Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Catalytic transformations of citral in a continuous flow over bifunctional Ru-MCM-41 extrudates

Zuzana Vajglová[1], Päivi Mäki-Arvela[1], Kari Eränen[1], Narendra Kumar[1], Markus Peurla[2], Dmitry Yu. Murzin[1*]

[1] *Åbo Akademi University, Johan Gadolin Process Chemistry Centre, Biskopsgatan 8, Turku/Åbo, Finland, 20500*
[2] *University of Turku, Turku, Finland, 20500*
[*] *dmurzin@abo.fi, corresponding author*

EXPERIMENTAL

Definitions

Normalized time is defined as follows:

$$t_N = t \cdot m_{cat} \cdot \frac{c_{Ru} \cdot D_{Ru}}{Mr_{Ru}} \left[h \cdot mol_{Ru(surface)}\right] \qquad (1)$$

where t is reaction time, m_{cat} is mass of catalyst, c_{Ru} is the concentration of Ru in the entire catalyst volume, D_{Ru} is Ru distribution and Mr_{Ru} is the molecular weight of ruthenium.

The liquid phase mass balance closure is defined as a sum of the concentration of citronellal at a certain time and the concentrations of products visible in the GC chromatogram divided by the initial concentration of citronellal, denoted as MB:[1-3]

$$MB\,(\%) = \frac{\Sigma m_i}{\Sigma m_0} * 100 \qquad (2)$$

$\sum m_i$ = sum of mass concentration of all components at different sampling times
$\sum m_0$ = sum of mass concentration of all components at time = 0
The reaction rates (r) and turnover frequency (TOF) are calculated as follows:

$$r_{extrudates} = \frac{\Delta\dot{n}}{m_{cat}} \left[\frac{mol}{s.g}\right] \qquad (3)$$

$$r_{powder\ catalyst} = \frac{\Delta n}{\Delta t.m_{cat}} \left[\frac{mol}{s.g}\right] \qquad (4)$$

$$TOF_{extrudates} = \frac{\dot{n}_{in} - \dot{n}_{out}}{n_{metal(surface)}} \left[\frac{1}{s}\right] \qquad (5)$$

$$TOF_{powder\ catalyst} = \frac{\Delta n \cdot V_l}{\Delta t.n_{metal(surface)}} \left[\frac{1}{s}\right] \qquad (6)$$

where $_{\text{extrudates}}$ is obtained over extrudates in trickle-bed reactor and $_{\text{powder catalyst}}$ is obtained over powder catalyst in a batch reactor, $\Delta\dot{n}$ denotes the change in molar flow rate of the feed at time zero and time t in a trickle bed reactor, $\Delta n/\Delta t$ reacted moles per time interval Δt in a batch reactor, m_{cat} is catalyst mass, V_l is liquid volume and $n_{metal(surface)}$ is moles of exposed measured metal.[1-4] Cumulative reaction rate and turn-over-frequency (r_{cum}, TOF_{cum}) at time t was calculated as differences to time zero, while the instantaneous reaction rate and turn-over-frequency (r_{inst}, TOF_{inst}) at time t were related to time t-1.

RESULTS AND DISCUSSION

Catalyst characterization results

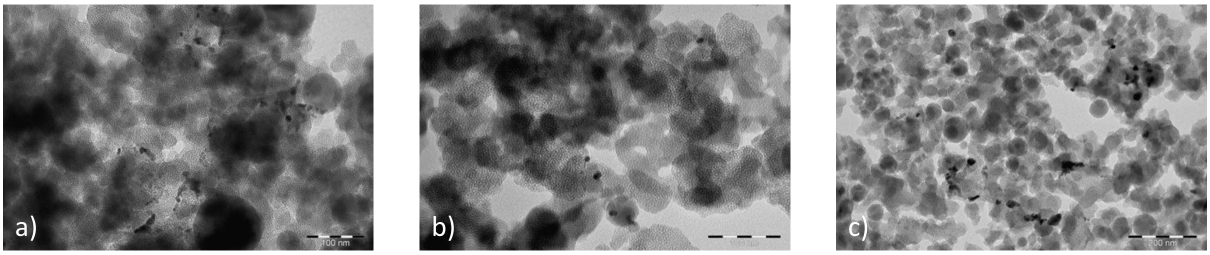

*Figure S1. TEM images of powder catalysts: a) Ru/(H-MCM-41+Bindzil) (**P-B**);[3] b) (Ru/Bindzil)+H-MCM-41 (**P-C**); c) (Ru/H-MCM-41)+Bindzil (**P-D**).*

