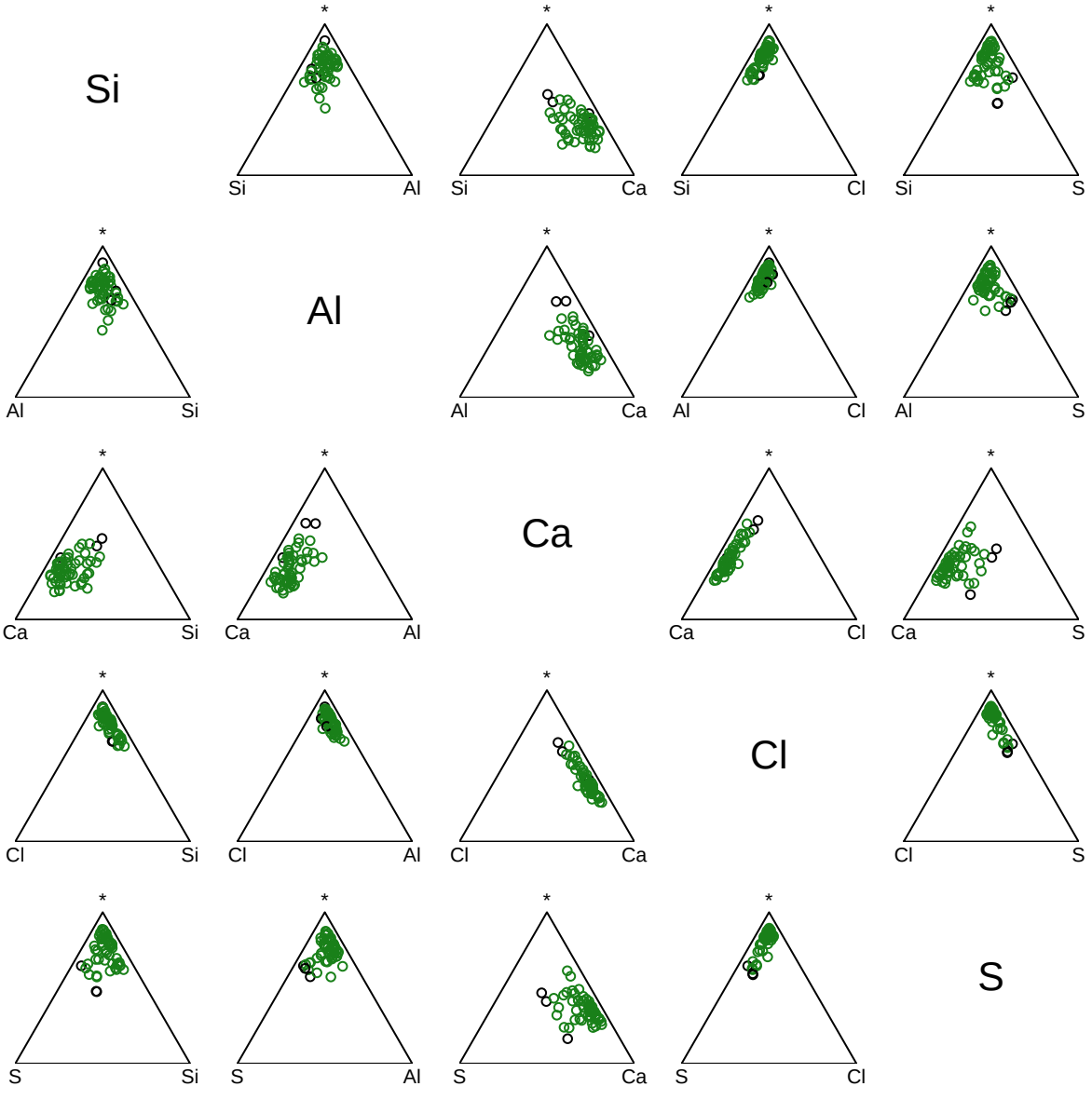
P

Si, Al, Ca, Cl, S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Si Cl
Si S
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Al Ca
Al Cl
Al S
Ca
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Cl S
S
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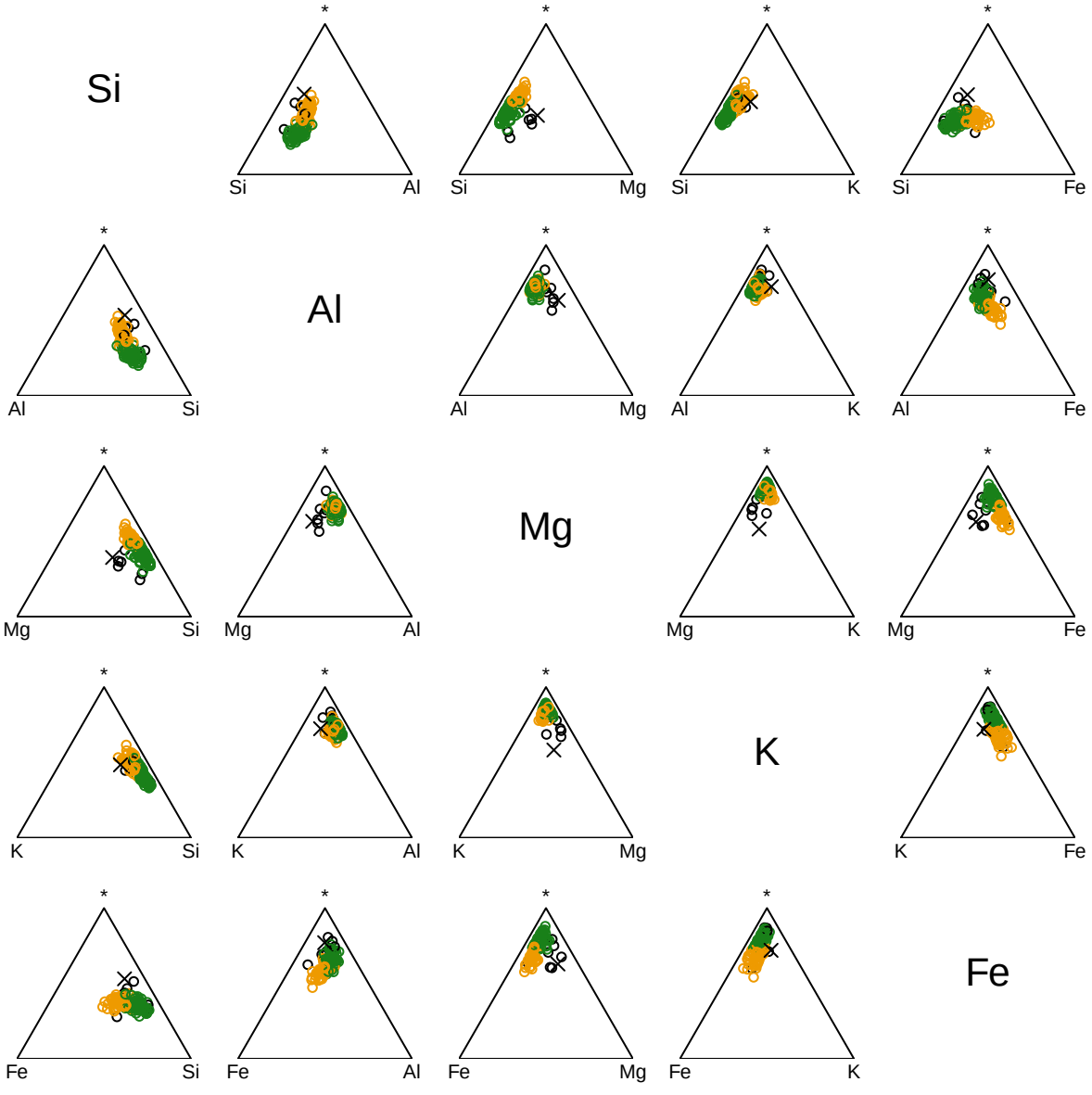
S Al
S Ca
S Cl

Si, Al, Mg, K, Fe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Al Fe
Mg
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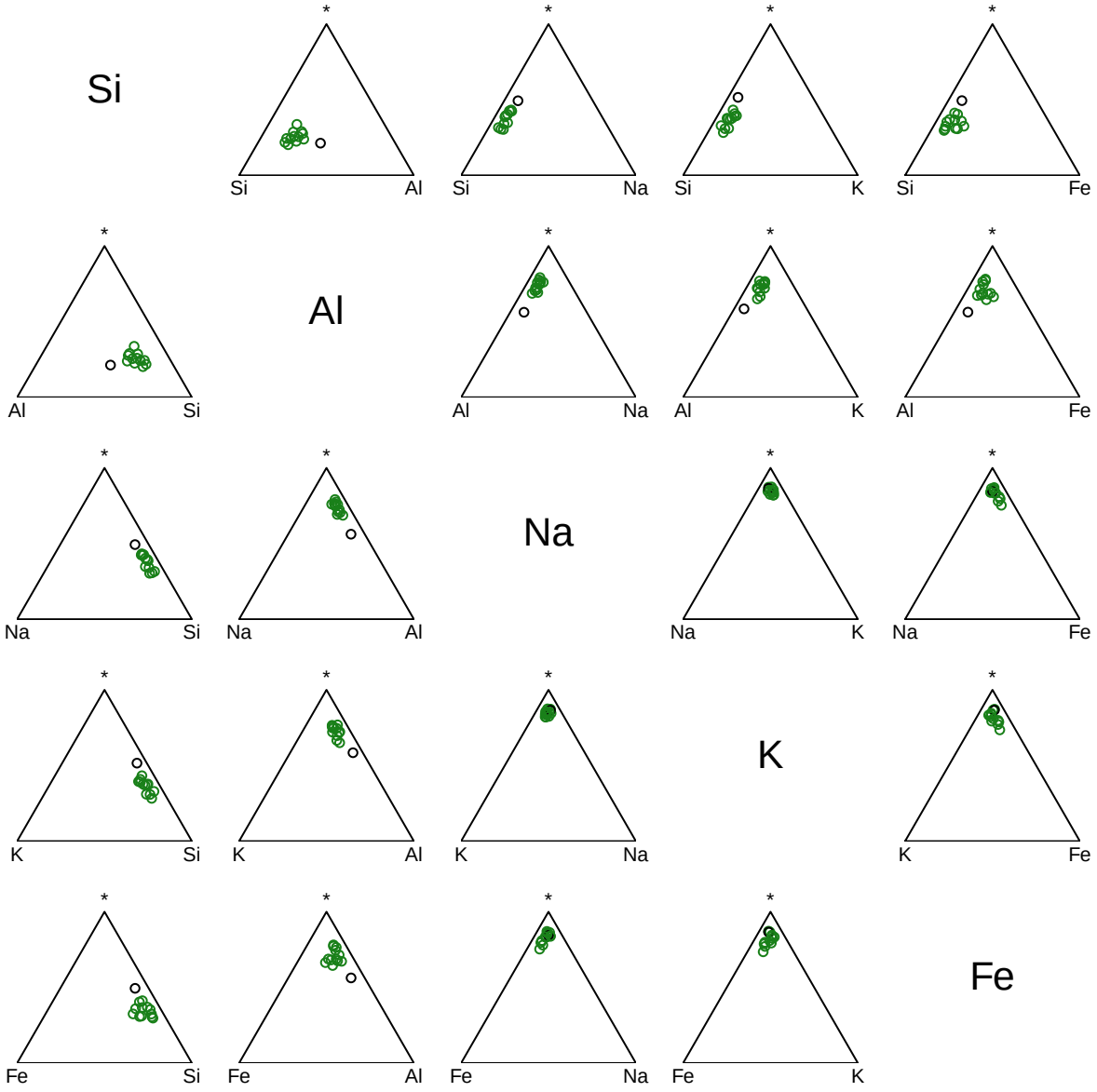
Fe K

Si, Al, Na, K, Fe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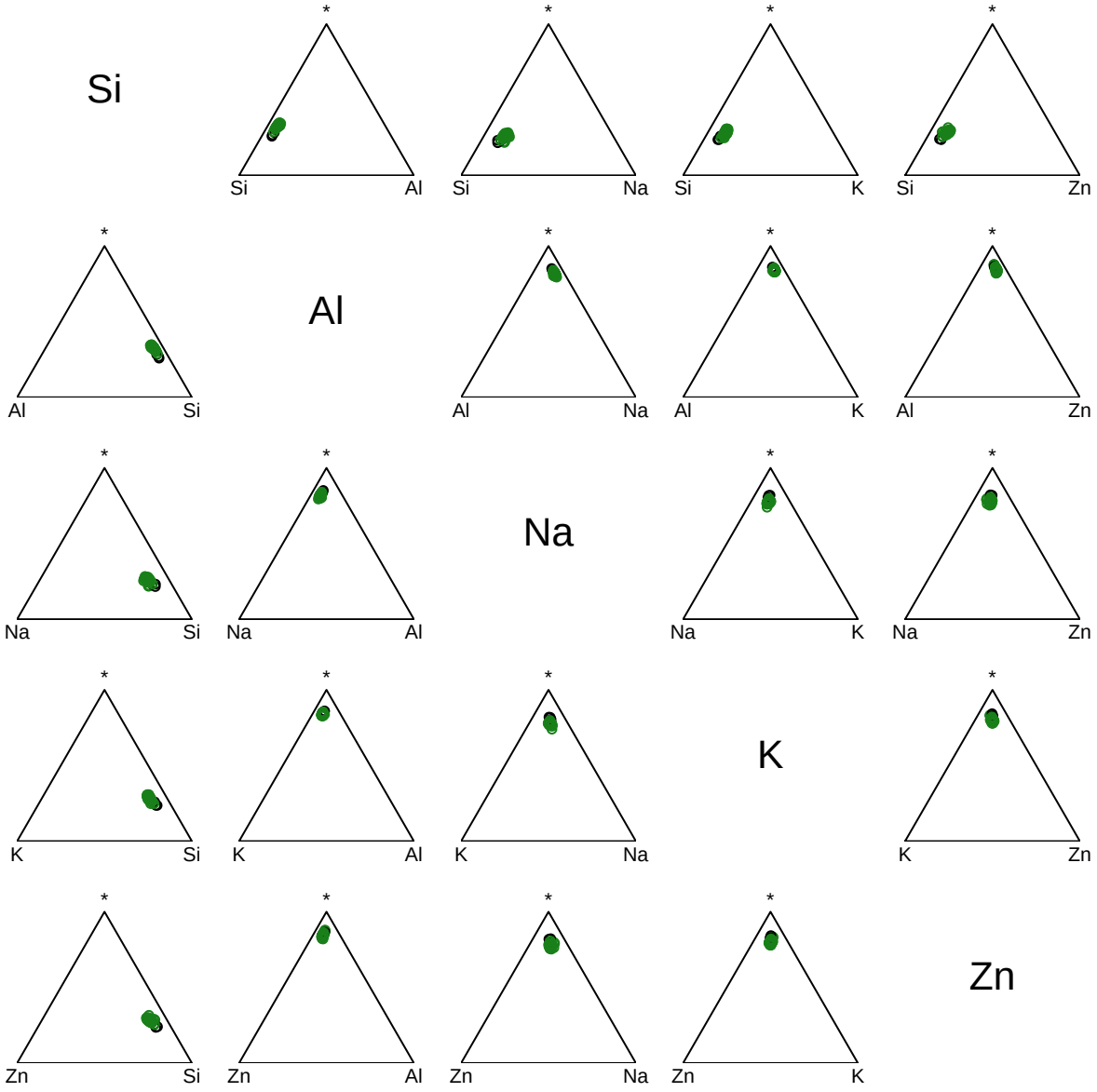
Fe Na
Fe K
Fe

