Assignment-3

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***Abstract*—This document explains the concept of balancing the chemical equations using linear algebra.**

Download all python codes from

https://github.com/vipulmalik8569/MT−EE5609

and latex-tikz codes from

https://github.com/vipulmalik8569/MT−EE5609

1 Problem

Write the balanced chemical equations for the following reaction :

$$BaCl_2 + K_2SO_4 \rightarrow BaSO_4 + KCl \tag{1.0.1}$$

2 Solution

We know that the number of atoms of each element remains the same, before and after a chemical reaction.

Equation (1.0.1) can be written as:

$$x_1BaCl_2 + x_2K_2SO_4 \rightarrow x_3BaSO_4 + x_4KCl \tag{2.0.1}$$

Element wise contribution in forming the respective chemical compound can be written in the form of equation as :

$$Ba : x_1 + 0x_2 - x_3 - 0x_4 = 0 \tag{2.0.2}$$
$$Cl : 2x_1 + 0x_2 - 0x_3 - 1x_4 = 0 \tag{2.0.3}$$
$$K : 0x_1 + 2x_2 - 0x_3 - 1x_4 = 0 \tag{2.0.4}$$
$$S : 0x_1 + 1x_2 - 1x_3 - 0x_4 = 0 \tag{2.0.5}$$
$$O : 0x_1 + 4x_2 - 4x_3 - 0x_4 = 0 \tag{2.0.6}$$

In matrix form this can be written as:

$$A\mathbf{x} = 0 \tag{2.0.7}$$

$$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 2 & 0 & 0 & -1 \\ 0 & 2 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 4 & -4 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.0.8}$$

Using Gaussian Elimination method :

$$\xleftrightarrow{R_2 \leftrightarrow R_5} \begin{pmatrix} 1 & 0 & -1 & 0 & : & 0 \\ 0 & 4 & -4 & 0 & : & 0 \\ 0 & 2 & 0 & -1 & : & 0 \\ 0 & 1 & -1 & 0 & : & 0 \\ 2 & 0 & 0 & -1 & : & 0 \end{pmatrix} \tag{2.0.9}$$

$$\xleftrightarrow{R_5 \leftarrow 2R_1 - R_5} \begin{pmatrix} 1 & 0 & -1 & 0 & : & 0 \\ 0 & 4 & -4 & 0 & : & 0 \\ 0 & 2 & 0 & -1 & : & 0 \\ 0 & 1 & -1 & 0 & : & 0 \\ 0 & 0 & -2 & 1 & : & 0 \end{pmatrix} \tag{2.0.10}$$

$$\xleftrightarrow[R_4 \leftarrow 4R_4 - R_2]{R_3 \leftarrow 2R_3 - R_2} \begin{pmatrix} 1 & 0 & -1 & 0 & : & 0 \\ 0 & 4 & -4 & 0 & : & 0 \\ 0 & 0 & 4 & -2 & : & 0 \\ 0 & 0 & 0 & 0 & : & 0 \\ 0 & 0 & -2 & 1 & : & 0 \end{pmatrix} \tag{2.0.11}$$

$$\xleftrightarrow{R_5 \leftrightarrow R_5} \begin{pmatrix} 1 & 0 & -1 & 0 & : & 0 \\ 0 & 4 & -4 & 0 & : & 0 \\ 0 & 0 & 4 & -2 & : & 0 \\ 0 & 0 & -2 & 1 & : & 0 \\ 0 & 0 & 0 & 0 & : & 0 \end{pmatrix} \tag{2.0.12}$$

$$\xleftrightarrow{R_4 \leftarrow 2R_4 - R_3} \begin{pmatrix} 1 & 0 & -1 & 0 & : & 0 \\ 0 & 4 & -4 & 0 & : & 0 \\ 0 & 0 & 4 & -2 & : & 0 \\ 0 & 0 & 0 & 0 & : & 0 \\ 0 & 0 & 0 & 0 & : & 0 \end{pmatrix} \tag{2.0.13}$$

Clearly the system is linearly dependent. Therefore by fixing the value of $x_4 = 2$, one of the possible vector $\mathbf{x}$ is:

$$\mathbf{x} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 2 \end{pmatrix} \tag{2.0.14}$$

Hence by putting the values of x_1, x_2, x_3, x_4 in equation (1.0.1) we get our balanced chemical equation as followes :

$$BaCl_2 + K_2SO_4 \rightarrow BaSO_4 + 2KCl \tag{2.0.15}$$