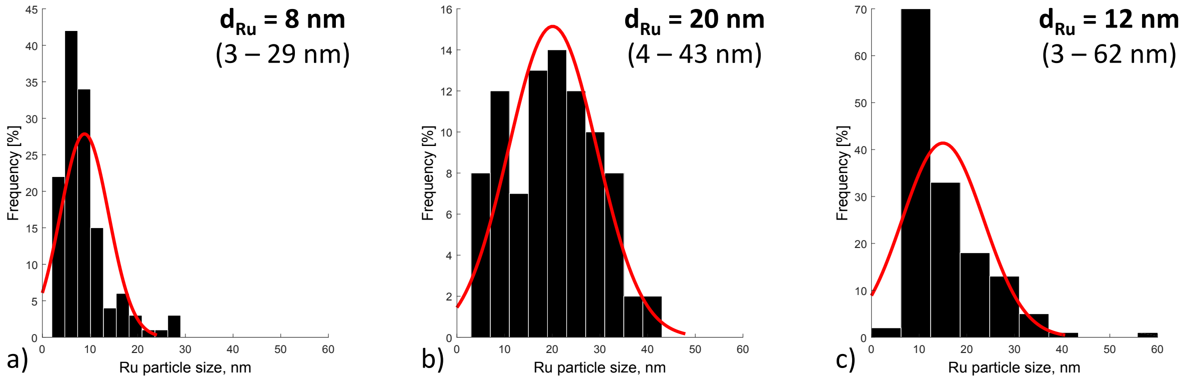

*Figure S2. Ru particle size distribution of powder catalysts: a) Ru/(H-MCM-41+Bindzil) (**P-B**);[3] b) (Ru/Bindzil)+H-MCM-41 (**P-C**); c) (Ru/H-MCM-41)+Bindzil (**P-D**).*

Table S1. Brønsted and Lewis acid sites. In parenthesis data for theoretical value calculated from the contribution of individual components.

Type	Brønsted acidity, µmol/g				Lewis acidity, µmol/g				Total acidity
	weak	*medium*	*strong*	∑	*weak*	*medium*	*strong*	∑	*µmol/g*
P[3]	41	19	24	84	20	14	21	56	140
Z	0	0	1	1	1	0	0	1	2
P*[3]	29 (29)	11 (13)	1 (17)	41 (59)	28 (14)	6 (10)	1 (15)	34 (40)	75 (99)
P-B[3]	18	4	0	21	41	3	0	44	65
P-C	37	0	0	37	32	0	0	32	69
P-D	28	0	0	28	15	0	0	15	44
E-A[3]	36	1	0	37	22	2	0	24	60
E-B[3]	31	0	0	31	21	0	0	21	51
E-C[3]	32	3	0	35	23	2	0	25	60

E-D[3]	29	0	0	29	22	0	0	22	52

P – powder catalyst; E - extrudates; **P-B** – Ru/(H-MCM-41+Bindzil); **P-C** – (Ru/Bindzil)+H-MCM-41; **P-D** – (Ru/H-MCM-41)+Bindzil; **E-A** – Ru/(H-MCM-41+Bindzil) *post* synthesis; **E-B** – Ru/(H-MCM-41+Bindzil*) in-situ* synthesis; **E-C** – (Ru/Bindzil)+H-MCM-41; **E-D** – (Ru/H-MCM-41)+Bindzil.

Catalytic results

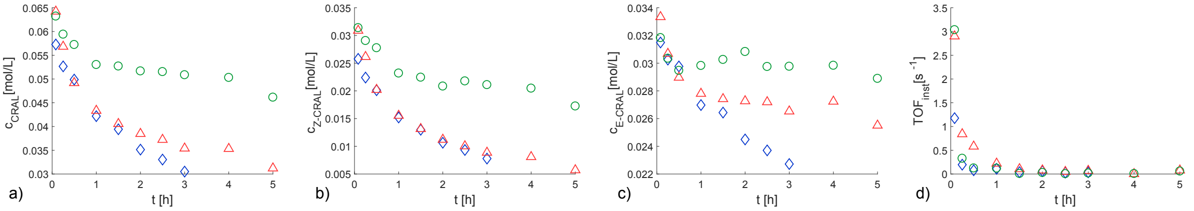

*Figure S3. Concentration profile as a function of reaction time: a) racemic mixture of citral, b) Z-citral, c) E-citral; d) Instantaneous turn-over-frequency as a function of reaction time. Legend: Ru/(H-MCM-41+Bindzil) (**P-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**P-C**, red triangle), Ru/(H-MCM-41)+Bindzil (**P-D**, green circle). Conditions: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst.*

