

Predominance and mineral stability diagrams are most useful if they are based on a full chemical speciation. The diagrams can then include a wide range of reactions of importance in environmental chemistry including adsorption and ion exchange reactions. They can also take into account the possible interactions between a large number of components and are able to model changes at a fixed total concentration of each component rather than under the commonly used but less realistic assumption of a fixed activity. A "hunt-and-track" algorithm is described that enables predominance and mineral stability diagrams to be constructed using any general-purpose speciation program. Examples are given using PHREEQC and Orchestra.