Si, Al, Na, K, Zn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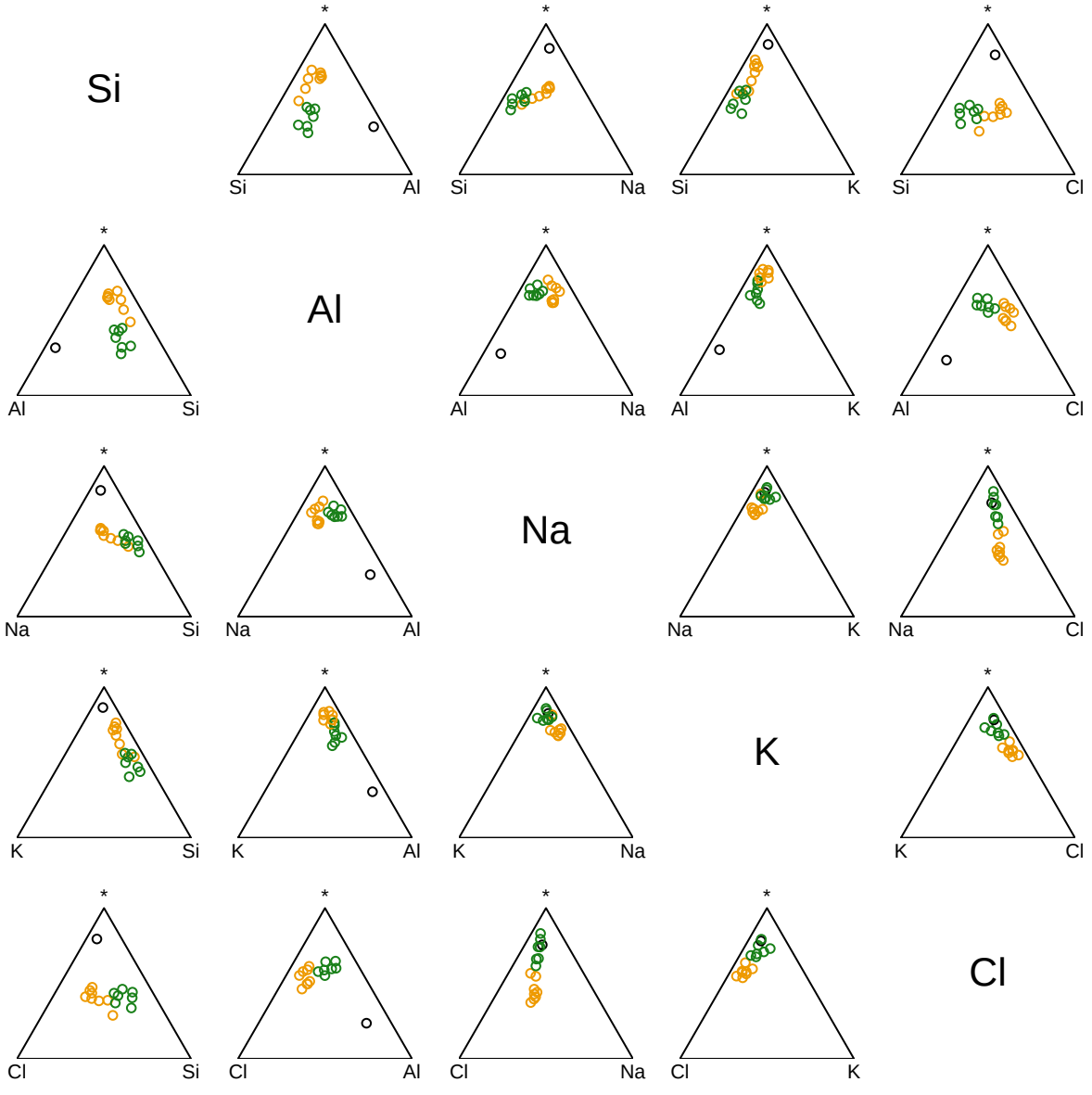
Si, Al, Na, K, Cl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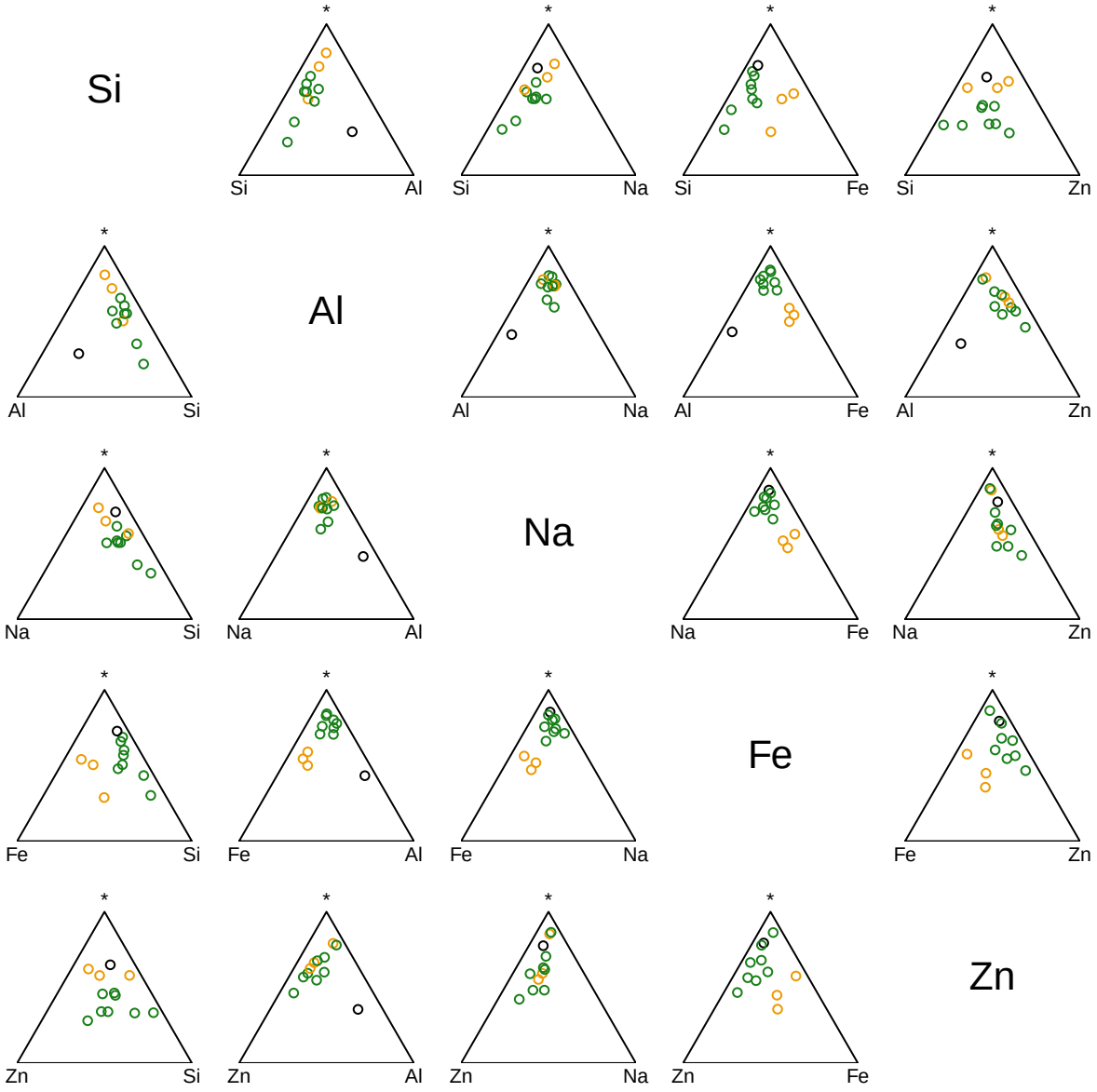
Si, Al, Na, Fe, Zn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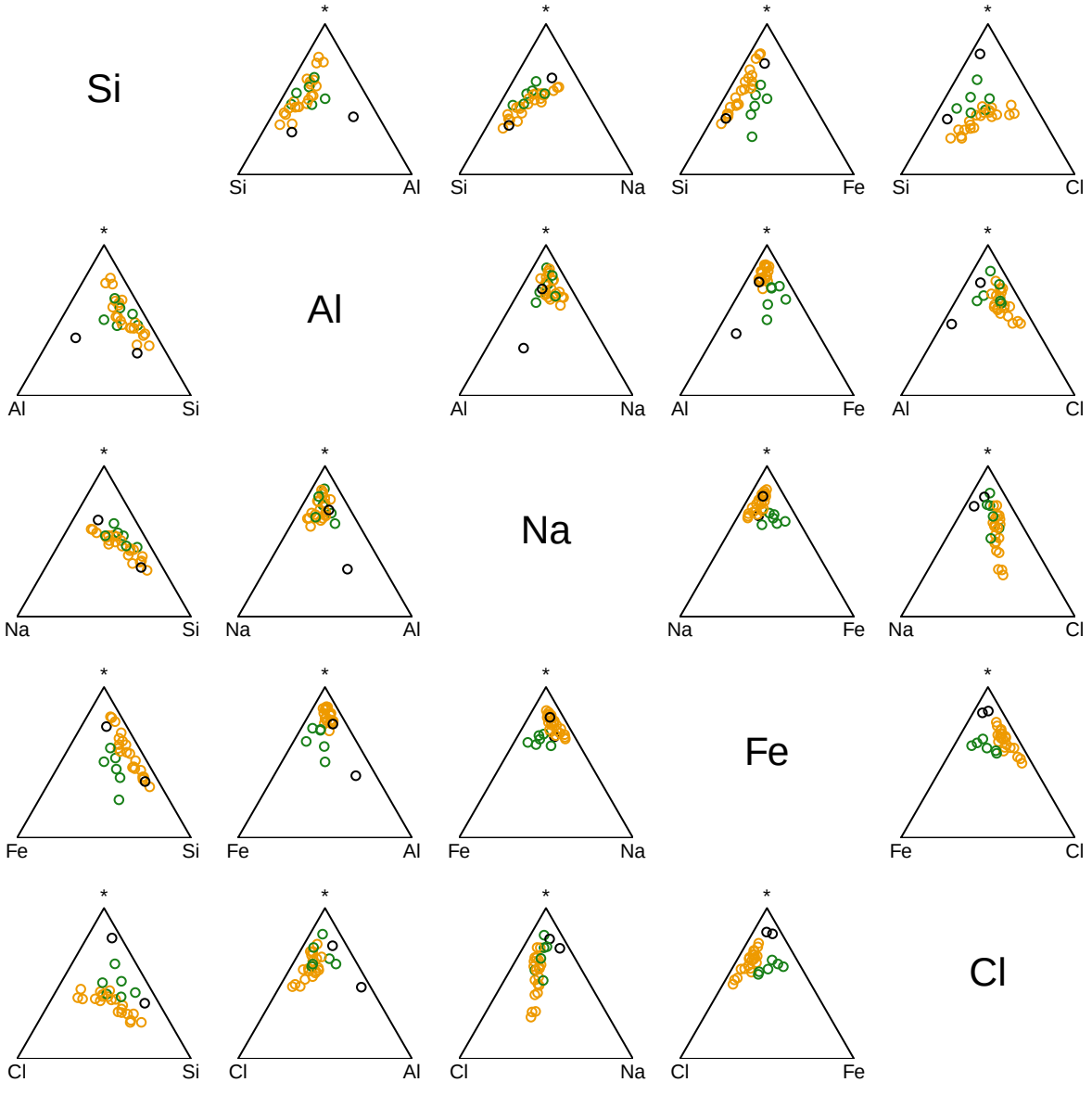
Si, Al, Na, Fe, Cl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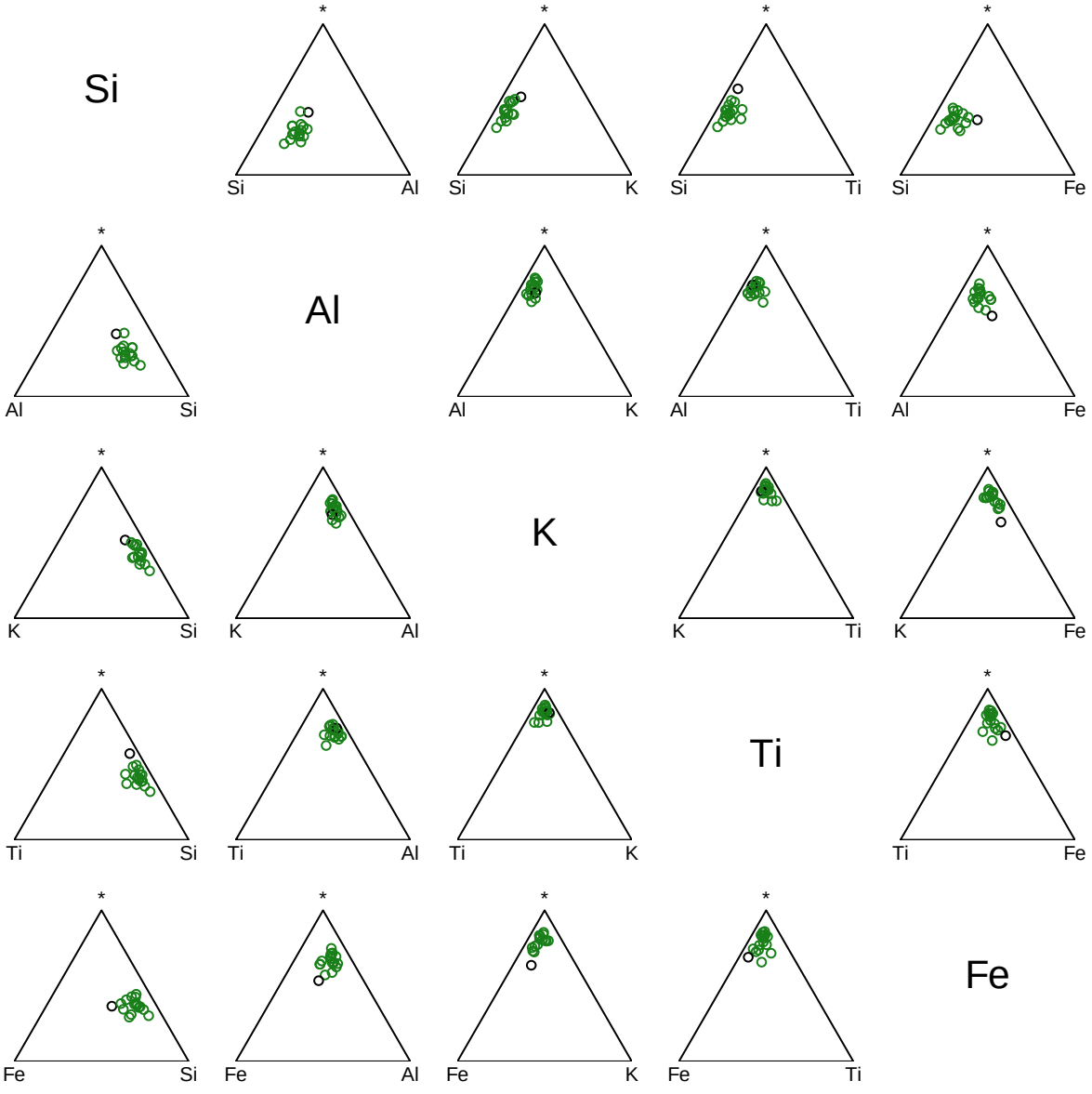
Si, Al, K, Ti, Fe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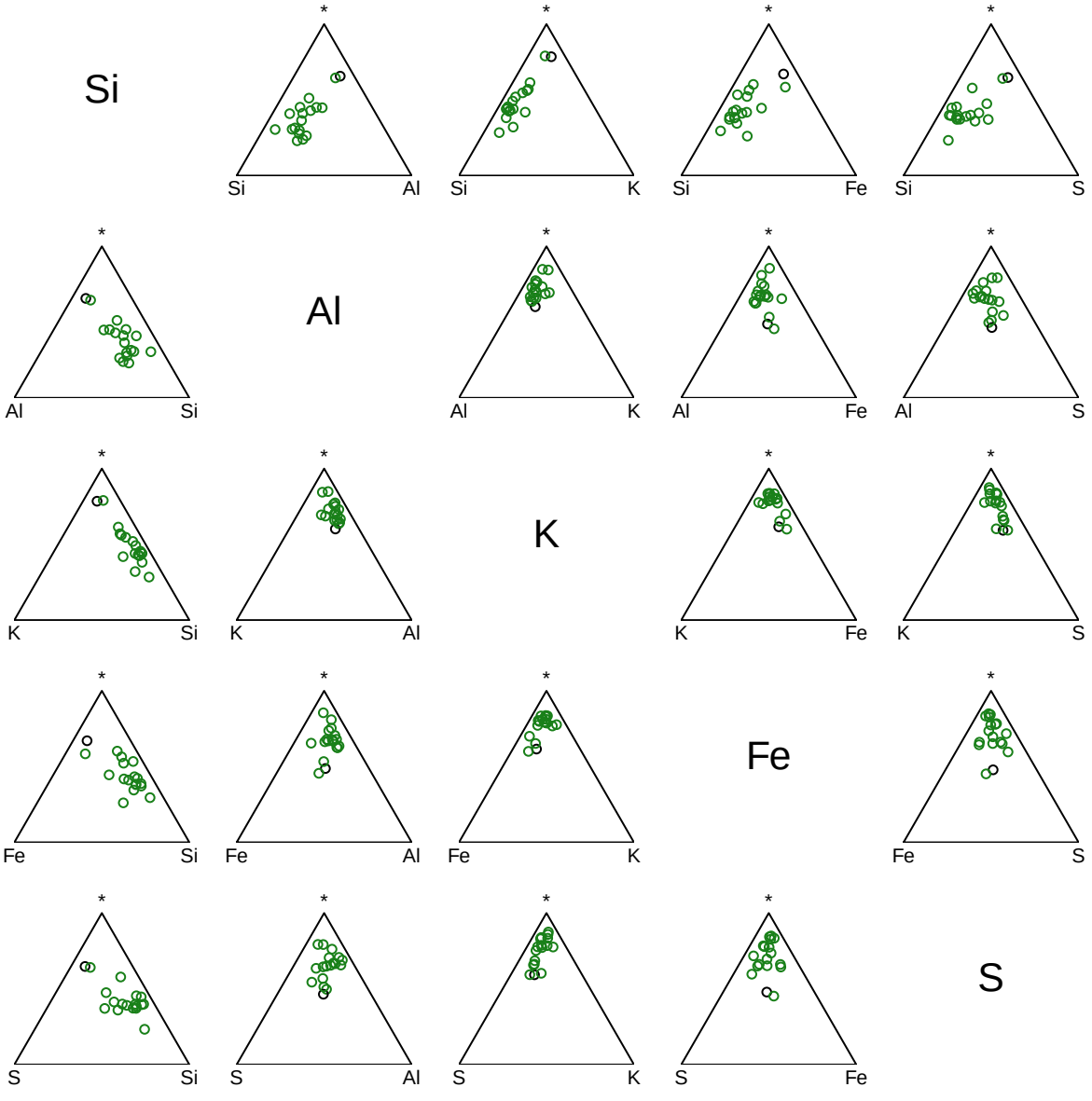
Si, Al, K, Fe, S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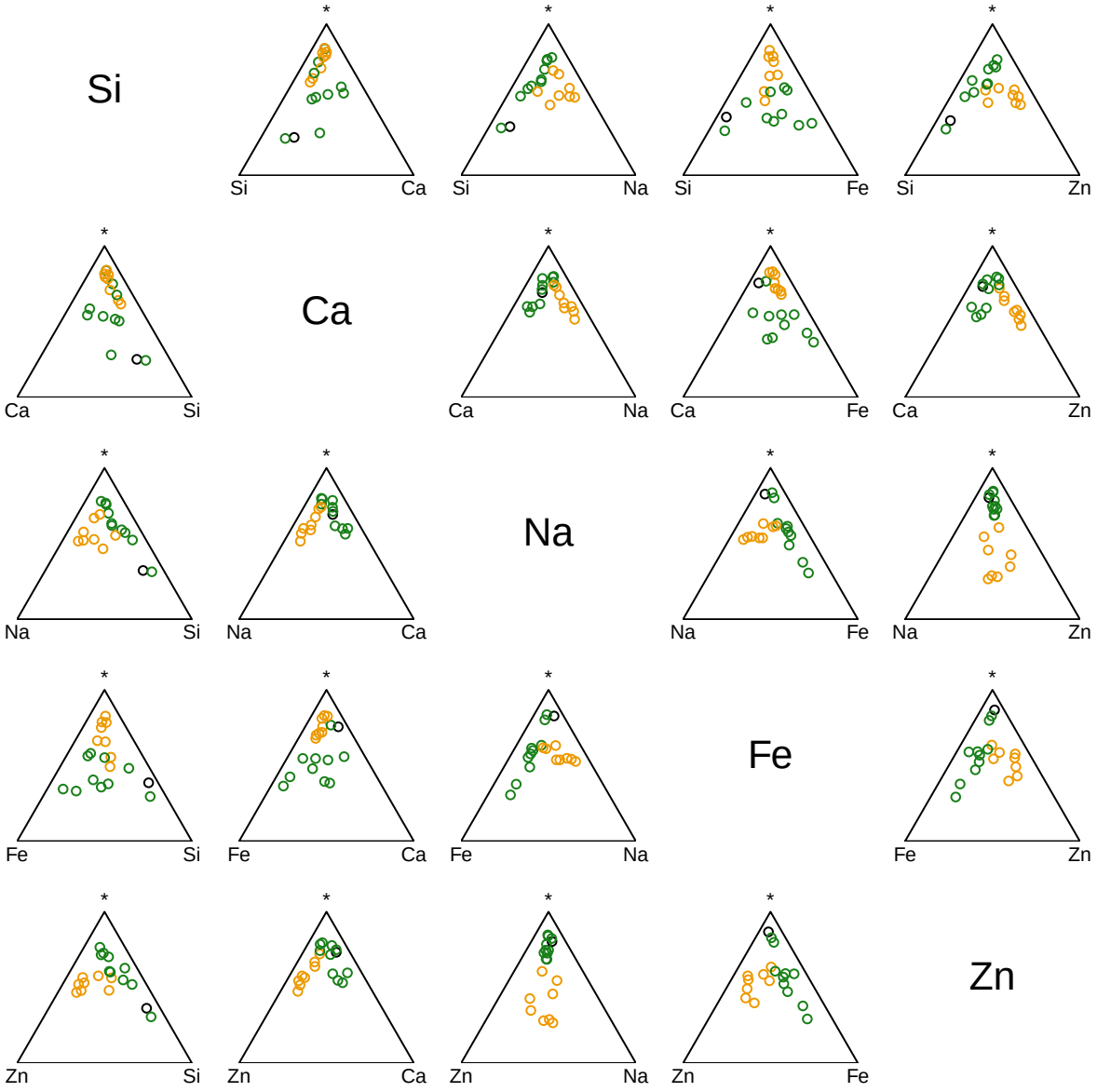
Si, Ca, Na, Fe, Zn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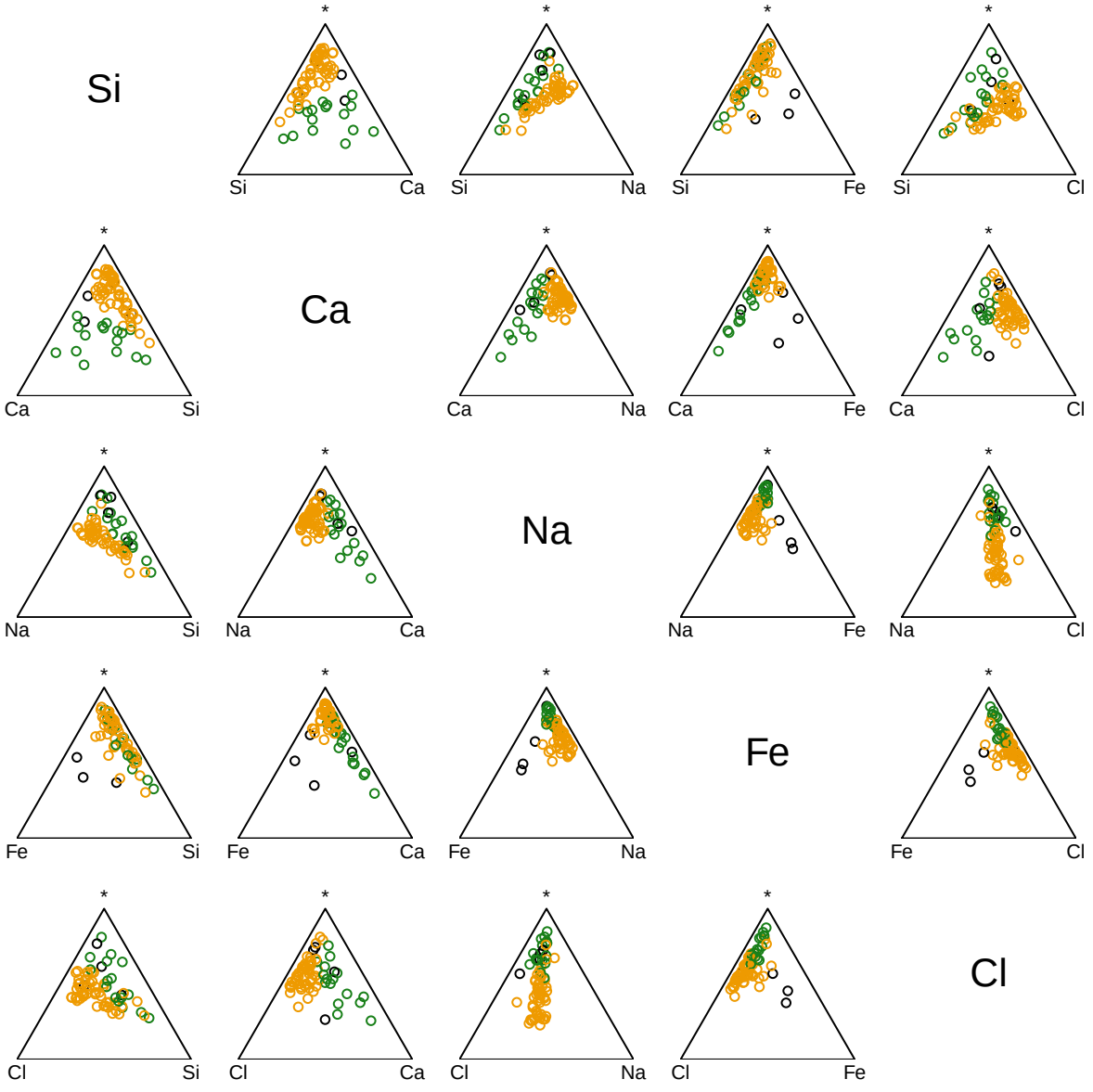
Si, Ca, Na, Fe, Cl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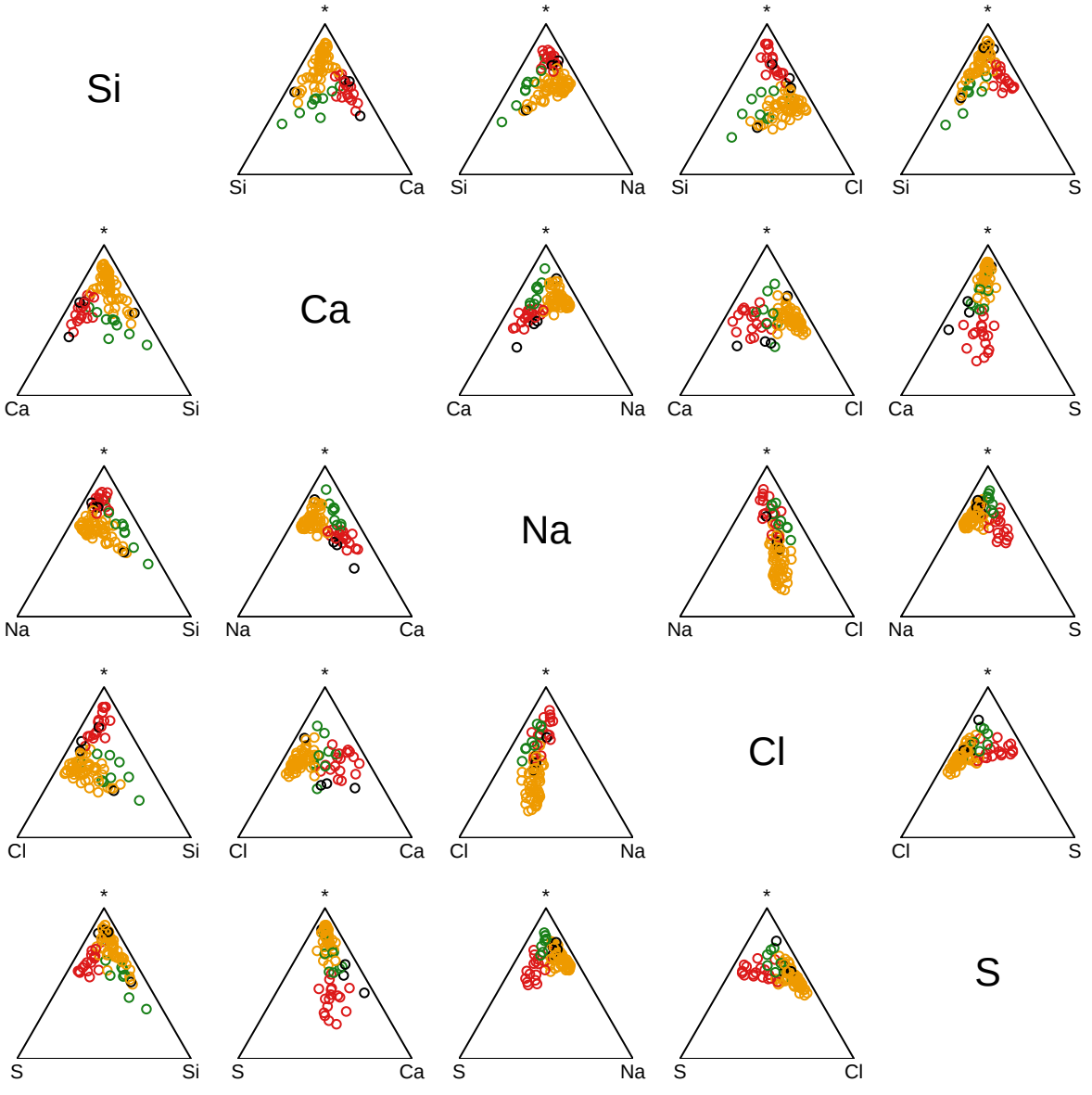
Si, Ca, Na, Cl, S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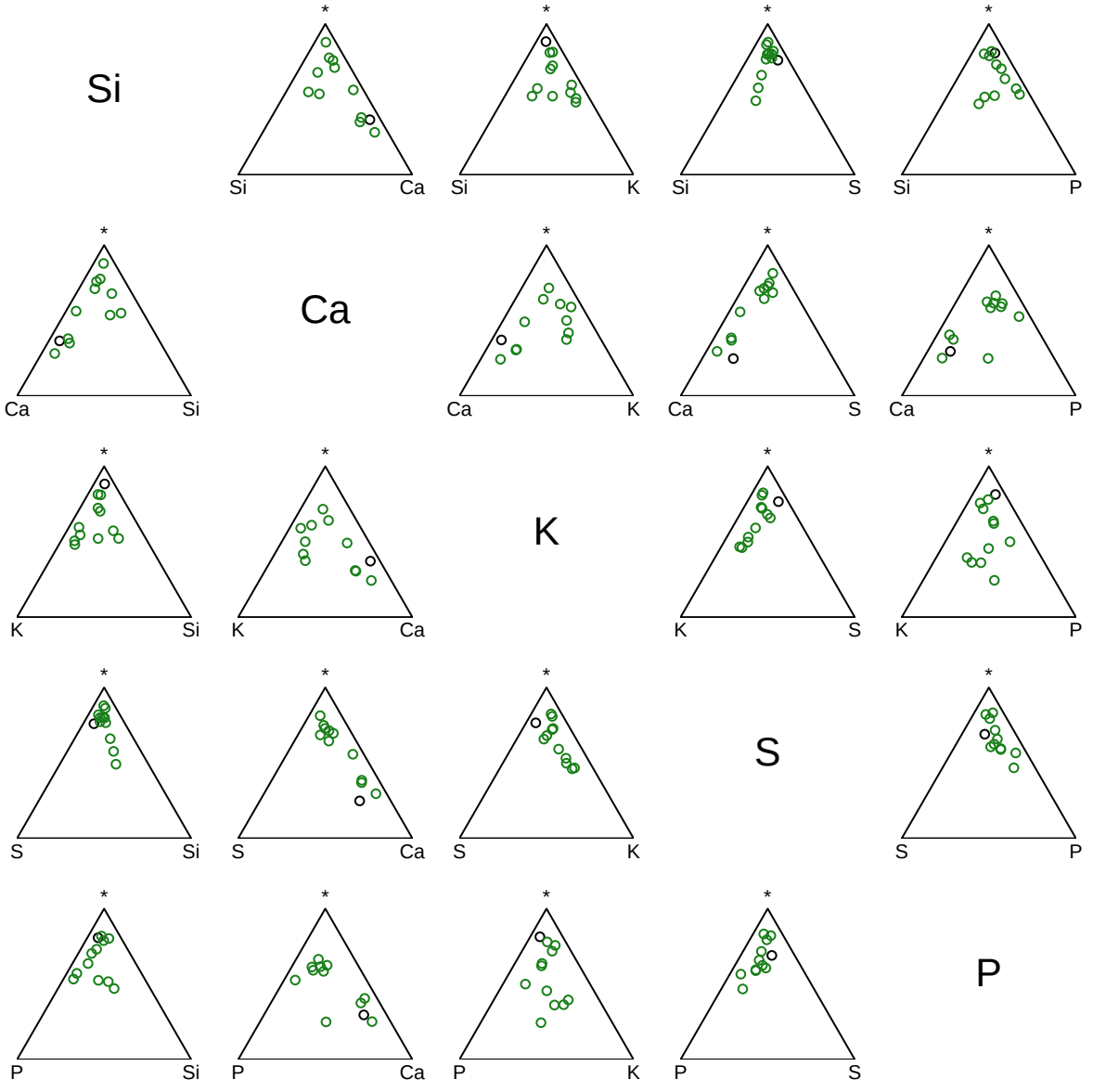
Si, Ca, K, S, P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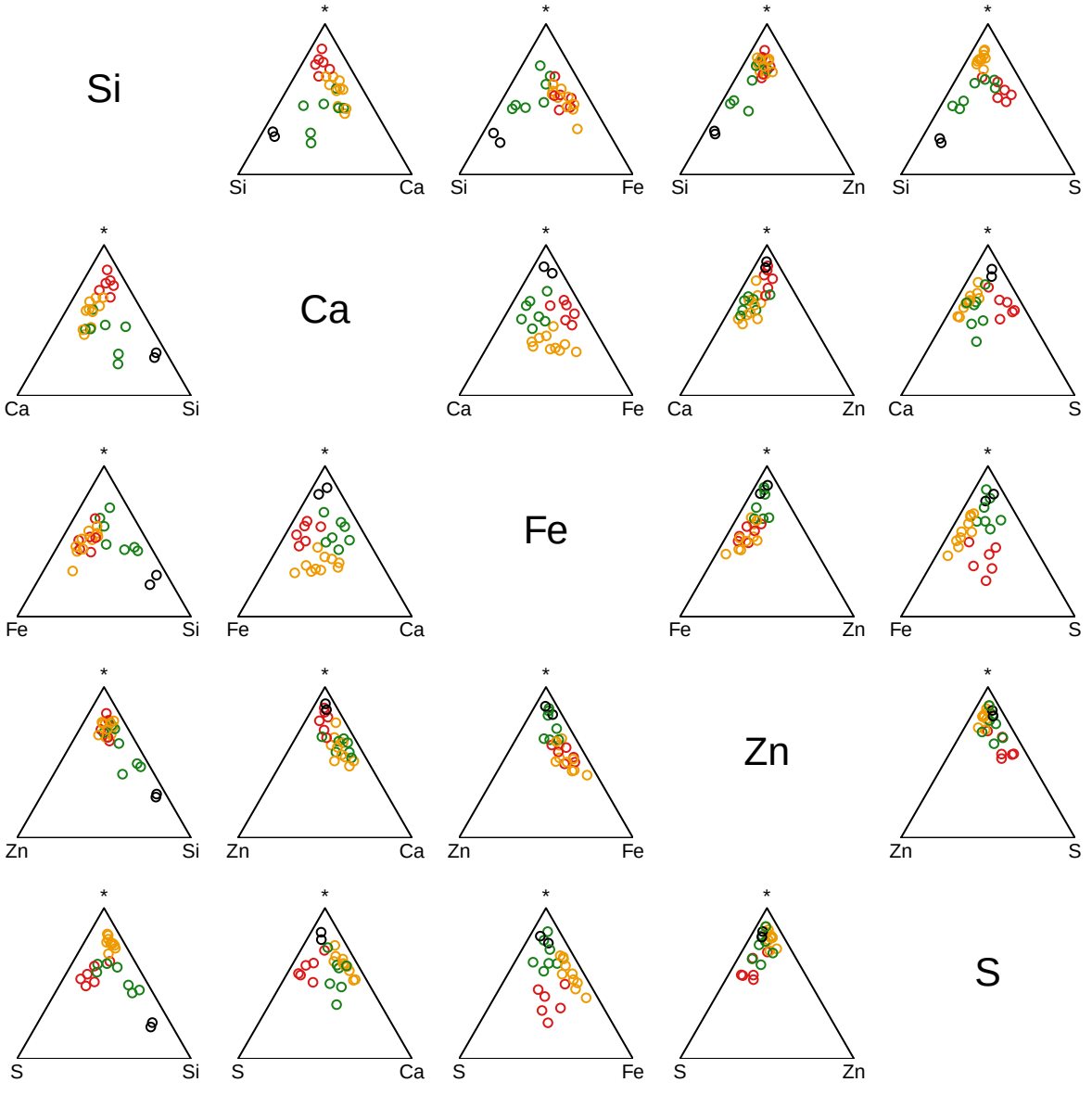
Si, Ca, Fe, Zn, S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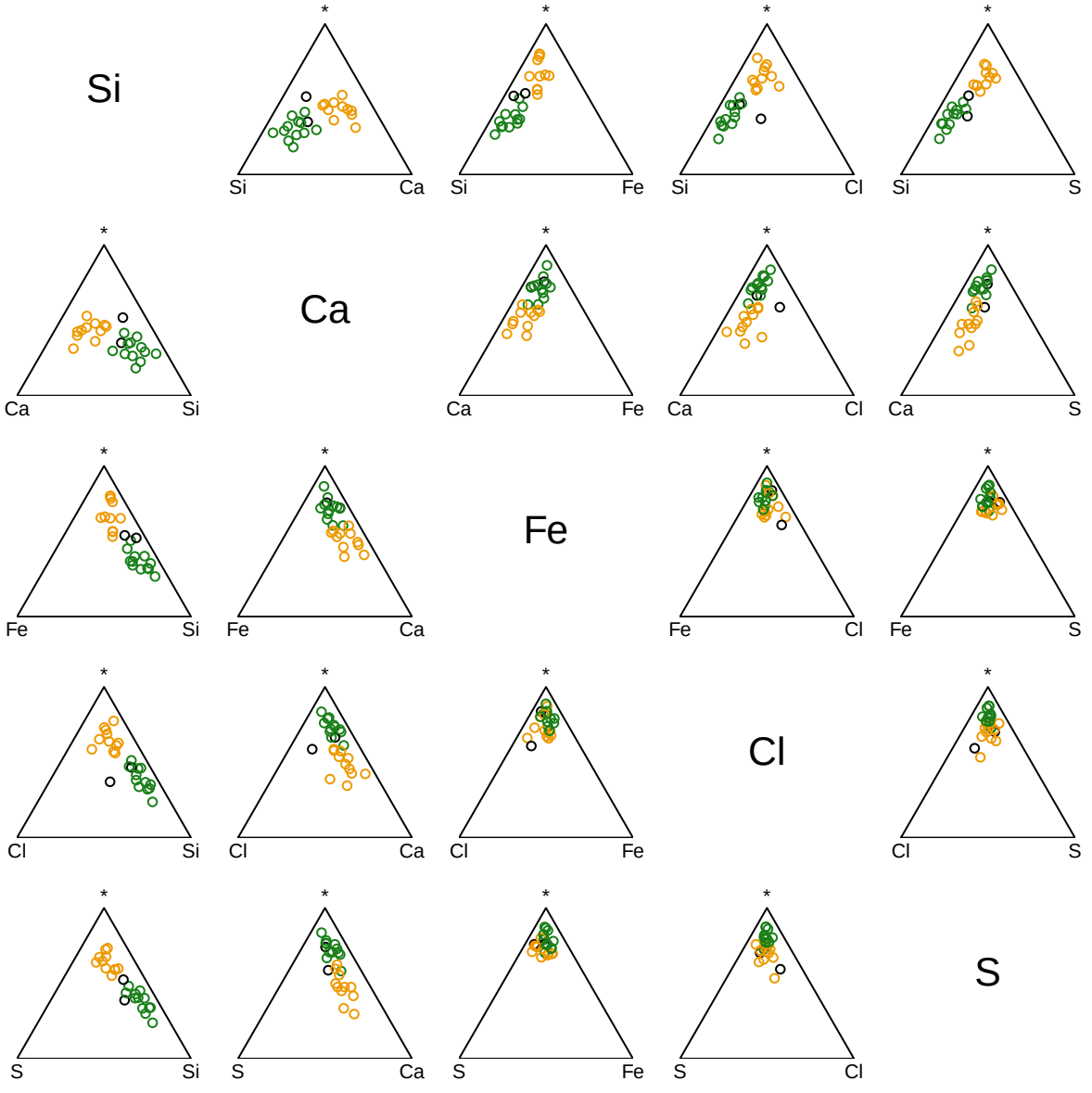
Si, Ca, Fe, Cl, S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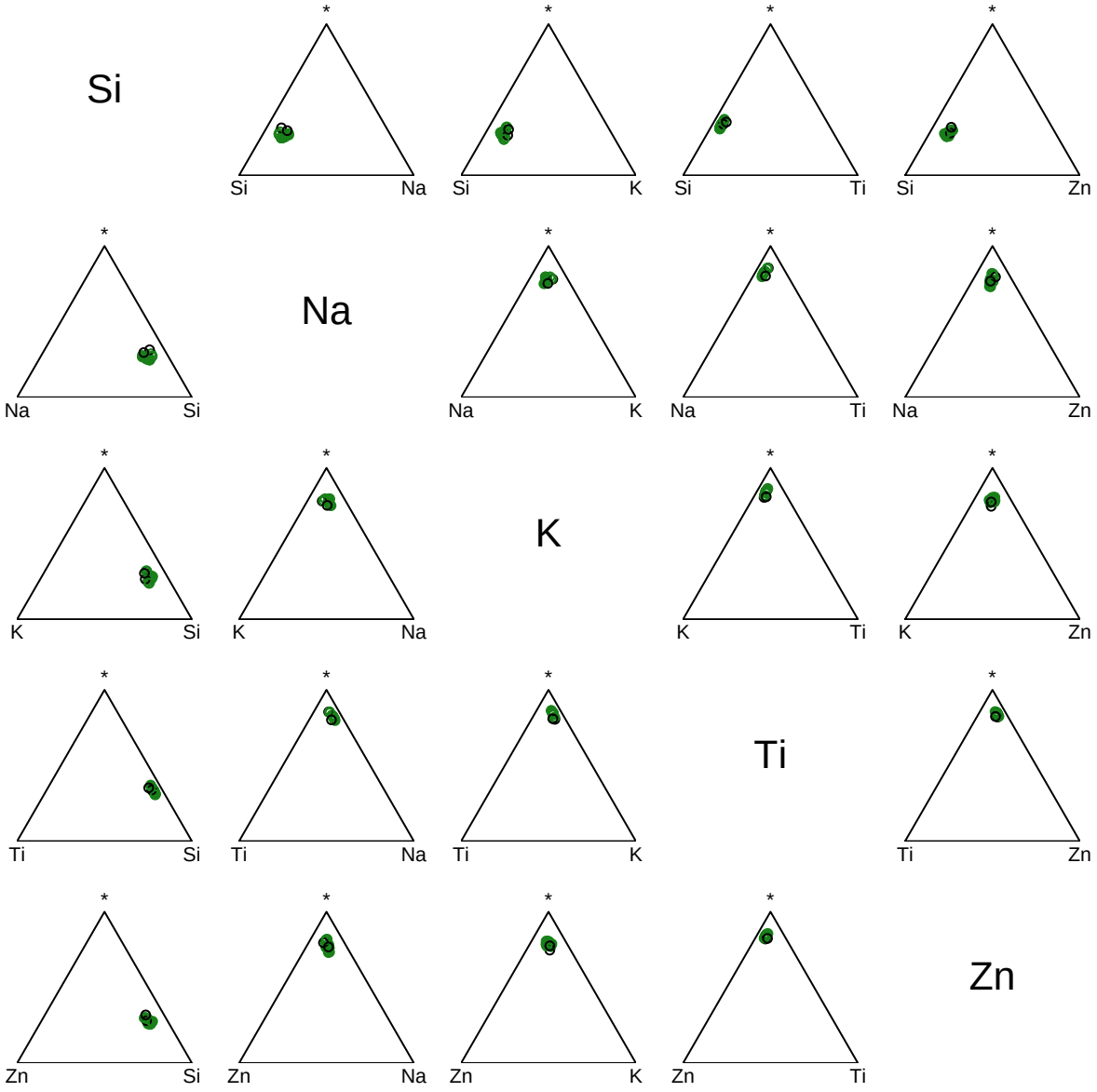
Si, Na, K, Ti, Zn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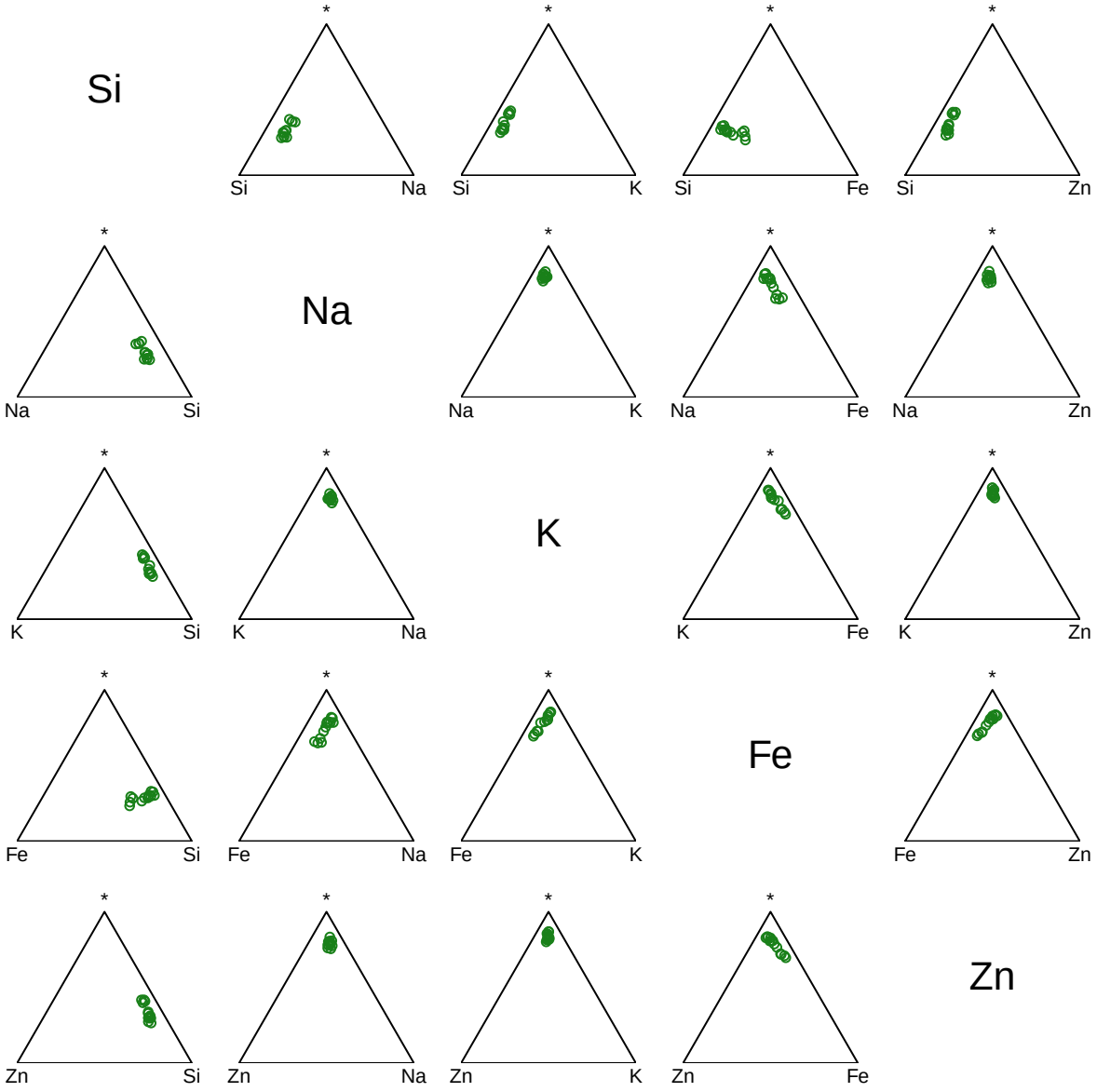
Si, Na, K, Fe, Zn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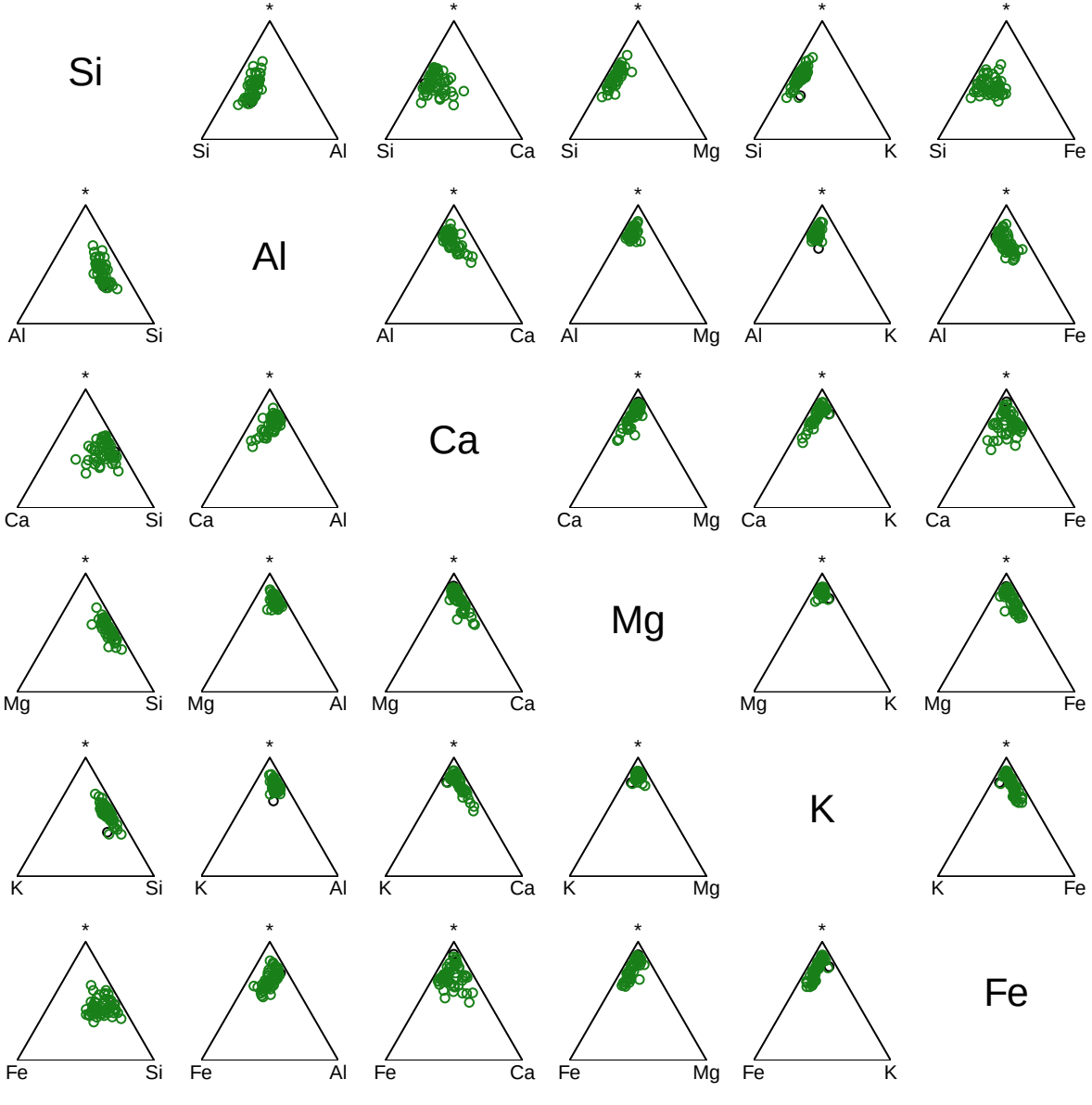
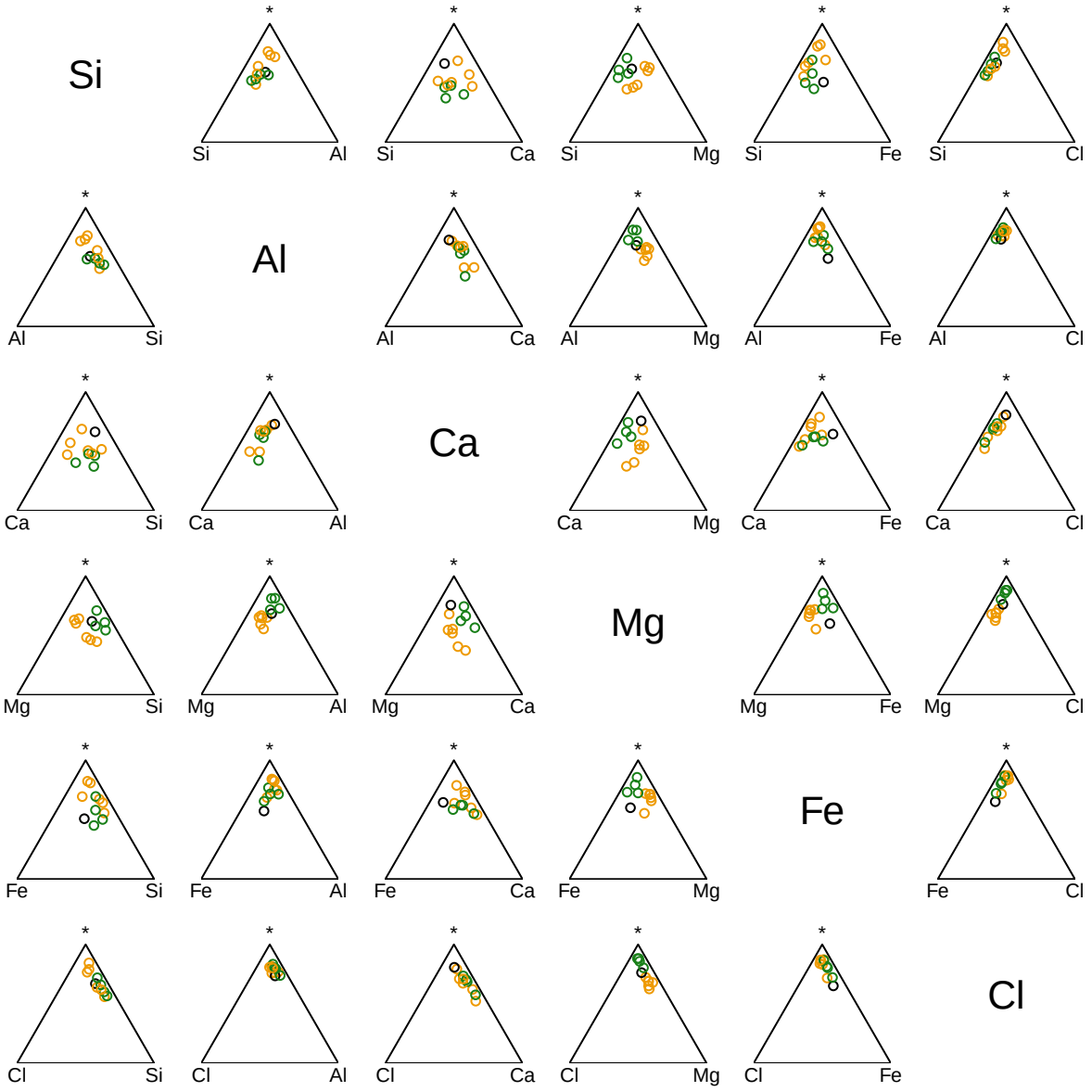
Zn Fe