Table S2. Citral transformation to menthol over Ru catalysts. Legend: t, TOS – reaction time, time-on-stream; X – conversion of citral; r – cumulative reaction rate; TOF – cumulative turnover frequency; η – effectiveness factor; PCU – percentage of catalyst utilization, ^{0} the initial time for powder catalyst and extrudates was 5 min and 30 min, respectively. Conditions for the batch experiment over the powder catalysts: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst. Conditions for the continuous experiment aver the extrudates: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 1 g of catalyst, 12.5 min of residence time.

Catalyst	**t, TOS***	**X**	**r^0_{cum}**	**$TOF^0{}_{cum}$**	**η^0**	**r_{cum}**	**TOF_{cum}**	**η**	**PCU**
-	*h*	*%*	*mol/s/g*	*1/s*	-	*mol/s/g*	*1/s*	-	*%*
P-B	3	59	$2.53\cdot10^{-5}$	1.449	-	$1.81\cdot10^{-6}$	0.104	-	-
P-C	5	58	$1.52\cdot10^{-5}$	2.329	-	$1.61\cdot10^{-6**}$	0.247^{**}	-	-
P-D	5	40	$2.10\cdot10^{-5}$	2.445	-	$1.09\cdot10^{-6**}$	0.127^{**}	-	-
E-A	0.2, 3*	70	$4.36\cdot10^{-7}$	0.025	0.02	$3.62\cdot10^{-7}$	0.021	0.20	19.8
E-B	0.2, 3*	66	$4.93\cdot10^{-7}$	0.056	0.02	$3.26\cdot10^{-7}$	0.037	0.18	35.8
E-C	0.2, 3*	66	$4.65\cdot10^{-7}$	0.056	0.03	$3.08\cdot10^{-7}$	0.037	0.19	15.0
E-D	0.2, 3*	64	$4.38\cdot10^{-7}$	0.037	0.02	$3.15\cdot10^{-7}$	0.027	0.29	21.1

**at 3 h of reaction time, P – powder catalyst; E - extrudates; P-B – Ru/(H-MCM-41+Bindzil); P-C – (Ru/Bindzil)+H-MCM-41; P-D – (Ru/H-MCM-41)+Bindzil; E-A – Ru/(H-MCM-41+Bindzil) *post* synthesis; E-B – Ru/(H-MCM-41+Bindzil*) in-situ* synthesis; E-C – (Ru/Bindzil)+H-MCM-41; E-D – (Ru/H-MCM-41)+Bindzil.

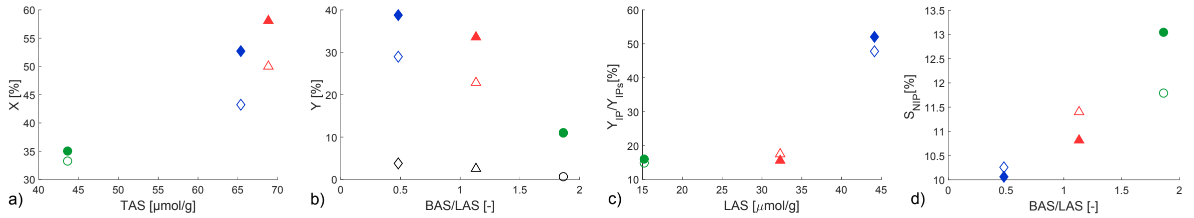

*Figure S4. a) Citral conversion as a function of total acidity, b) total yield as a function of Brønsted to Lewis acid sites ratio, c) stereoselectivity of isopulegol as a function of Lewis acidity, d) Selectivity of neoisopulegol as a function of Brønsted to Lewis acid sites ratio. Legend: Ru/(H-MCM-41+Bindzil) (**P-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**P-C**, red triangle), Ru/(H-MCM-41)+Bindzil (**P-D**, green circle); at normalized time* *of 1.5·10⁻⁶ h·mol$_{Ru(surface)}$ (black open symbols), 3.5·10⁻⁶ h·mol$_{Ru(surface)}$ (open symbols), 7·10⁻⁶ h·mol$_{Ru(surface)}$ (filled symbols). Conditions: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst.*

