

A STUDY OF CHLOROBENZENE PYROLYSIS

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Supplementary Description

1) Temperature profiles measured in tubular reactor

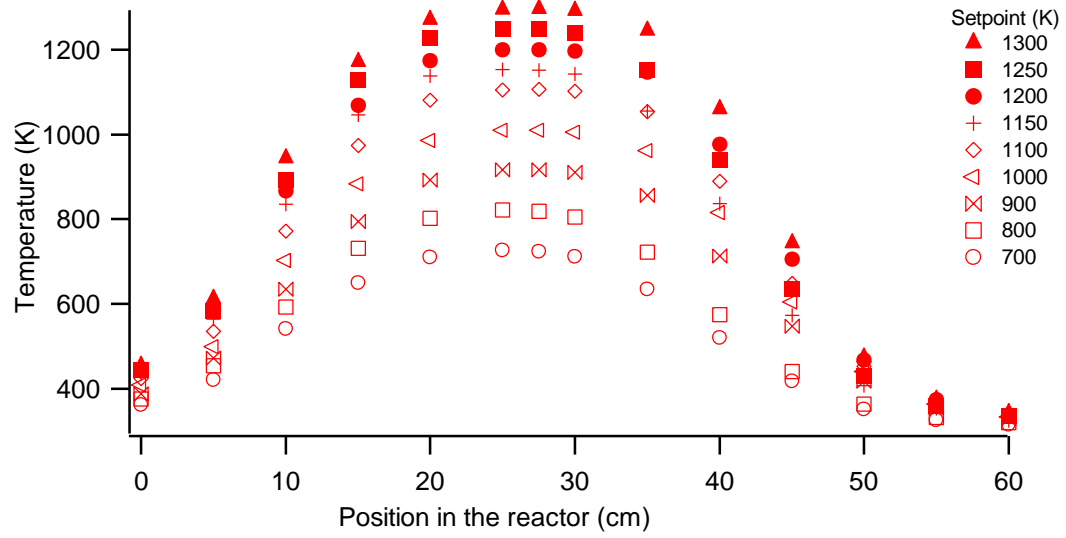


Figure S1: Measured temperature profile in TR.

2) Discussion about plug flow reactor assumption

According to Villiermaux [1], the results obtained with a Tubular Reactor are very close to the theoretic results of a Plug Flow Reactor when the values of the Peclet number are above 100.

The Peclet number, Pe , is given as follows:

$$Pe = \frac{L^2}{D\tau + \frac{QL}{48\pi D}}$$

With L : length of the reactor

τ : residence time

D : molecular diffusion coefficient

Q : flow rate of the fluid in the reactor

The Pe number in our reactor according to the set temperatures is given in the table S1:

Table S1: Values of the Peclet number during the pyrolysis of chlorobenzene (0.5% chlorobenzene inlet mole fraction, $\tau = 2$ s, $P = 106.7$ kPa) in TR.

T (K)	Pe
423	484
500	410
600	341
650	315
700	293
725	282
750	273
775	264
800	256
825	248
850	241
875	234
900	228
925	221
950	216
975	210
1000	205
1025	200
1050	195
1075	190
1250	164