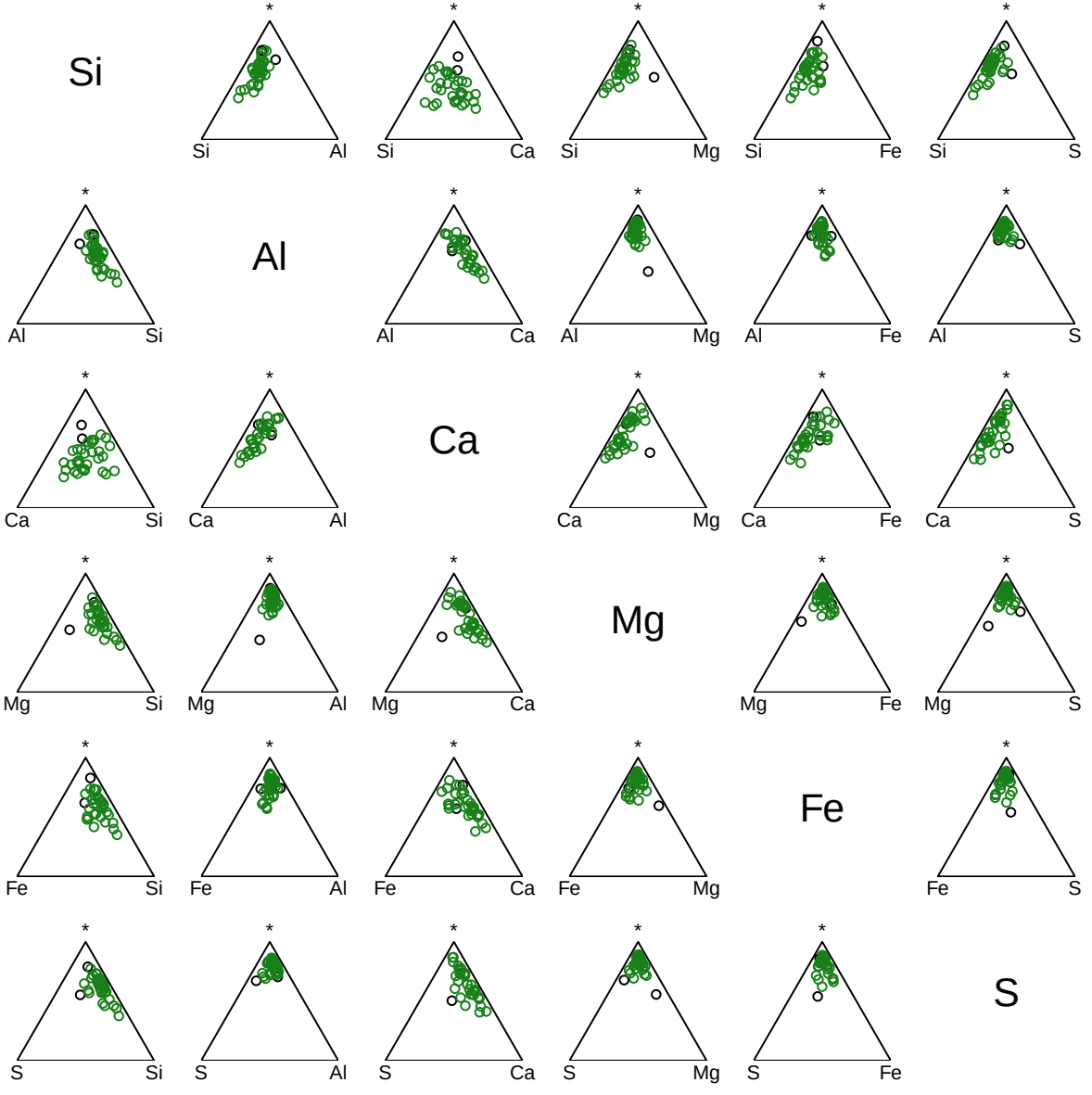
Si, Al, Ca, Mg, K, Fe



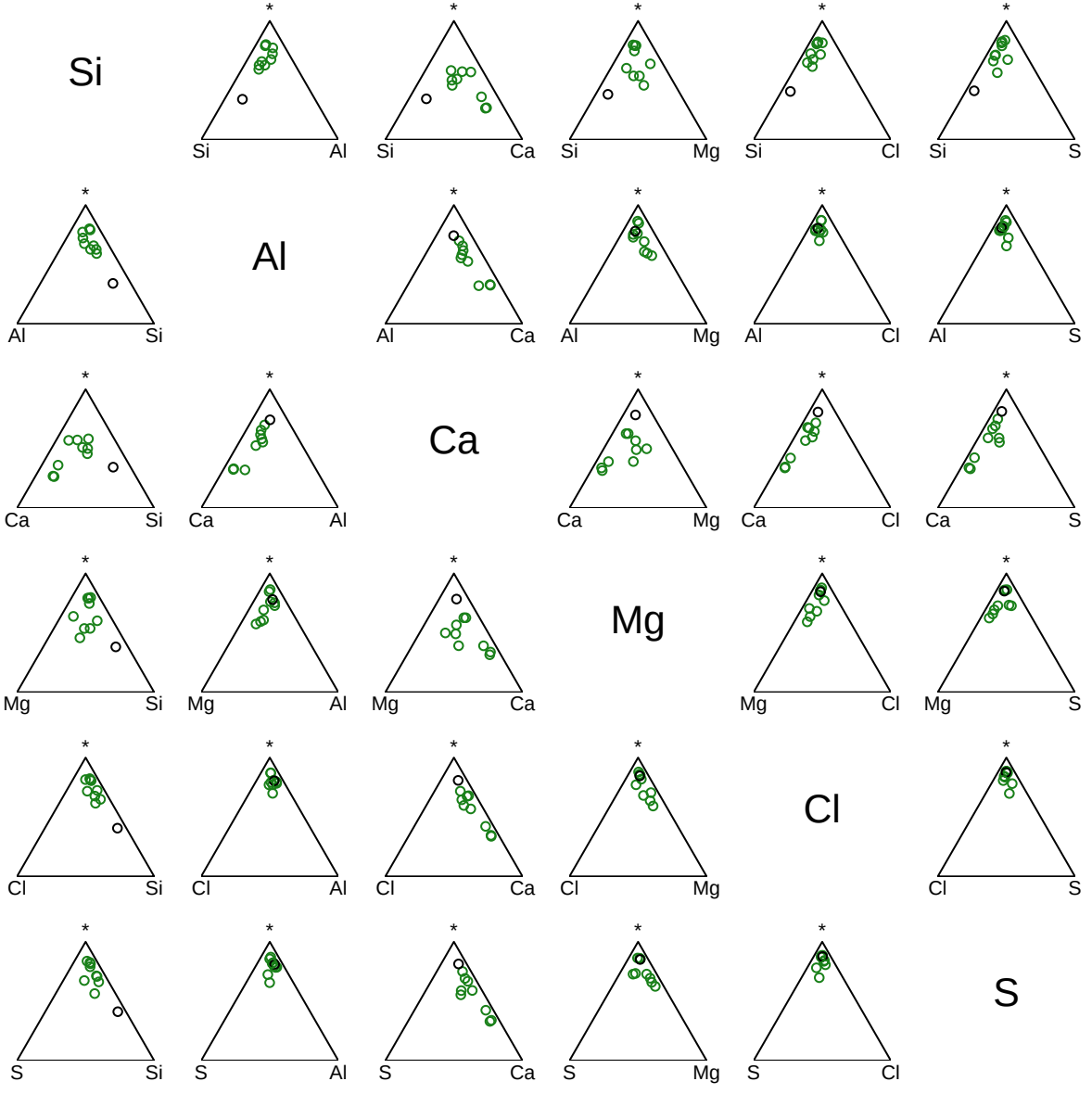
Si, Al, Ca, Mg, Fe, Cl



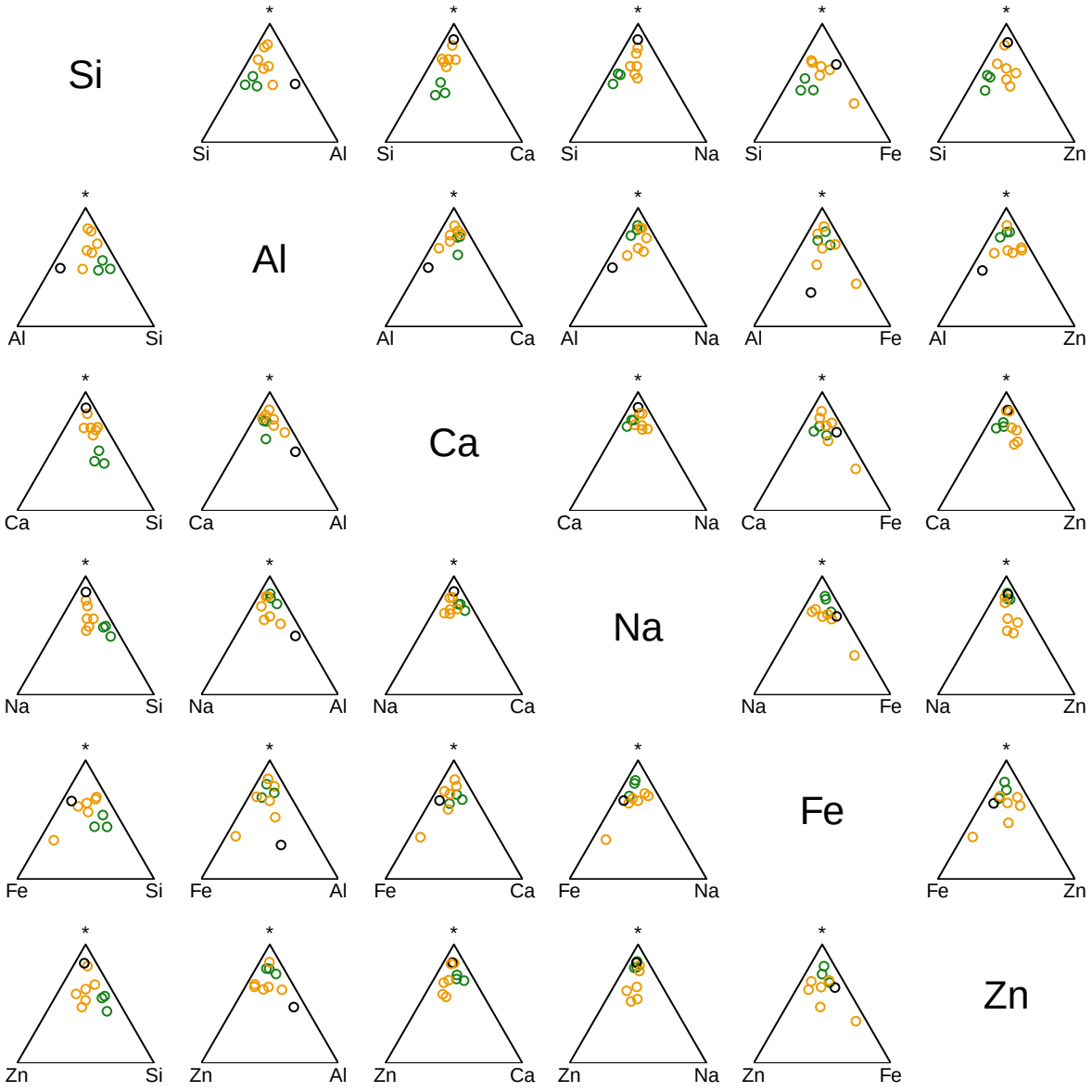
Si, Al, Ca, Mg, Fe, S



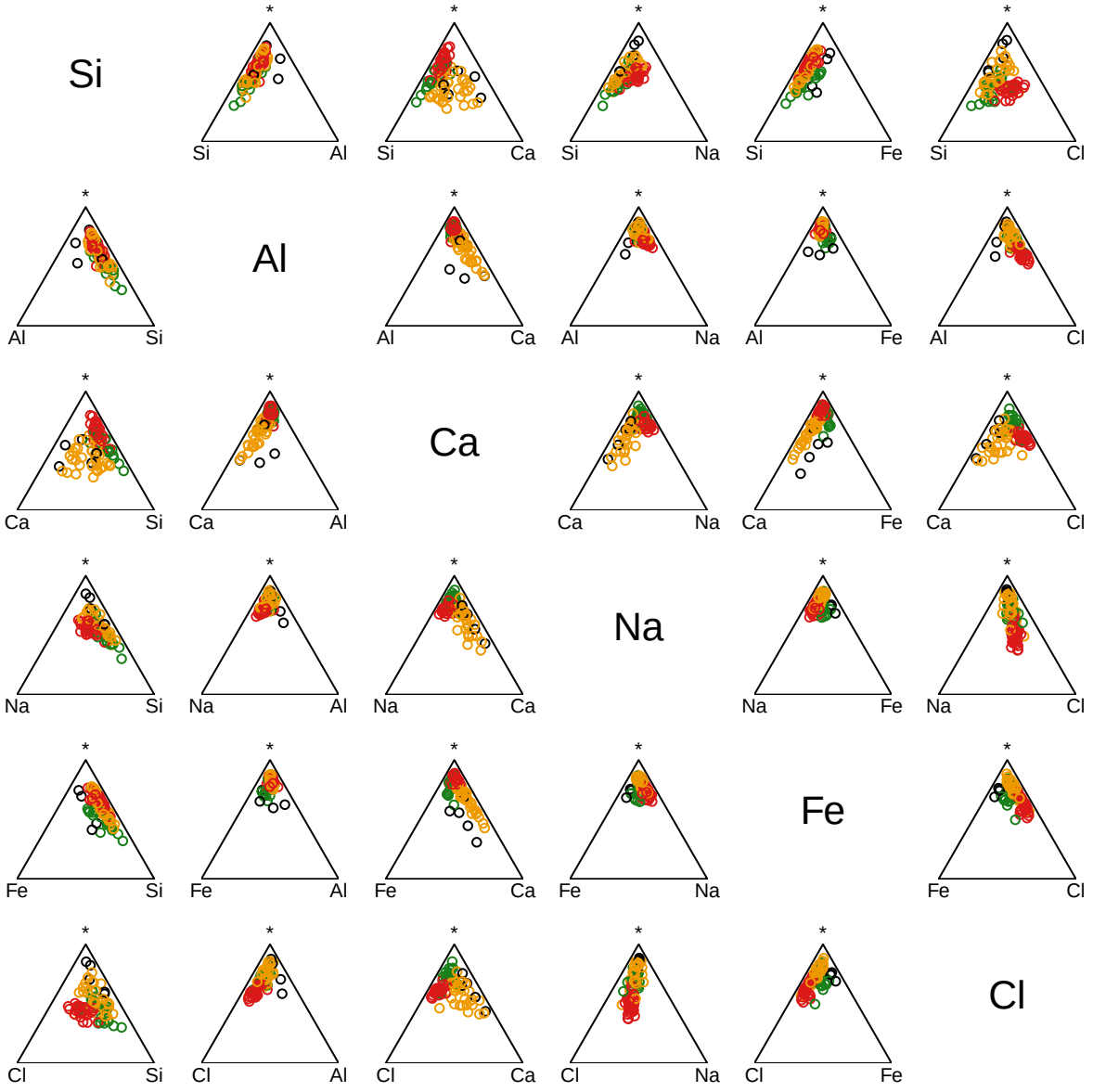
Si, Al, Ca, Mg, Cl, S



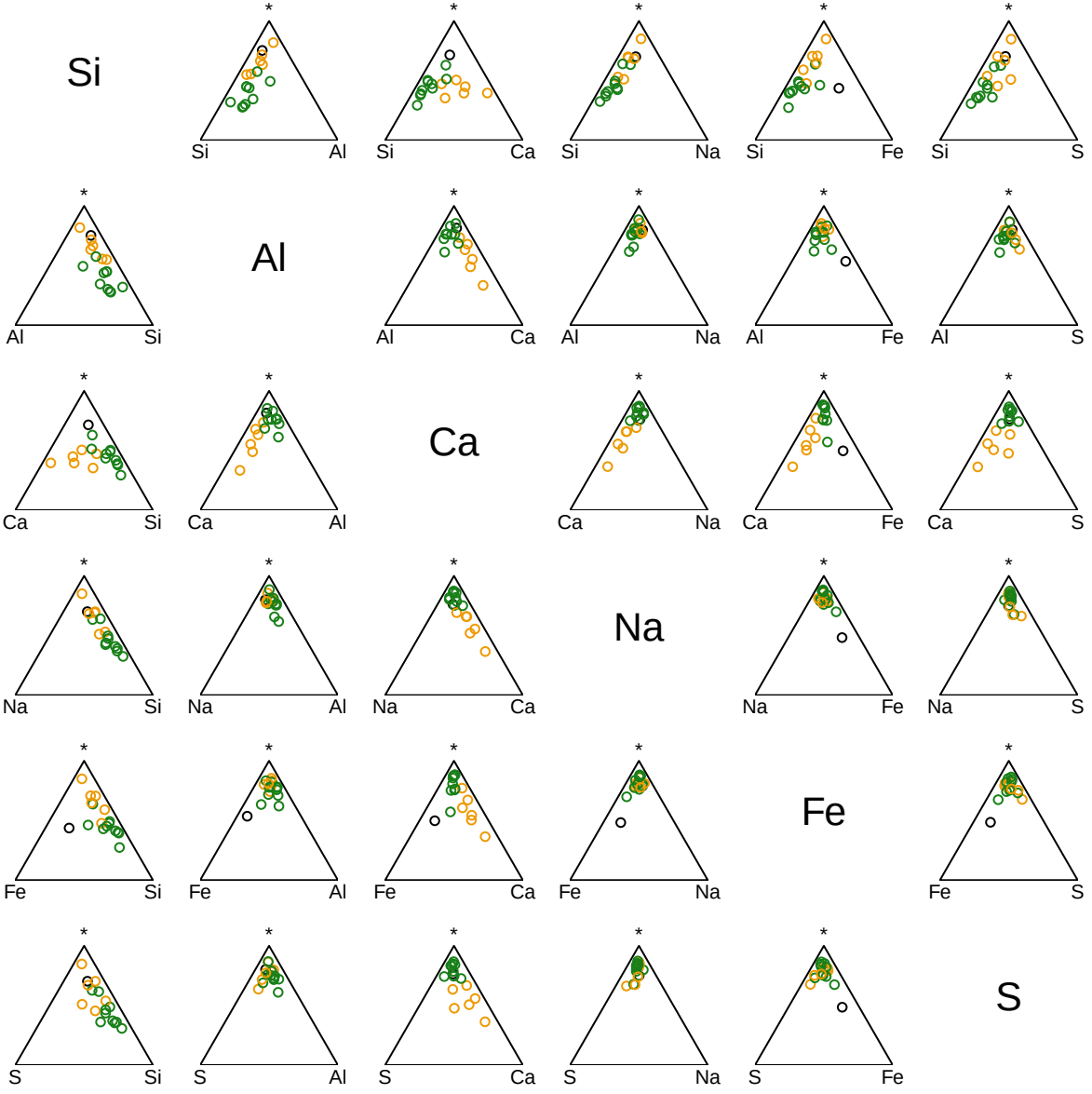
Si, Al, Ca, Na, Fe, Zn



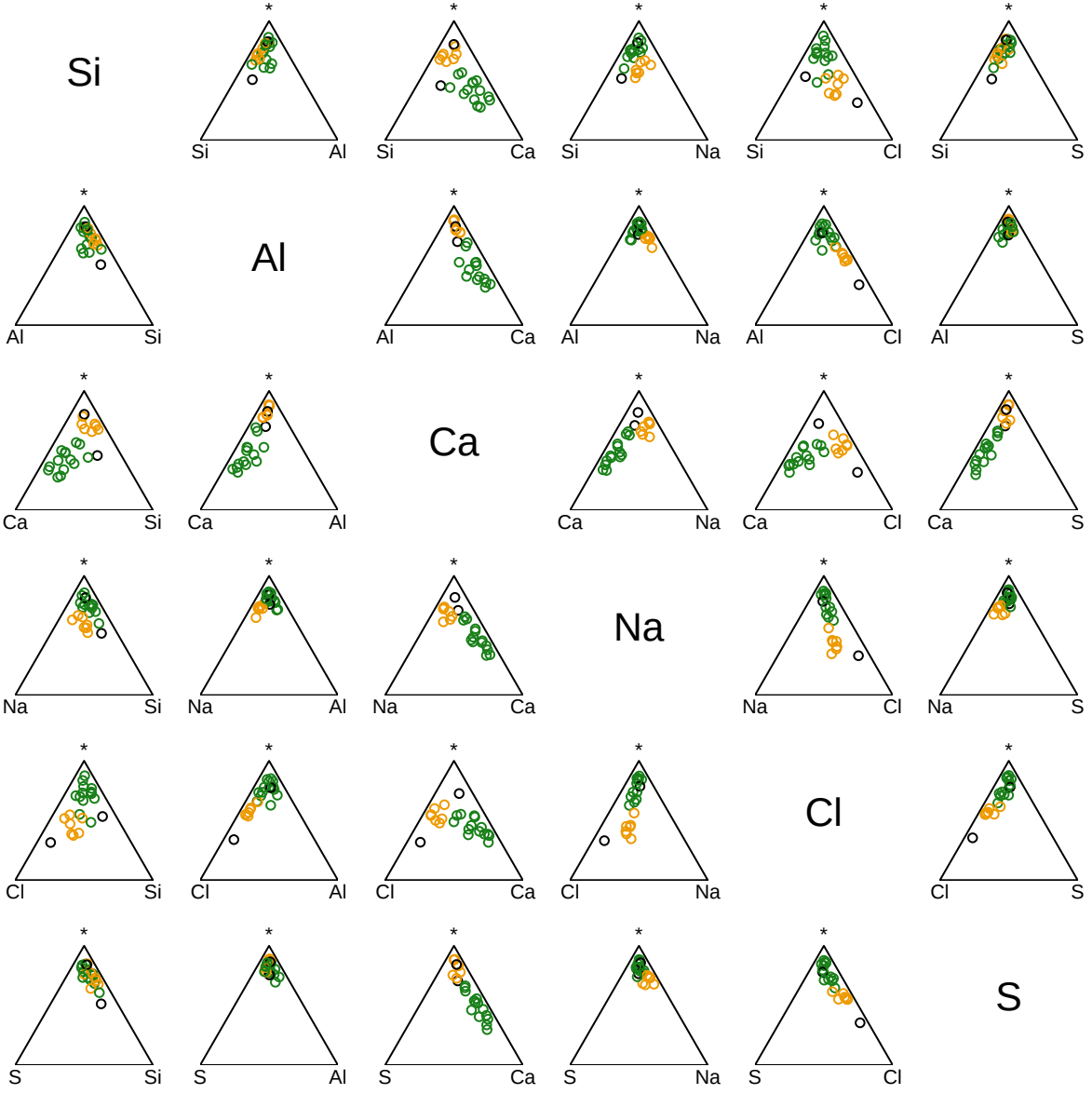
Si, Al, Ca, Na, Fe, Cl



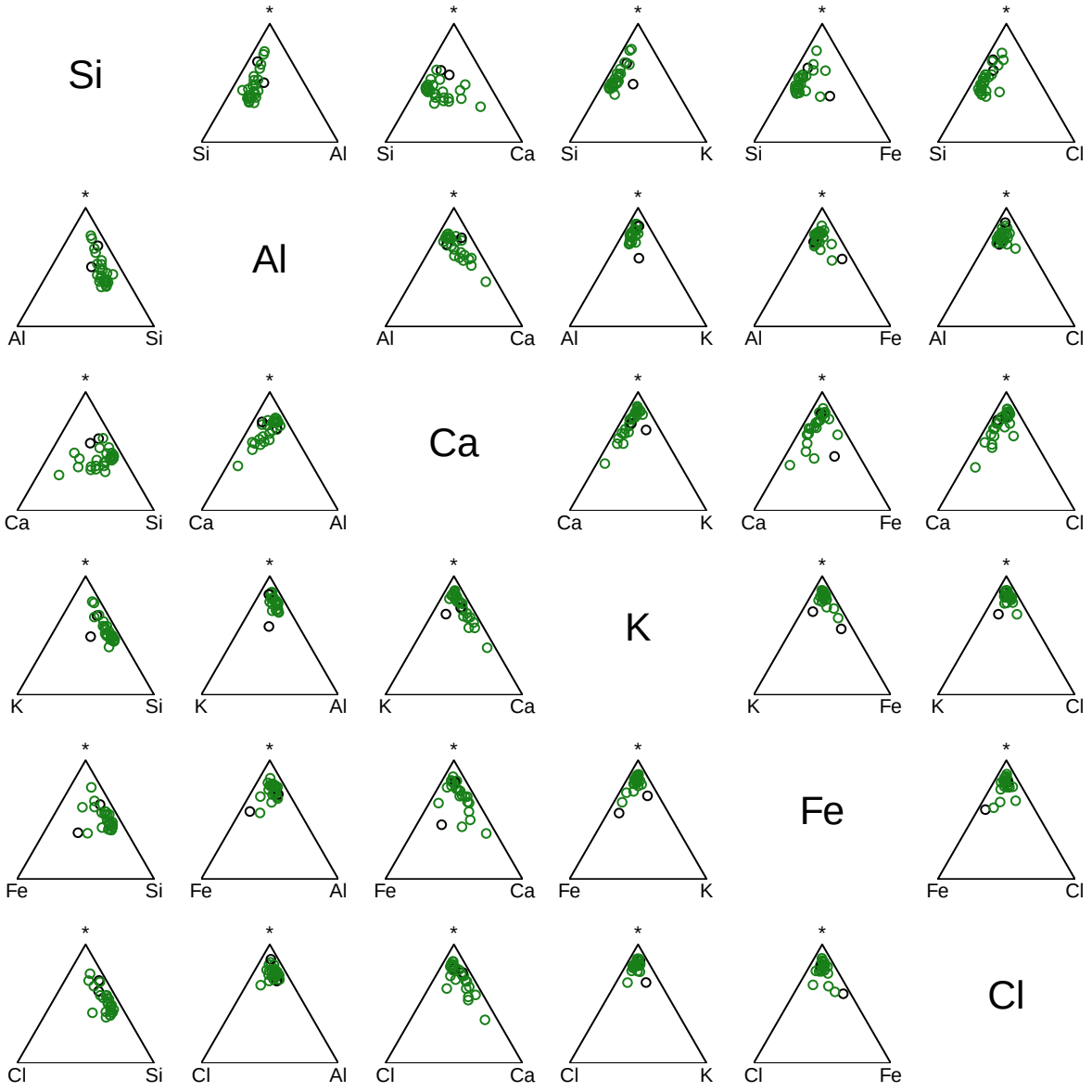
Si, Al, Ca, Na, Fe, S



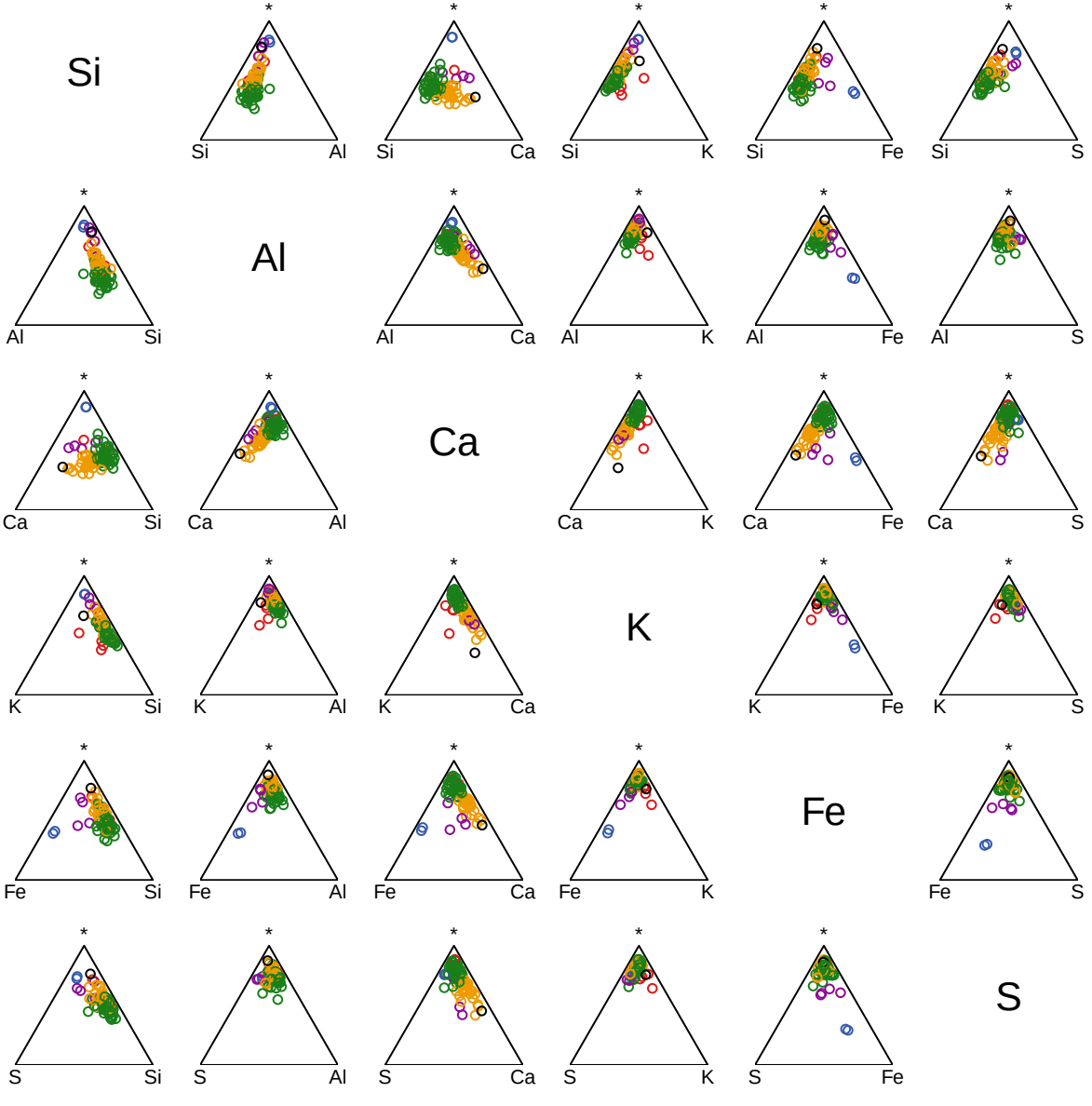
Si, Al, Ca, Na, Cl, S



Si, Al, Ca, K, Fe, Cl



Si, Al, Ca, K, Fe, S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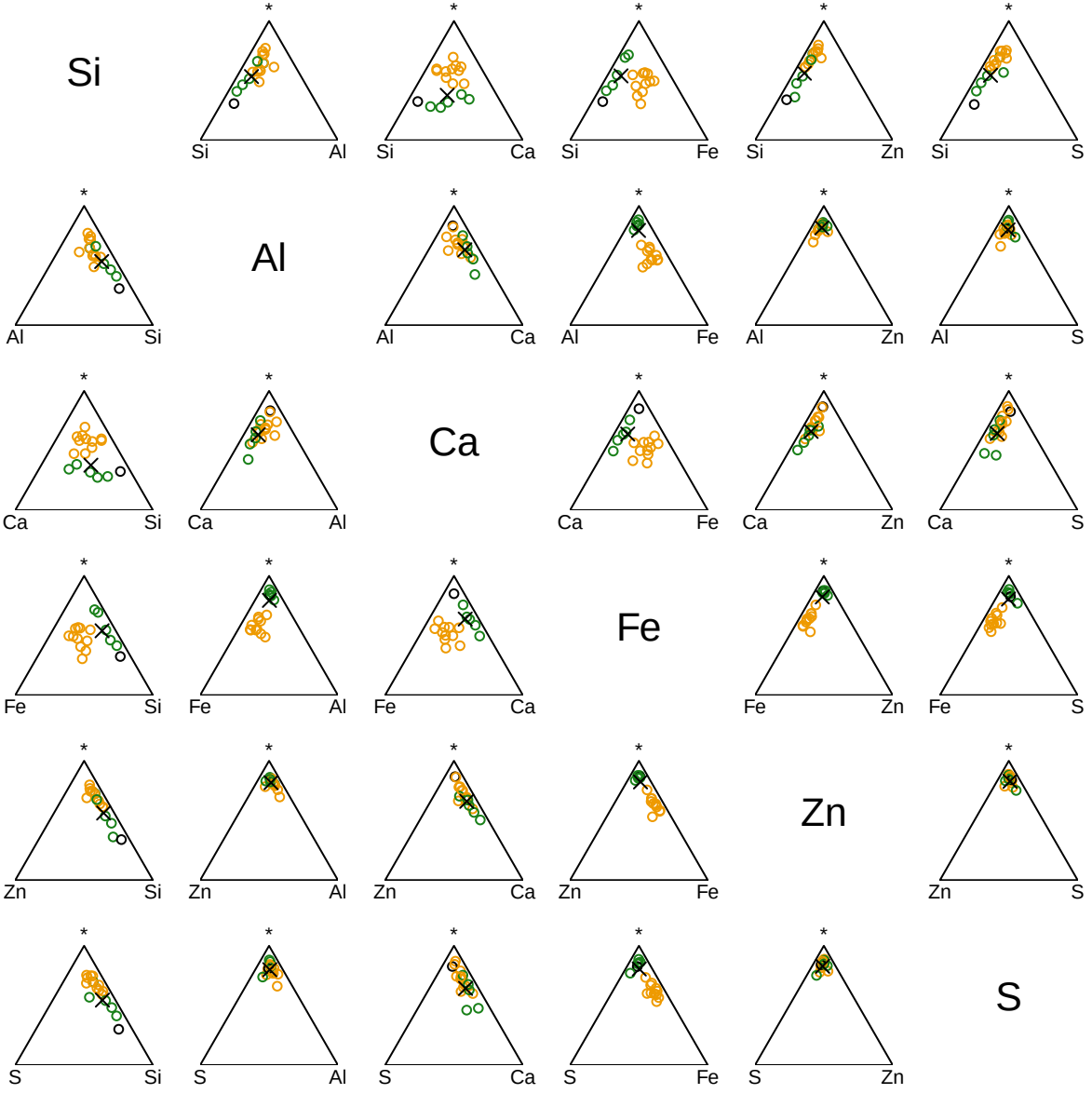
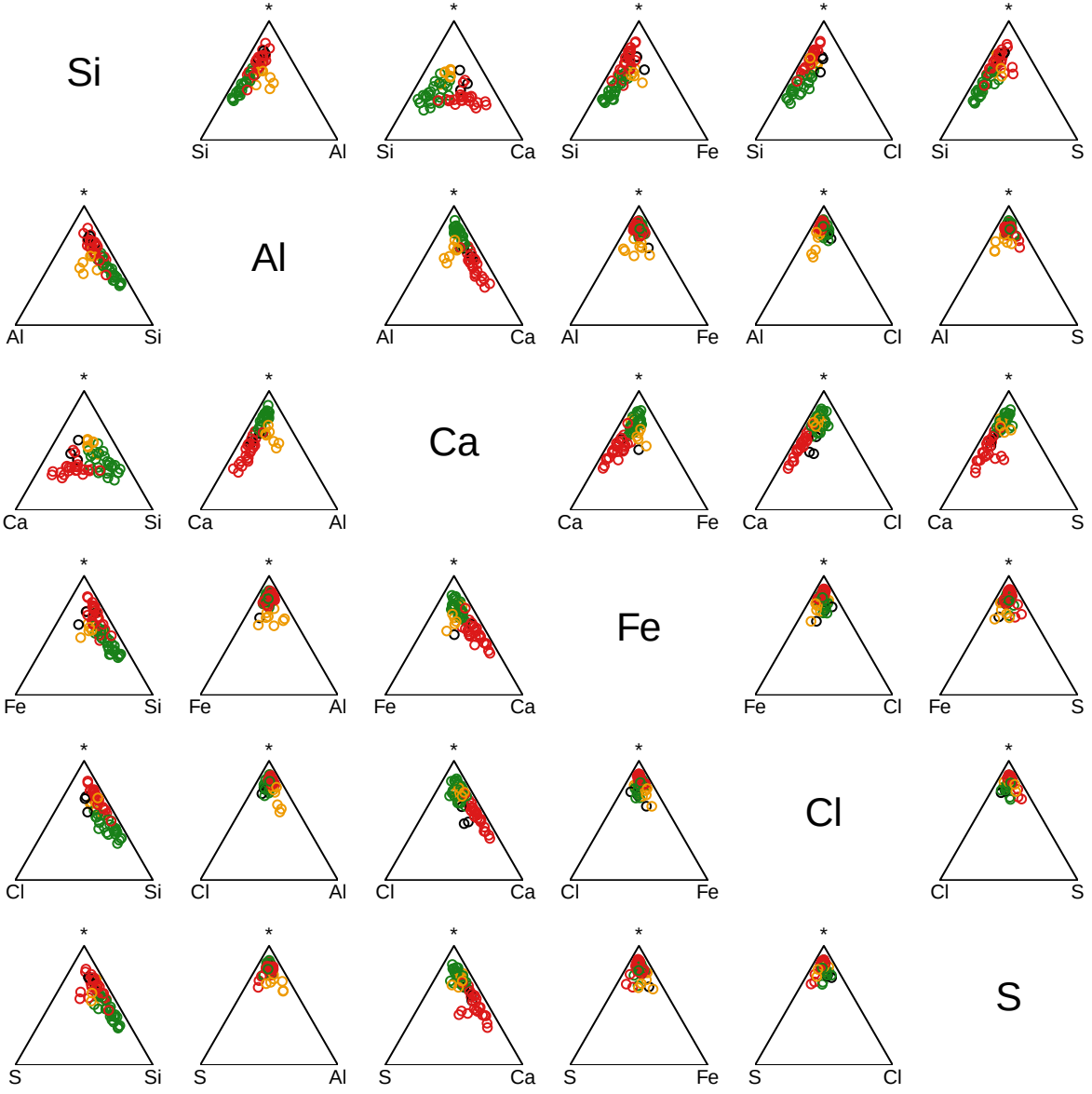
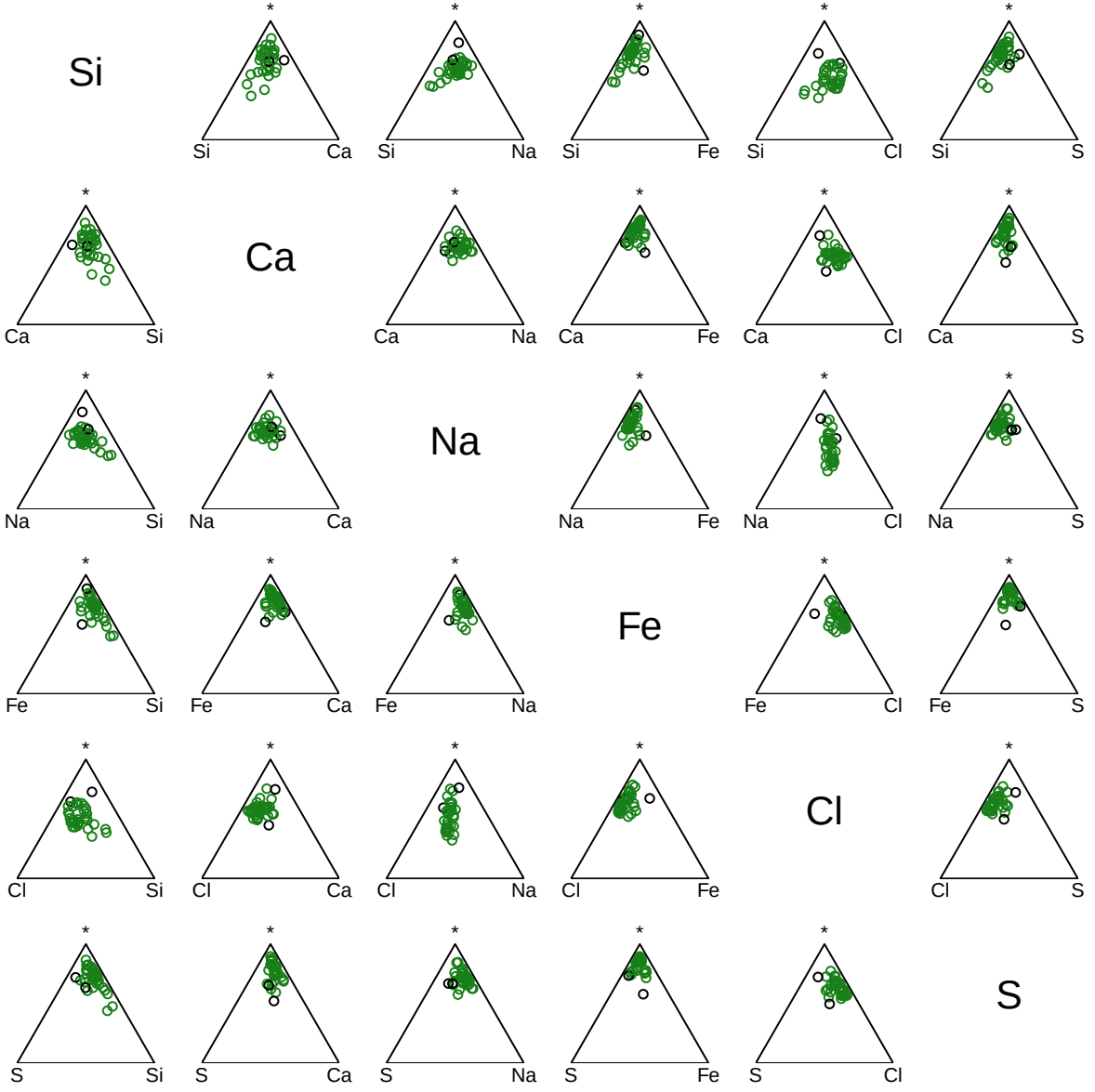
Si, Al, Ca, Fe, Zn, S



