Hydrogenation of Alkynyl Substituted Aromatics Over Rhodium/Silica.

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Supplementary Data.

The activation energy for phenylacetylene was determined by measuring the first order rate constants over a temperature range of 313 – 343 K.

Temp (K)	1/T	k (min^{-1})	ln(k)
313	0.0031949	0.023	-3.7723
323	0.0030960	0.049	-3.0159
333	0.0030030	0.0781	-2.5498
343	0.0029155	0.1614	-1.8239

The linear relationship between 1/T and ln(k) was analysed:

	Regression Output:		
Constant			17.887046345159
Std Err of Y Est			0.0879413729418242
R Squared			0.992293301549774
No. of Observations			4
Degrees of Freedom			2

X Coefficient(s)		-6774.33531303681	
Std Err of Coef.		422.149077676783	

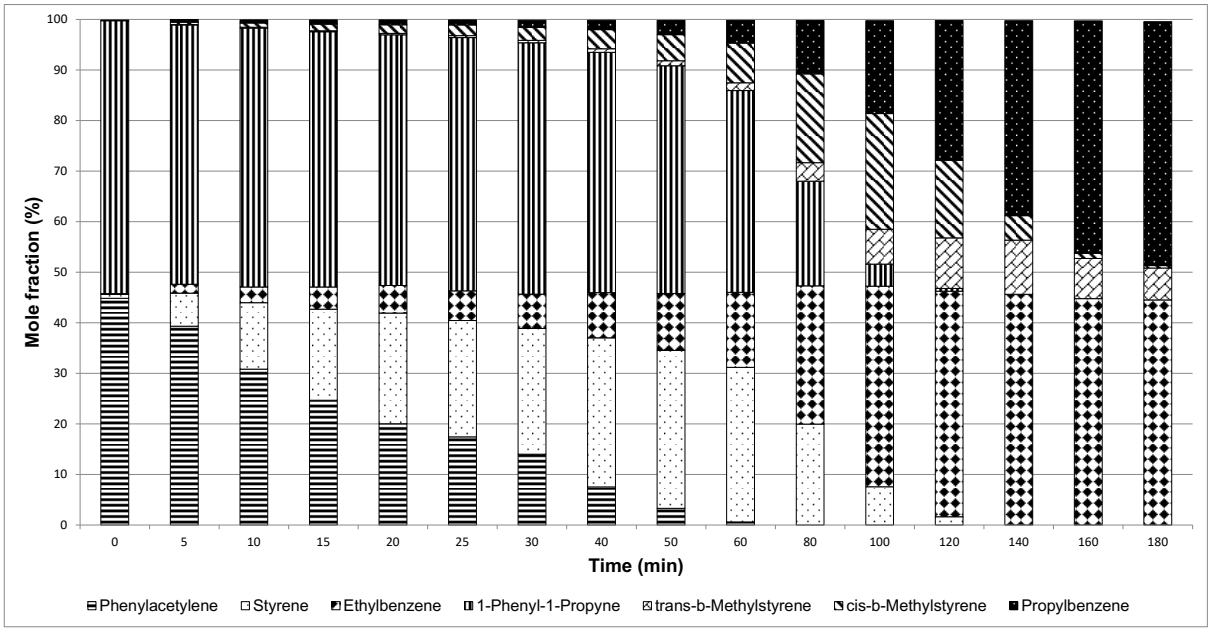
From the x-coefficient an activation energy of 56.3 kJ.mol^{-1} was calculated with an error of ±3.5 kJ.mol^{-1}.

The activation energy for 1-phenyl-1-propyne was determined by measuring the first order rate constants over a temperature range of 313 – 343 K.

Temp (K)	1/T	k (min^{-1})	ln(k)
313	0.0031949	0.0294	-3.52676
323	0.0030960	0.04899	-3.01614
333	0.0030030	0.0923	-2.38271
343	0.0029155	0.1028	-2.27497

The linear relationship between 1/T and ln(k) was analysed:

	Regression Output:		
Constant			15.4689378985295
Std Err of Y Est			0.0645851416470318
R Squared			0.99365048224137
No. of Observations			3
Degrees of Freedom			1
X Coefficient(s)		-5953.64964972949	
Std Err of Coef.		475.923140475551	

From the x-coefficient an activation energy of 49.5 kJ.mol^{-1} was calculated with an error of ±4.0 kJ.mol^{-1}.

The reaction profile for the phenylacetylene/1-phenyl-1-propyne competitive hydrogenation is shown in the figure.