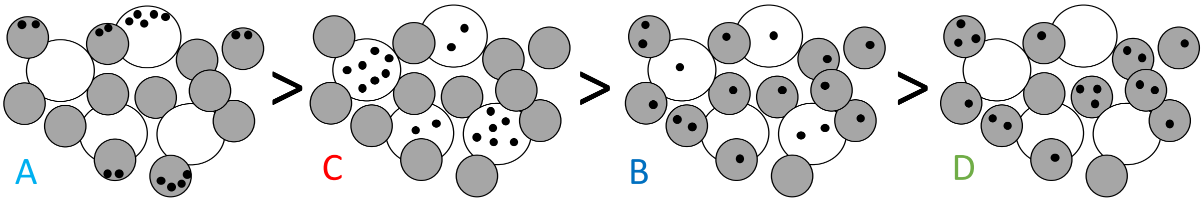

Figure S5. A schematic picture of the catalysts employed in this study, showing different distances between the metal and acid sites: a) A – Ru/(H-MCM-41+bindzil-50/80), post synthesis; b) C – (Ru/bindzil-50/80)+H-MCM-41, in-situ synthesis; c) B - Ru/(H-MCM-41+bindzil-50/80), in-situ synthesis; d) D – (Ru/H-MCM-41)+bindzil-50/80, in-situ synthesis. Legend: H-MCM-41 (grey circle), bindzil-50/80 (white circle), Ru (black dots) [3, 5].

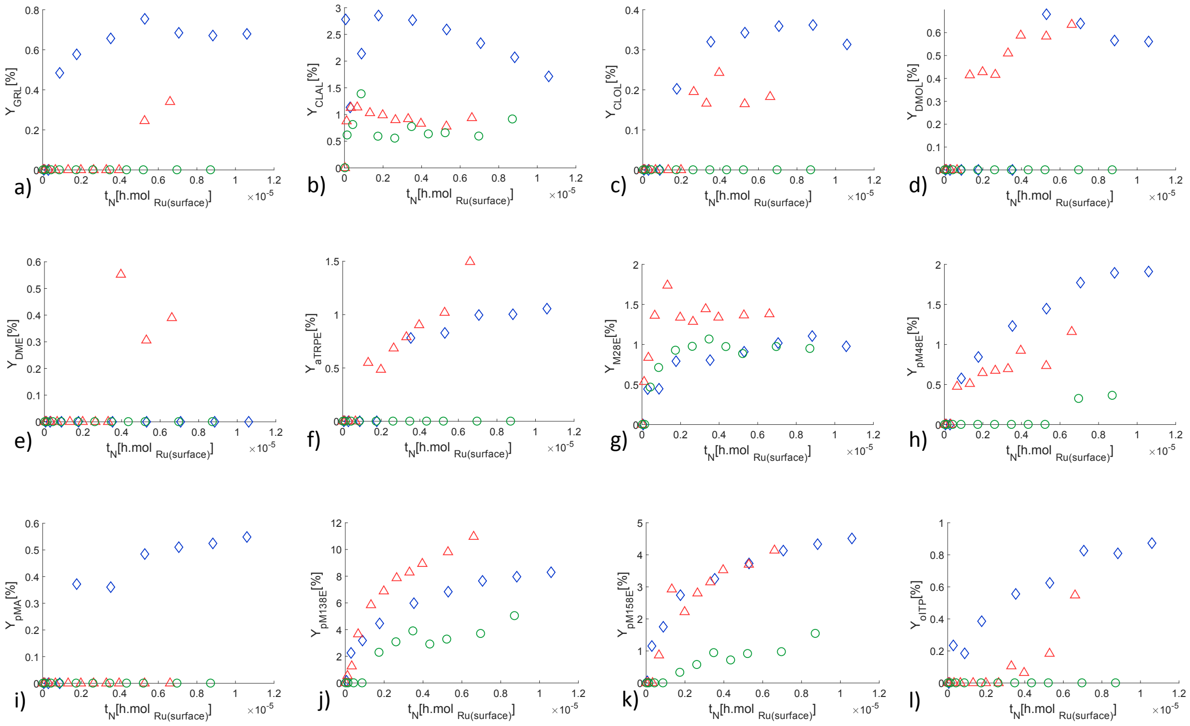

*Figure S6. Product distribution in citral transformation to menthol over powder catalyst in a batch reactor: a) geraniol, b) citronellal, c) citronellol, d) 3,7-dimethyloctan-1-ol, e) 2,6-dimethyloctane, f) α-terpinolene, g) metha-2,8-diene, h) p-menth-4(8)-ene, i) p-menthane, j) p-mentha-1,3,8-triene, k) p-mentha-1,5,8-triene, l) o-isopropenyltoluene. Legend: Ru/(H-MCM-41+Bindzil) (**P-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**P-C**, red triangle), Ru/(H-MCM-41)+Bindzil (**P-D**, green circle). Conditions: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst.*