3) A typical IRTF spectrum obtained during the chlorobenzene pyrolysis

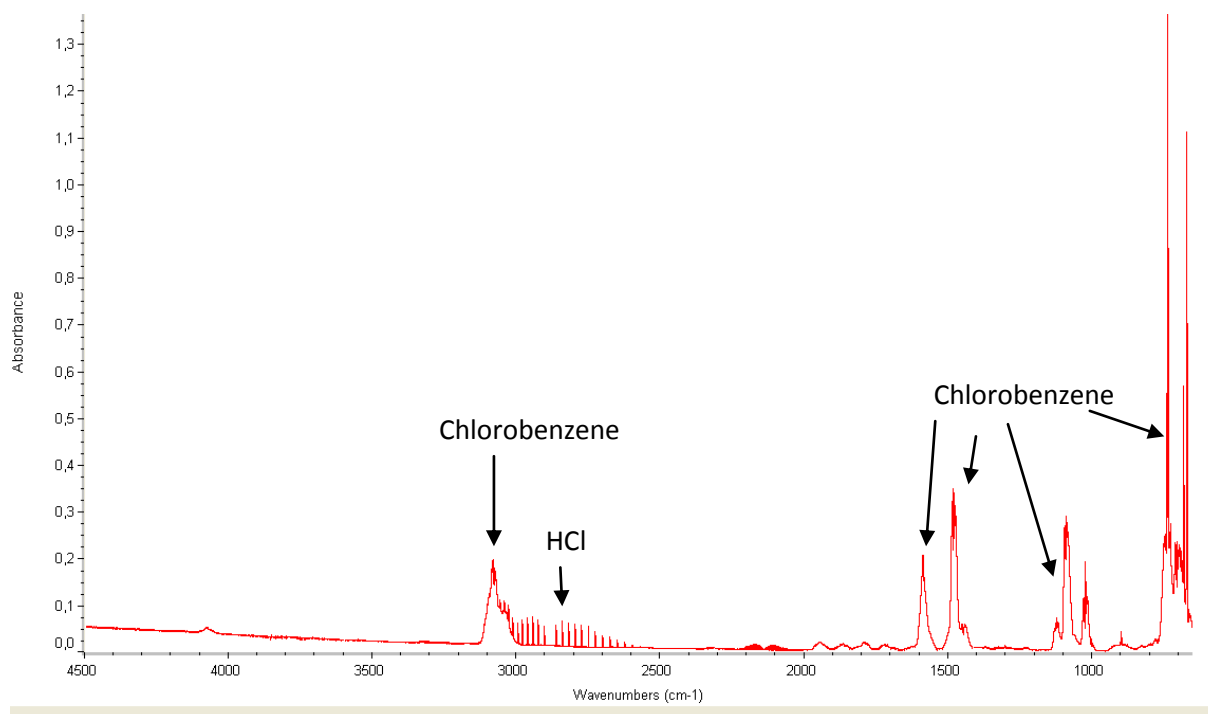


Figure S2: IRTF spectrum obtained during the chlorobenzene pyrolysis in TR (0.5% chlorobenzene inlet mole fraction, $\tau = 2$ s, $P = 106.7$ kPa, $T = 1150$ K).

4) Calculated enthalpies, entropies, heat capacities as well as optimized geometries for species and transition state structures

Table 2: Calculated Enthalpies, $\Delta_f H_{298}^0$ for Radicals in the Chlorobenzene System

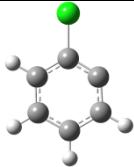
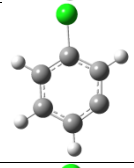
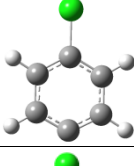
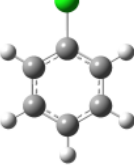
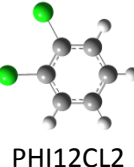
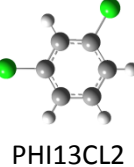
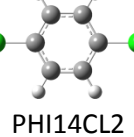
<i>Species</i>	Reactions	ΔH_{f298}^0 (kcal mol ⁻¹)
		B3LYP/6-311G(d,p)
	$\text{R2PHICL} + \text{CH}_3\bullet \rightarrow \text{PhCl} + \text{CH}_4$ $\text{R2PHICL} + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\bullet + \text{HCl}$ Average	75.73 73.86 74.79
	$\text{R3PHICL} + \text{CH}_3\bullet \rightarrow \text{PhCl} + \text{CH}_4$ $\text{R3PHICL} + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\bullet + \text{HCl}$ Average	74.23 72.36 73.30
	$\text{R4PHICL} + \text{CH}_3\bullet \rightarrow \text{PhCl} + \text{CH}_4$ $\text{R4PHICL} + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\bullet + \text{HCl}$ Average	74.96 73.09 74.03
 PHICL	Taken from [2]	13.01
 PHI12CL2	Taken from [3].	7.89
 PHI13CL2		6.72
 PHI14CL2		5.88

