

## Kinetic modelling of Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Cl catalysts formulation changes in *n*-heptane reforming: supplementary information

### Kinetic model validation: complements

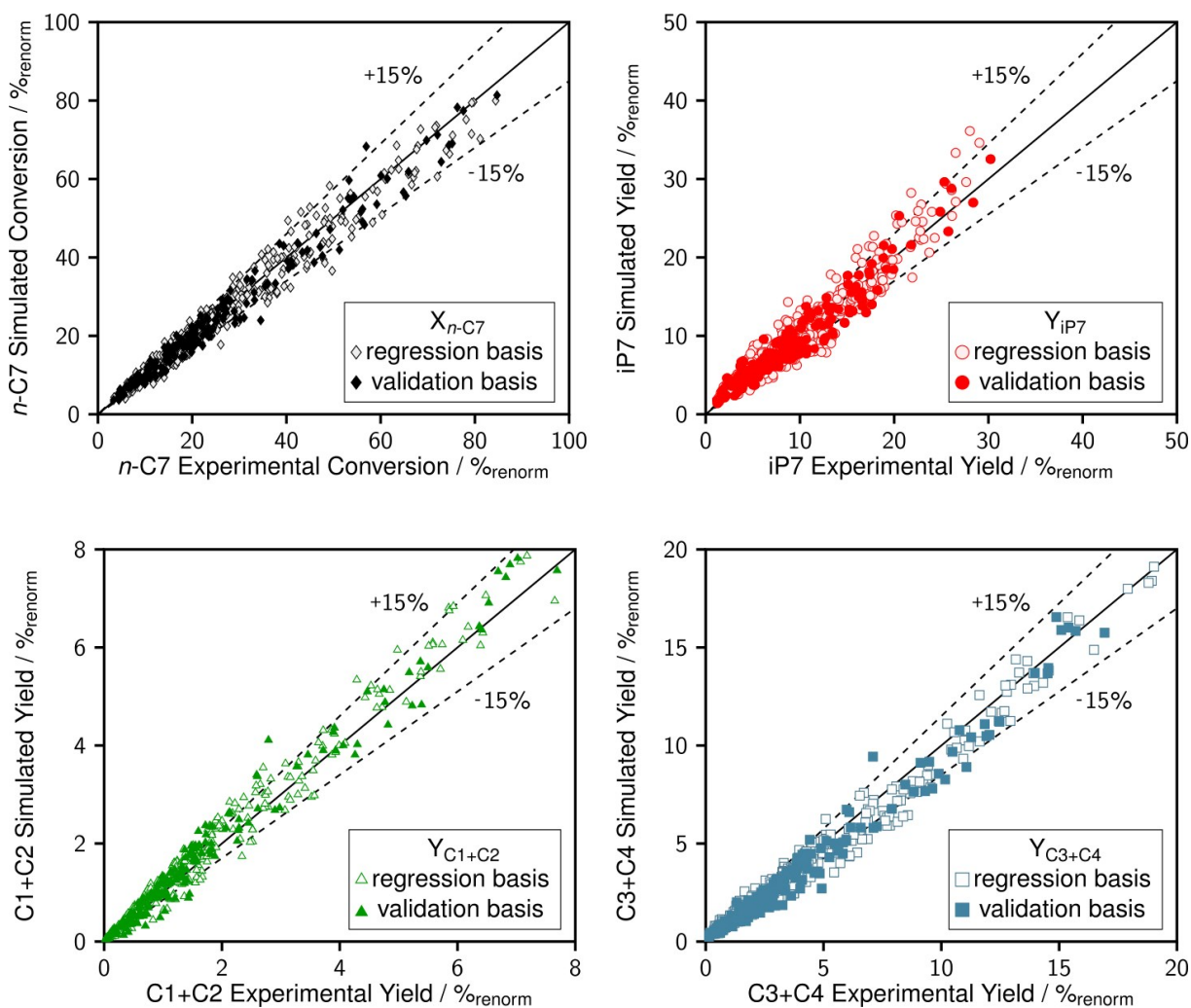


Figure 1: Parity plots obtained with the nine T-flat catalysts.

