Supplementary Material (ESI) for Green Chemistry

Bisoxazoline-Functionalised Enantioselective Monolithic Mimi-Flow-reactors: Development of Efficient Processes from batch to Flow Conditions

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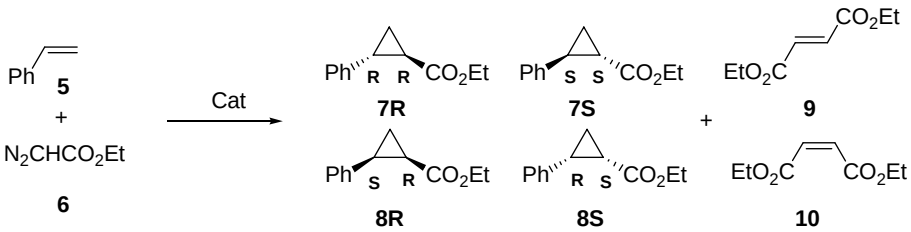
Kinetic calculation BOX

Continuous cyclopropanation reaction between **5** (EDA) and **6** (STR) in CH_2Cl_2.
The main reagents and products involved in the reaction path are:

% 1.Styrene: STR
% 2.Ethyl diazetate : EDA
% 3.Fumarate: FMT
% 4.Maleate: MLT
% 5.Trans-cyclopropane_a: CPTa 7R
% 6.Trans-cyclopropane_b: CPTb 7S
% 7.Cis-cyclopropane_a: CPCa 8R
% 8.Cis-cyclopropane_b: CPCb 8S



The sequence of reactions used was:

$$r_1 = k_1 \cdot c_2^{2.2} \quad (1)$$
$$r_2 = k_2 \cdot c_2^{1.6} \quad (2)$$
$$r_3 = k_3 \cdot c_1 \cdot c_2^{1.6} \quad (3)$$
$$r_4 = k_4 \cdot c_1 \cdot c_2^{4.0} \quad (4)$$
$$r_5 = k_5 \cdot c_1 \cdot c_2^{1.5} \quad (5)$$
$$r_6 = k_6 \cdot c_1 \cdot c_2^{1.5} \quad (6)$$

The different mass balance equations for a fixed bed catalytic reactor are:

$$\frac{dc_1}{d\tau} = -r_3 - r_4 - r_5 - r_6 \quad (7)$$
$$\frac{dc_2}{d\tau} = -2 \cdot r_1 - 2 \cdot r_2 - r_3 - r_4 - r_5 - r_6 \quad (8)$$

$$\frac{dc_3}{d\tau} = +r_1 \quad (9)$$

$$\frac{dc_3}{d\tau} = +r_1 \quad (10)$$

$$\frac{dc_4}{d\tau} = +r_2 \quad (11)$$

$$\frac{dc_5}{d\tau} = +r_3 \quad (12)$$

$$\frac{dc_6}{d\tau} = +r_4 \quad (13)$$

$$\frac{dc_7}{d\tau} = +r_5 \quad (14)$$

$$\frac{dc_8}{d\tau} = +r_6 \quad (15)$$

Final values of the parameters were:

k_1=0.117 $L^{1.2}\cdot mol^{-1.2}\cdot min^{-1}$

k_2=0.0475 $L^{0.6}\cdot mol^{-0.6}\cdot min^{-1}$

k_3=0.0350 $L^{0.6}\cdot mol^{-0.6}\cdot min^{-1}$

k_4=0.120 $L^{3}\cdot mol^{-3}\cdot min^{-1}$

k_5=0.0232 $L^{0.5}\cdot mol^{-0.5}\cdot min^{-1}$

k_6=0.0070 $L^{0.5}\cdot mol^{-0.5}\cdot min^{-1}$