

The chemist's toolkit 12

Determinants

A pair of simultaneous equations of the form

$$a_1x + b_1y = 0 \quad \text{and} \quad a_2x + b_2y = 0$$

has non-trivial solutions ($x = y = 0$ is a trivial solution) only if the determinant of the coefficients, D , is equal to zero, where

$$D = \begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix} = a_1b_2 - b_1a_2 \quad \text{2} \times \text{2 Determinant}$$

The rule can be extended to three or more simultaneous equations of a similar form (such as $a_1x + b_1y + c_1z = 0$, etc). Thus, a 3×3 determinant is evaluated by expanding it as a sum of 2×2 determinants:

$$D = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = a_1 \begin{vmatrix} b_2 & c_2 \\ b_3 & c_3 \end{vmatrix} - b_1 \begin{vmatrix} a_2 & c_2 \\ a_3 & c_3 \end{vmatrix} + c_1 \begin{vmatrix} a_2 & b_2 \\ a_3 & b_3 \end{vmatrix} \quad \text{3} \times \text{3 Determinant}$$

and there are non-trivial solutions only if $D = 0$. Note the sign change in alternate columns (b_1 occurs with a negative sign in the expansion).

An important property of a determinant is that if any two rows or any two columns are interchanged, then the determinant changes sign:

$$\text{Exchange columns: } \begin{vmatrix} b & a \\ d & c \end{vmatrix} = bc - ad = -(ad - bc) = - \begin{vmatrix} a & b \\ c & d \end{vmatrix}$$

$$\text{Exchange rows: } \begin{vmatrix} c & d \\ a & b \end{vmatrix} = cb - da = -(ad - bc) = - \begin{vmatrix} a & b \\ c & d \end{vmatrix}$$

An implication is that if any two columns or rows are identical, then the determinant is zero.

If the simultaneous equations are of the form

$$a_1x + b_1y = k_1 \quad \text{and} \quad a_2x + b_2y = k_2$$

with k_1 and k_2 nonzero, use **Cramer's rule**, that $x = D_x/D$ and $y = D_y/D$, where

$$D_x = \begin{vmatrix} k_1 & b_1 \\ k_2 & b_2 \end{vmatrix}, \quad D_y = \begin{vmatrix} a_1 & k_1 \\ a_2 & k_2 \end{vmatrix}$$

with analogous expressions for equations in more unknowns. Note that for simultaneous equations of this form, there are non-trivial solutions only if $D \neq 0$.