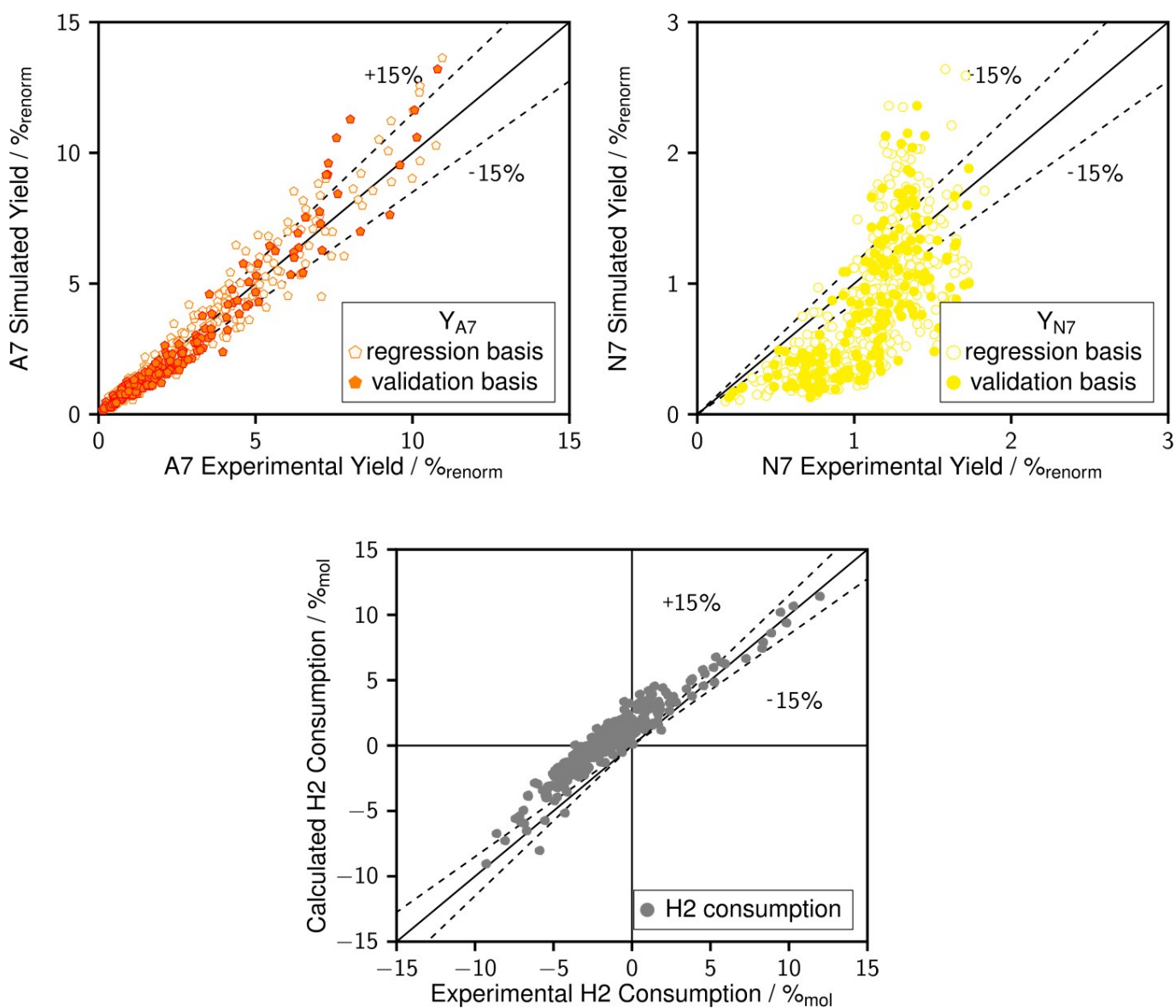


Figure 2: Parity plots obtained with the nine T-flat catalysts.

