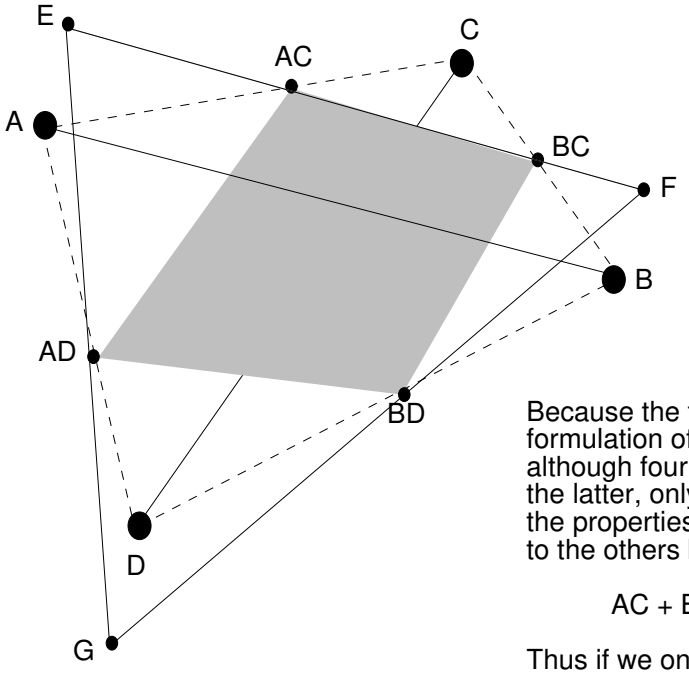
Multisite Solutions

In perplex a "multisite" solution is any solution that is described by more endmembers than the number of components actually necessary to define the composition space of the solution. As an example consider the solution (A,B)(C,D) where A and B mix on one site and C and D mix on another, since each site is binary the solution has only two independent compositional variables and therefore could be described as a ternary (single−site) solution among three endmembers, e.g., E, F, and G.



Although the ternary EFG solution is perfectly valid and can be easily formulated, the use of imaginary endmembers make some people uncomfortable; hence multisite formulations. Multisite models require as many endmembers as there are possible endmember site populations; thus 4 endmembers, AC, AD, BC, BD, are necessary to describe (A,B)(C,D).

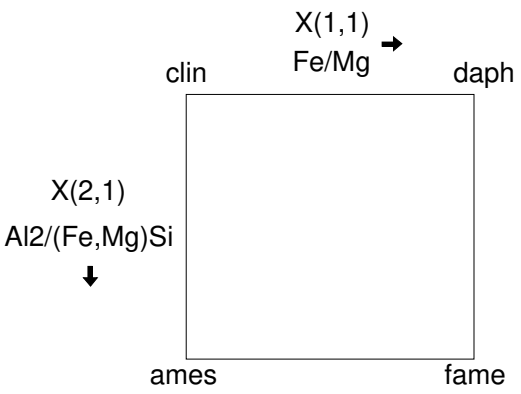
Because the ternary formulation EFG and the multisite formulation of (A,B)(C,D) are both valid, it follows that although four endmembers are necessary to describe the latter, only 3 of these endmembers are indepedent, the properties of the fourth endmember being related to the others by mass balance relation:

$$AC + BD = BC + AD$$

Thus if we only have data for the endmembers AC, BC, and BD the properties of AD can be computed (you can do this in FRENDLY) as:

$$AD = AC + BD - AD$$

Tschermaks and Fe Solution in Clinochlore



As a specific example of a multisite solution for perplex consider Tschermaks and FeMg−1 solution in chlorite (this is discussed in some detail on page 4 of the program documentation).

The key to entering this model into perplex is understanding how the order in which you enter the endmebers determines the compositional variables for the solution. The first endmember read is considered to have the the first species on all sites; the second name has the second species on the first site, and the first species on all the remaining sites. If the first site is binary, then the next endmember MUST be the one with the second species on the first site and the first species on the second site.

If the second site is also binary (as in chlorite) then the fourth, and final, name is the endmember with the second species on both sites.

Thus, entering the chlorite endmbers in the order clin, daph, ames, fames implies that the first "site" (actually it is not a crystallographic site) describes Fe/Mg mixing with Mg being the first species and that the second "site" describes the extent of Tschermaks substitution with the first "species" or "molecule" on the second site being Al2 and the second species being (Mg,Fe)Si (note that this determined entirely from the first two endmembers entered). The Fe/Mg ratio of the tschermaks substitution is accounted for by the first site. X(1,1) is thus X(Mg) relative to clinochlore, X(1,2) is X(Fe), X(2,1) is X(Tschermaks), and X(2,2) is X(inverse Tschermaks). When perplex creates names for the chlorite pseudocompounds it writes the first tow letters of the first endmember, followed by the mole fractions (in percent) of the first species on the first site and the first species on the second site, i.e., cl99−99 is essentially pure clinochlore and cl50−90 would be a chlorite with X(Mg) = 0.5 and X(Ts) = 0.1. For more information on naming conventions see chapter 4 of the tutorial and chapter 4 of the documentation.