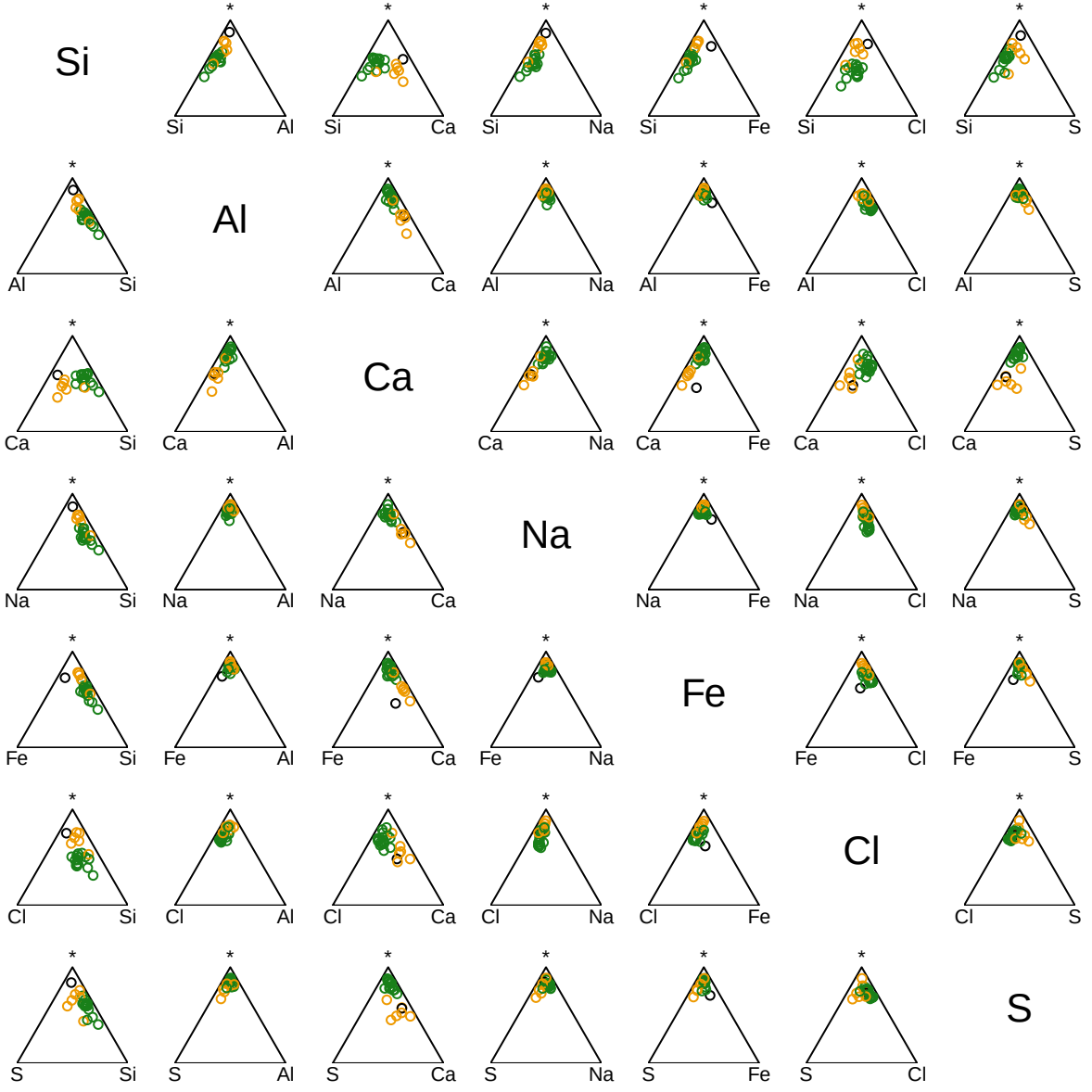
Si, Al, Ca, Fe, Cl, S



Si, Ca, Na, Fe, Cl, S

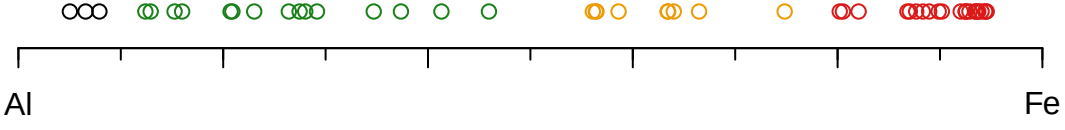


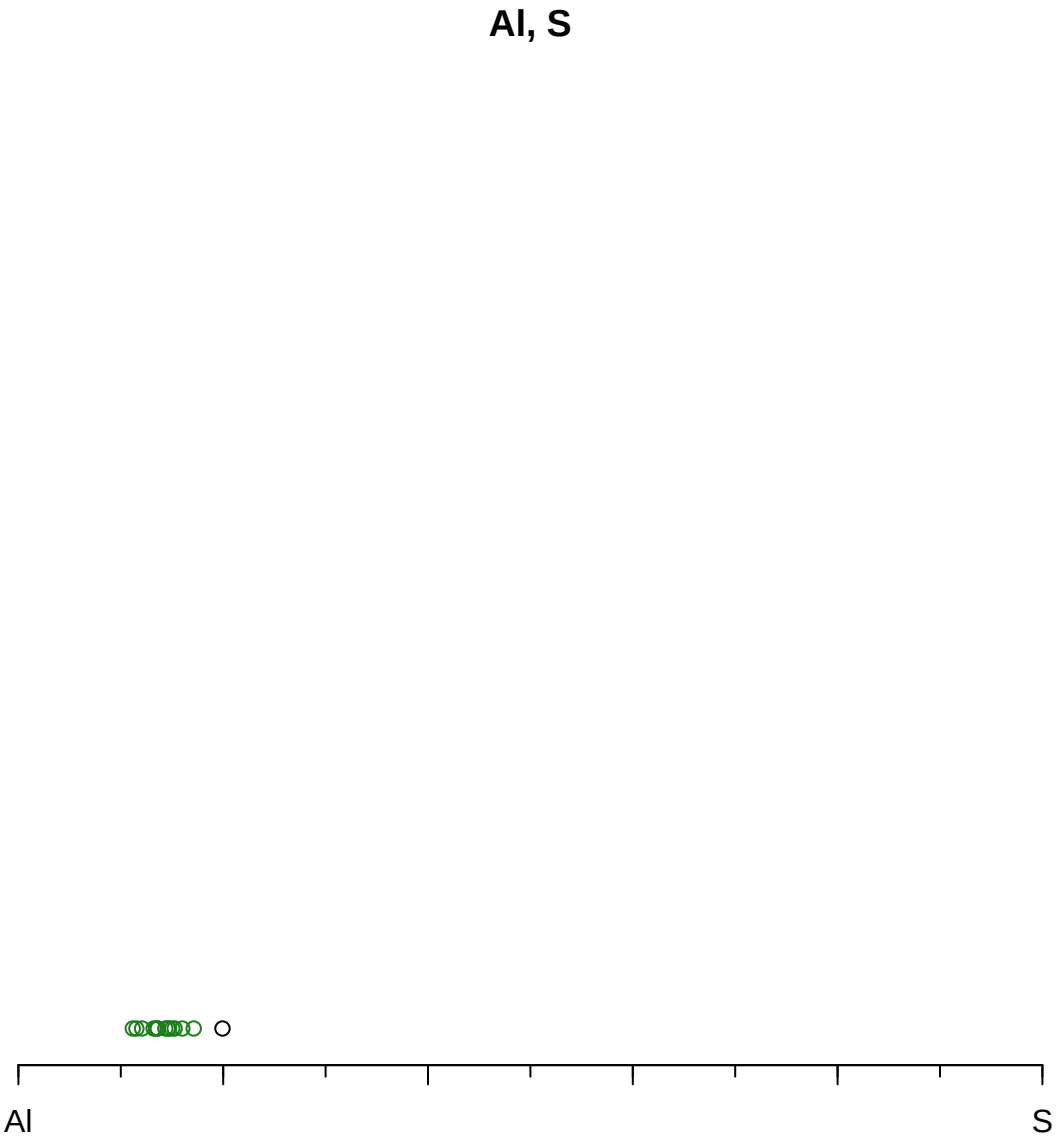
Si, Al, Ca, Na, Fe, Cl, S



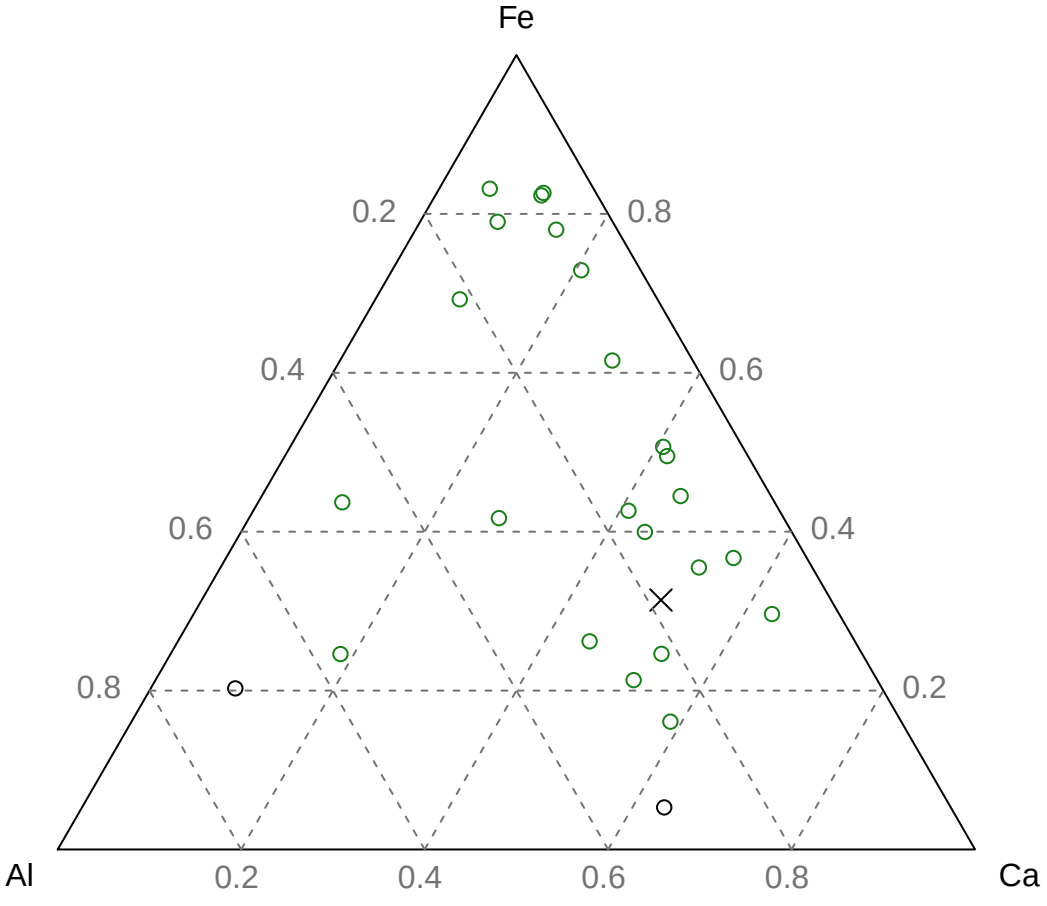
Al, Ca

Al, Fe




Al, S
Al
S

Al, Ca, Fe



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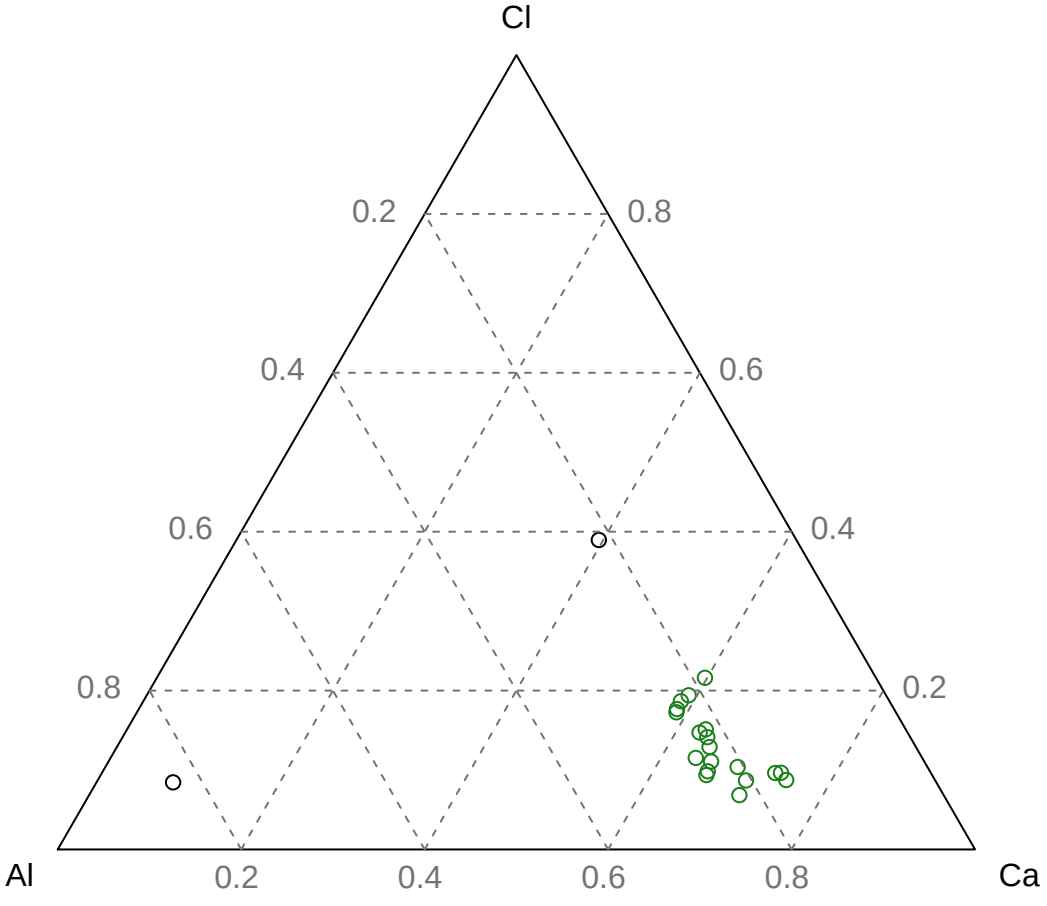
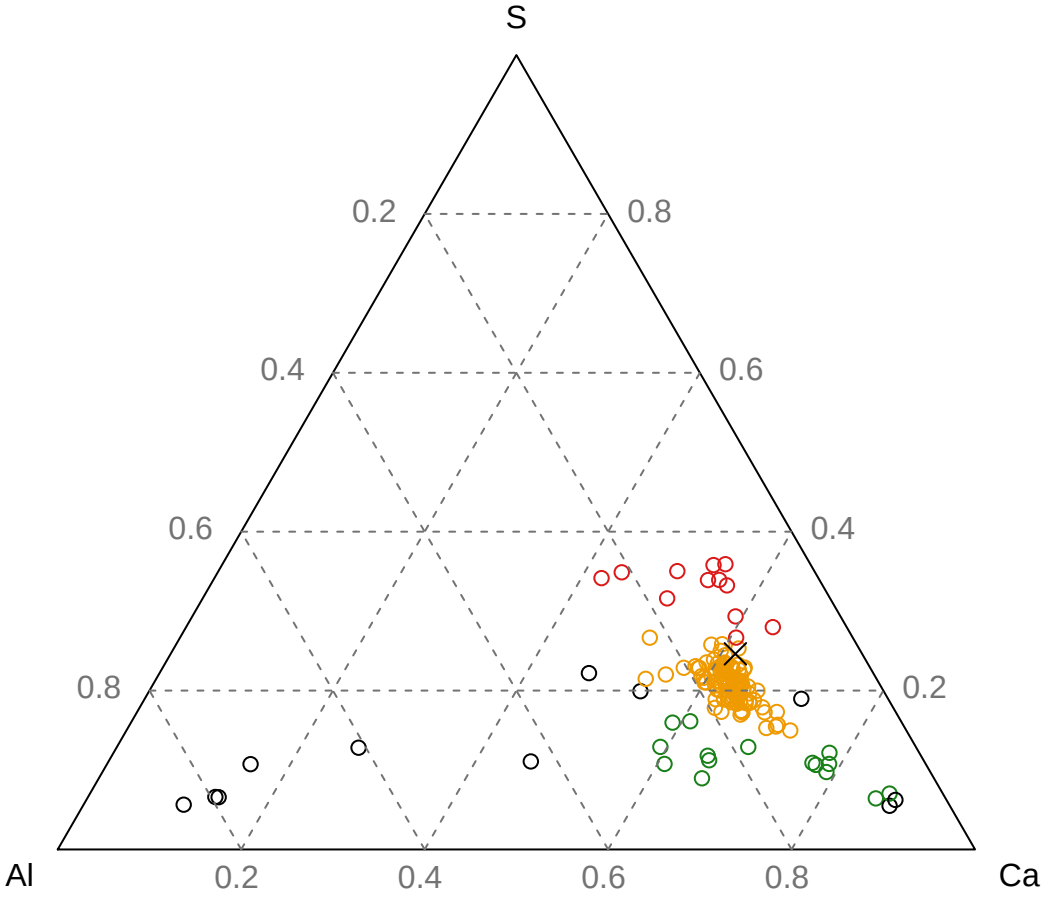
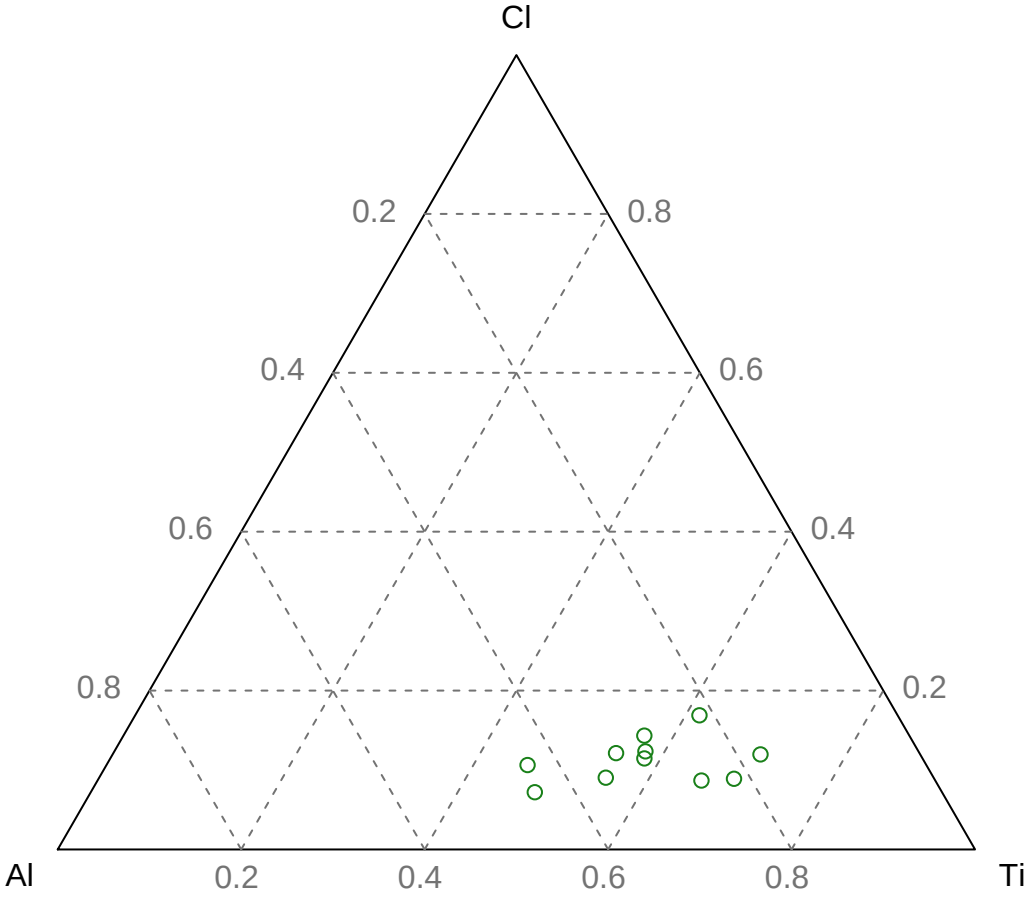


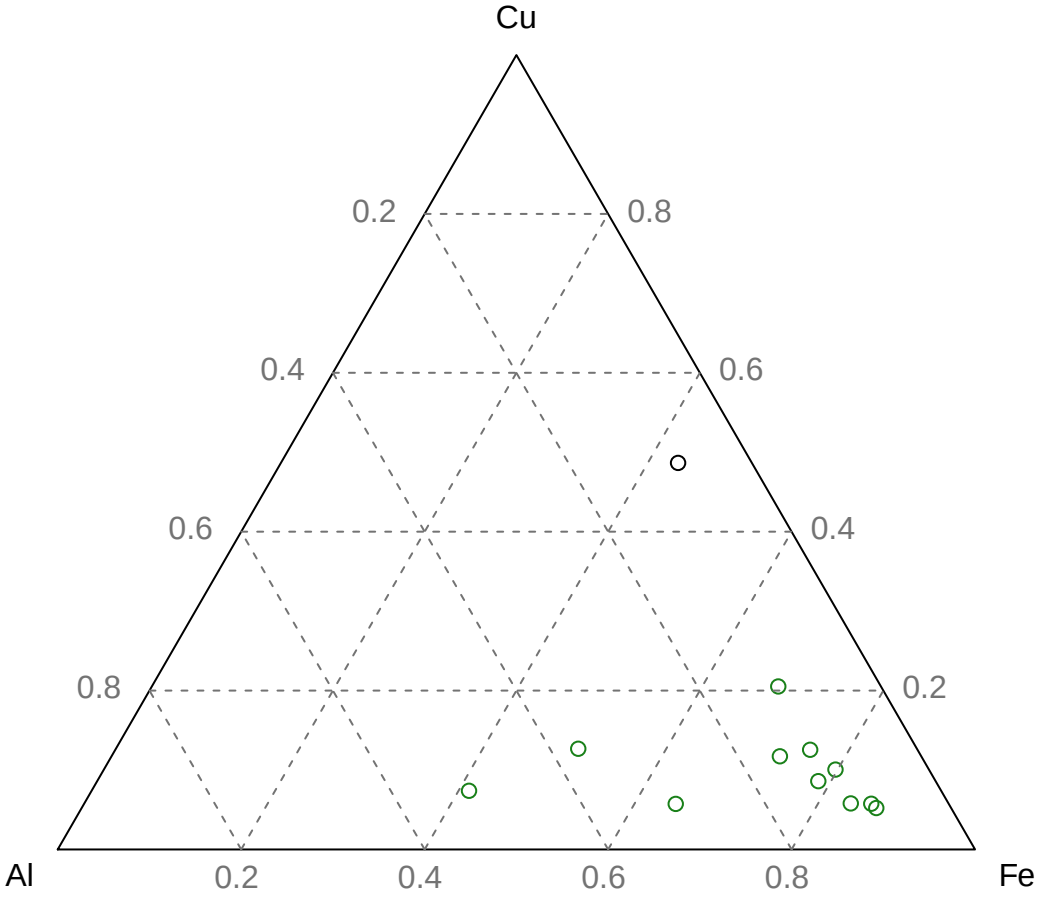
Al, Ca, S



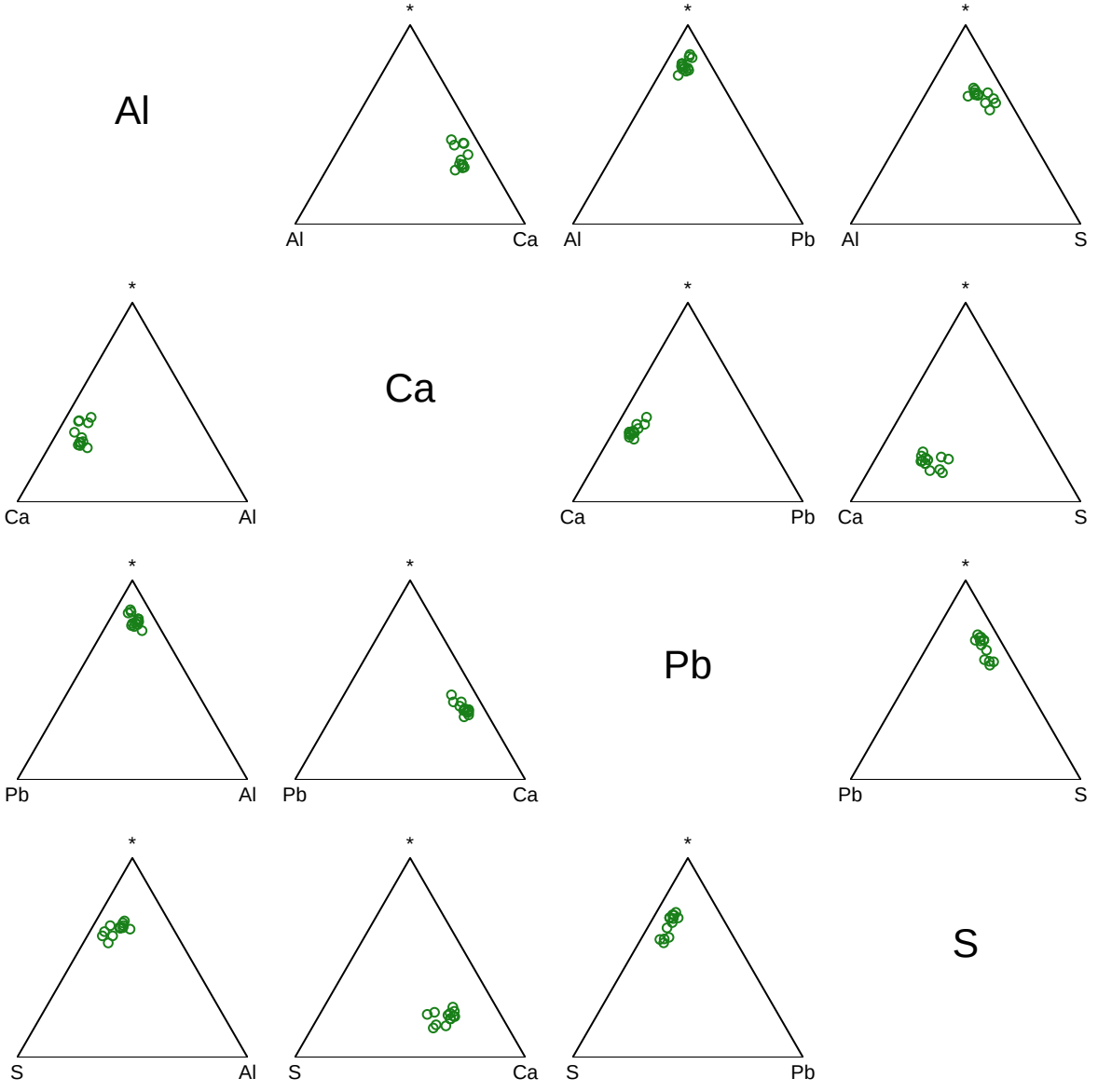
Al, Ti, Cl



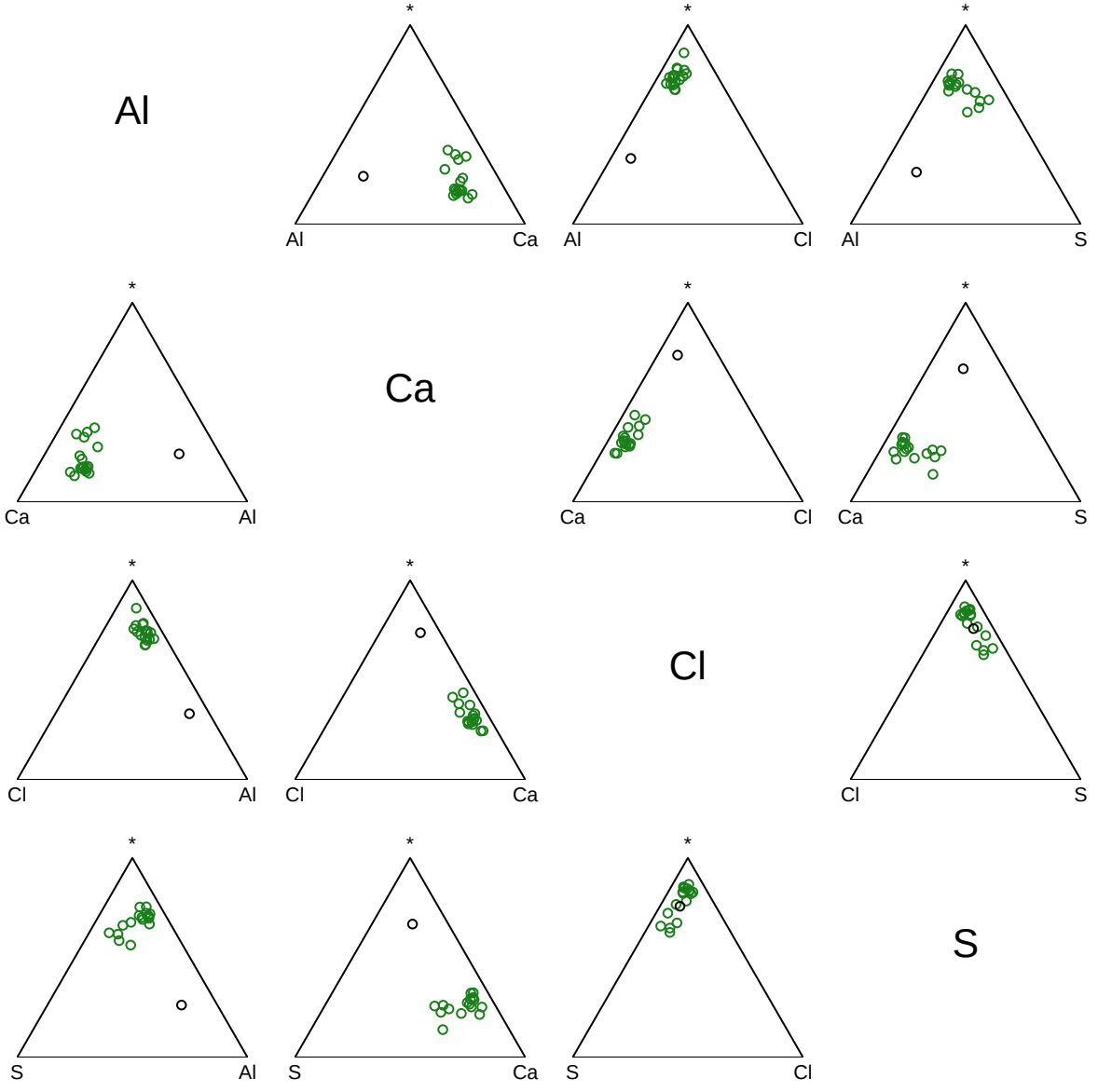
Al, Fe, Cu



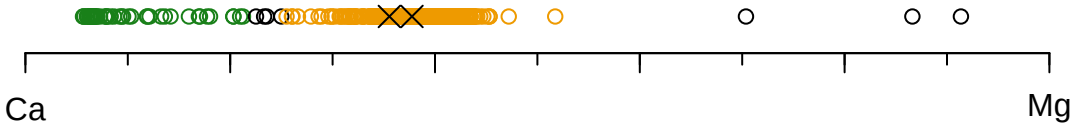
Al, Ca, Pb, S



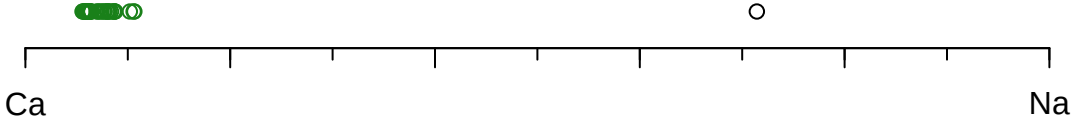
Al, Ca, Cl, S



Ca, Mg



Ca, Na



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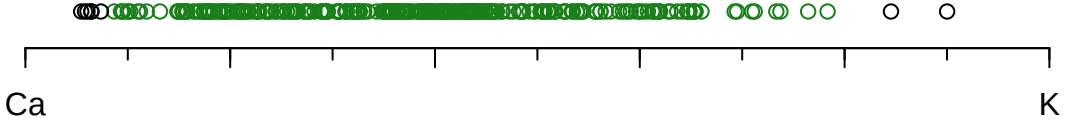
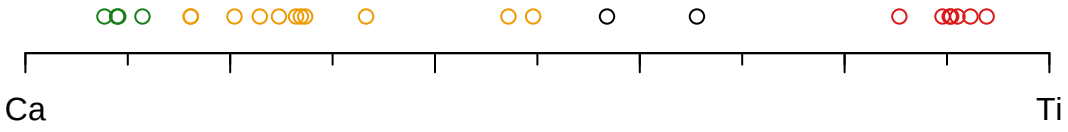
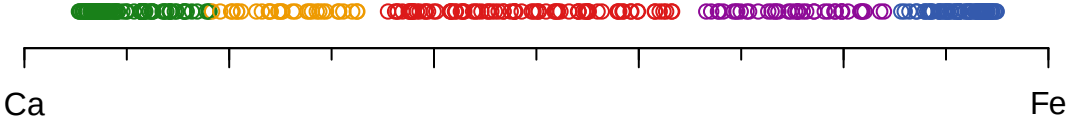


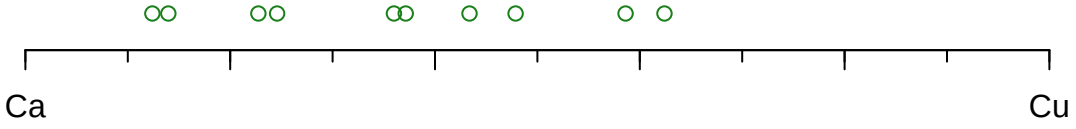
Ca, Ti



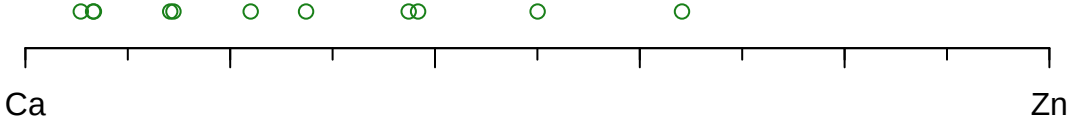
Ca, Fe



Ca, Cu



Ca, Zn



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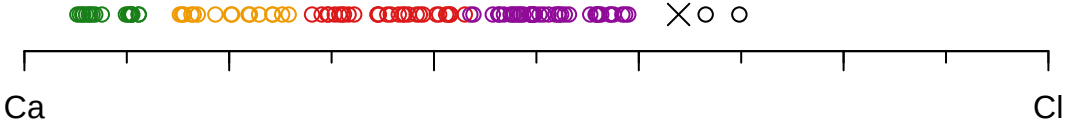

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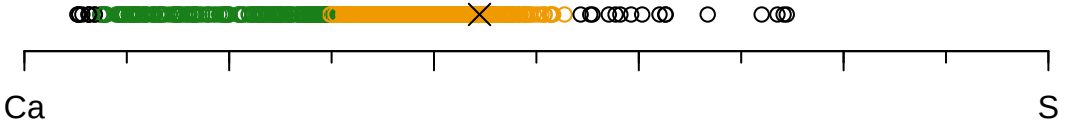
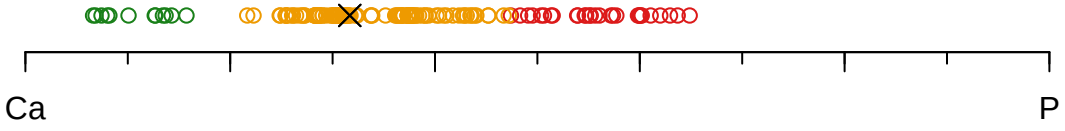


Ca, P



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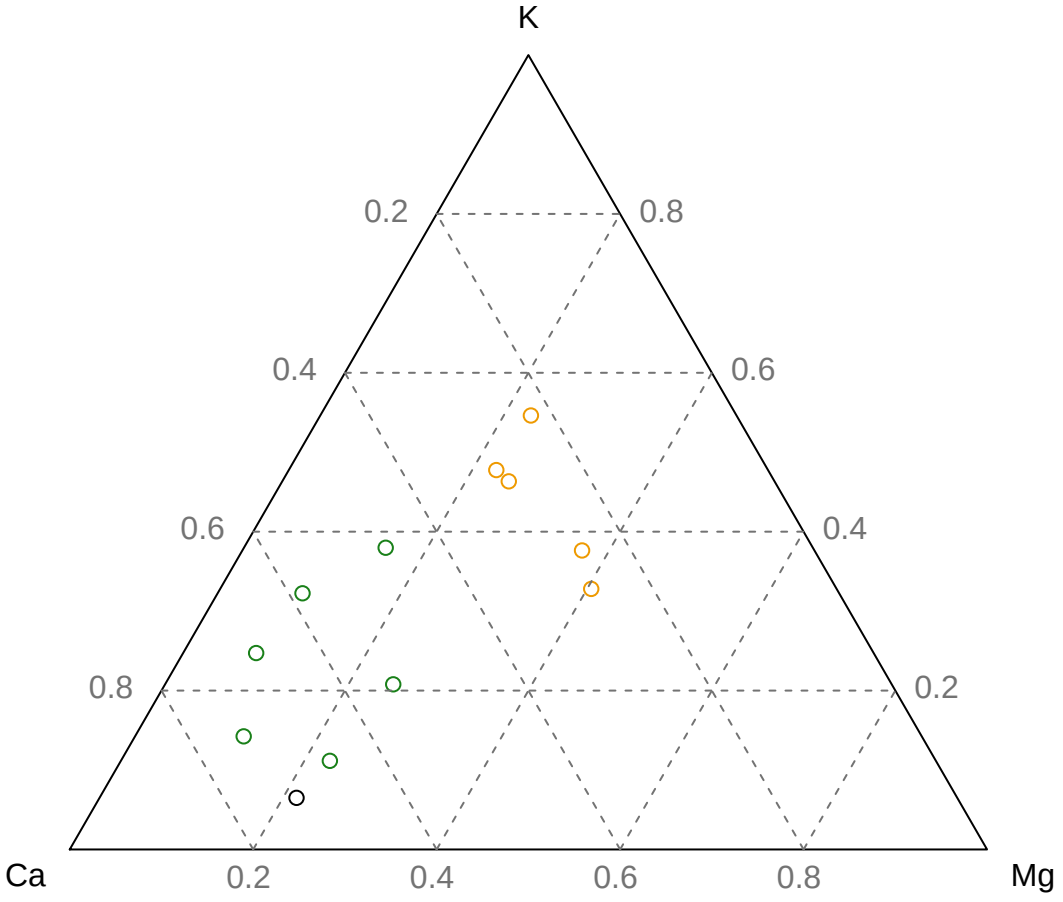

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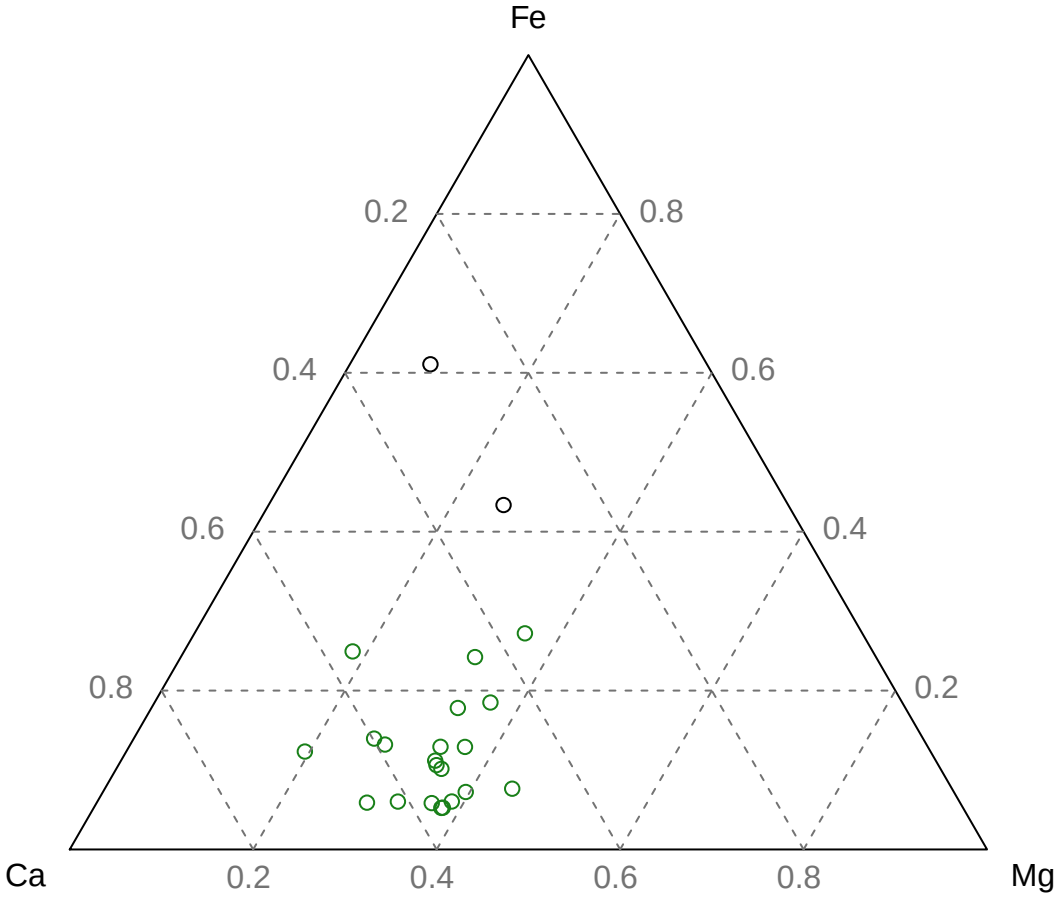
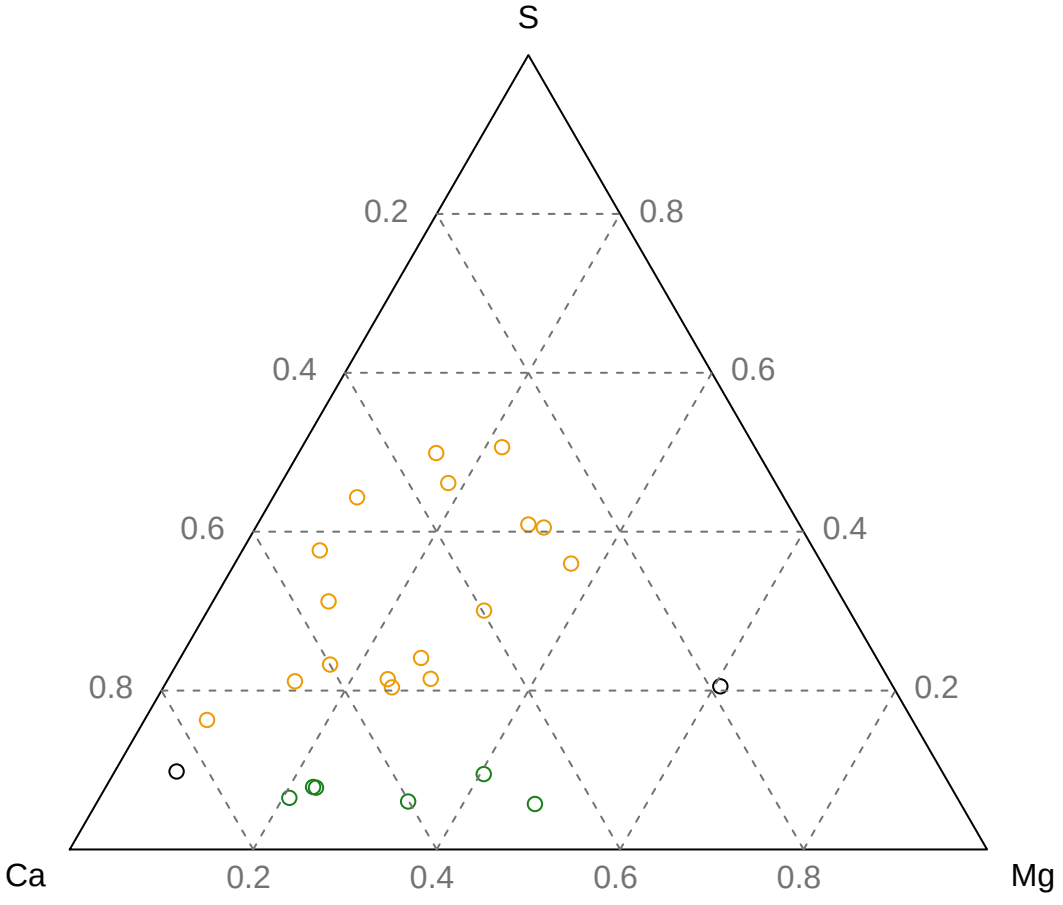