Table S3. Stereoselectivity to isopulegol isomers in menthol synthesis from citral. Legend: isopulegol (IP), neoisopulegol (NIP), isoisopulegol (IIP), neoisopulegol (NIP). Conditions for the batch experiment over the powder catalysts: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst. Conditions for the continuous experiment aver the extrudates: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 1 g of catalyst, 12.5 min of residence time.

	t, TOS*	**Y_{IPs}**	**Y_{IP}/Y_{IPs}**	**Y_{NIP}/Y_{IPs}**	**Y_{IIP}/Y_{IPs}**	**Y_{NIIP}/Y_{IPs}**
	h	%				
P-B	3	13.0	54	33	14	0
P-C	5	5.4	15	67	19	0
P-D	5	3.9	15	46	21	18

E-A	0.2, 3*	6.7	55	36	9	0
E-B	0.2, 3*	4.4	45	39	14	0
E-C	0.2, 3*	3.6	33	47	19	0
E-D	0.2, 3*	4.5	42	42	16	0

P – powder catalyst; E - extrudates; P-B – Ru/(H-MCM-41+Bindzil); P-C – (Ru/Bindzil)+H-MCM-41; P-D – (Ru/H-MCM-41)+Bindzil; E-A – Ru/(H-MCM-41+Bindzil) *post* synthesis; E-B – Ru/(H-MCM-41+Bindzil*) in-situ* synthesis; E-C – (Ru/Bindzil)+H-MCM-41; E-D – (Ru/H-MCM-41)+Bindzil.

Table S4. Stereoselectivity to menthol isomers in menthol synthesis from citral. Legend: menthol (ME), neomenthol (NME), isomenthol (IME), neoisomenthol (NIME). Conditions for the batch experiment over the powder catalysts: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst. Conditions for the continuous experiment aver the extrudates: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 1 g of catalyst, 12.5 min of residence time.

	t, TOS*	**Y_{MEs}**	**Y_{ME}/Y_{MEs}**	**Y_{NME}/Y_{MEs}**	**Y_{IME}/Y_{MEs}**	**Y_{NIME}/Y_{MEs}**
	h	%				
P-B	3	1.8	22	0	44	33
P-C	5	2.8	21	0	61	21
P-D	5	1.0	0	0	100	0
E-A	0.2, 3*	9.1	66	23	0	12
E-B	0.2, 3*	2.9	66	14	0	21
E-C	0.2, 3*	1.3	62	0	38	0
E-D	0.2, 3*	2.3	52	0	22	26

P – powder catalyst; E - extrudates; P-B – Ru/(H-MCM-41+Bindzil); P-C – (Ru/Bindzil)+H-MCM-41; P-D – (Ru/H-MCM-41)+Bindzil; E-A – Ru/(H-MCM-41+Bindzil) *post* synthesis; E-B – Ru/(H-MCM-41+Bindzil*) in-situ* synthesis; E-C – (Ru/Bindzil)+H-MCM-41; E-D – (Ru/H-MCM-41)+Bindzil.

