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# Energy Economy as a Measure of Efficiency in Sustainable Chemical Processes

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## Abstract

Ever since the seminal publication by Barry M. Trost in 1991 on atom-economy, other chemists interested in catalysis, including transition metal catalysis and organocatalysis, have been inspired by the Trost-Method.


**Keywords:** Atom economy, Step economy, Redox economy

## Introduction

In view of the indisputable climate change concomitant with rapidly increasing CO2 concentrations in the atmosphere, sustainability is an issue of paramount importance for humans and all other forms of life. Indeed, not only traditional chemical companies, but essentially all other corporations engaging in commercial businesses claim sustainability (often denoted as greenness). Even sports events such as football teams or car racing claim sustainability! Numerous scientific articles report sustainability as the goal of the research. Moreover, the titles of a number of scientific journals contain the word "green".

But it is not at all clear what the words "sustainable" or "green" actually mean nor how sustainability can be measured. Atom economy in the search for synthetic efficiency in organic and pharmaceutical chemistry as proposed by Trost1 in 1991 constituted a seminal step forward which inspired synthetic organic chemists to view efficiency as an issue of paramount importance [2]. This was followed by the idea of step economy as championed by Wender and coworkers [3]. Finally, redox economy as emphasized by Hoffmann and Baran also deserves special mention [1].

Yet all of the above approaches have their specific limitations and caveats. As a chemist, I focus in this review on chemical processes, and propose energy economy as the central and decisive parameter in the fight against manmade climate change. It begins with a short description of atom, step and redox economy.

### Atom Economy

Atom economical chemical transformations are ensured whenever two reaction partners join together without forming any side-products that have to be laboriously separated and subjected to a costly disposal procedure (Equation 1a). Classical examples are the Diels-Alder and the 1,3-dipolar cycloadditions. In an atom uneconomical process, an undesired side-product is formed, often in stoichiometric amounts (Equation 1b). A typical reaction is the Wittig olefination.

a) $A + B \rightarrow C$ atom economical Equation 1

b) $A + B \rightarrow C + D$ atom uneconomical

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## Step Economy

The proposal of atom economy served as the inspiration to suggest step economy. Chemists engaging in the synthesis of natural products have traditionally strived for devising synthetic pathways that are characterized by as few as possible steps. This was systematized by proposing step economy, in which the discovery of new reactions played a central role (Figure 1) [3].

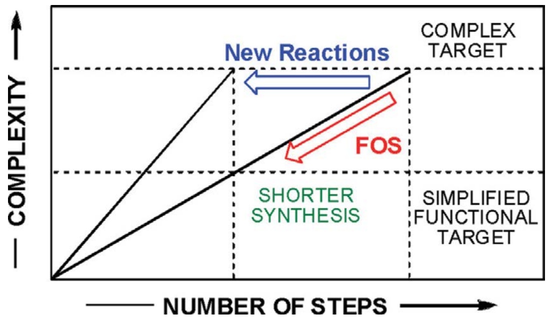


**Figure 1:** Schematic representation of step economy (Wender, Verma et al. 2007).

## Redox Economy

Chemists have seldomly thought about redox economy. For example, for a century or longer it was customary to react benzene or other aromatic compounds with chlorine or bromine, such halogenation forming a halogenated aromatic such as chlorobenzene (oxidation). The halo-benzene is then reacted with magnesium in a reduction step with formation of the respective Grignard reagent, which in turn can be used to perform additions to aldehydes or ketones. Finding a way to add benzene or other aromatics directedly to aldehydes or ketones would be much more efficient. A general scheme of redox economy is shown in Figure 2 [1].

All three types of "economies" as summarized above play an important role in modern synthetic organic chemistry and should be continued to be considered in future efforts, ideally in combination with catalysis. Nevertheless, an atom economical reaction using transition metal catalysts or organocatalysts may require excessive energy in the formation of the catalysts and in the downstream workup. In such cases, claiming sustainability appears problematic. The same applies to many enzyme-based syntheses of otherwise useful products. Finally, $CO_2$ capture seems like a positive development, but it ignores the energy used up for this purpose.

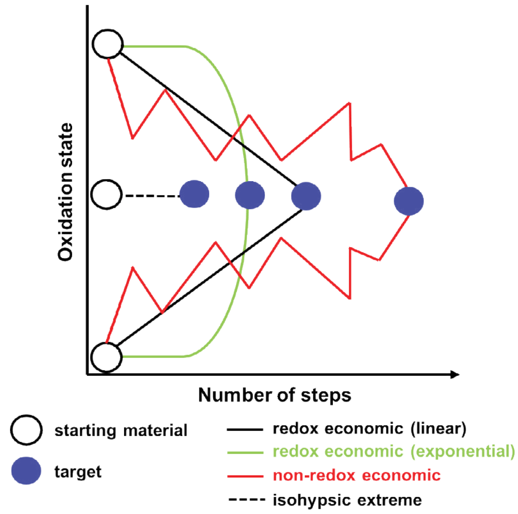


**Figure 2:** Schematic representation of redox economy (Burns, Baran et al. 2009).

Today's societies in the developed or less developed parts of the world increasingly continue to require more and more energy, the operation of cell-phones being an example. Moreover, researchers at universities and at companies are rapidly developing advanced super computers which literally "eat up" huge, if not astronomical amounts of energy. Notwithstanding their benefits, they are detrimental in the fight to curb the highly negative aspects of climate change.

I therefore suggest that synthetic organic chemists should consider energy economic issues in all of their efforts. Quantification may be difficult, but it would nevertheless constitute an important step forward.

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