Ca, Mg, S



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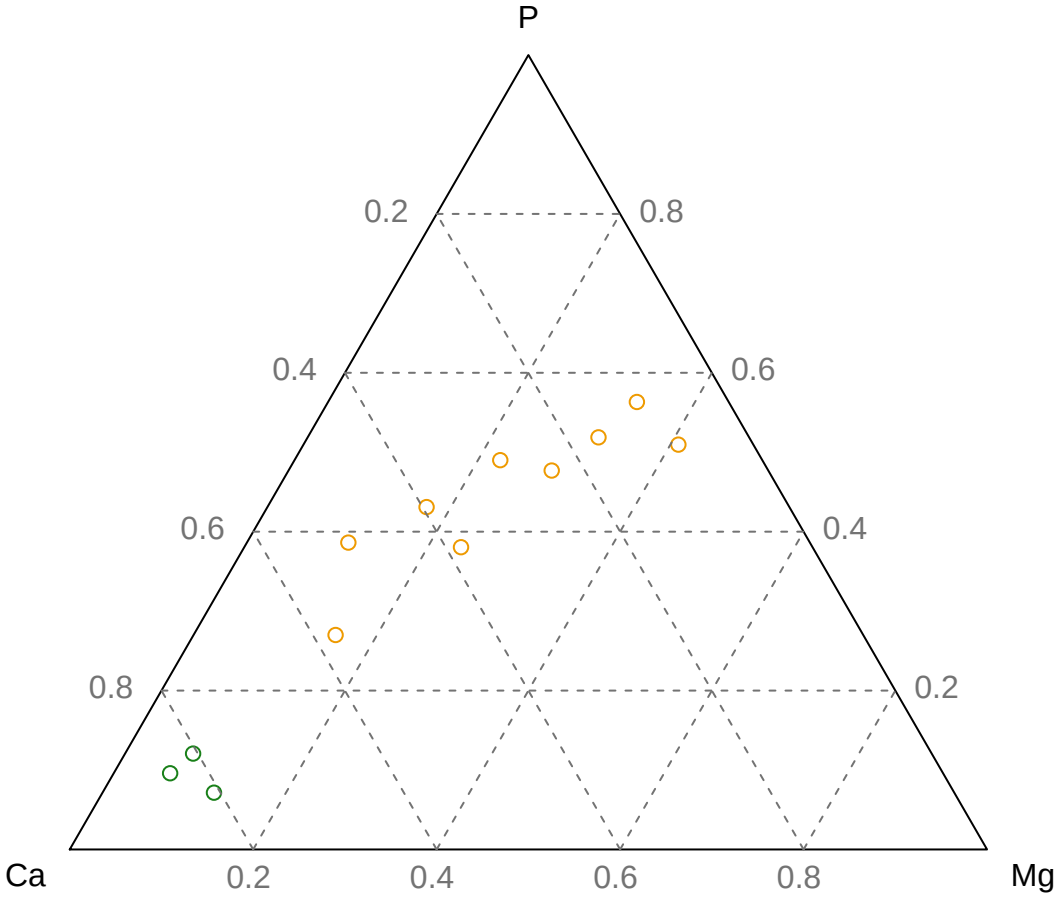

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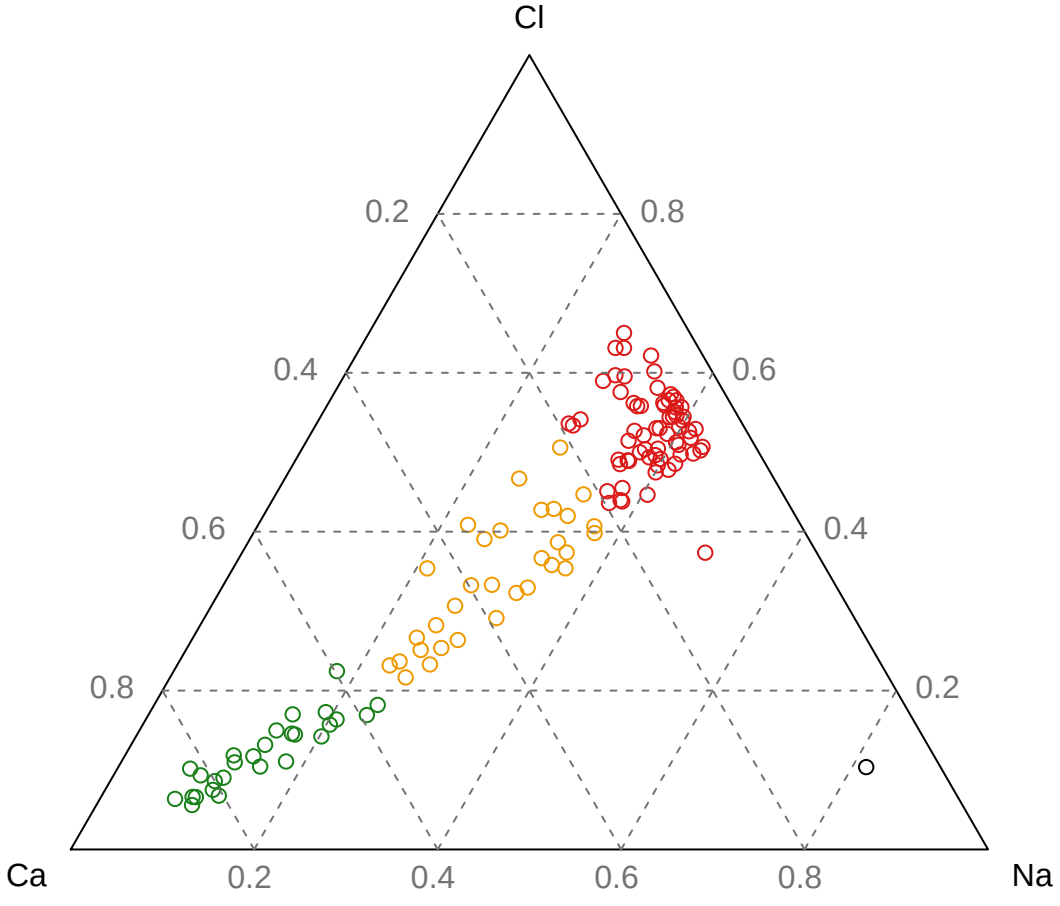

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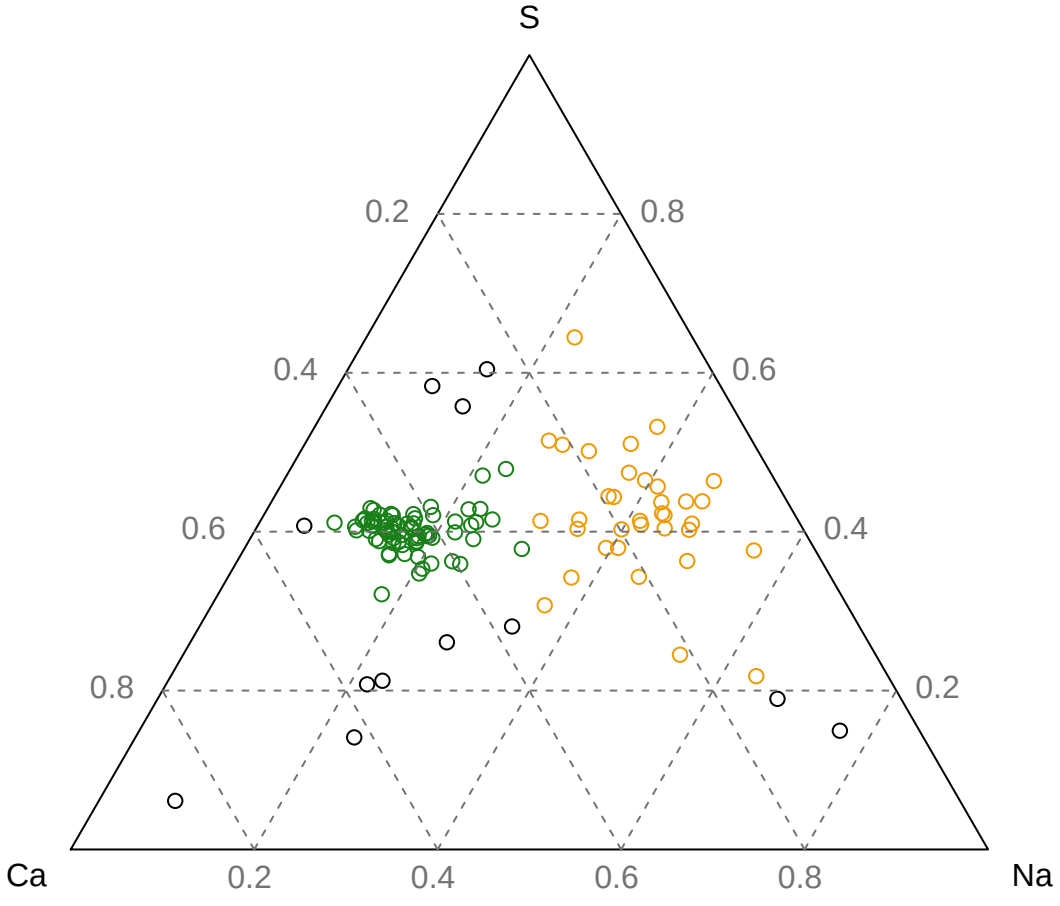

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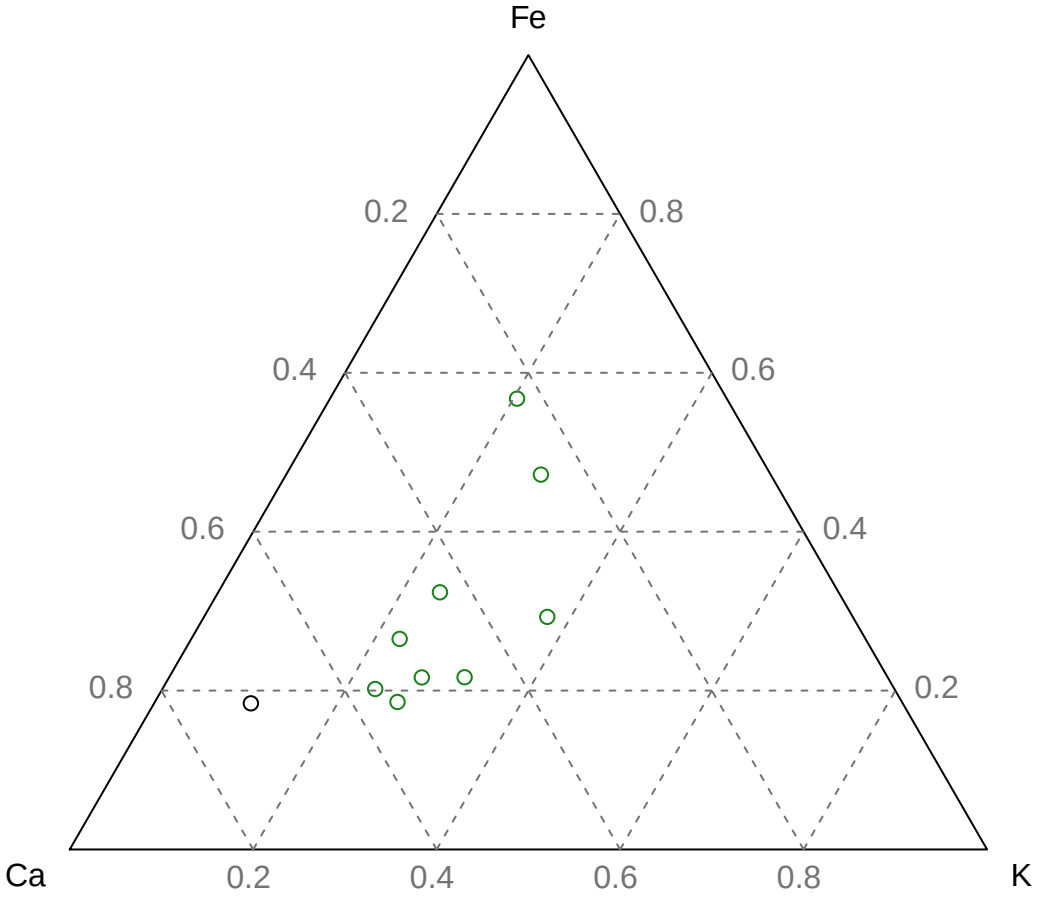

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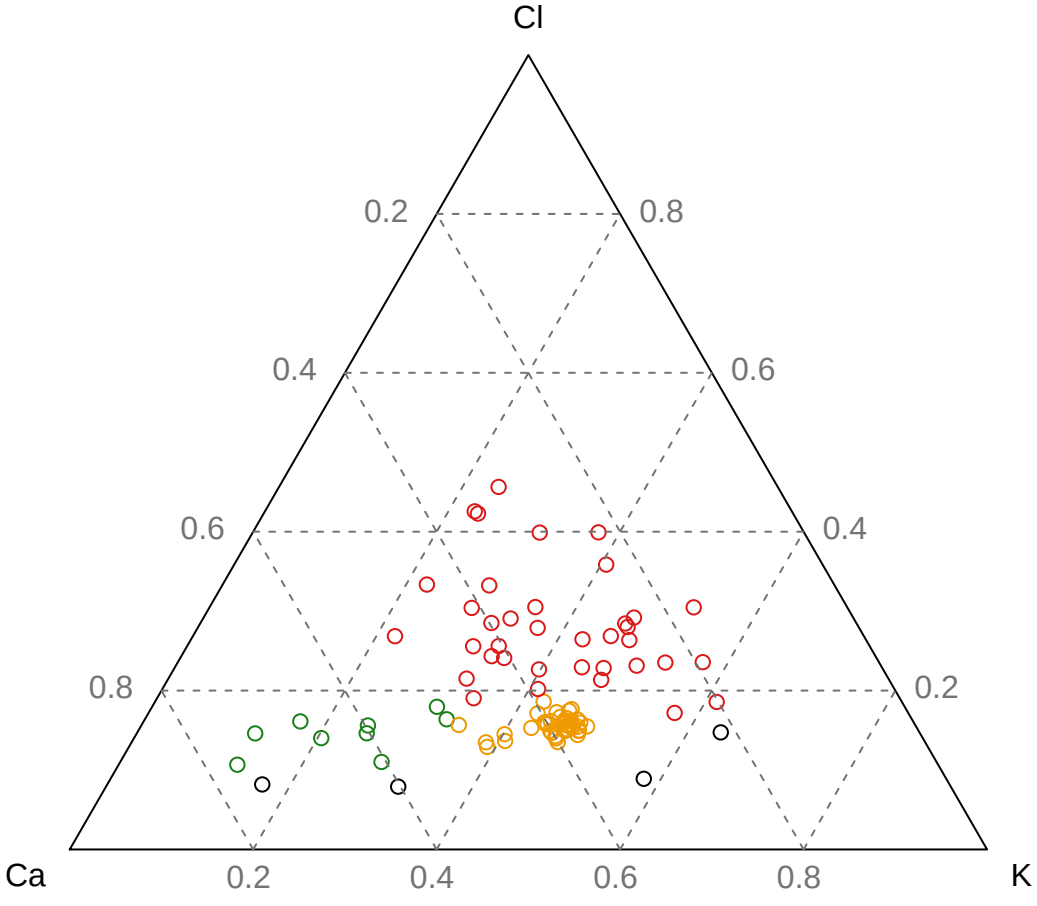

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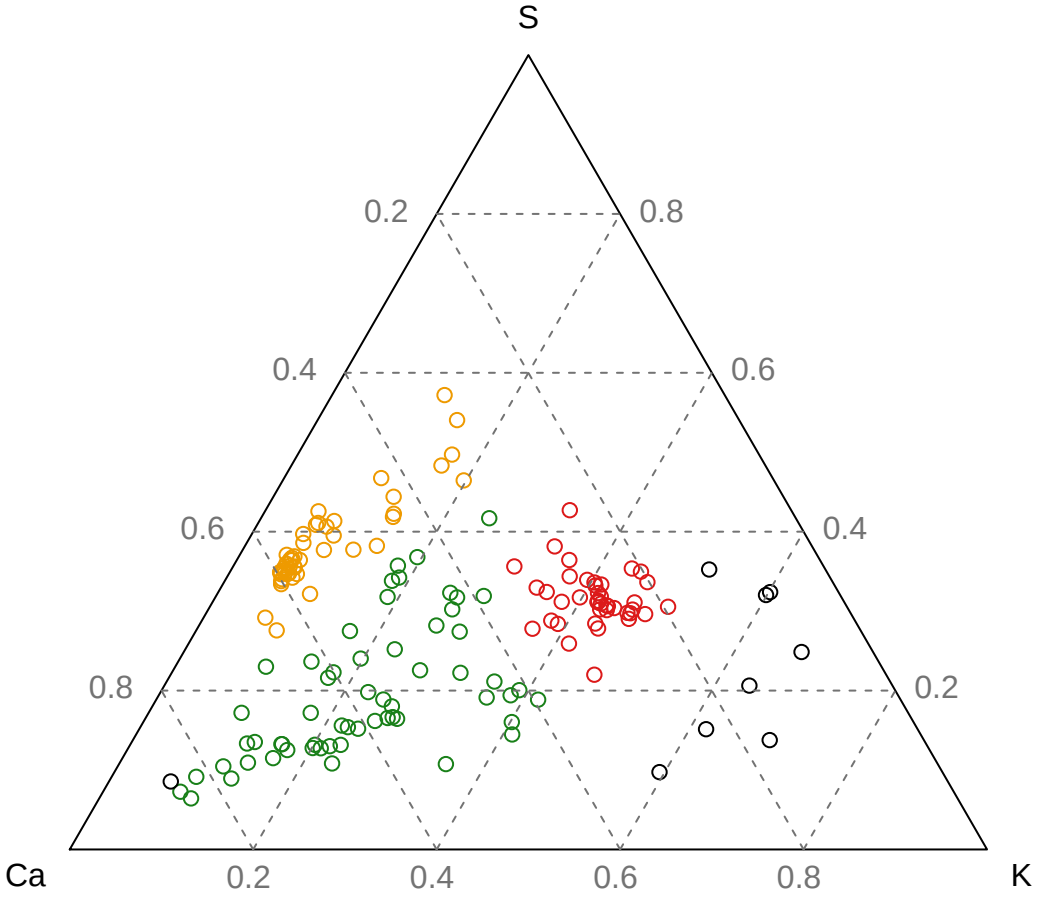

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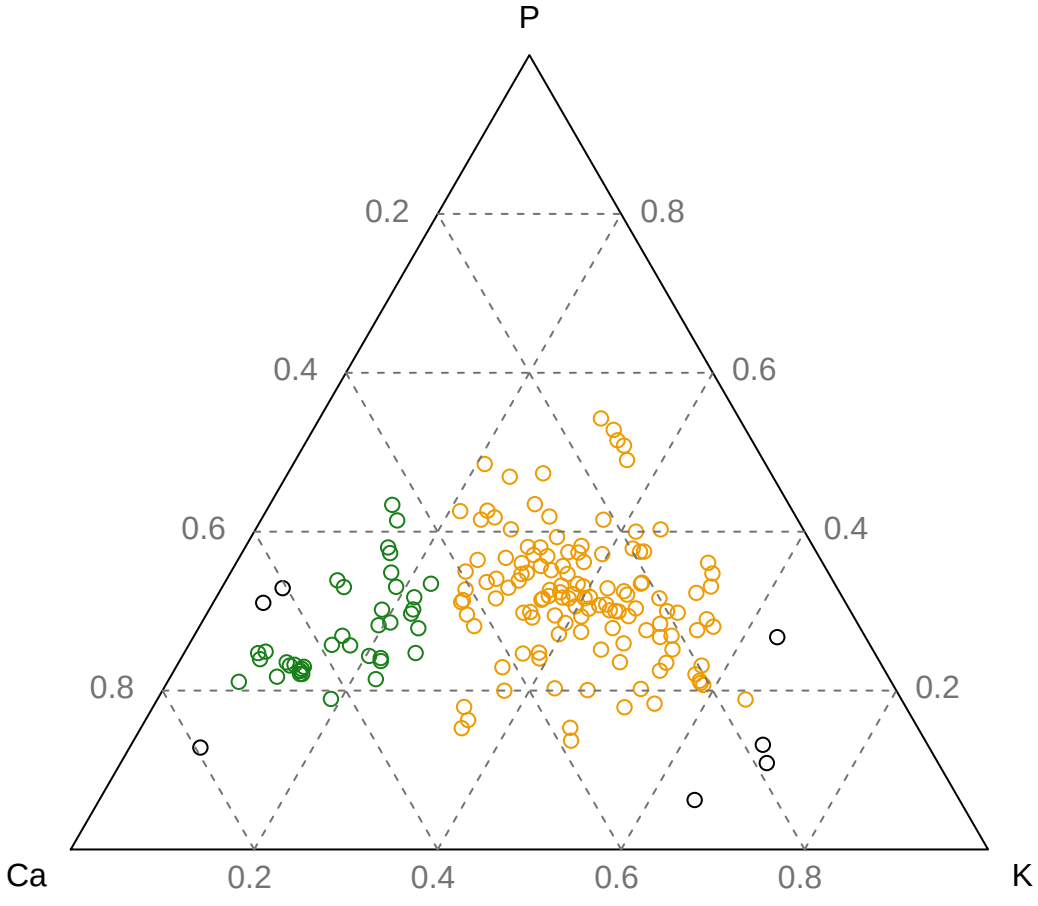

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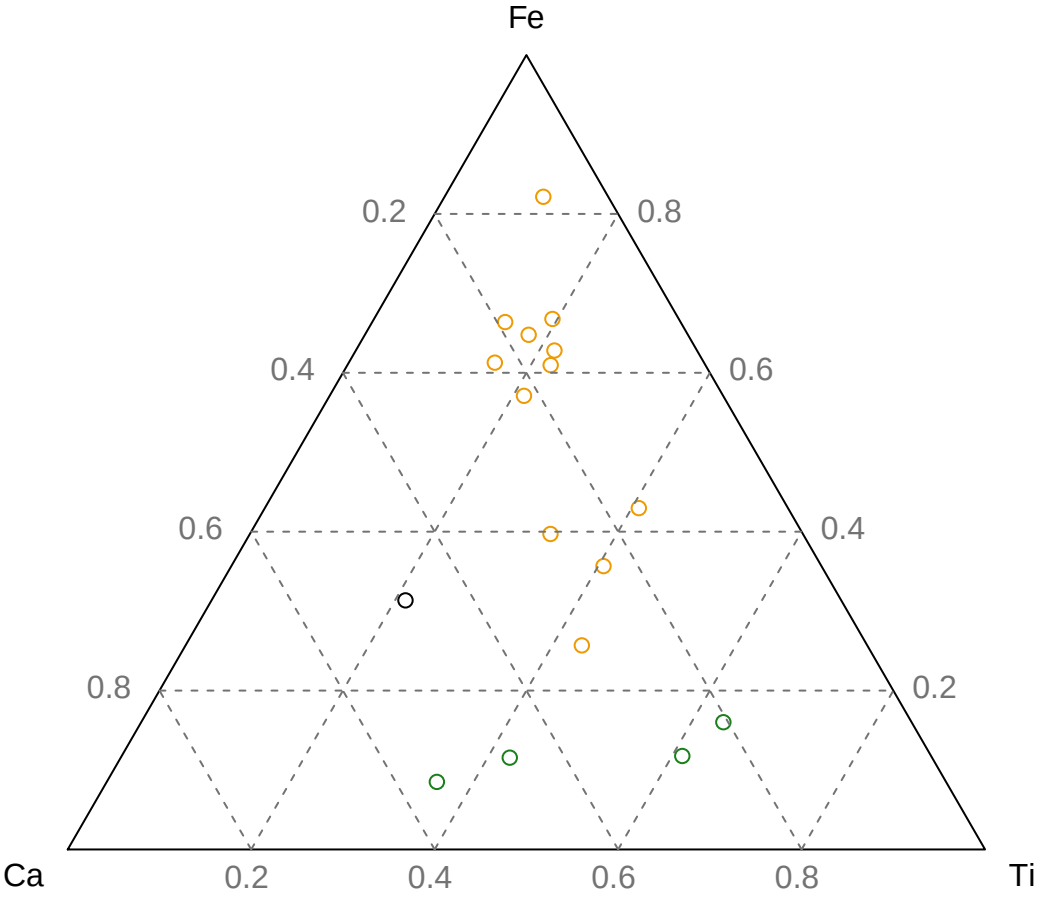

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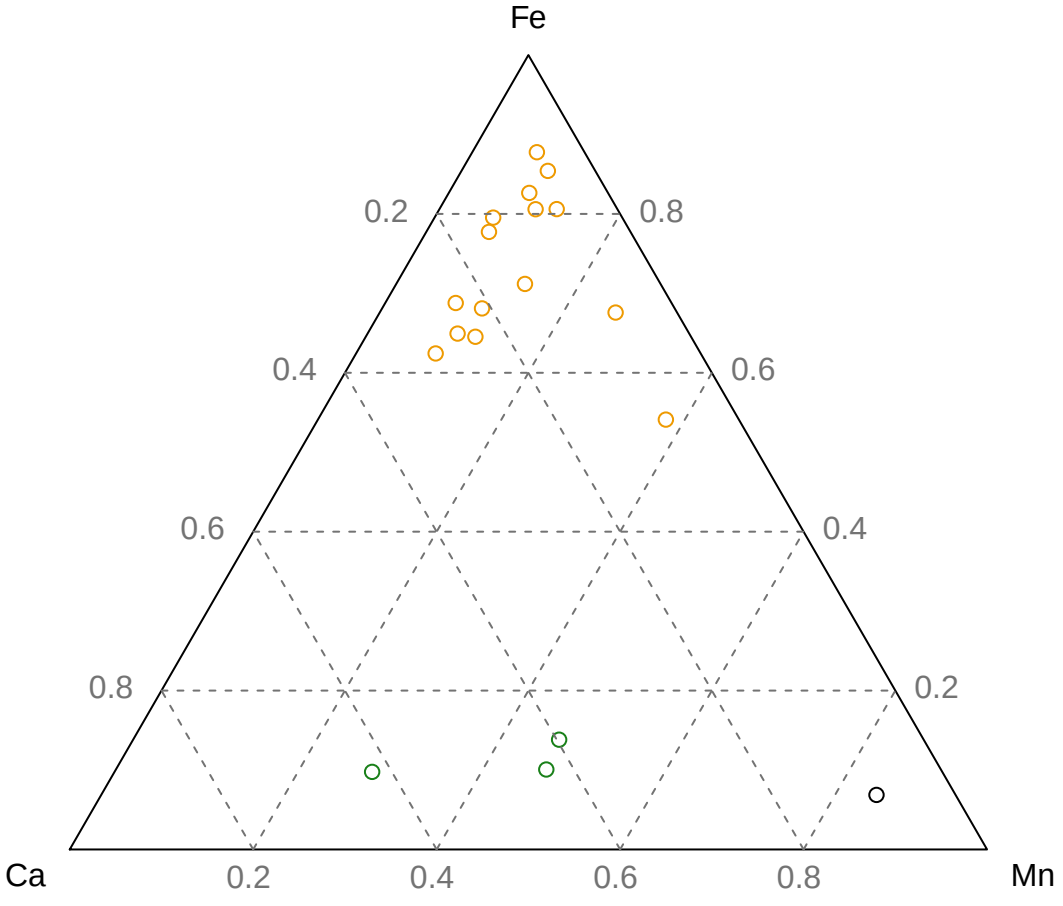

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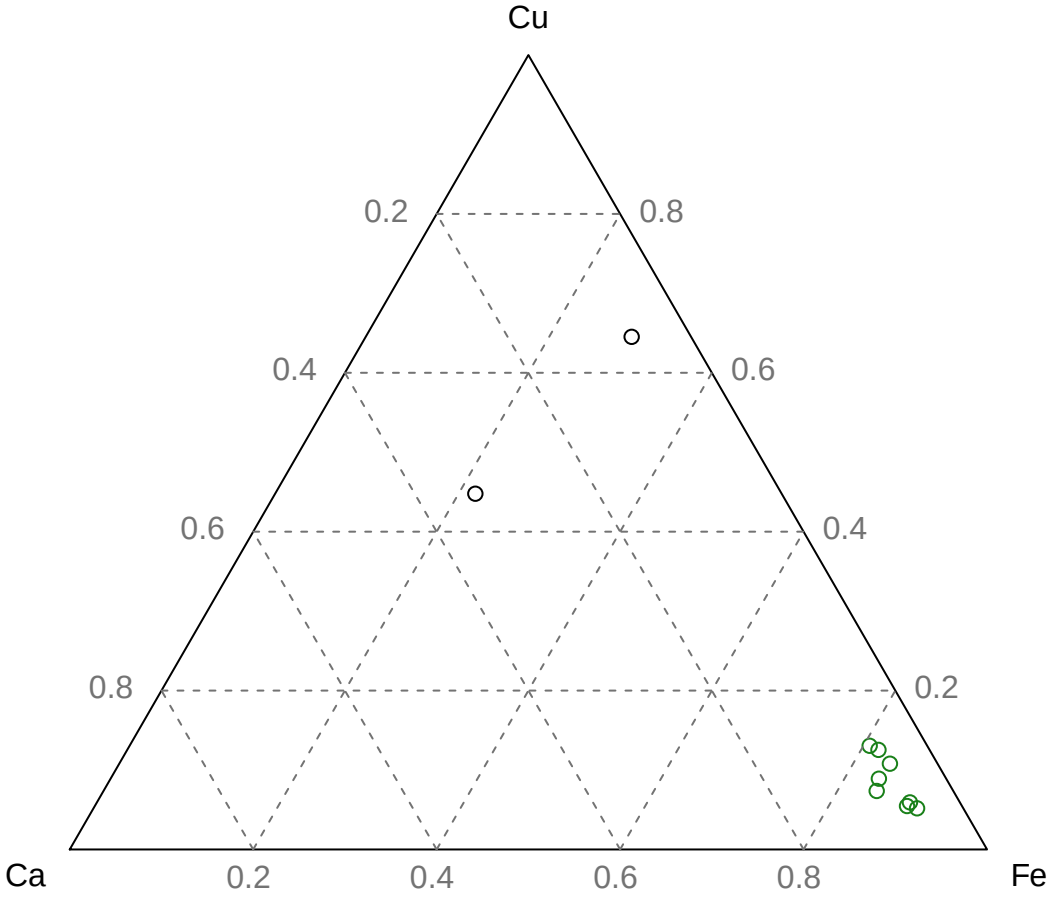

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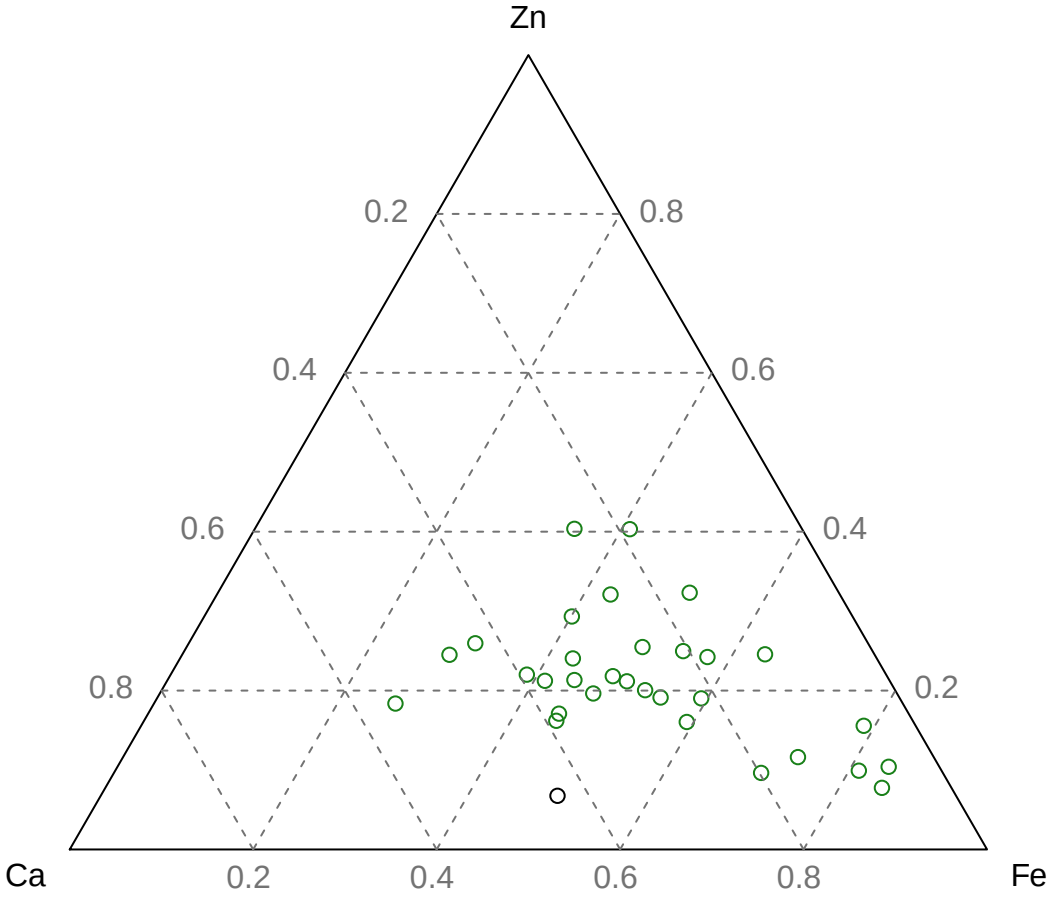

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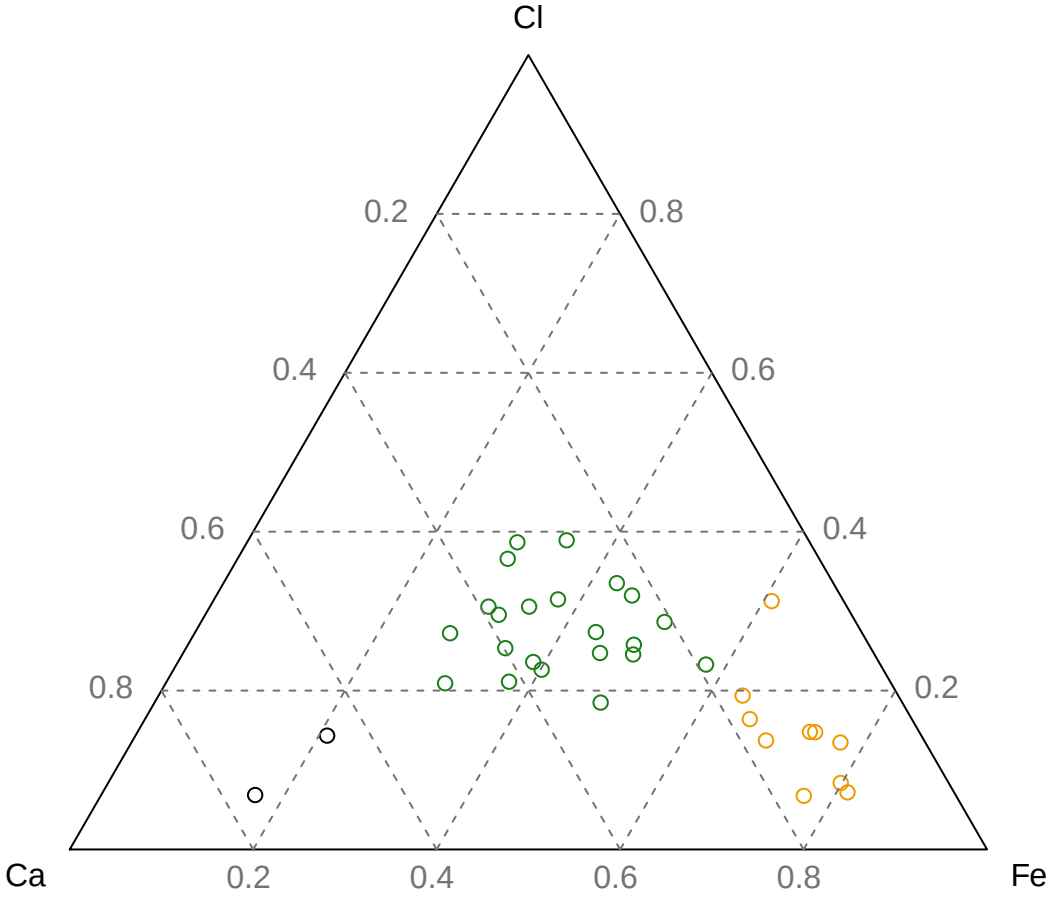

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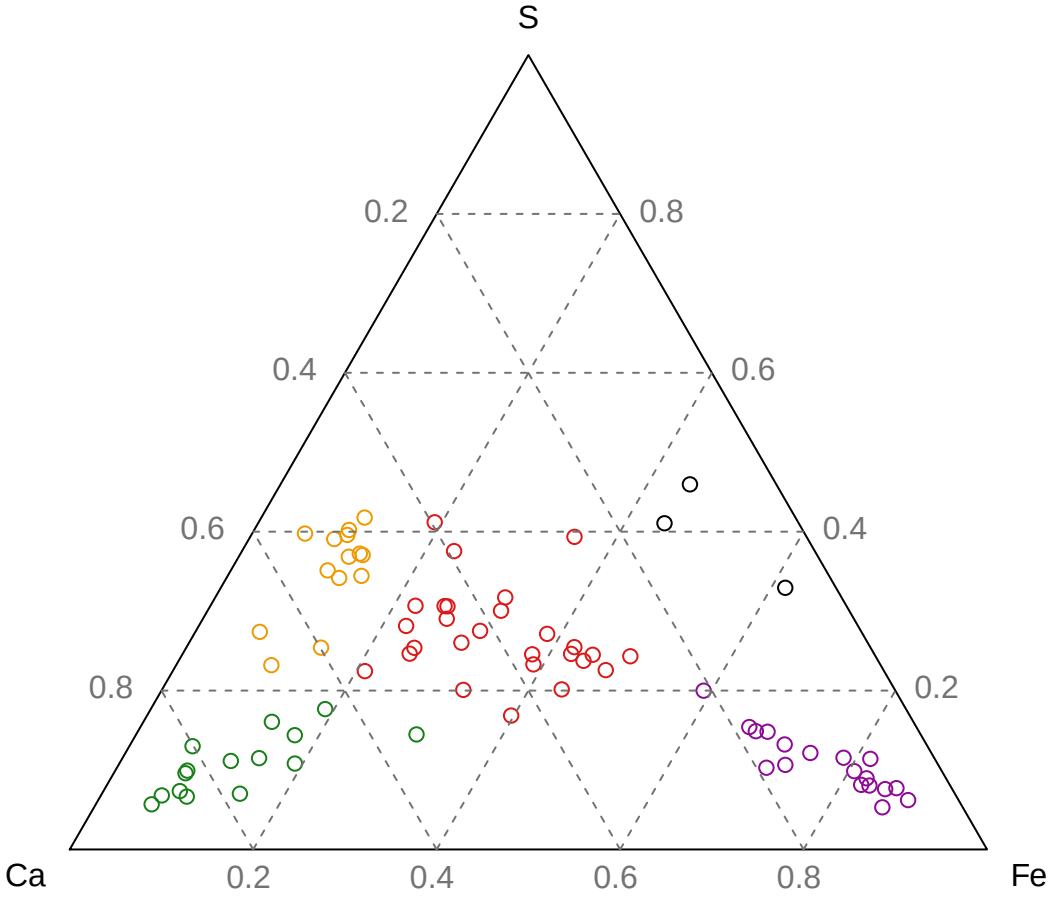

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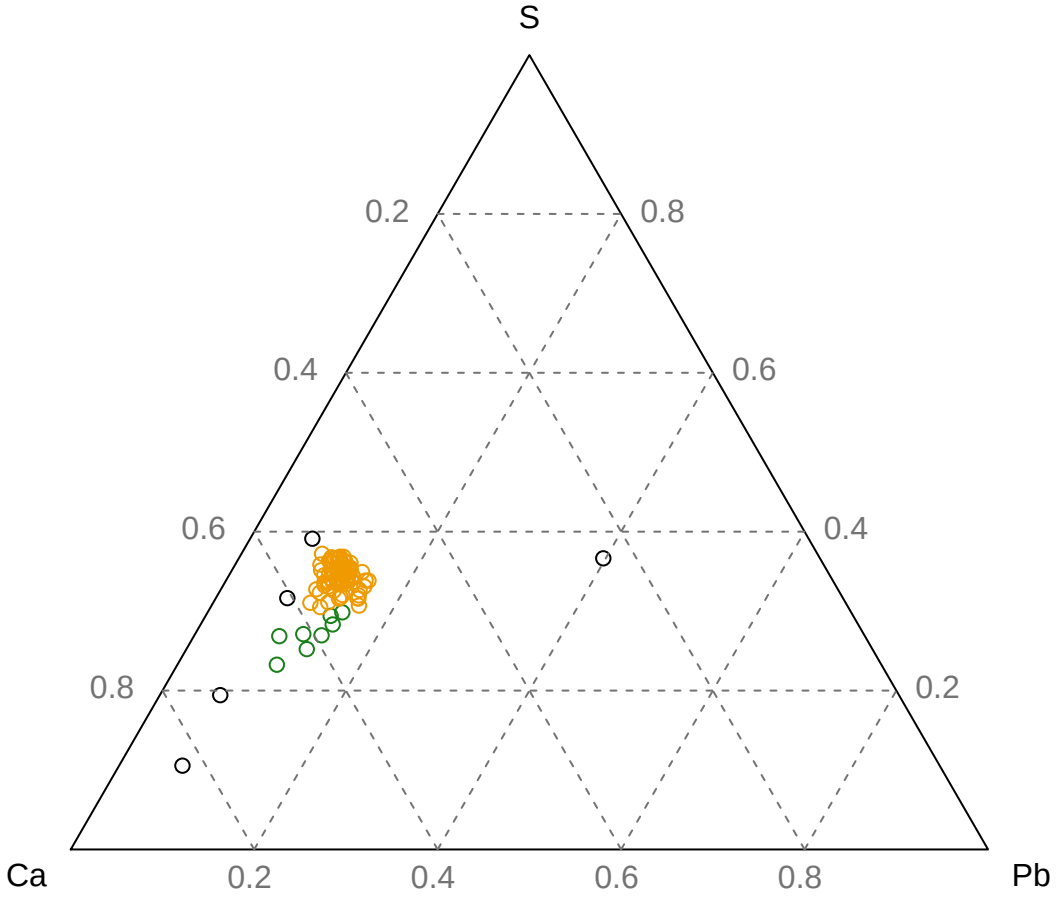