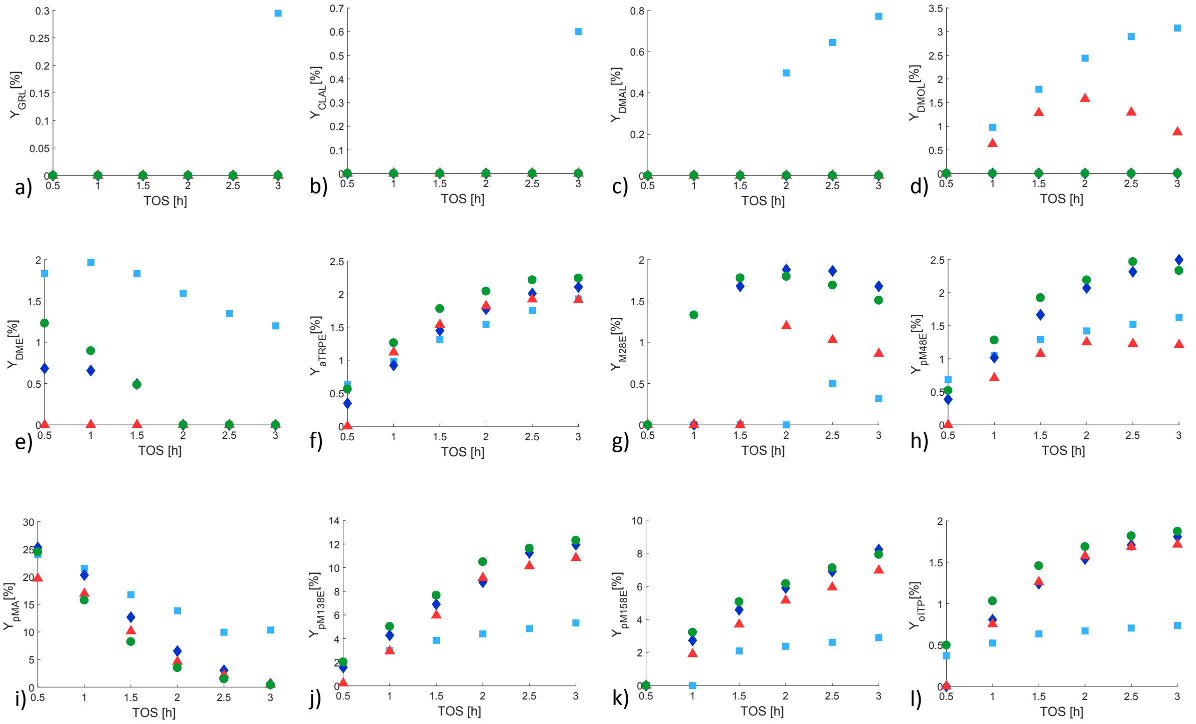

*Figure S7. Product distribution in citral transformation to menthol over extrudates in a trickle-bed reactor: a) geraniol, b) citronellal, c) 3,7-dimethyloctanal, d) 3,7-dimethyloctan-1-ol, e) 2,6-dimethyloctane, f) α-terpinolene, g) mentha-2,8-diene, h) p-menth-4(8)-ene, i) p-menthane, j) p-mentha-1,3,8-triene, k) p-mentha-1,5,8-triene, l) o-isopropenyltoluene. Legend: Ru/(H-MCM-41+Bindzil), post synthesis (**E-A**, light blue square), Ru/(H-MCM-41+Bindzil), in-situ synthesis (**E-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**E-C**, red triangle), Ru/(H-*

*MCM-41)+Bindzil (**E-D**, green circle). Conditions: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 1 g of catalyst, 12.5 min of residence time.*

Tables 5 and 6 present the collected catalytic results of citral transformation from both the batch and trickle-bed reactor over Ru-powder catalysts (0.2 g) and extrudates (1 g) with controlled metal location, respectively, under 70 °C, 10 bar with 0.086 M of the initial citral (Z-/E-CRAL = 1) concentration in cyclohexane.

Table S5. Citral transformation to menthol over Ru catalysts. Legend: t – reaction time, TOS – time-on-stream, X – conversion, MB – liquid phase mass balance closure, Y – total yield, Y_{ACP} – yield of acyclic hydrogenation products, Y_{DFP} – yield of defunctionalization products, Y_{CP} – yield of cyclic products (MEs+IPs+DFP), Y_{DM} – yield of dimeric ethers and heavy components, Y_{MEs} – yield of menthols, Y_{IPs} – yield of isopulegols. Conditions for the batch experiment over the powder catalysts: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst. Conditions for the continuous experiment aver the extrudates: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 1 g of catalyst, 12.5 min of residence time.

Cat.	**t, TOS***	**X**	**MB**	**Y**	**Y_{ACP}**	**Y_{DFP}**	**Y_{CP}**	**Y_{DM}**	**Y_{MEs}**	**Y_{IPs}**	**CP/ACP**	**IP/ME**	**Z-/E-CRAL**
-	*h*	%									-		
P-B	3.0	59	81	40	3.3	22.3	37.1	0.0	1.8	13.0	11	7.2	0.34
P-C	5.0	58	76	34	3.8	21.5	29.7	0.0	2.8	5.4	8	1.9	0.22
P-D	5.0	40	74	14	0.9	8.4	13.3	0.0	1.0	3.9	15	3.9	0.60
E-A	0.2, 3*	70	79	49	5.9	27.2	43.0	0.0	9.1	6.7	7	0.7	0.64
E-B	0.2, 3*	66	82	48	0.0	31.6	38.9	9.4	2.9	4.4	-	1.5	0.35
E-C	0.2, 3*	66	65	32	0.9	25.7	30.6	0.0	1.3	3.6	34	2.8	0.28
E-D	0.2, 3*	64	78	42	0.0	31.3	38.1	4.4	2.3	4.5	-	2.0	0.31

