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Effect of isomerization on the performance of aromatic hydrogen storage systems possessing different condensation extents

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1. Materials and methods

1.1 Procedure of hydrogenation and dehydrogenation.

The hydrogenation of Santowax-R mixture was carried out in a PARR-5500 laboratory high-pressure autoclave (V = 600 cm^3) at 180 °C, under hydrogen pressure of 7.093 MPa and stirring at the rate of 500–600 rpm. The dehydrogenation of fully saturated substrates was carried out in a flow catalytic setup according to the previously reported procedure.[S1] The main criterion for the comparison of different substrates was their ability to release the maximum amount of hydrogen during the dehydrogenation reaction under other conditions remaining the same. The hydrogen volume (dm^3 min^{-1}) released in the dehydrogenation process within 1 h of time on the stream was used as a measure of activity. At least three measurements have been done in every controlled point. The deviations did not exceed $\pm$5% in all cases. In order to purify hydrogen from possible impurities, a special combination of condensors and filters, including membranes, was used.

1.2 Procedure of catalyst preparation.

A Pt/C (3 wt.%) catalyst was prepared using a Sibunit carbon carrier *via* supporting platinum from an aqueous solution of [H_2PtCl_6] (ω(Pt) = 36.3%) by the incipient-wetness method according to the known procedure.[S2] This catalyst was evaluated in preliminary tests and showed a high activity in the both hydrogenation and dehydrogenation reactions.[S1] The pre-

activation of catalyst included reduction in a hydrogen flow (the flow rate of 40–50 ml min^{-1}) for 2 h at 320 °C.

Table S1 Comparison of sterical isomers of decalin and perhydroterphenyl.

Substrate	*Cis*-		*Trans*-	
	C(%)	T_m/ºC	*C*(%)	T_m/ºC
Decalin	39	–31.5	61	–43.2
Perhydroterphenyl				
o-isomer	25	16–19[S3]	75	47[S3]
m-isomer	20	20–25[S3]	80	62[S3]
p-isomer	55	48[S3]	45	162[S3]

Table S2 Experimental data on equilibrium constants K_{eq} of reactions (I–VII).

Equilibrium constant, K_{eq}	Dehydrogenation temperature, *T*/ ºC			
	280	300	320	340
K_I	-	1.85	9.98	7.51
K_{II}	3.08	7.02	19.95	24.00
K_{III}	1.78	3.09	8.58	10.31
K_{IV}	1.74	2.27	2.33	2.32
K_V	2.48	2.69	1.96	1.84
K_{VI}	2.04	2.50	1.35	1.30
K_{VII}	0.59	1.10	0.93	0.90

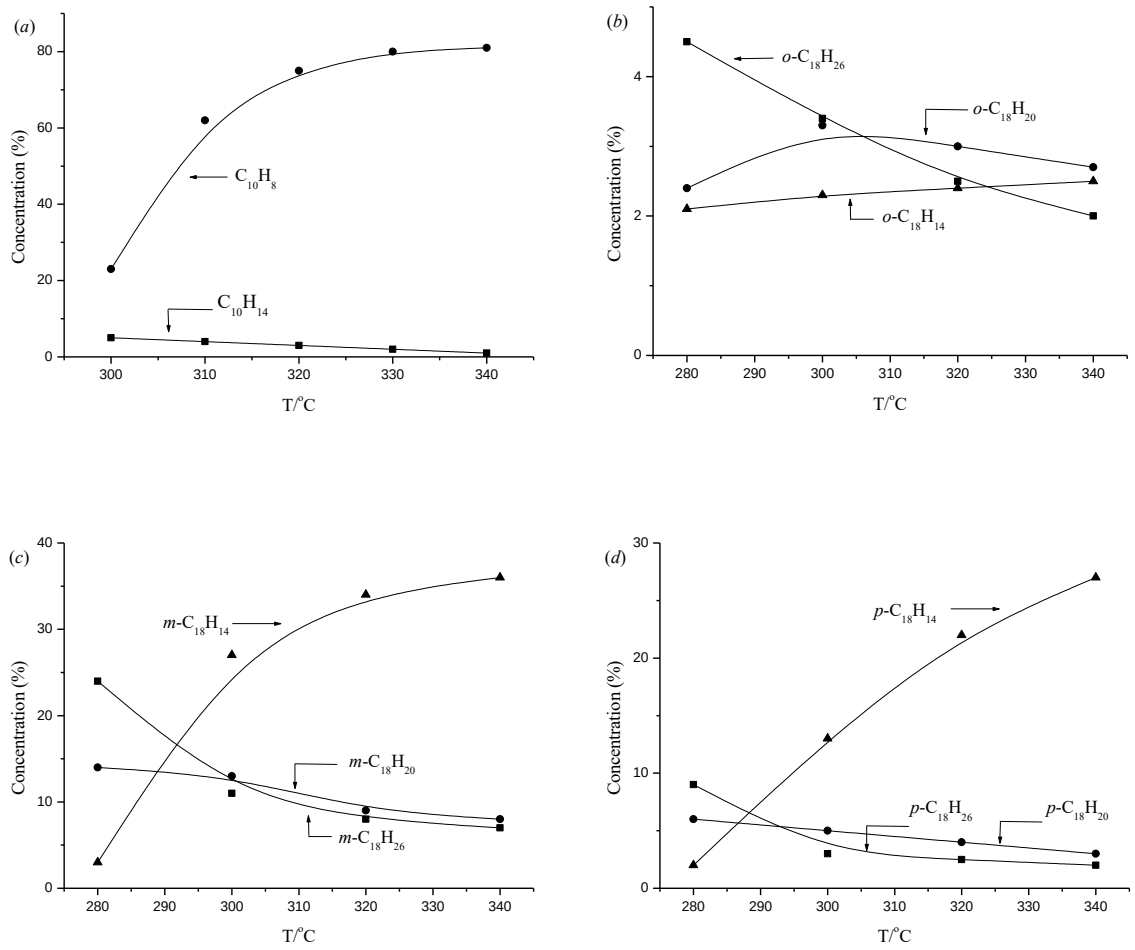

Figure S1 Dependences of the concentrations of partially dehydrogenated and final products of dehydrogenation of (*a*) decalin and the mixture of (*b*) *o*-, (*c*) *m*- and (*d*) *p*-isomers of perhydroterphenyl on the reaction temperature (V_L = 1 h^{-1}, P = 1 atm).

References

S1 A. N. Kalenchuk, V. I. Bogdan, S. F. Dunaev and L. M. Kustov, *Fuel Proc. Tech.*, 2018, **169**, 94.

S2 A. N. Kalenchuk, V. I. Bogdan, S. F. Dunaev and L. M. Kustov, *Int. J. Hydrogen Energy*, 2018, **43**, 6191.

S3 W. Brugel, E. Kuss, T. Pollmann and H. Stegemeyer, *J. Mol. Struct.*, 1967, **1**, 61.