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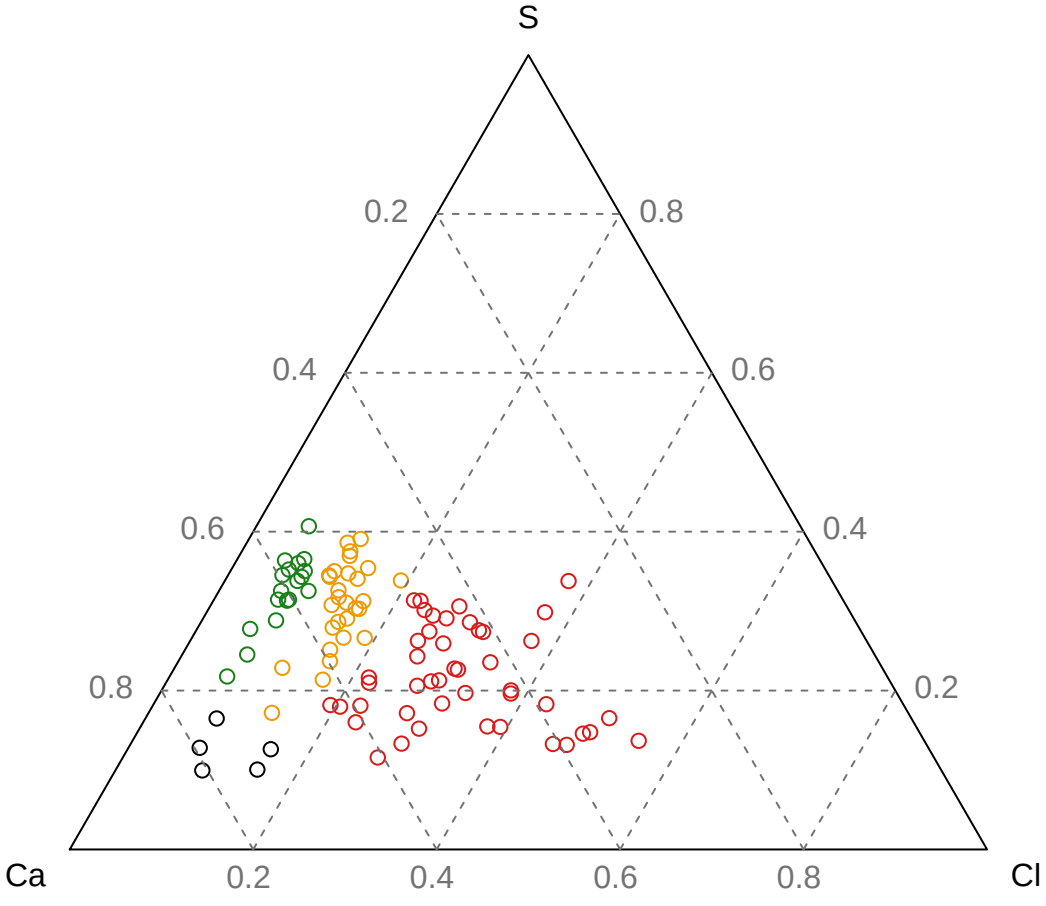
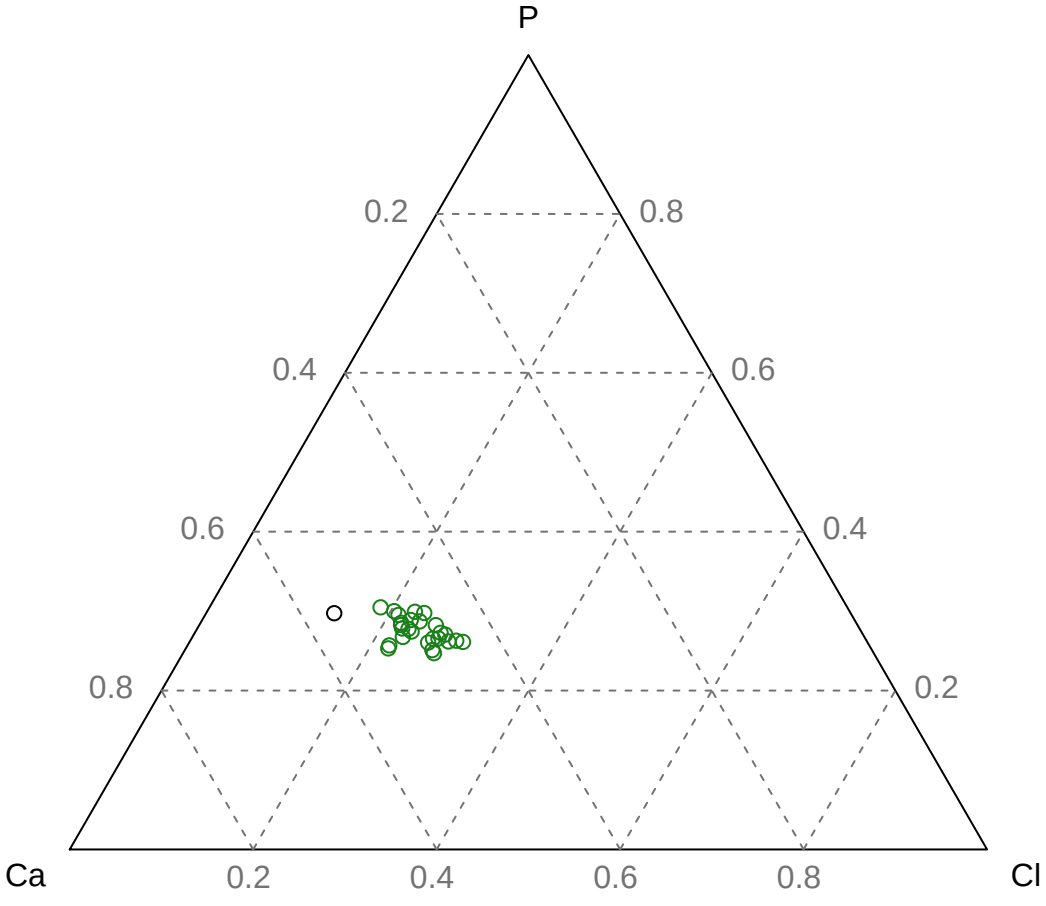


Ca, Cl, P



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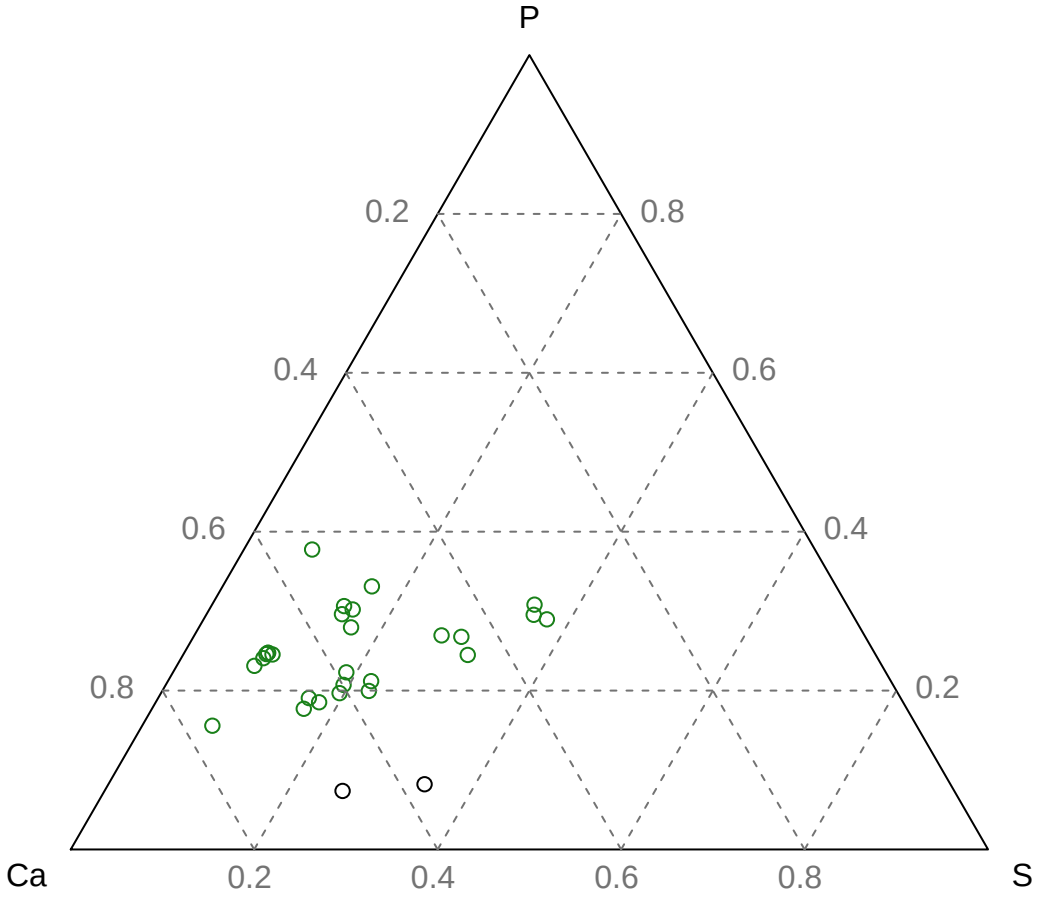
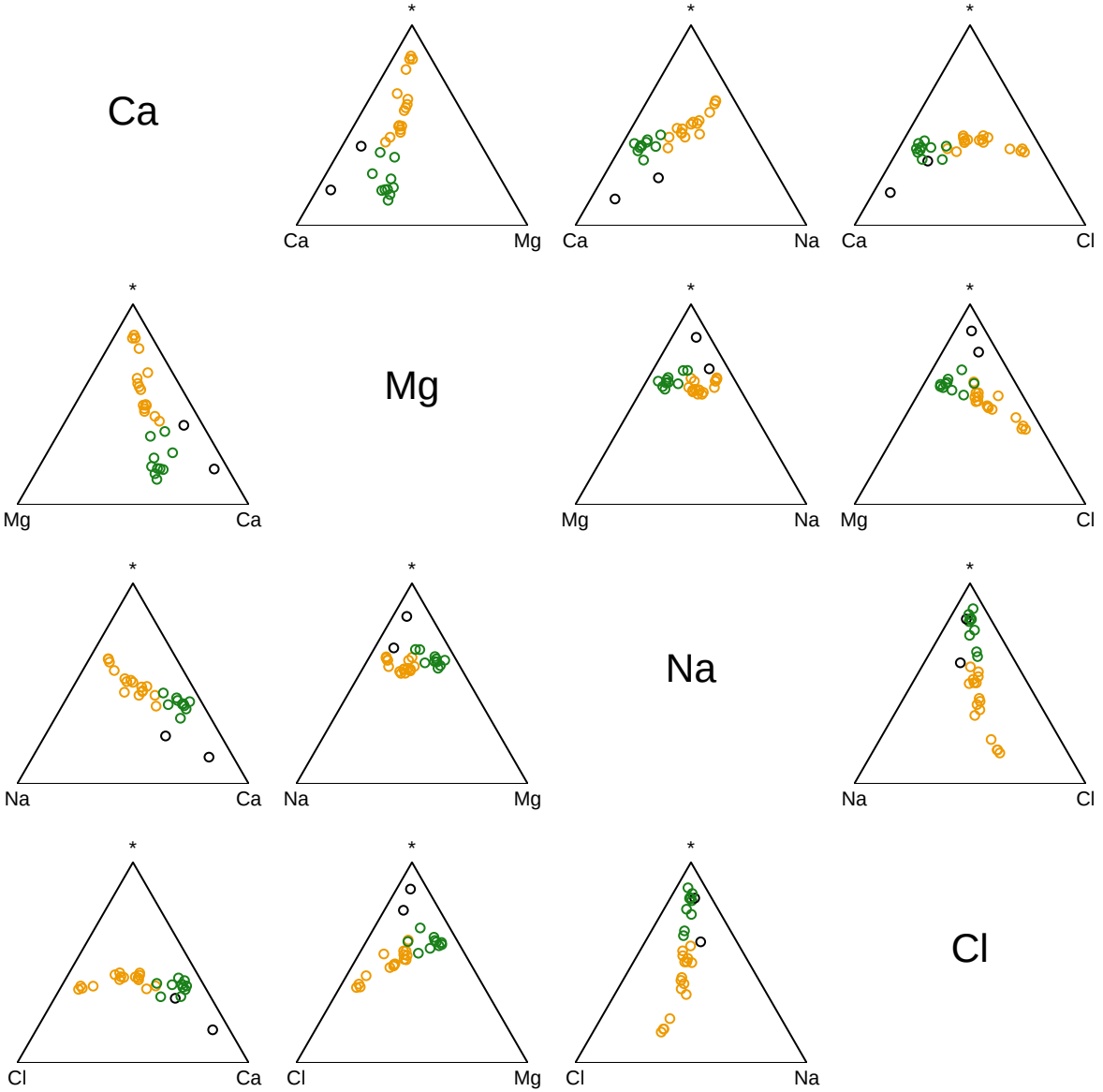


Ca, Mg, Na, Cl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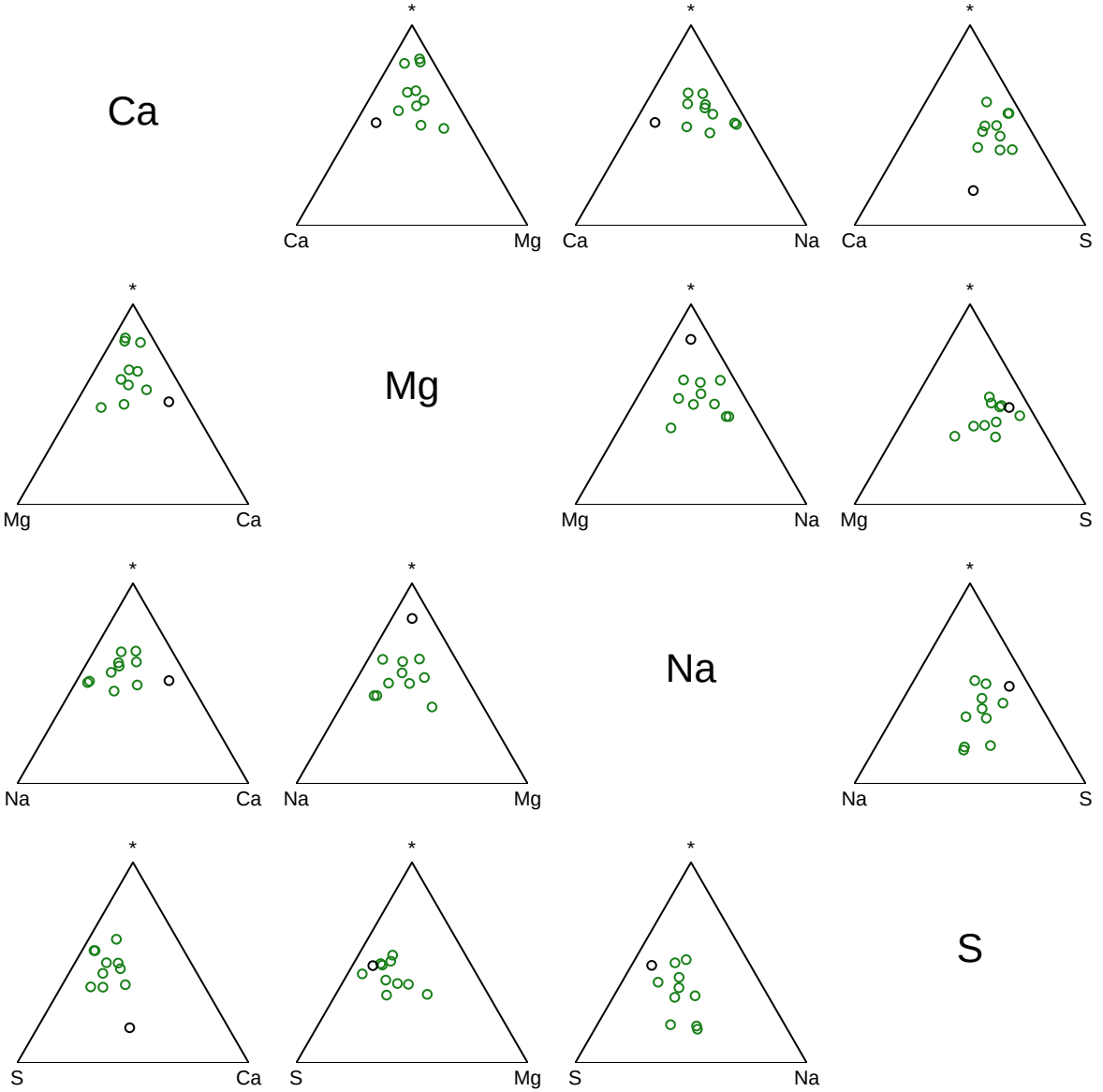
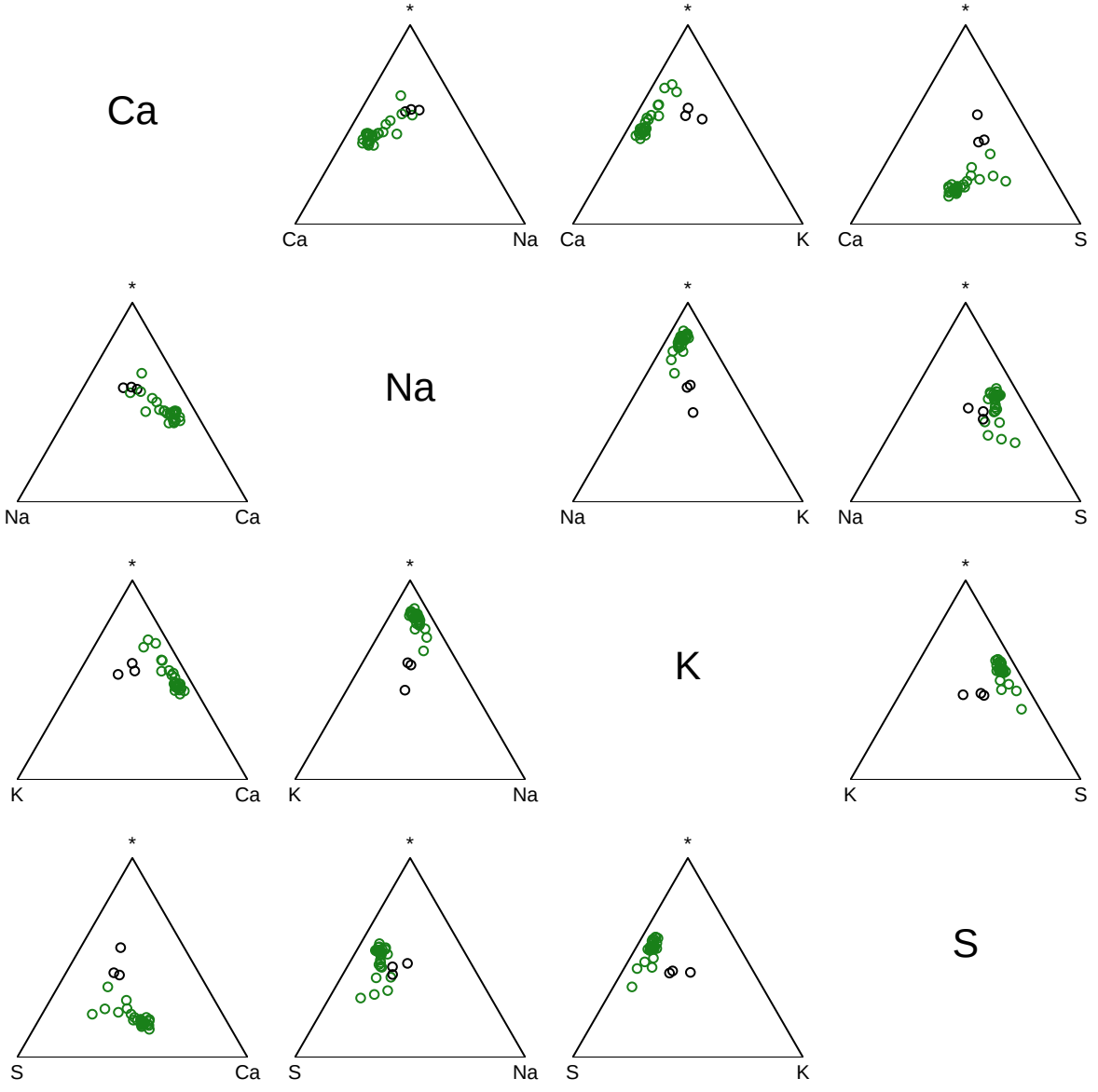
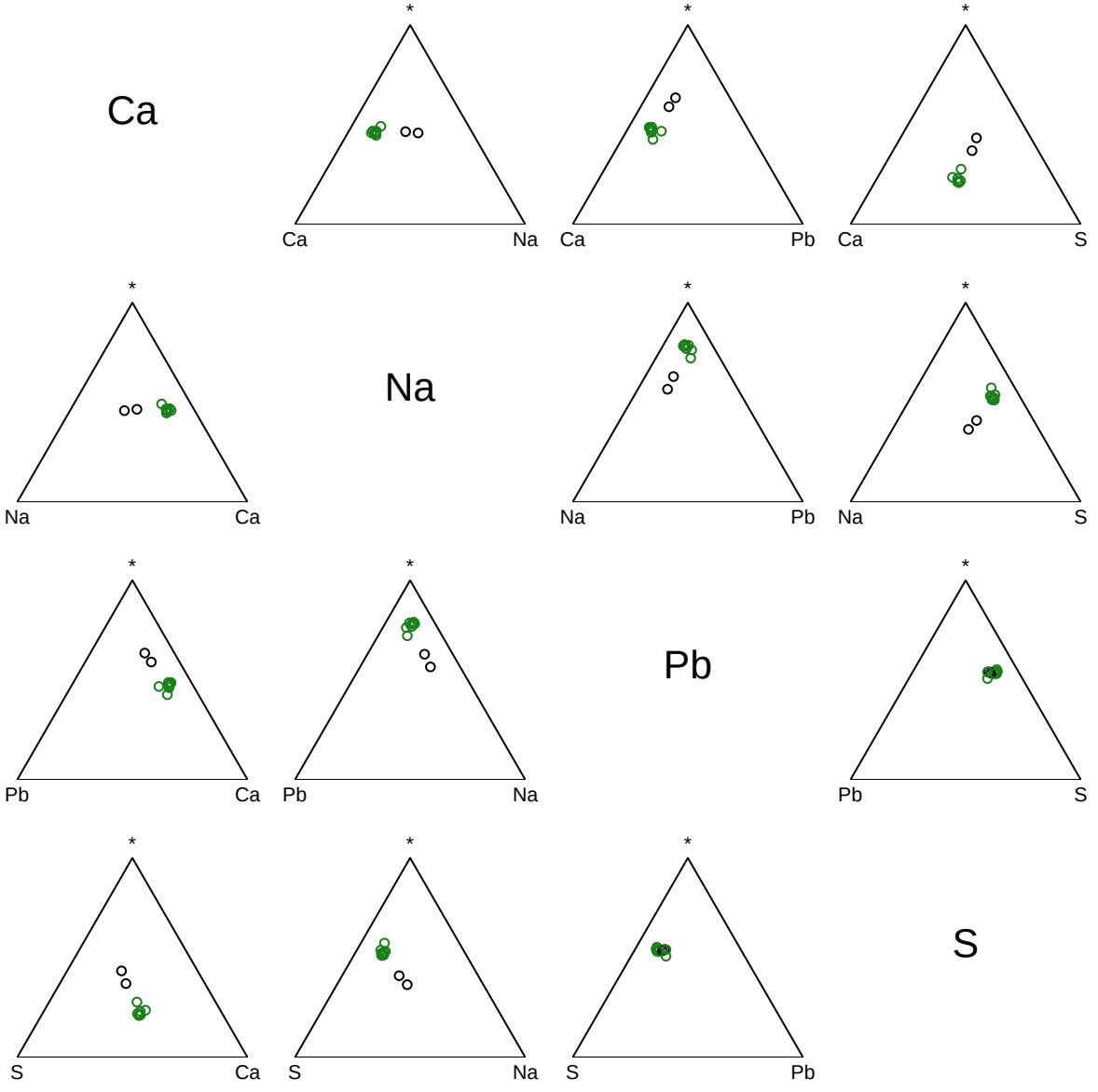
Ca, Mg, Na, S



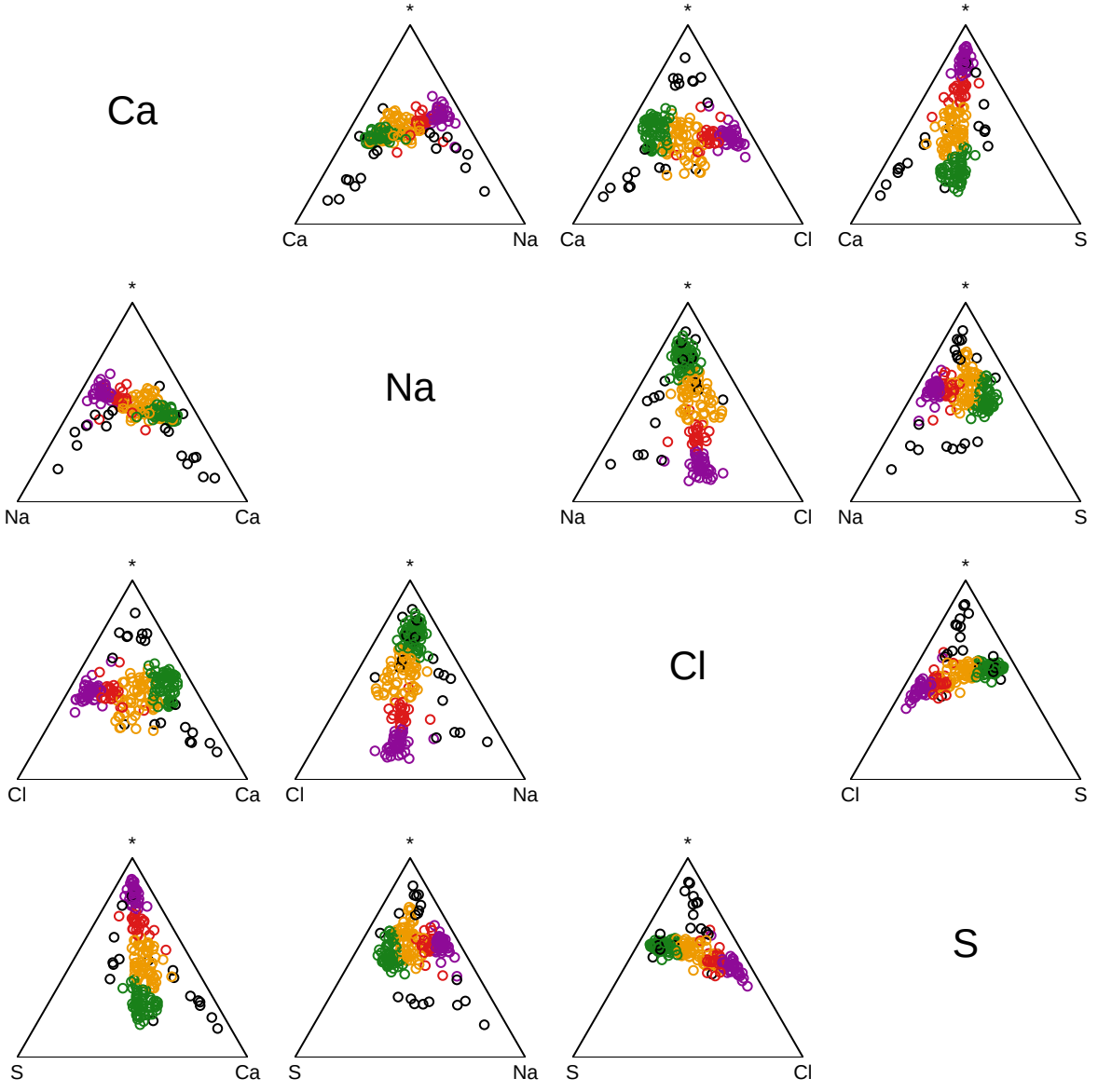
Ca, Na, K, S



Ca, Na, Pb, S



Ca, Na, Cl, S



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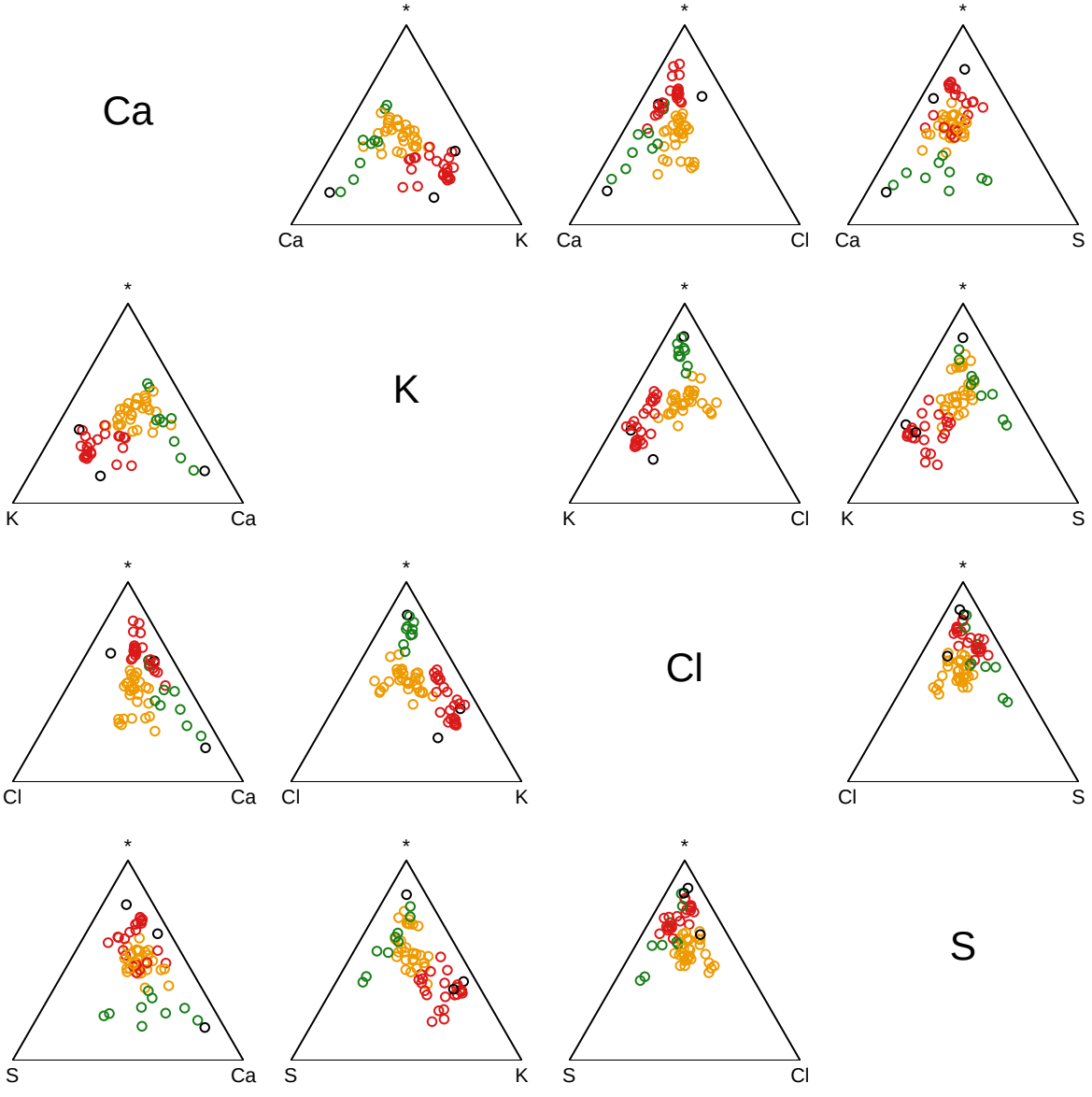
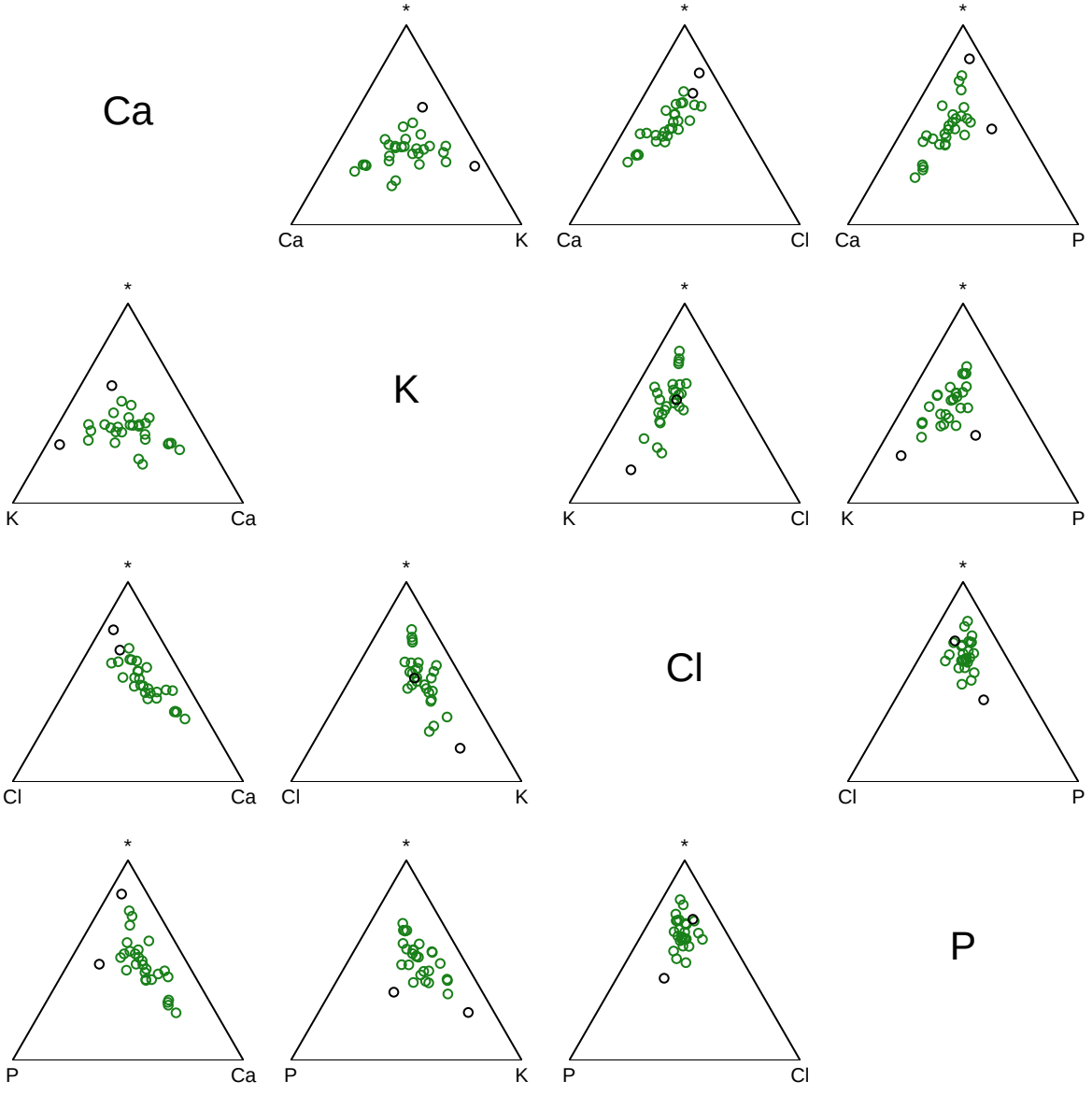


