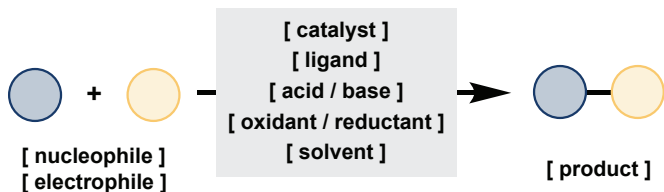


**A****B**

*(fingerprint length, number of components)*  
*fingerprint matrix*

*(number of components, 1)*  
*weight array*

$$\begin{bmatrix} \text{nucleophile FP} \\ \text{electrophile FP} \\ \text{catalyst FP} \\ \text{ligand FP} \\ \text{acid / base FP} \\ \text{oxidant / reductant FP} \\ \text{solvent FP} \end{bmatrix}^{-1} \cdot \begin{bmatrix} w_n \\ w_e \\ w_c \\ w_l \\ w_{ab} \\ w_{or} \\ w_s \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ \cdot \\ \cdot \\ b_{\text{len(fp)}} \end{bmatrix}$$

*(fingerprint length, 1)*  
*reaction fingerprint*