



Phase determination by isomorphous replacement. Structure factors are plotted in the complex plane, as in Figure 13-34. (a) A single heavy-atom derivative. The circle with radius F_{PH} represents the parent crystal, with measured intensity and unknown phase. The circle with radius F_{PH} represents the isomorphous heavy-atom-containing crystal, with measured intensity and unknown phase. The vector F_{H} is calculated from the heavy-atom position that had been determined from a difference Patterson synthesis. Because F_{H} is calculated, both its phase and its amplitude are known. Equation 13-102 will be satisfied by F_{P} , F_{H} , and F_{PH} when F_{P} lies at the origin, but F_{PH} is located at the end of F_{H} as shown. Therefore, the two circles are displaced, and they intersect at two positions: A and B. These positions define two possible values for the phase of F_{P} : ϕ_{a} and ϕ_{b} . (b) Inclusion of a second heavy-atom derivative. Its scattering amplitude yields a circle (colored) of radius F_{PH} centered at the end of the vector F_{H} , which is calculated from the known position of the heavy atom. This circle also intersects F_{P} circle at two places: B and C. Because one intersection (B) is the same as an intersection found with the first heavy atom, the only phase choice for F_{P} consistent with both derivatives is ϕ_{b} . [After D. Eisenberg, in The Enzymes, 3rd ed., vol. 1, ed. P. D. Boyer (New York: Academic Press, 1970), p. 1.]