Ca, K, Cl, P



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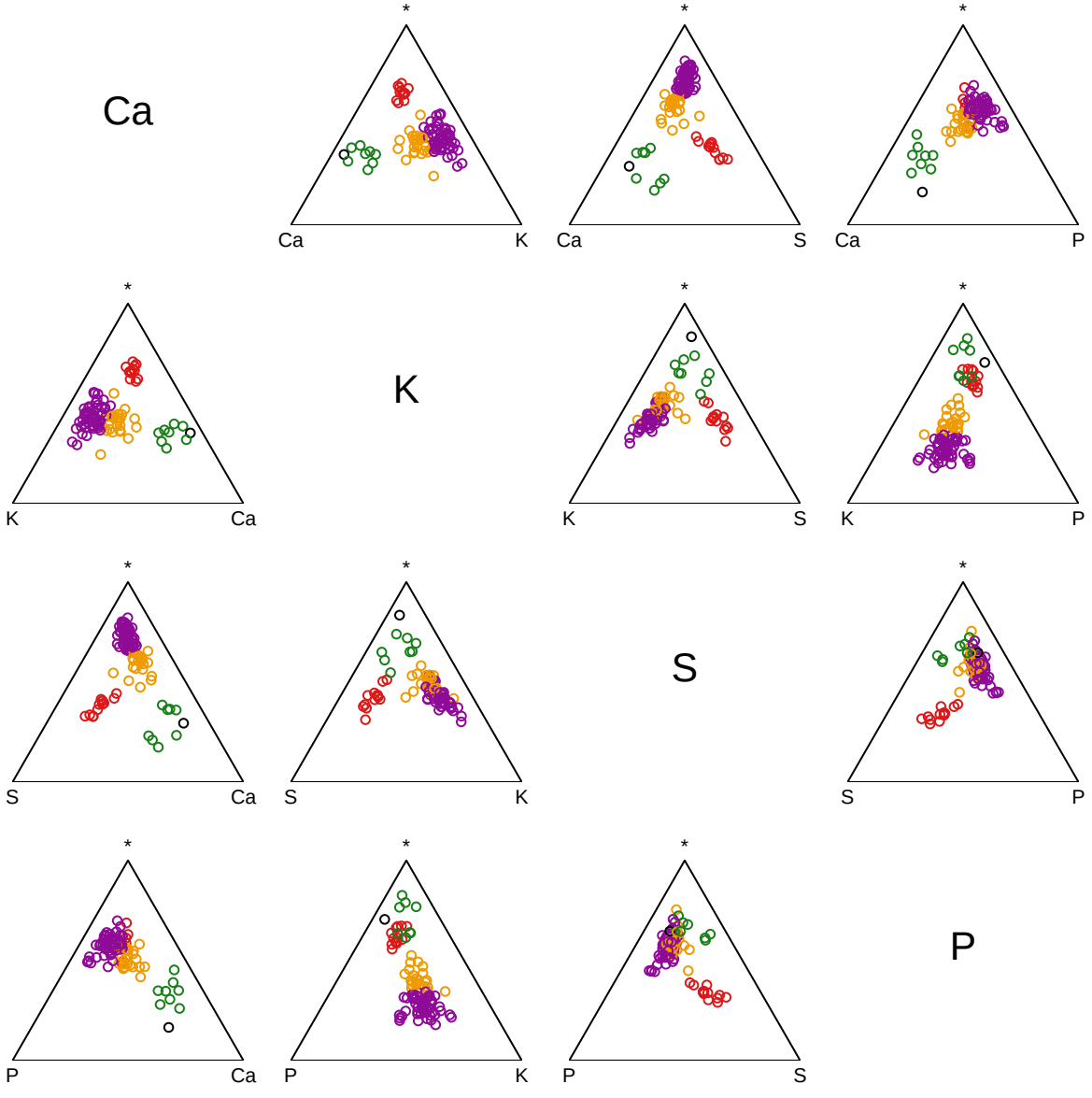
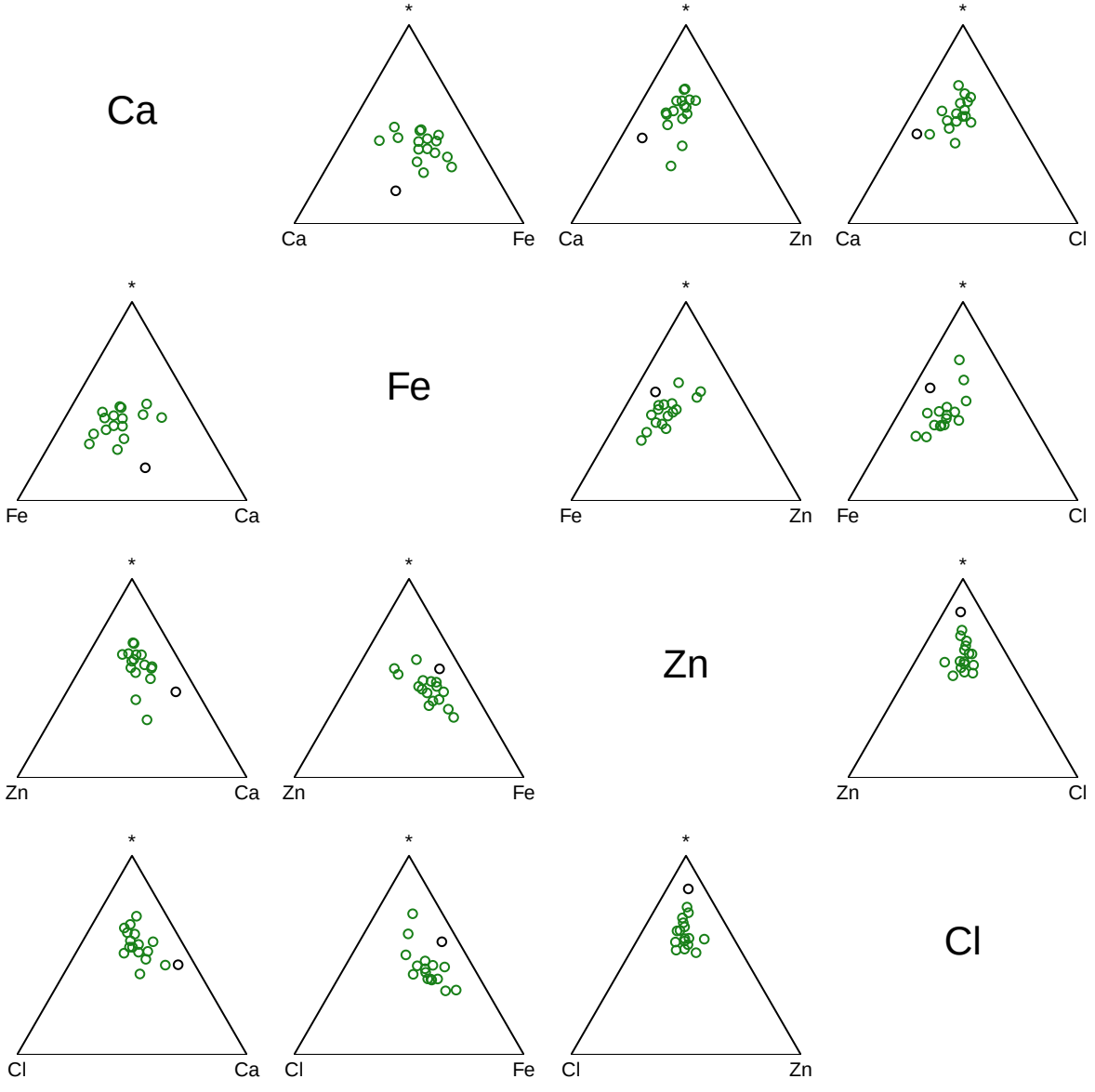


Ca, Fe, Zn, Cl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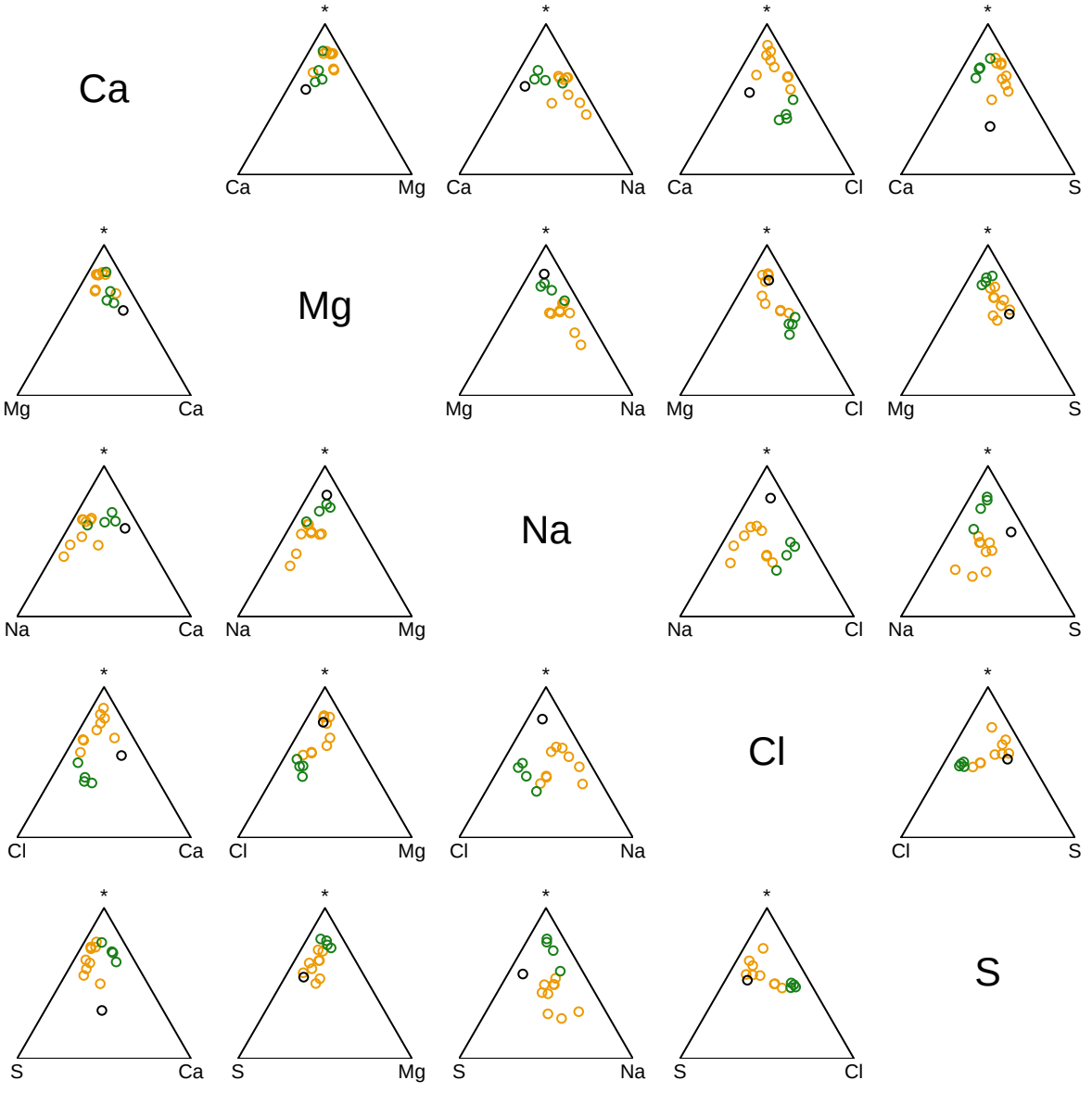
Ca, Mg, Na, Cl, S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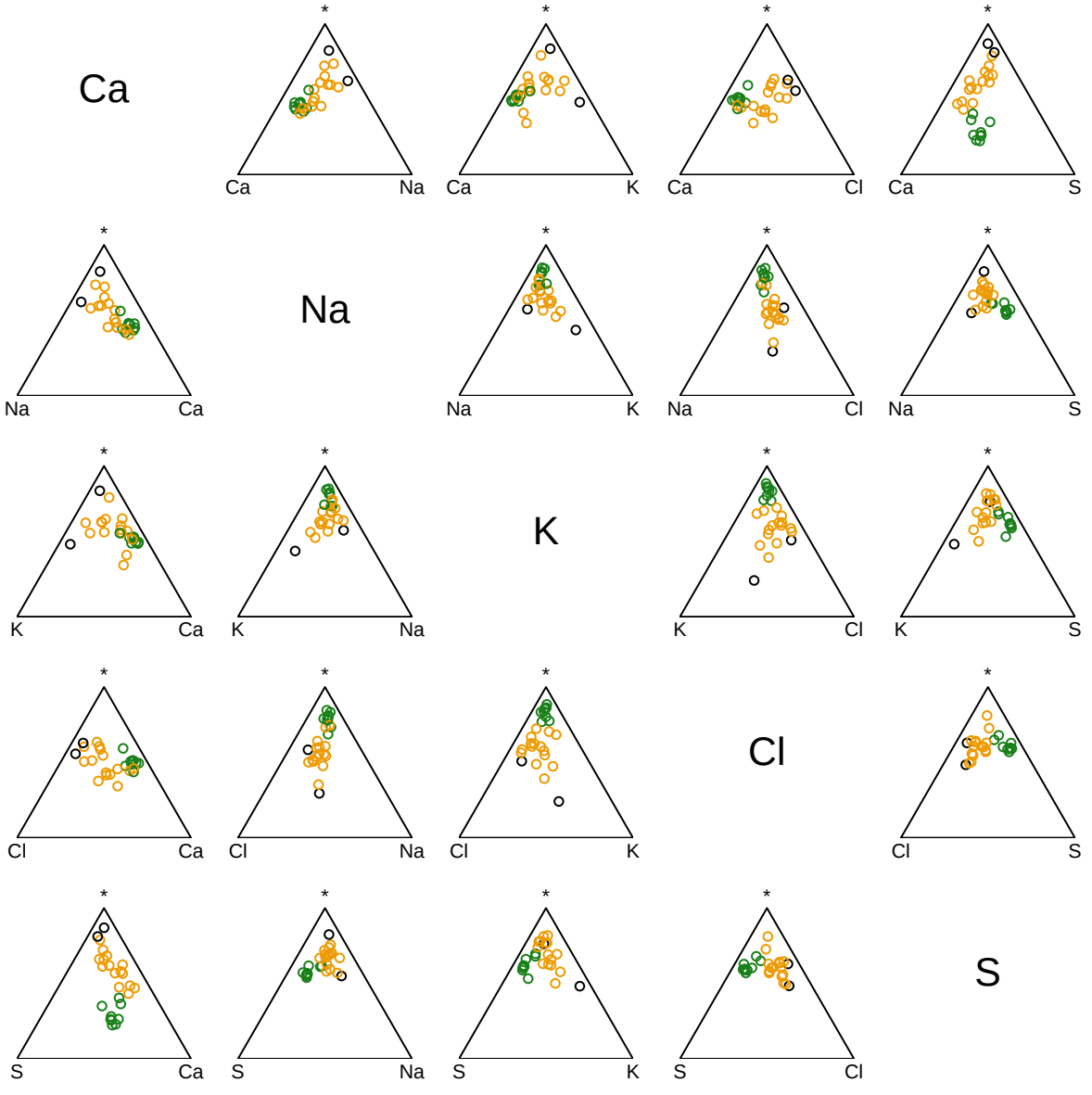
Ca, Na, K, Cl, S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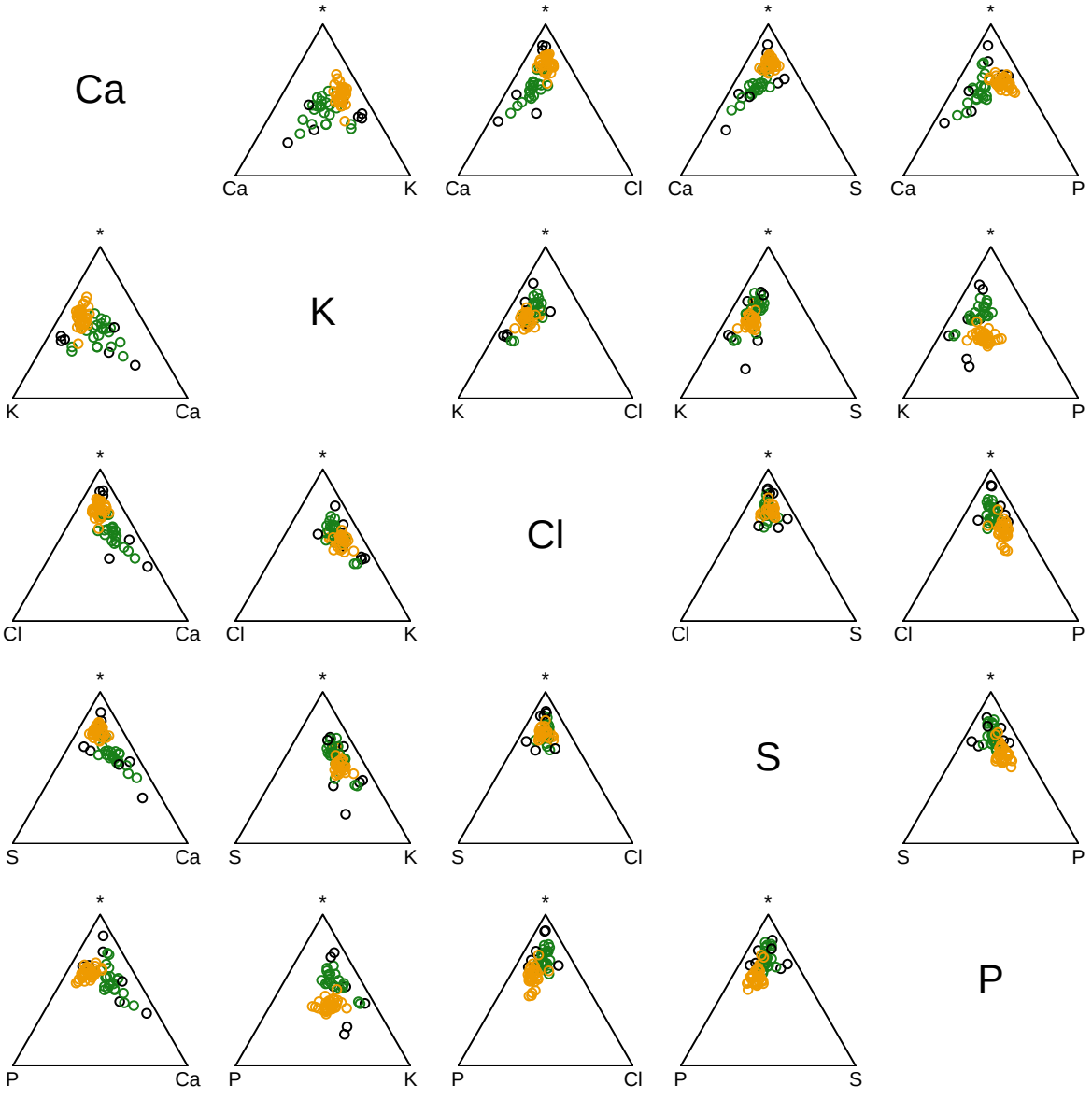
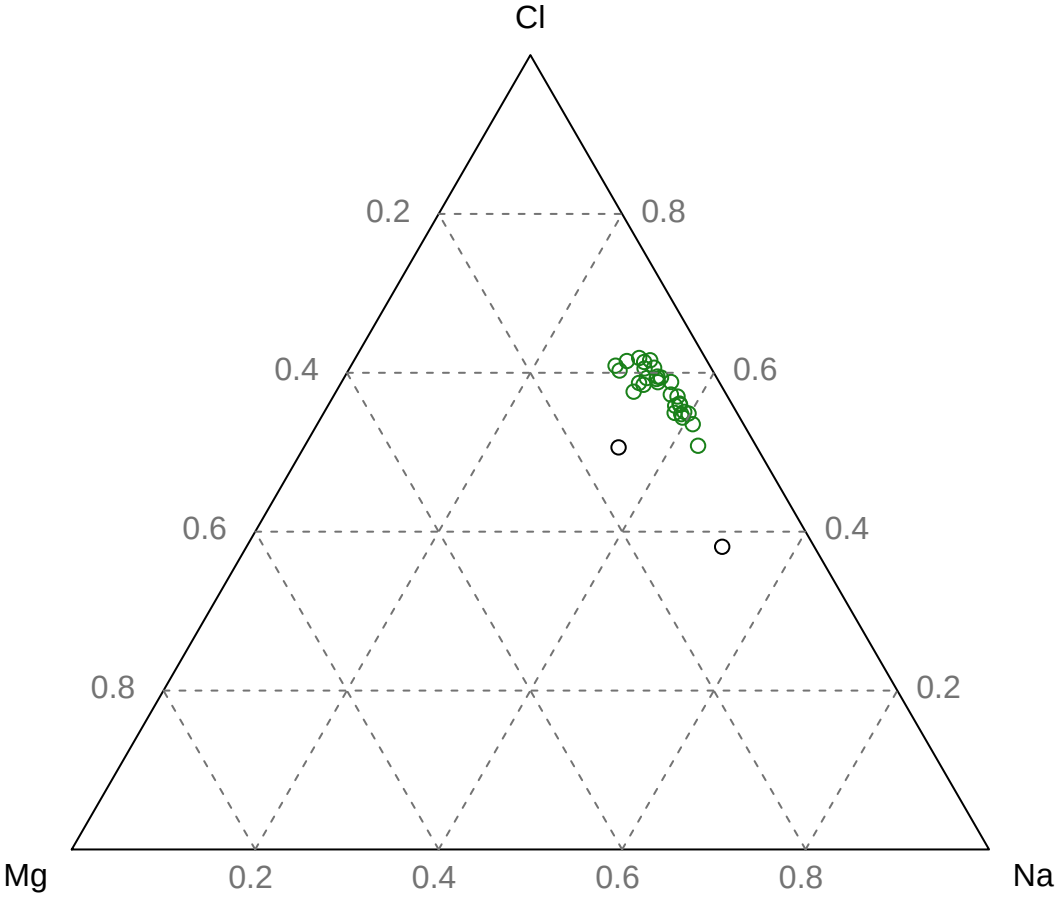
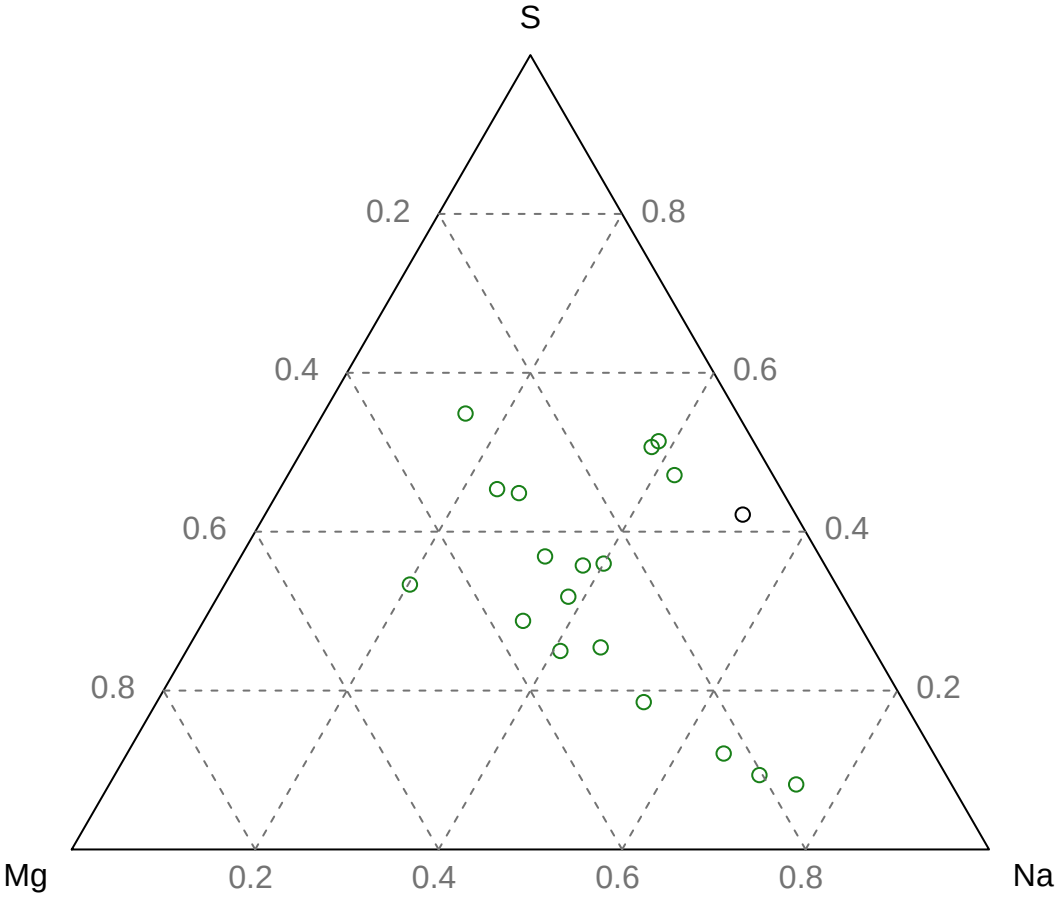
Ca, K, Cl, S, P



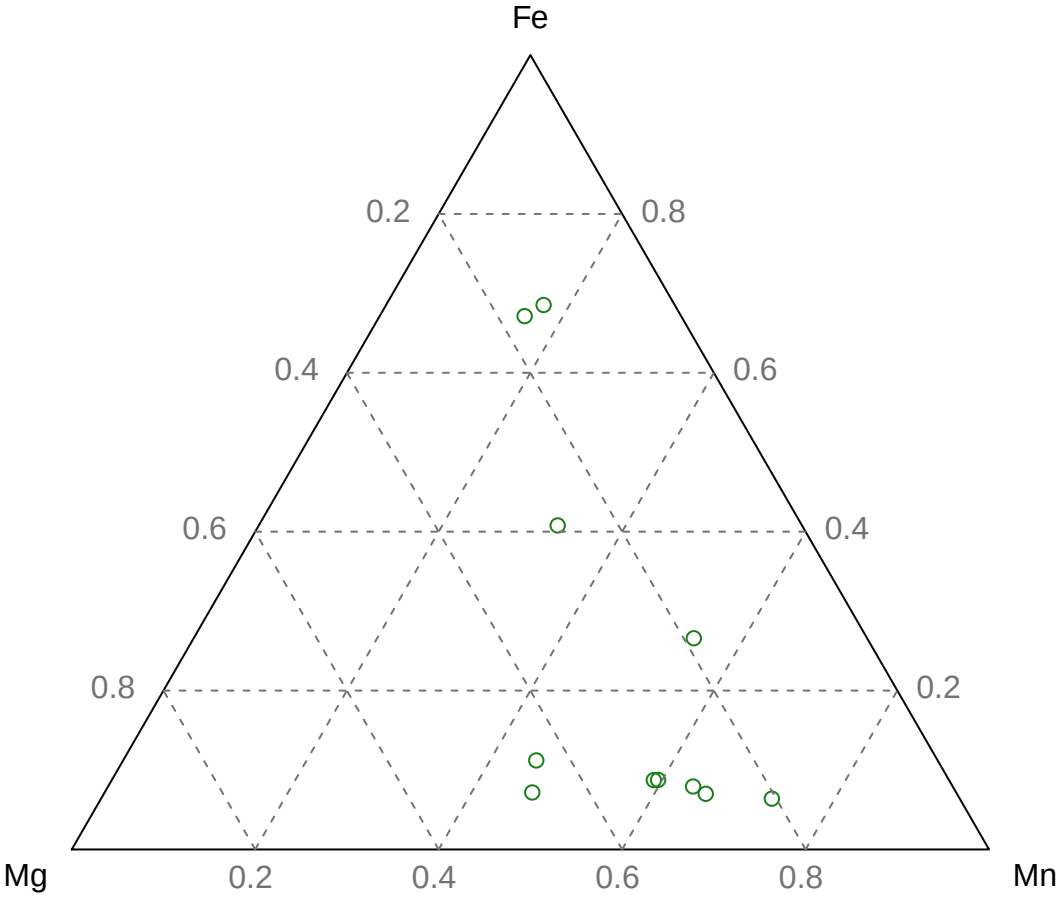
Mg, Na, Cl



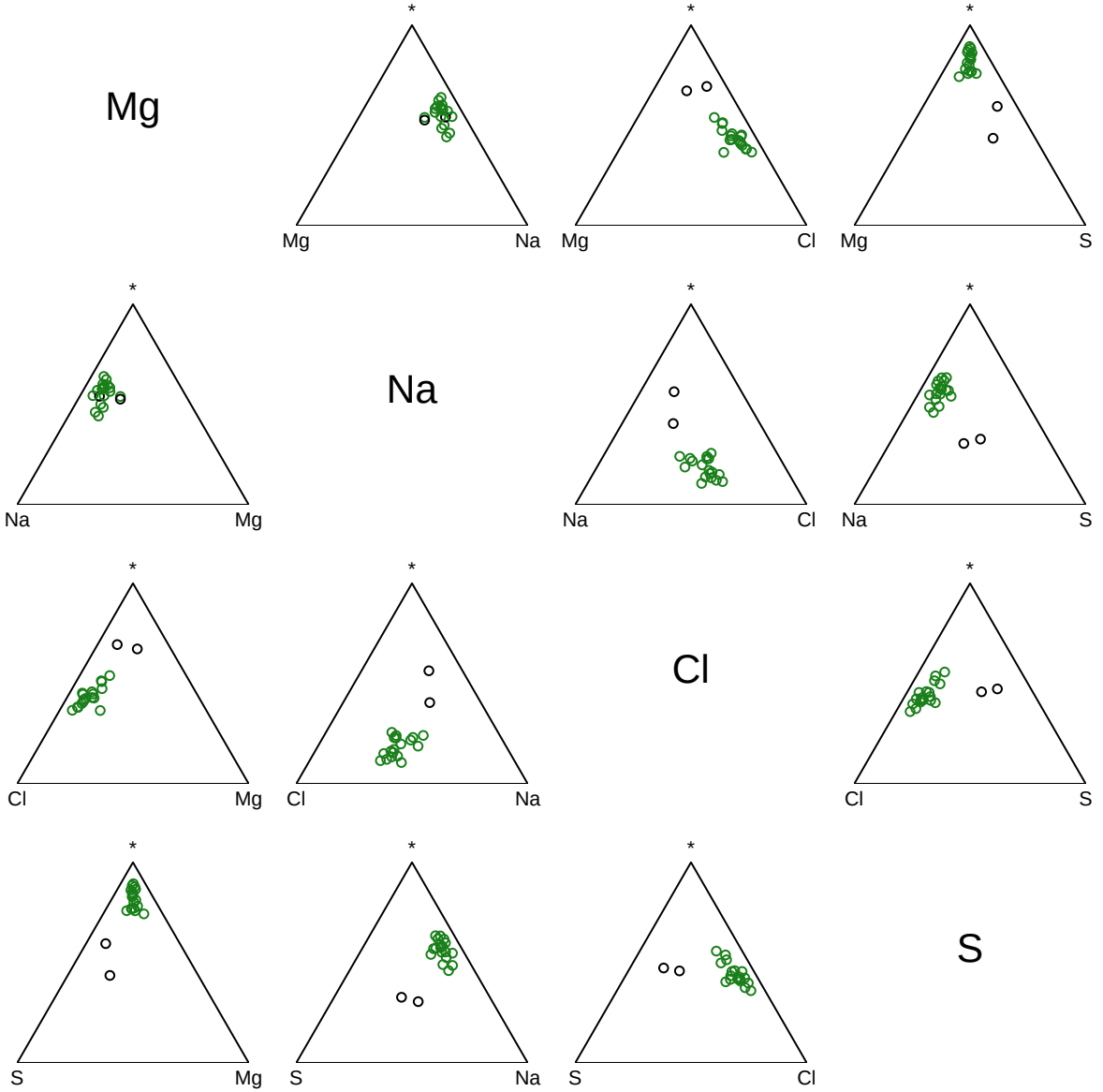
Mg, Na, S



Mg, Mn, Fe



Mg, Na, Cl, S



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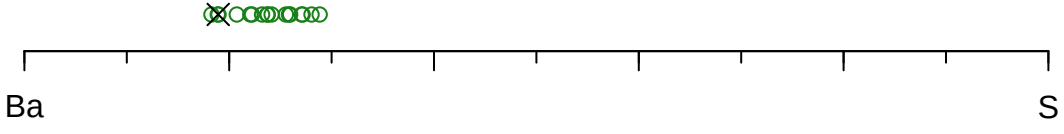
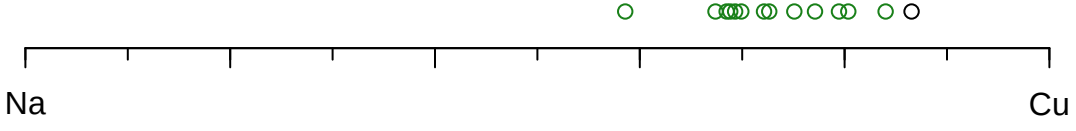
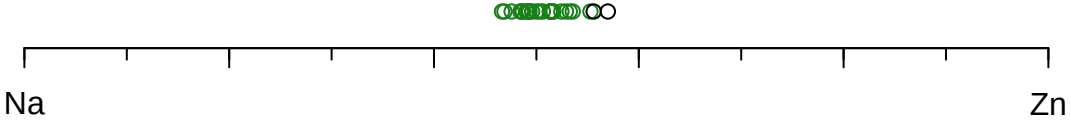