P – powder catalyst; E - extrudates; P-B – Ru/(H-MCM-41+Bindzil); P-C – (Ru/Bindzil)+H-MCM-41; P-D – (Ru/H-MCM-41)+Bindzil; E-A – Ru/(H-MCM-41+Bindzil) *post* synthesis; E-B – Ru/(H-MCM-41+Bindzil*) in-situ* synthesis; E-C – (Ru/Bindzil)+H-MCM-41; E-D – (Ru/H-MCM-41)+Bindzil.

Table S6. Citral transformation to menthol over Ru catalysts. Legend: t – reaction time, TOS – time-on-stream, ACP – acyclic hydrogenation products, DFP – defunctionalization products, Y_{GRL} – yield of geraniol, Y_{CLAL} – yield of citronellal, Y_{DMAL} – yield of 3,7-dimethyloctanal, Y_{CLOL} – yield of citronellol, Y_{DMOL} – yield of 3,7-dimethyloctan-1-ol, Y_{DME} – 2,6-dimethyloctane, $Y_{\alpha TRPE}$ – α-terpiolene, Y_{LMN} – yield of limonene, Y_{M28E} – yield of mentha-2,8-diene, Y_{pM48E} – yield of p-menth-4(8)-ene, Y_{pMA} – yield of p-menthane, Y_{pM138E} – yield of p-mentha-1,3,8-triene, Y_{pM158E} – yield of p-mentha-1,5,8-triene, Y_{oC} – yield of o-cymene, Y_{oIPT} – yield of o-isopropenyltoluene. Conditions for the batch experiment over the powder catalysts: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst. Conditions for the continuous experiment aver the extrudates: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 1 g of catalyst, 12.5 min of residence time.

Cat.	**t, TOS***	**ACP**						**DFP**								
		Y_{GRL}	**Y_{CLAL}**	**Y_{DMAL}**	**Y_{CLOL}**	**Y_{DMOL}**	**Y_{DME}**	**$Y_{\alpha TRPE}$**	**Y_{LMN}**	**Y_{M28E}**	**Y_{pM48E}**	**Y_{pMA}**	**Y_{pM138E}**	**Y_{pM158E}**	**Y_{oC}**	**Y_{oIPT}**
-	*h*	%														
P-B	3.0	0.7	1.7	0.0	0.3	0.6	0.0	1.1	0.0	1.0	1.9	0.5	8.3	4.5	2.4	0.9
P-C	5.0	0.3	0.9	0.0	0.2	0.6	0.4	1.5	0.0	1.4	1.2	0.0	11.0	4.1	0.0	0.5

P-D	5.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.4	0.0	5.0	1.5	0.0	0.0
E-A	0.2, 3*	0.3	0.6	0.8	0.0	3.1	1.2	1.9	1.9	0.3	1.6	10.4	5.3	2.9	1.8	0.7
E-B	0.2, 3*	0.0	0.0	0.0	0.0	0.0	0.0	2.1	0.0	1.7	2.5	0.6	11.9	8.2	2.2	1.8
E-C	0.2, 3*	0.0	0.0	0.0	0.0	0.9	0.0	1.9	0.0	0.9	1.2	0.4	10.8	7.0	1.3	1.7
E-D	0.2, 3*	0.0	0.0	0.0	0.0	0.0	0.0	2.2	0.0	1.5	2.3	0.4	12.3	7.9	2.1	1.9

P – powder catalyst; E - extrudates; P-B – Ru/(H-MCM-41+Bindzil); P-C – (Ru/Bindzil)+H-MCM-41; P-D – (Ru/H-MCM-41)+Bindzil; E-A – Ru/(H-MCM-41+Bindzil) *post* synthesis; E-B – Ru/(H-MCM-41+Bindzil*) in-situ* synthesis; E-C – (Ru/Bindzil)+H-MCM-41; E-D – (Ru/H-MCM-41)+Bindzil.