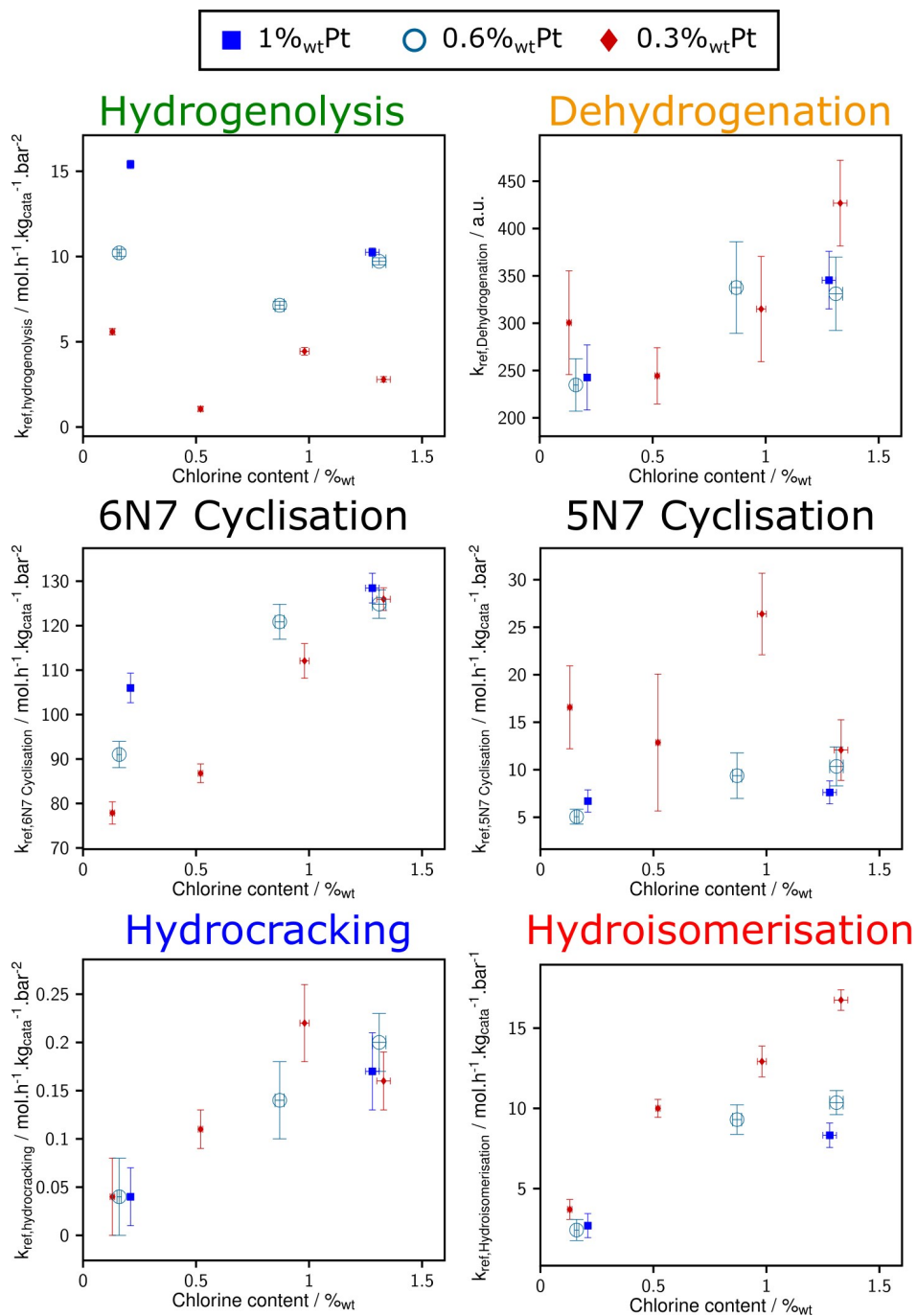


Figure 3: Reference rate constants fitted on T-flat catalysts.

