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Data Article

Equilibrium data for the cross-metathesis of methyl oleate with cinnamaldehyde

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ABSTRACT

Here we present equilibrium data for the cross-metathesis of methyl oleate (MO) with cinnamaldehyde (CA) obtained experimentally from liquid-phase catalytic tests conducted at 323 K. The reaction was carried out in batch reactors, using different reactant molar ratios and the 2nd generation Ru Hoveyda-Grubbs complex as catalyst. Reaction mixtures at the equilibrium were analyzed by gas chromatography. Equilibrium constants were determined by assuming unitary activity coefficients for a cinnamaldehyde/methyl oleate equimolar ratio, and the validity of that approximation was evaluated by calculating the equilibrium conversions for different reactant molar ratios.

Specifications Table

Subject area	*Chemical Engineering*
More specific subject area	*Organometallic catalysis, Functionalized Olefin Cross Metathesis*
Type of data	*Figure, Table*
How data was acquired	*Gas Chromatograph, Agilent 6850 Chromatograph (FID). Schlenck-type glass reactor for catalytic tests.*

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Data format	*Analyzed*
Experimental factors	*The equilibrium in the cross-metathesis of methyl oleate with cinnamaldehyde was achieved in a Schlenck-type reacter under inert atmosphere at 323 K and different cinnamaldehyde/methyl oleate initial molar ratios.*
Experimental features	*Catalytic tests in batch reactor, monitored by gas chromatography*
Data source location	*INCAPE (Instituto de Investigaciones en Catálisis y Petroquímica), Santa Fe, Argentina* https://goo.gl/maps/K8UENtWYqUk
Data accessibility	*Data are accessible with the article*
Related research article	P. Nieres, A.F. Trasarti, C.R. Apesteguía, Valorisation of plant oil derivatives via metathesis reactions: study of the cross-metathesis of methyl oleate with cinnamaldehyde, Mol. Catal. (2018) *in press*

Value of the data

- The cross metathesis of methyl oleate with cinnamaldehyde is an attractive route for the synthesis of various useful intermediates and compounds for fine chemistry and polymer industry [1].
- Equilibrium data for MO/cinnamaldehyde reaction (unpublished to date) are relevant to improve the yield in cross-metathesis products, in competition with the MO self-metathesis reaction.
- Theoretical and experimental equilibrium conversions presented here allow other researchers to extend analyses for cross metathesis of unsaturated fatty acid methyl esters with functionalized olefins.

1. Data

Table 1 lists the retention times and flame ionization detector (FID) response factors relative to n-dodecane (internal standard) for all the reactants and products detected during the catalytic tests. Fig. 1 shows a typical gas chromatogram identifying the reactants methyl oleate (MO) and cinnamaldehyde (CA), and the products 2-undecenal (2UAL), methyl 11-oxo-9-undecenoate (11UDE), 1-decenylbenzene (1DB), 9-octadecene (9OCT), methyl 10-phenyl-9-decenoate (10DE), dimethyl 9-octadecen-1,18-dioate (9OD).

Table 2 shows the reactions involved in the MO/CA cross-metathesis, while the expressions of the corresponding equilibrium constants K_i^{Eq} are given in Table 3. The experimental values obtained at 323 K for each compound at equilibrium for different initial reactant molar ratios ($R_{CA/MO}$) are collected in Table 4. The values of reaction equilibrium constants at 323 K and $R_{CA/OM} = 1$ were calculated using the experimental data of Table 4 and are presented in Table 5. Finally, we used the K_i^{Eq} values of

Table 1
Retention times and FID response factors for reactants and products.

Substance	Retention time (min)	Response factor[a]
n-dodecane (STD)	13.55	1
cinnamaldehyde (CA)	14.39	0.62
2-undecenal (2UAL)	15.92	0.83
methyl 11-oxo-9-undecenoate (11UDE)	20.14	1.13
1-decenylbenzene (1DB)	21.10	0.80
9-octadecene (9OCT)	21.46	1.38
methyl 10-phenyl-9-decenoate (10DE)	24.51	1.11
methyl oleate (MO)	24.66	1.28
dimethyl 9-octadecen-1,18-dioate (9OD)	27.69	1.20

[a] Relative to n-dodecane (internal standard)