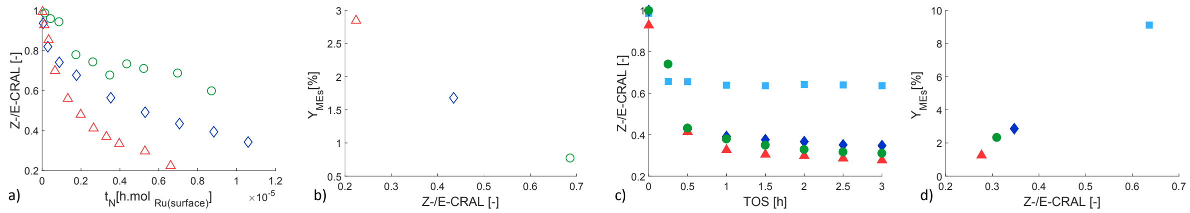

*Figure S8. Ratio of Z-citral to E-citral as a function of the time for: a) powder catalysts, c) extrudates. Yield of menthols as a function of the ratio of Z-citral to E-citral: b) powder catalysts at normalized time of 7·10-6 h·molRu$_{(surface)}$, d) extrudates at 3 h of TOS. Legend of powder catalyst: Ru/(H-MCM-41+Bindzil) (**P-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**P-C**, red triangle), Ru/(H-MCM-41)+Bindzil (**P-D**, green circle). Legend of extrudates: Ru/(H-MCM-41+Bindzil), post synthesis (**E-A**, light blue square), Ru/(H-MCM-41+Bindzil), in-situ synthesis (**E-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**E-C**, red triangle), Ru/(H-MCM-41)+Bindzil (**E-D**, green circle). Conditions for the batch experiment over the powder catalysts: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst. Conditions for the continuous experiment aver the extrudates: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 1 g of catalyst, 12.5 min of residence time.*

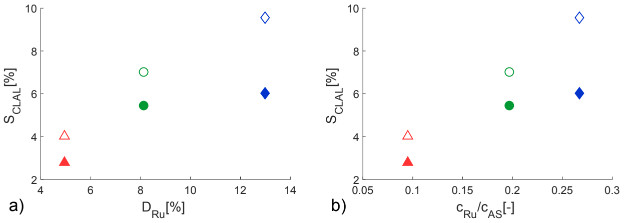

*Figure S9. Selectivity of citronellal as a function of a) Ru dispersion, b) ratio of Ru concentration to acidity. Legend: Ru/(H-MCM-41+Bindzil) (**P-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**P-C**, red triangle), Ru/(H-MCM-41)+Bindzil (**P-D**, green circle); at normalized time of 3.5·10^{-6} h·mol$_{Ru(surface)}$ (open symbols), 7·10^{-6} h·mol$_{Ru(surface)}$ (filled symbols). Conditions: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst.*

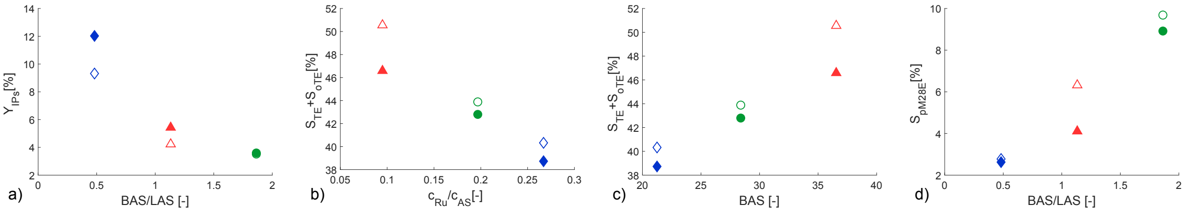

*Figure S10. a) Yield of isopulegols as a function of Brønsted to Lewis acid sites ratio, b, c) Selectivity of p-menthatrienes, o-cymene and o-isopropenyltoluene as a function of ratio of Ru concentration to acidity and Brønsted acidity, d) Selectivity of p-mentha-2,8-diene as a function of Brønsted to Lewis acid sites ratio. Legend: Ru/(H-MCM-41+Bindzil) (**P-B**, dark blue diamond), Ru/(Bindzil)+H-MCM-41 (**P-C**, red triangle), Ru/(H-MCM-41)+Bindzil (**P-D**, green circle); at normalized time of 3.5·10^{-6} h·mol$_{Ru(surface)}$ (open symbols), 7·10^{-6} h·mol$_{Ru(surface)}$ (filled symbols). Conditions: 70 °C, 10 bar of H_2, 0.086 M initial concentration of citral in cyclohexane, 0.2 g of catalyst.*

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