❖ Optical Purity

Optical purity or the enantiomeric excess (ee) may simply be defined as the purity measurement used for chiral compounds and reflects the extent to which a sample contains one enantiomer in greater amounts than another enantiomer.

The enantiomeric excess of the racemic mixture 0%, whereas a single completely pure enantiomer has an enantiomeric excess of 100%. A sample having 60% of one enantiomer and 40% of the other has an ee of 20% (60% − 40%). The general expression for optical purity may be given by the following relation.

$$Optical\ purity = \%\ ee = \frac{\alpha_{obs}}{\alpha_{max}} = \frac{[R] - [S]}{[R] + [S]} \times 100 \tag{7}$$

Where α_{obs} and α_{max} are the observed angle of rotation of plane-polarized light by the racemic mixture under consideration and maximum angle of rotation that it could rotate when R is replaced by S enantiomer and vice-versa, respectively. The symbol $[R]$ and $[S]$ are simply the percentage of R and S enantiomer, respectively.

Furthermore, the percentage of major and minor enantiomers can be obtained if the enantiomeric excess is known as given below.

$$\%\ of\ major\ enantiomer = \frac{100 + \%\ ee}{2} \tag{8}$$

Similarly

$$\%\ of\ minor\ enantiomer = \frac{100 - \%\ ee}{2} \tag{9}$$

In an ideal situation, each component's contribution to the total magnitude of optical rotation is directly proportional to the corresponding mole fraction, and therefore, the optical purity should be identical to the enantiomeric excess. This gives rise to the informal usage of the two terms as interchangeable, especially due to the fact that optical purity was the conventional route of measuring enantiomeric excess. Nevertheless, other methods like NMR spectroscopy and chiral column chromatography are now quite popular for measuring the amount of each enantiomer separately.

The success of asymmetric synthesis is also quantified using enantiomeric excess. In the case of diastereomers mixtures, analogous definitions (diastereomeric excess) are employed for measurement. The term 'enantiomeric excess' was presented by Morrison and Mosher in 1971 in their paper entitled "Asymmetric Organic Reactions", indicating its historic ties with optical rotation. It has been proposed that the concept of 'enantiomeric excess' should be changed by that of 'enantiomeric ratio' which means S:R or S/R because the determination of optical purity has already been replaced by other experimental techniques which directly measure R and S for simplistic mathematical treatments. The same can be said for replacing the 'diastereomeric excess by 'diastereomeric ratio; though it seems very far from practice.

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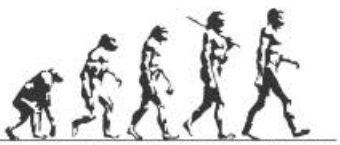

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