Indices for chemical reactions

Simple indices

In synthetic organic chemistry yield and purity are common indices, characterizing the quality of a chemical transformation. The yield Y is defined as the quotient of the actual amount of product obtained from the reaction (actual yield) and the amount of product which could have theoretically been obtained if the total of limiting reagent R had been transformed according to the stoichiometric equation (theoretical or stoichiometric yield), presuming 100 % purity of the reagents.

If n_R is the amount of the limiting reagent before the reaction and a_P and a_R are the stoichiometric coefficients of product *P* and limiting reagent *R*, the yield is given by

(1)

$$Y = \frac{n_\mathrm{P} a_\mathrm{R}}{n_\mathrm{R} a_\mathrm{P}}$$

If n_P is the amount after purification, it is called the final yield. Generally, the yield defined by this equation will be expressed as a percentage (percent yield or percentage yield).

Before actually performing the reaction, one can already derive the so-called atom economy from the stoichiometric equation. The atom economy expresses which fraction of the summed atomic masses on the left hand side of the equation appear in the product. By virtue of this definition, it is an evaluation of a synthetic approach from an economic point of view. The concept of atom economy was introduced by B. M. Trost in 1995 [1].

The purity of the product is determined by Thin Layer Chromatography (TLC), Gas Chromatography (GC) or High Performance Liquid Chromatography (HPLC) and is also generally expressed as a percentage. However, it should be noted that each analytical system has its limitations. For example, in gas chromatography only substances which evaporate at temperatures of up to 250 °C without decomposition can be analysed.

The mass efficiency e_S of a reaction we define as the ratio of the mass of the obtained and purified product m_P divided by the sum of the masses of all substances introduced to a reaction mixture during the experiment:

(2)

$$e_{\mathrm{S}} = \frac{m_{\mathrm{P}}}{\sum_i m_i}$$

where index i runs over all used substances. Coolants like cooling water or ice, not commixing with the reaction mixture are not taken into consideration accoring to our convention. Accounting for such substances is the task of the more detailed method of input analysis. e_S like it is defined here is similar to the inverse of the E factor (environmental factor) as it was introduced by R. Sheldon in 1994 [2]. We are using an efficiency index so that a higher value actually indicates an improvement.

The energy efficiency e_E of a reaction is defined in analogy as the ratio of the mass of the obtained and purified product m_P divided by the sum of the energy consumed during the experiment:

(3)

$$e_{\mathrm{E}} = \frac{m_{\mathrm{P}}}{\sum_k E_k}$$

where index *k* runs over all separately measurable energy consumptions, i.e. in general the consumed electrical energy. In this measure the energy used to produce ice for cooling is included. Important hints for the measurement of such energy contributions are presented in the NOP article Energiemessung - Energiekennzahlen.

Atom economy, mass efficiency and energy efficiency are automatically calculated for the NOP experiments and can be found under menu entry "Evaluation", submenu entry "Indices" on the page of each experiment (Beispiel-Link).

Environmental Assessment Tool for Organic Syntheses (EATOS)

A substance based evaluation of chemical reactions (including multistep reactions) can be conducted with the Environmental Assessment Tool for Organic Syntheses (EATOS, Website EATOS) [3] möglich.

This approach is based on Sheldons E factor (cf. above), i.e. on the total amount of substances entering a reaction in relation to the product obtained. For each of the used substances an environmental load factor Q is defined which is derived from MAK values (Maximum workplace concentrations in Germany), hazard symbols, R-phrases (cf. NOP article R- and S-Phrases), LD_{50} values and LC_{50} values, but optionally also from costs, depending on the evaluation focus of the user. The Environmental Index EI, used mostly for comparative evaluation of different synthetic pathways and techniques is calculated as the sum of all substance masses multiplied by their respective Q factor.

This evaluation concept was implemented in a freely available and platform independent software. The program also calculates the atom economies and Sheldon's E factor for the entered reactions.

You can find a short description of the evaluation approach EATOS as well as an application to the comparison of experiment 4010 with an alternative method in the NOP article "Bewertung der Umweltverträglichkeit von chemischen Reaktionen". We are also offering a Manual Bedienungs- und Benut-zungsanleitung für EATOS in German.

References

[1] B. M Trost. Angew. Chem. Int. Ed. Engl, 34:259 – 281, 1995.

[2] R. Sheldon. Chemtech, 24(3):38 – 47, 1994.

[3] M. Eissen and J. O. Metzger. Environmental performance metrics for daily use in synthetic chemistry. Chem. Eur. J., 8(16):3580 – 3585, 2002.

update 22. August 2012