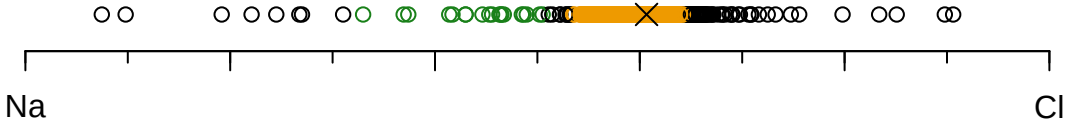
Na, Cu



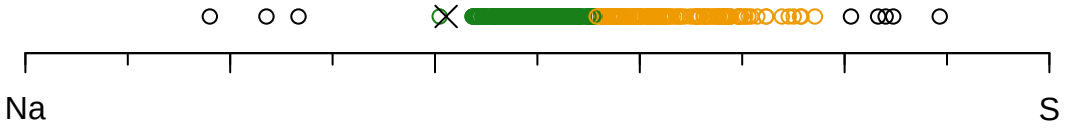
Na, Zn



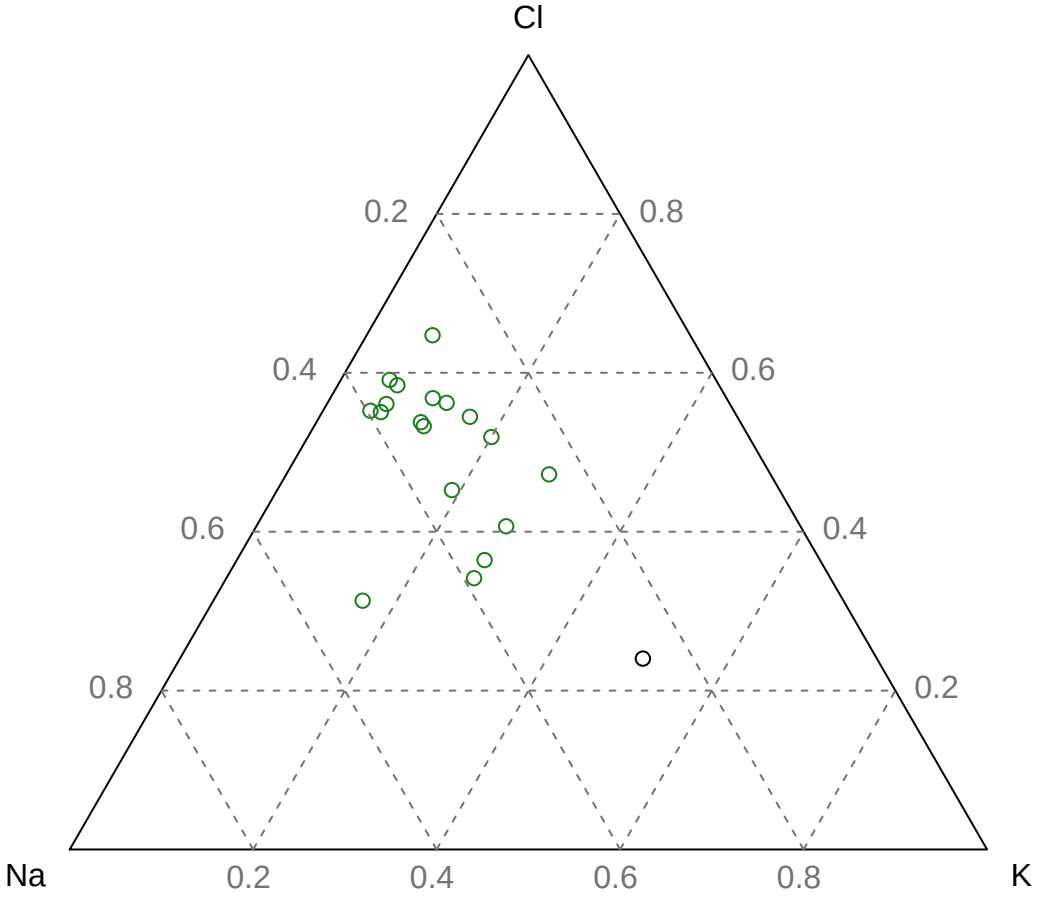
Na, Cl



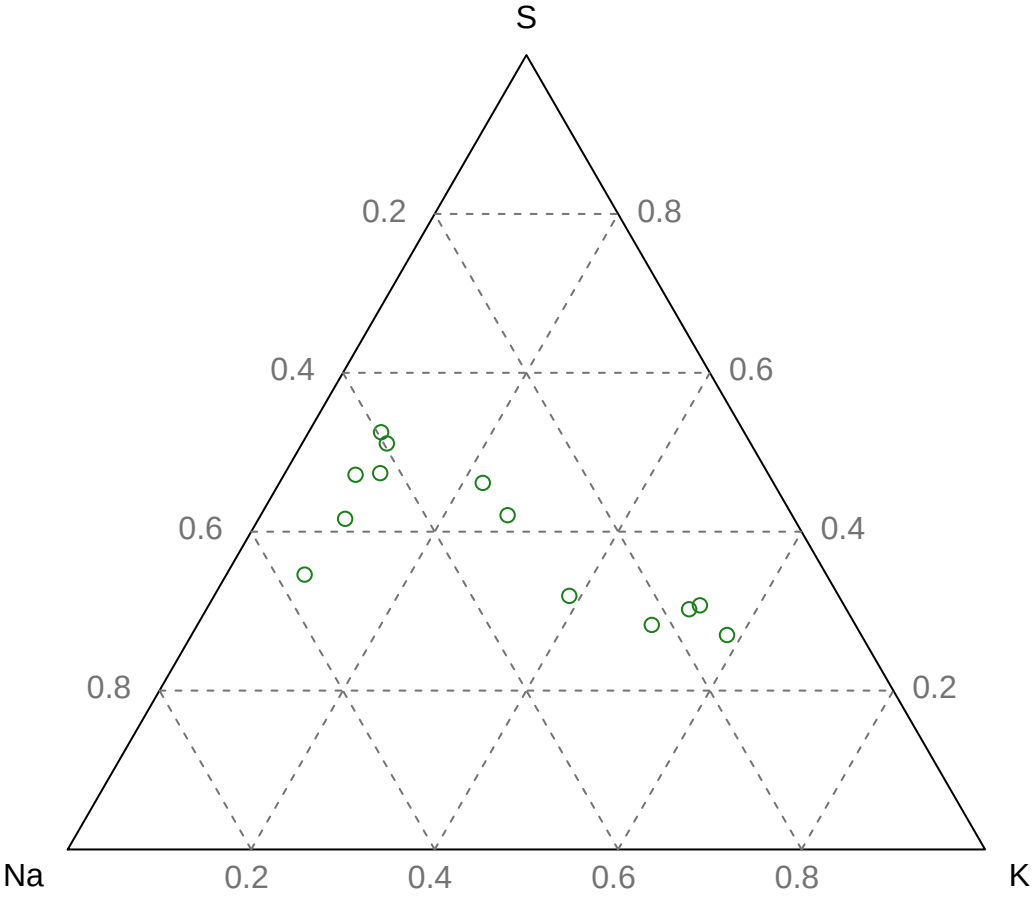
Na, S



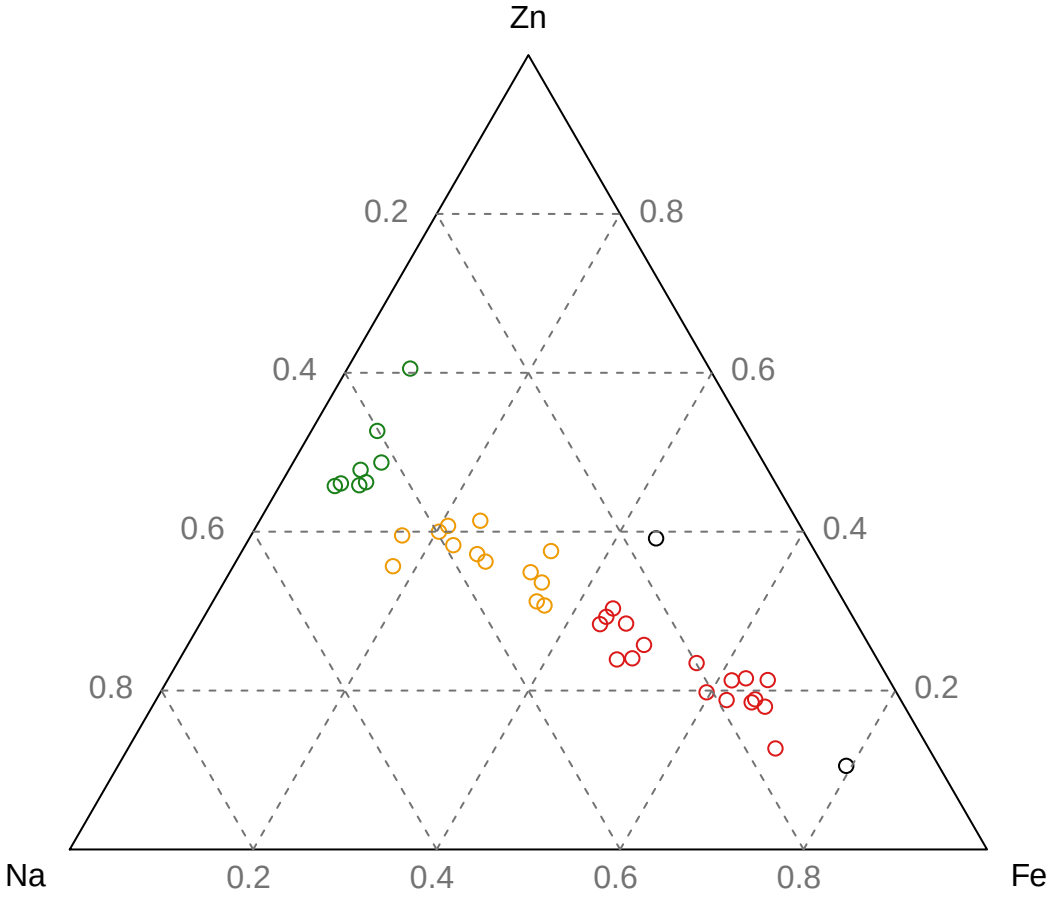
Na, K, Cl



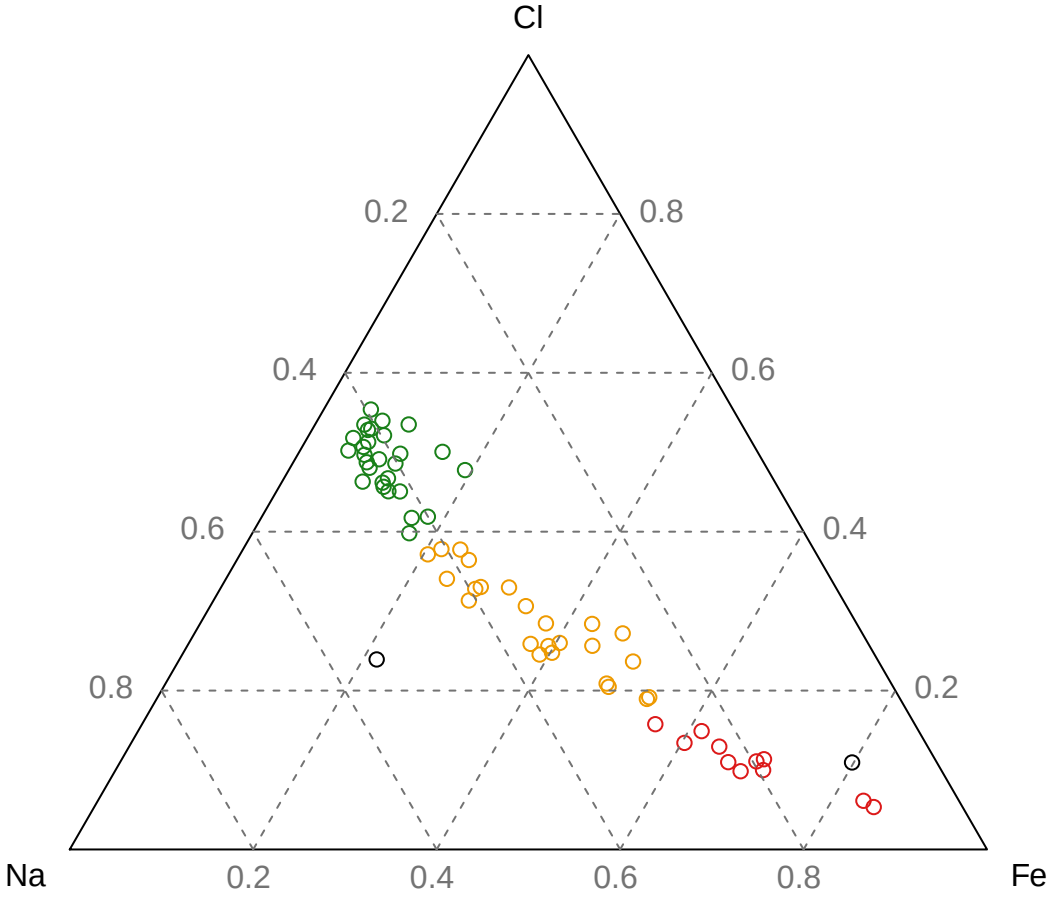
Na, K, S



Na, Fe, Zn



Na, Fe, Cl



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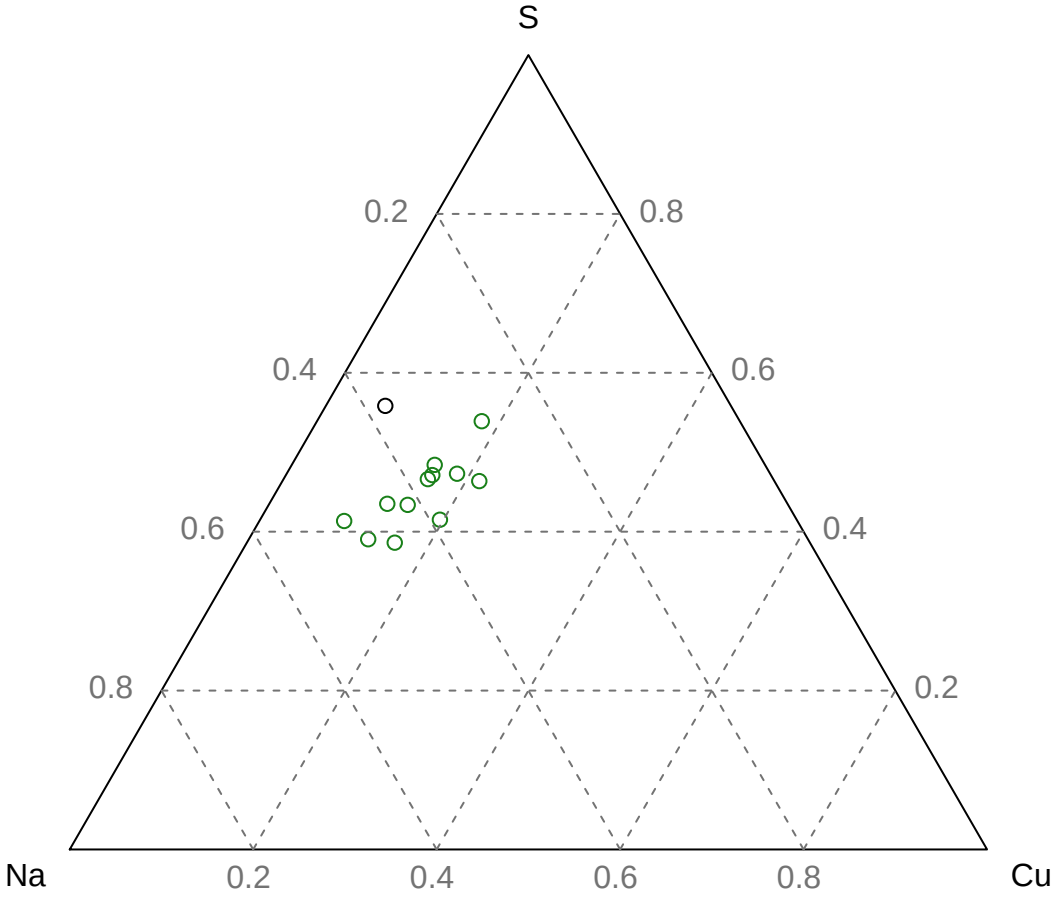
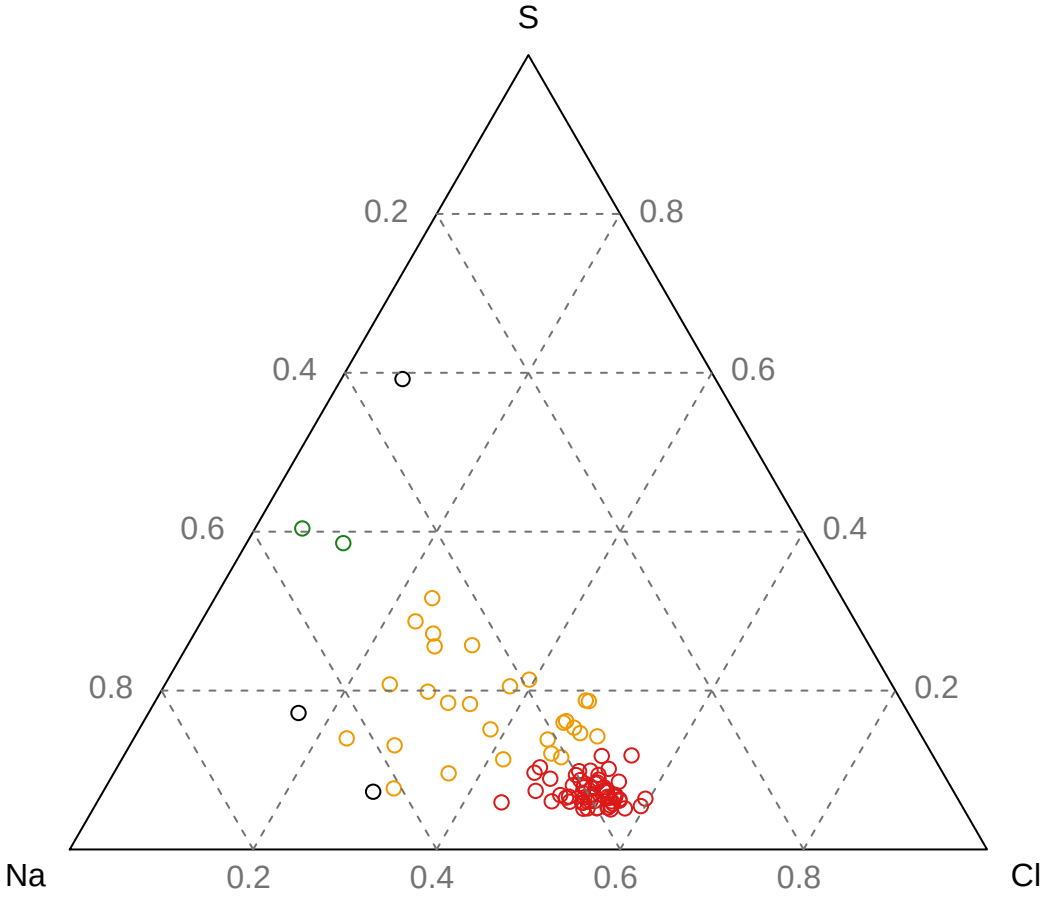
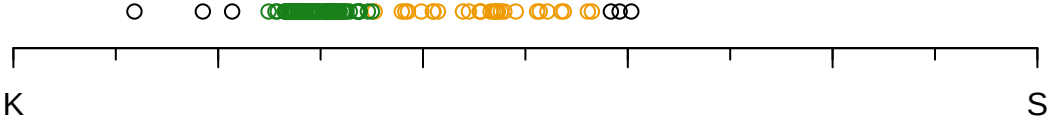


Na, Cl, S

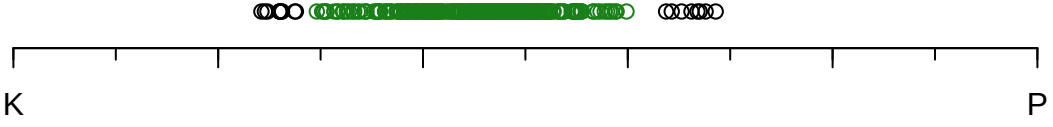


K, Cl

K, S



K, P



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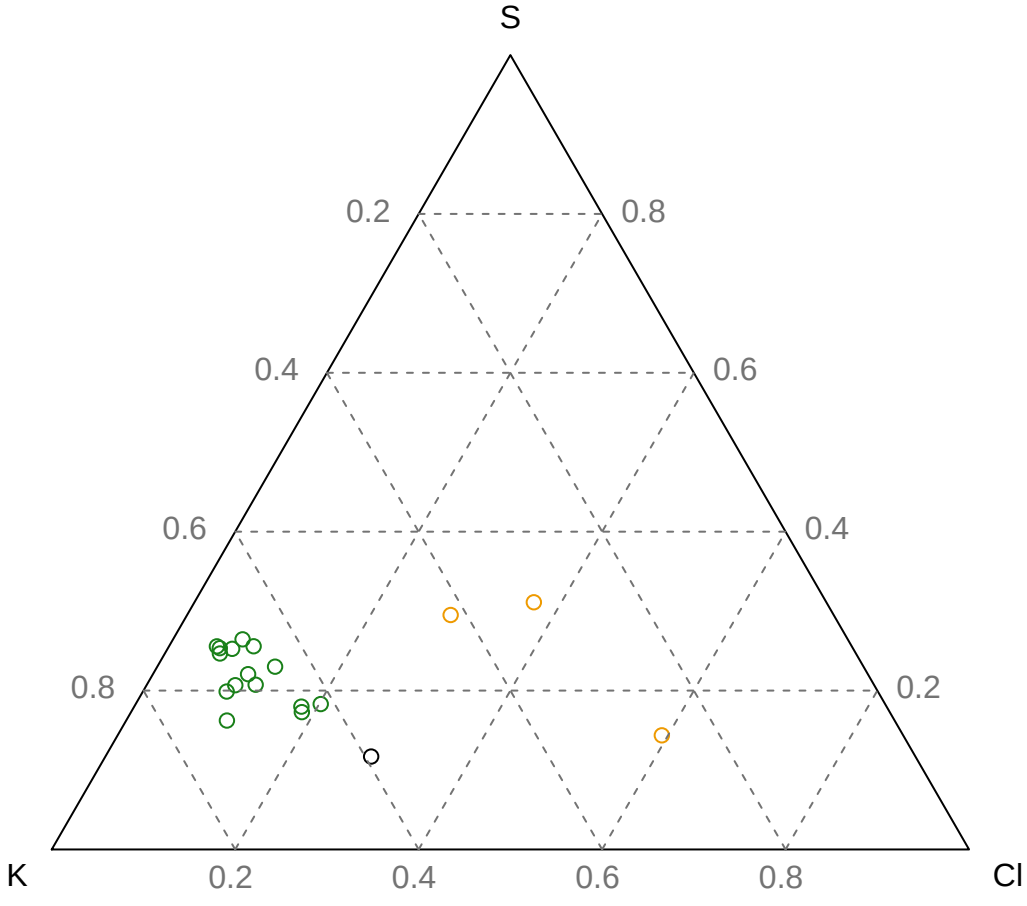
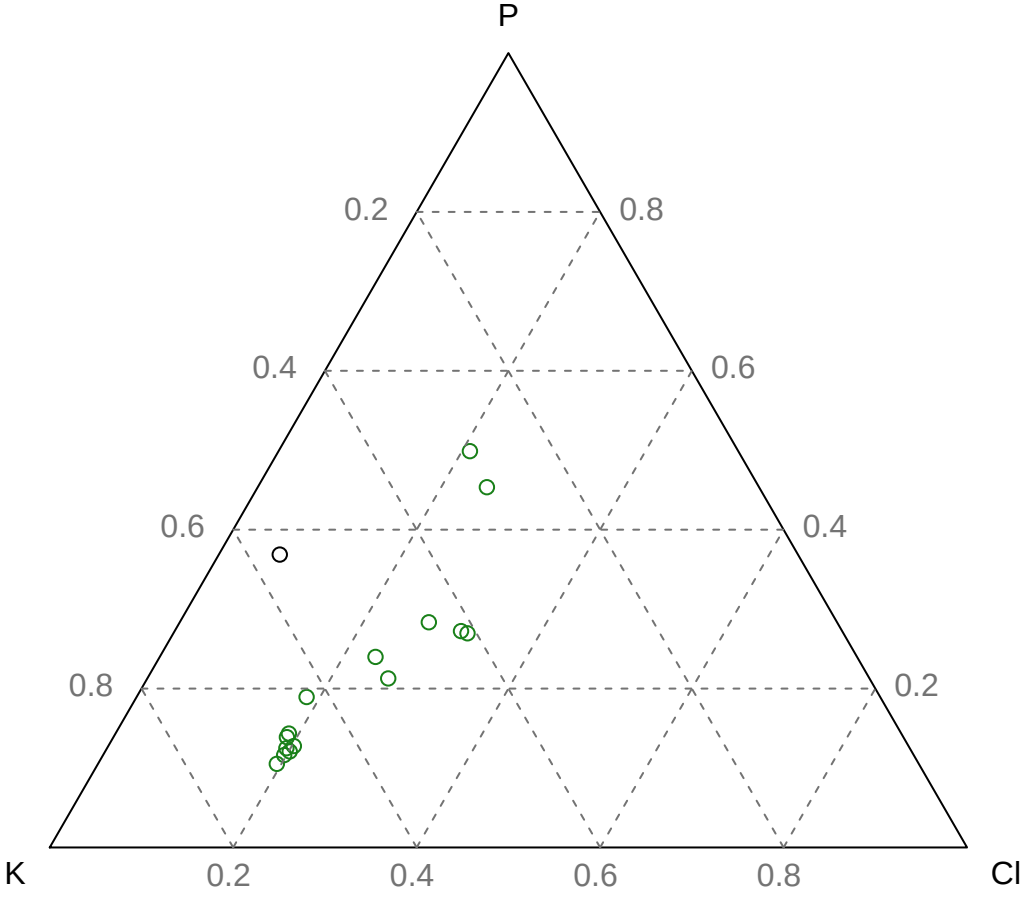
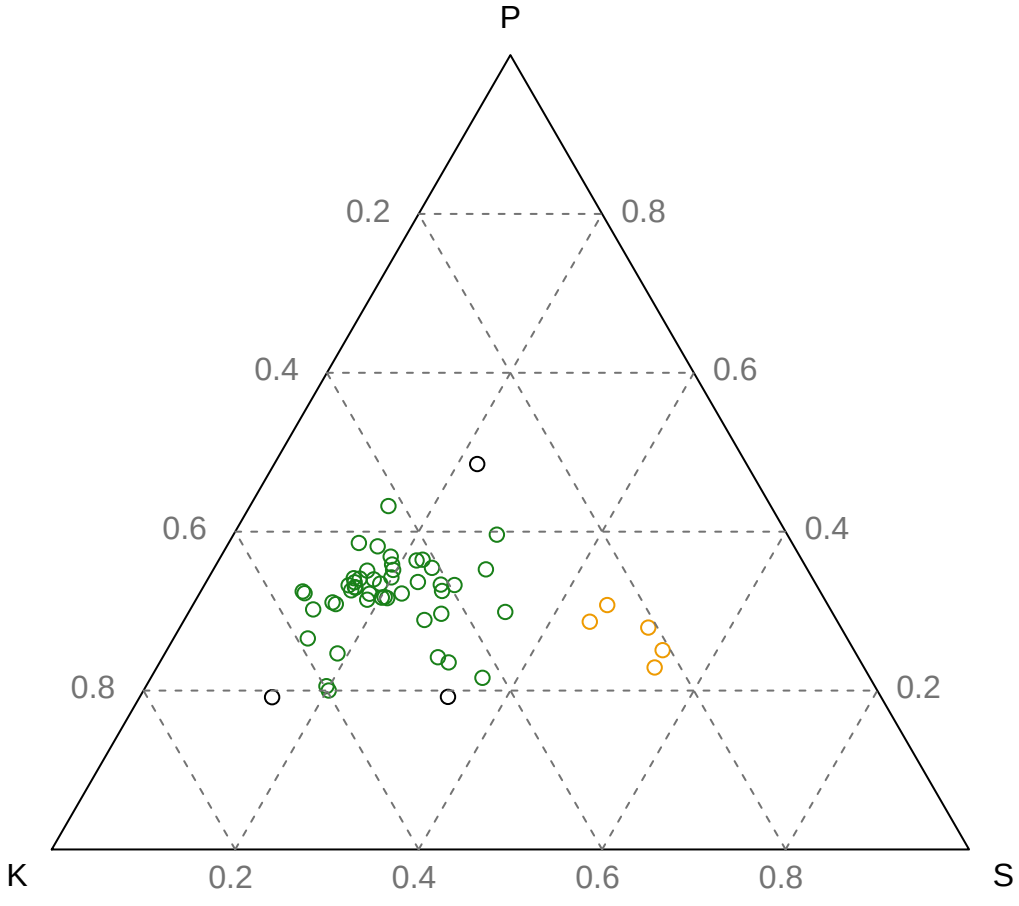


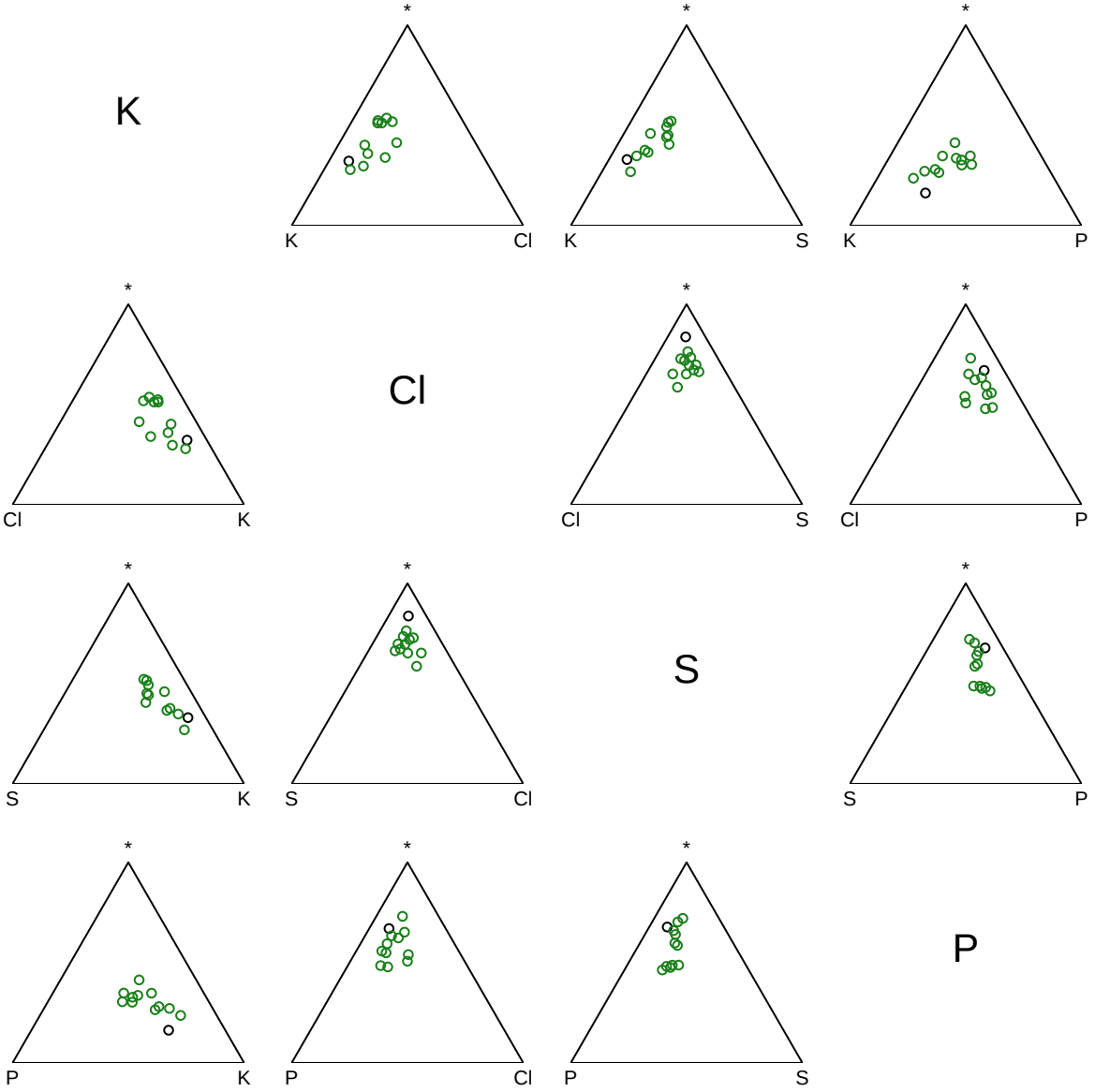
K, Cl, P



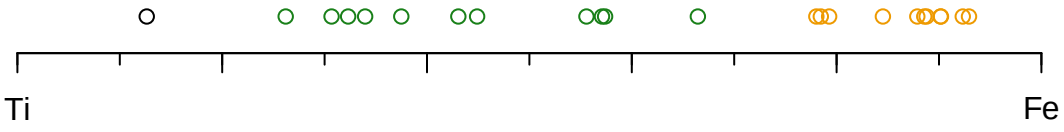
K, S, P



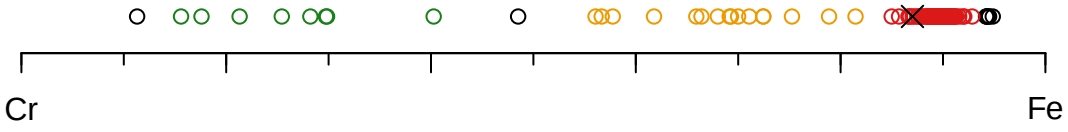
K, Cl, S, P



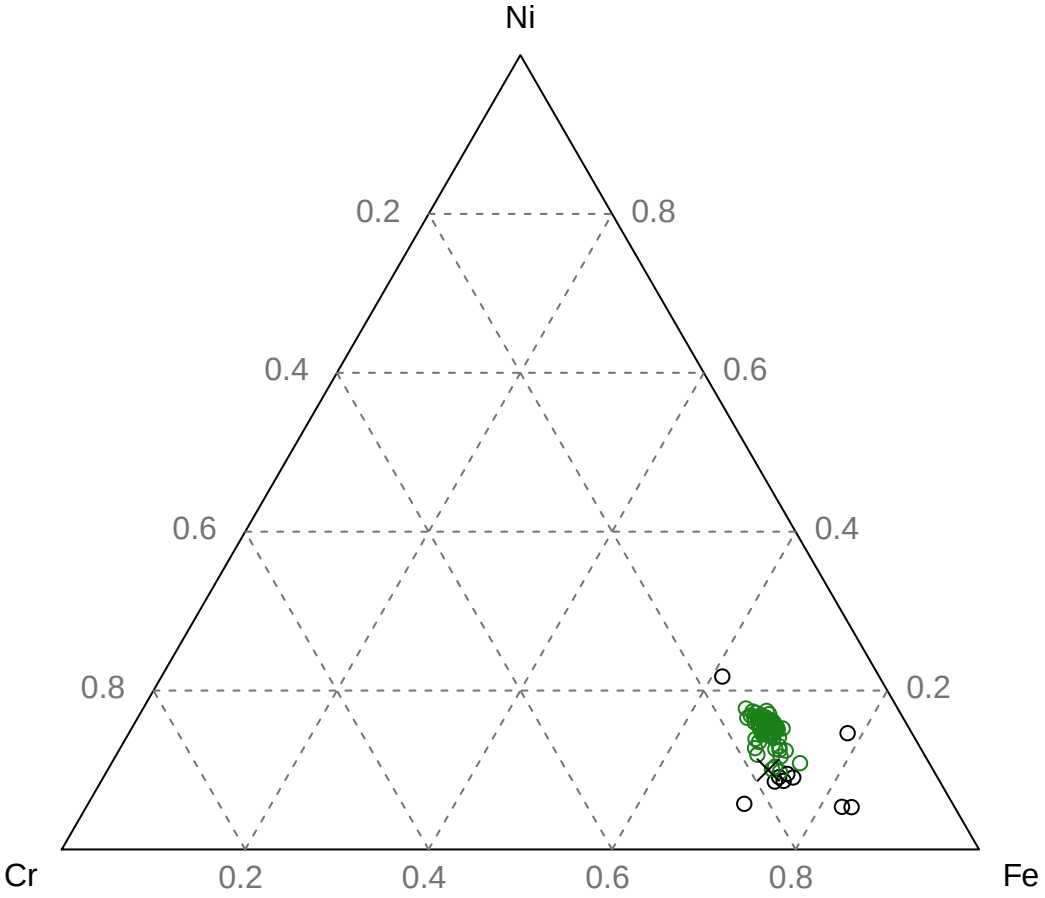
Ti, Fe



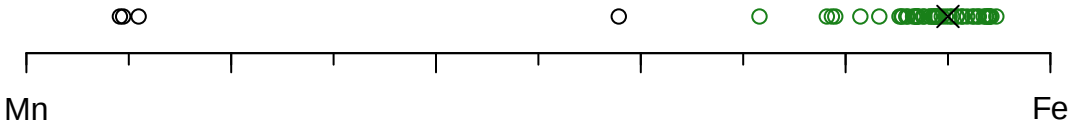
Cr, Fe



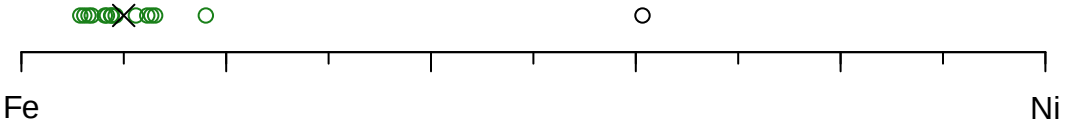
Cr, Fe, Ni



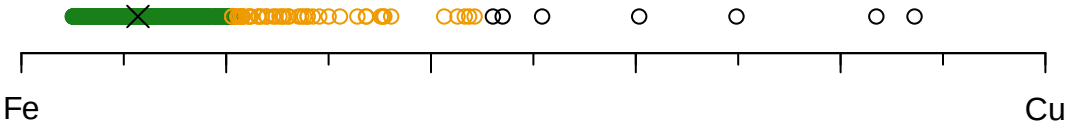
Mn, Fe



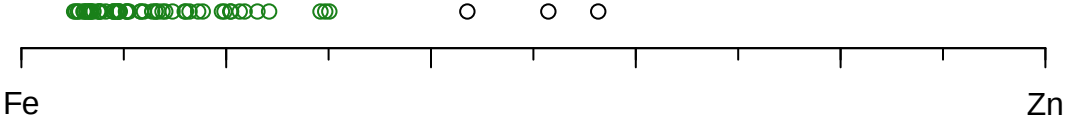
Fe, Ni



Fe, Cu



Fe, Zn



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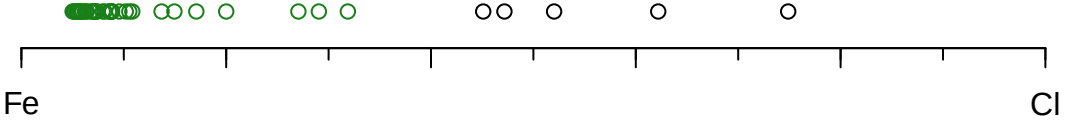
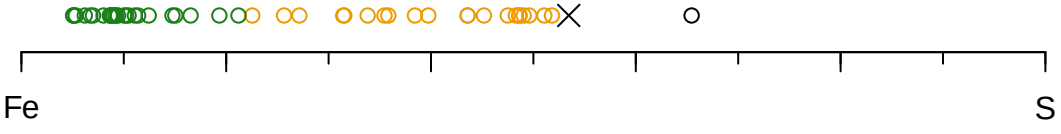
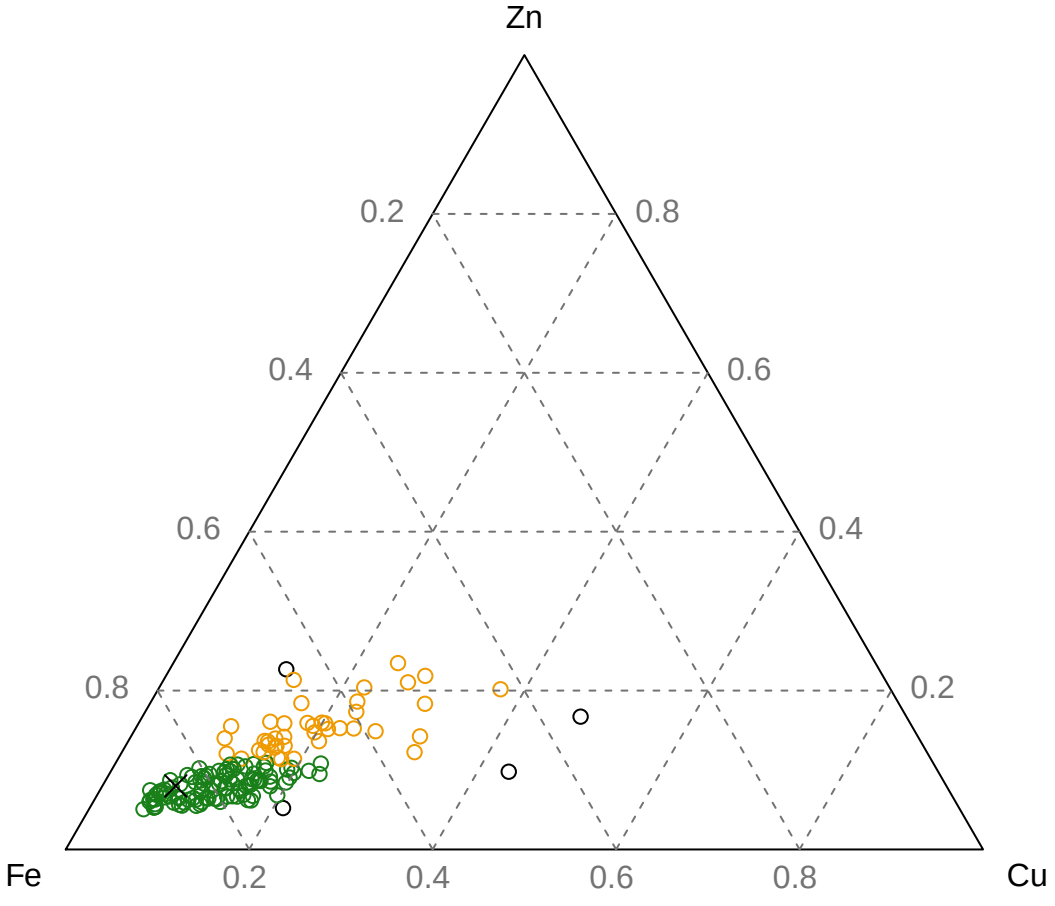


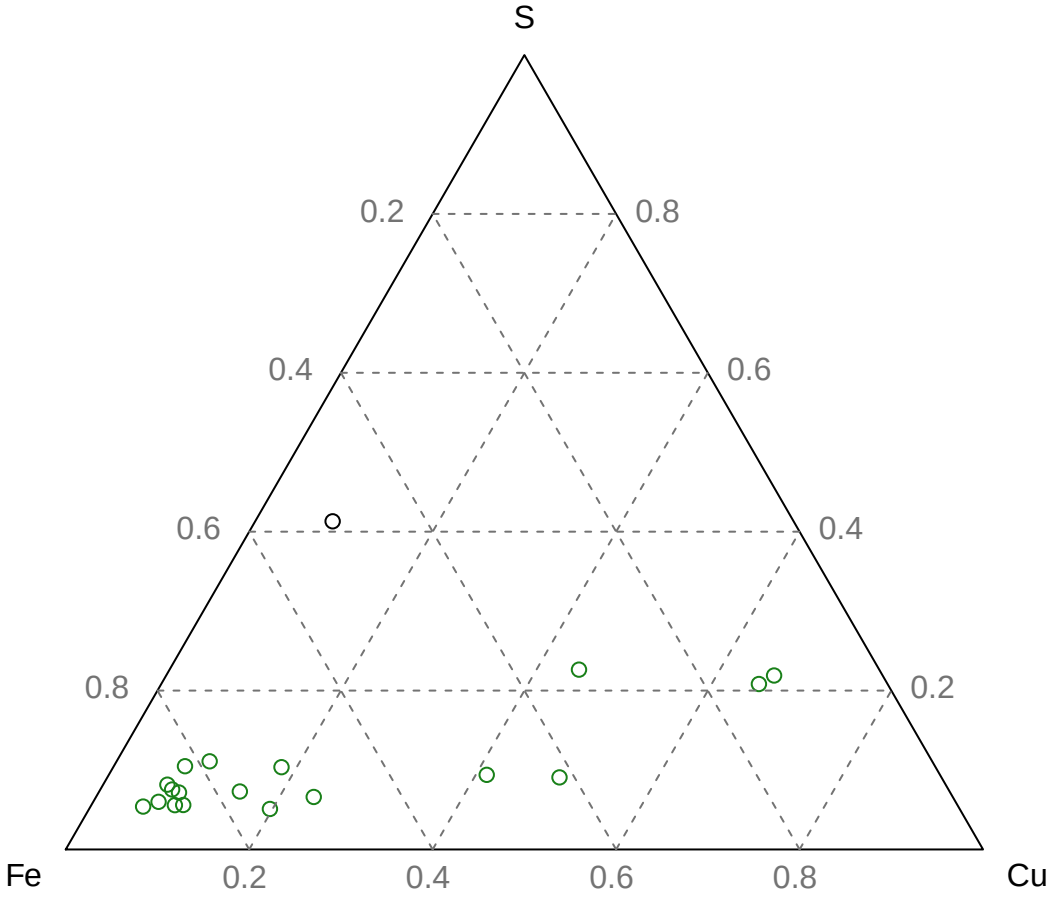
Fe, S



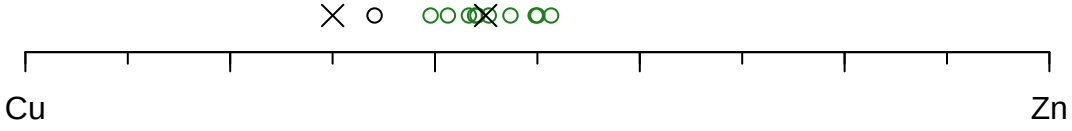
Fe, Cu, Zn



Fe, Cu, S



Cu, Zn



Supplementary File 1

Biplots show the particles in the projection plane of the two first principal components of the original coordinates. The colors of the circles represent the subclasses the corresponding particles belong to and are coded the same way as in fig. 4 and 5. The projected original coordinate axes are plotted in grey. By construction, the particles have the largest spread in this projection among all possible 2D projections. The biplot on the left is based on the particles in ILR transformed coordinates and demonstrates the separation of the particles best. The biplot on right is constructed from the original elementary coordinates, so that an interpretation in terms of elemental composition is possible.

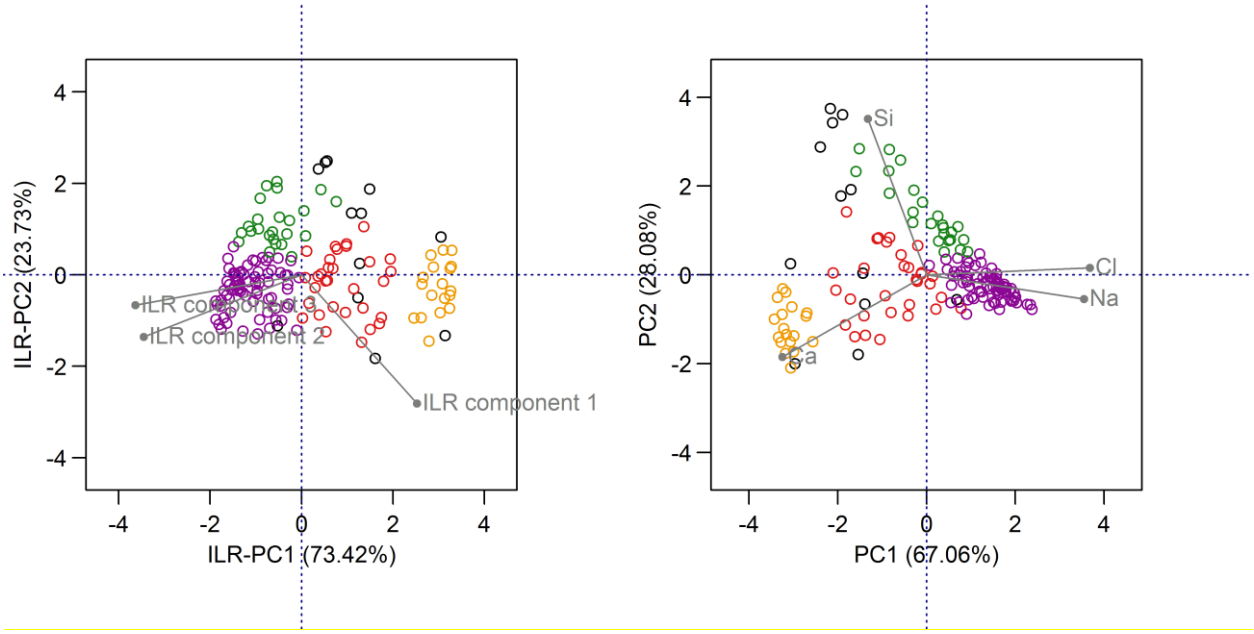


Figure 8. Biplots of the particles of the Si-Ca-Na-Cl main class in ILR transformed (left) and elemental coordinates (right). The subclasses the particles belong to are color-coded as described in fig. 4 of the publication.