## Reference rate constants fitted parameters

		P-egg_Pt0.3_Cl1.4	P-egg_Pt0.3_Cl1	P-egg_Pt0.3_Cl0.5	P-egg_Pt0.3_Cl0.1	P-egg_Pt0.6_Cl1.4	P-egg_Pt0.6_Cl1	P-egg_Pt0.6_Cl0.5	P-egg_Pt0.6_Cl0.1	P-egg_Pt1.0_Cl1.4	P-egg_Pt1.0_Cl0.1
kref,Hydrogenolysis	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	2.9	3.1	1.7	2.8	6.2	7.0	1.7	7.5	7.5	8.2
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	2.8	3.0	1.6	2.7	6.0	6.8	1.6	7.2	7.3	8.0
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	3.0	3.2	1.7	2.9	6.3	7.2	1.8	7.7	7.7	8.4
kref,Hydrocracking	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	0.1	0.1	0.1	0.0	0.2	0.2	0.1	0.1	0.2	0.2
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	0.1	0.1	0.0	0.0	0.2	0.2	0.1	0.0	0.2	0.1
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	0.2	0.2	0.1	0.0	0.2	0.2	0.1	0.1	0.3	0.2
kref,6N7cyclisation	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	104.4	96.8	86.7	64.1	116.2	110.8	93.3	79.5	122.4	88.0
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	101.3	93.9	84.0	62.1	112.8	107.4	90.6	77.0	119.0	85.4
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	107.4	99.6	89.4	66.1	119.7	114.1	96.0	82.0	125.9	90.5
kref,5N7cyclisation	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	38.5	37.0	37.3	14.6	30.2	25.3	44.6	10.9	35.3	17.5
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	29.6	28.3	27.5	11.4	23.4	19.5	34.2	8.6	28.7	14.4
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	47.3	45.6	47.0	17.8	37.0	31.1	55.0	13.2	41.8	20.6
kref,Hydroisomerisation	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-1</sup>	17.1	15.2	11.8	5.4	16.8	15.2	13.1	3.1	18.3	7.1
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-1</sup>	16.2	14.3	11.1	5.0	15.8	14.4	12.4	2.8	17.3	6.5
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-1</sup>	18.1	16.0	12.5	5.8	17.7	16.1	13.9	3.4	19.4	7.6
kref,Naiphth,Dehydrogenation	a.u	386.9	347.2	389.1	277.5	446.4	414.1	373.3	281.7	560.3	363.1
Low Confidence Value	a.u	349.7	313.9	347.5	249.4	402.8	373.0	338.1	254.2	514.0	333.8
High Confidence Value	a.u	424.1	380.4	430.8	305.5	490.1	455.3	408.5	309.2	606.7	392.3

		T-flat_Pt0.3_Cl1.3	T-flat_Pt0.3_Cl0.9	T-flat_Pt0.3_Cl0.5	T-flat_Pt0.3_Cl0.1	T-flat_Pt0.6_Cl1.3	T-flat_Pt0.6_Cl0.9	T-flat_Pt0.6_Cl0.1	T-flat_Pt1_Cl1.3	T-flat_Pt1_Cl0.1
kref,Hydrogenolysis	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	2.8	4.4	1.1	5.6	9.7	7.1	10.2	10.2	15.4
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	2.7	4.3	1.0	5.5	9.6	7.0	10.1	10.1	15.3
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	2.9	4.6	1.1	5.7	9.8	7.3	10.3	10.4	15.5
kref,Hydrocracking	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	0.2	0.2	0.1	0.0	0.2	0.1	0.0	0.2	0.0
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	0.1	0.2	0.1	0.0	0.2	0.1	0.0	0.1	0.0
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	0.2	0.2	0.1	0.1	0.2	0.2	0.1	0.2	0.1
kref,6N7cyclisation	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	125.9	112.1	86.8	77.9	124.8	120.9	91.0	128.4	106.0
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	124.7	110.1	85.7	76.6	123.2	118.9	89.5	126.8	104.3
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	127.2	114.0	87.8	79.1	126.4	122.8	92.5	130.1	107.6
kref,5N7cyclisation	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	12.1	26.4	12.9	16.6	10.3	9.4	5.1	7.6	6.7
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	10.5	24.2	9.3	14.4	9.3	8.2	4.7	7.0	6.1
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-2</sup>	13.7	28.5	16.5	18.8	11.4	10.6	5.4	8.2	7.3
kref,Hydroisomerisation	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-1</sup>	16.8	12.9	10.0	3.7	10.4	9.3	2.4	8.3	2.7
Low Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-1</sup>	16.4	12.4	9.7	3.4	10.0	8.8	2.1	7.9	2.3
High Confidence Value	mol.h <sup>-1</sup> .kg <sub>cats</sub> <sup>-1</sup> .bar <sup>-1</sup>	17.1	13.4	10.3	4.0	10.7	9.8	2.8	8.7	3.1
kref,Naiphth,Dehydrogenation	a.u	426.8	314.9	244.3	300.5	331.1	337.6	234.8	345.4	242.6
Low Confidence Value	a.u	404.2	287.2	229.5	273.1	311.7	313.4	220.9	330.2	225.4
High Confidence Value	a.u	449.4	342.7	259.2	327.9	350.5	361.8	248.6	360.6	259.9

Figure 4: Reference rate constants fitted on P-egg and T-flat catalysts. 6N cyclisation parameters were not statistically relevant.