Table 3: Calculated ΔH_{TS} in the Chlorobenzene System

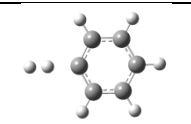
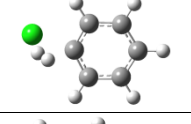
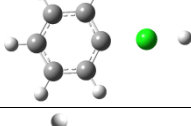
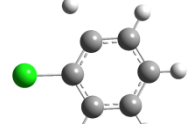
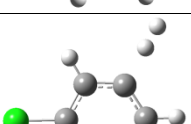
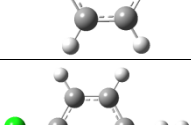
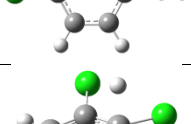
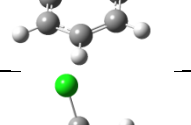
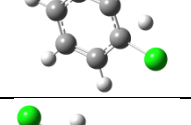
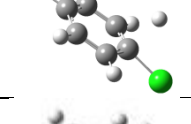
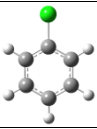
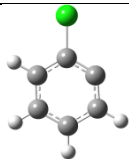
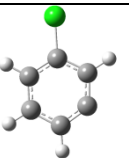
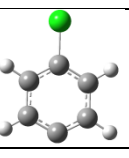
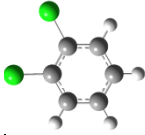
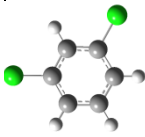
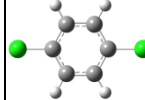
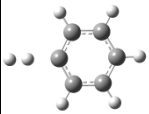
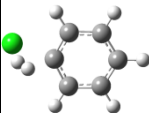
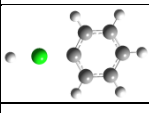
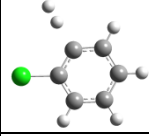
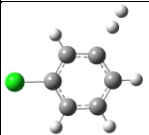
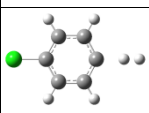
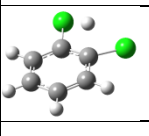
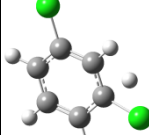
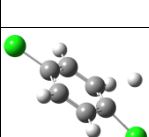
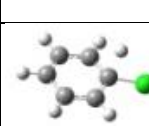
<i>Transition state Structures</i>	Reactions Adduct \rightarrow TS \rightarrow Products	ΔH_{TS} (kcal mol ⁻¹)
		B3LYP/6-311G(d,p)
	$C_6H_5\bullet + H_2 \rightarrow TS1$ $TS1 \rightarrow C_6H_6 + H\bullet$ Average	85.50 80.51 83.01
	$PHICL + H_2 \rightarrow TS2$ $TS2 \rightarrow C_6H_6 + HCL$ Average	87.59 85.48 86.53
	$PHICL + H\bullet \rightarrow TS3$ $TS3 \rightarrow C_6H_5\bullet + HCL$ Average	74.40 77.28 75.84
	$PHICL + H\bullet \rightarrow TS4$ $TS4 \rightarrow R2PHICL + H_2$ Average	75.44 79.25 77.34
	$PHICL + H\bullet \rightarrow TS5$ $TS5 \rightarrow R3PHICL + H_2$ Average	74.06 77.87 75.96
	$PHICL + H\bullet \rightarrow TS6$ $TS6 \rightarrow R4PHICL + H_2$ Average	74.60 78.40 76.50
	$PHICL + CL\bullet \rightarrow TS7$ $TS7 \rightarrow PHI12CL_2 + H$ Average	67.89 66.99 67.44
	$PHICL + CL\bullet \rightarrow TS8$ $TS8 \rightarrow PHI13CL_2 + H$ Average	65.98 66.43 66.20
	$PHICL + CL\bullet \rightarrow TS9$ $TS9 \rightarrow PHI14CL_2 + H$ Average	65.67 65.36 65.51
	$PHICL + H\bullet \rightarrow TS10$ $TS10 \rightarrow C_6H_6 + Cl$ Average	73.87 70.97 72.42

Table 4: Calculated Thermochemical Properties of Species and Transition State Structures^a

Species	$\Delta_f H_{298}^0$ ^b	S_{298}^0 ^b	Cp (T) cal/mole K							
			300 K	400 K	500 K	600 K	800 K	1000 K	1500 K	
 PHICL	13.01	74.89	23.61	30.65	36.48	41.10	47.78	52.33	58.91	
 R2PHICL	74.79	76.27	23.19	29.60	34.84	38.97	44.85	48.79	54.39	
 R3PHICL	73.30	76.13	23.25	29.69	34.94	39.06	44.91	48.83	54.40	
 R4PHICL	74.03	76.10	23.24	29.67	34.92	39.04	44.90	48.82	54.40	
 PHI2CL2	7.89	81.78	27.37	34.21	39.75	44.09	50.25	54.34	60.14	
 PHI3CL2	6.72	82.10	27.48	34.31	39.84	44.16	50.29	54.36	60.14	
 PHI4CL2	5.88	83.49	27.47	34.30	39.82	44.14	50.27	54.36	60.13	

^aThermodynamic properties are referred to a standard state of an ideal gas at 1 atm;^b $\Delta_f H_{298}^0$ in kcal mol⁻¹; S_{298}^0 in cal mol⁻¹ K⁻¹

Table 5: Calculated Thermochemical Properties of Transition State Structures^a

Species		$\Delta_f H_{298}^0$ ^b	S_{298}^0 ^b	Cp (T) cal/mole K						
				300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
	TS1	83.01	69.48	20.45	27.18	32.86	37.44	44.28	49.08	56.19
	TS2	86.53	81.39	28.41	36.61	43.14	48.21	55.46	60.41	67.69
	TS3	75.84	82.68	27.66	34.76	40.60	45.22	51.88	56.39	62.93
	TS4	77.34	81.03	27.78	35.08	41.02	45.70	52.40	56.92	63.34
	TS5	75.96	80.92	27.76	35.08	41.04	45.73	52.46	56.97	63.38
	TS6	76.50	81.04	27.80	35.11	41.05	45.73	52.44	56.95	63.36
	TS7	67.44	84.87	30.03	37.42	43.26	47.76	54.08	58.24	64.08
	TS8	66.20	85.20	30.18	37.56	43.38	47.86	54.14	58.27	64.09
	TS9	65.51	85.25	30.16	37.53	43.34	47.83	54.11	58.26	64.08
	TS10	72.42	79.58	26.07	33.65	39.73	44.56	51.42	56.06	62.73

^aThermodynamic properties are referred to a standard state of an ideal gas at 1 atm;^b $\Delta_f H_{298}^0$ in kcal mol⁻¹; S_{298}^0 in cal mol⁻¹ K⁻¹

Table 6: Optimized structures

R2PHICL	R3PHICL	R4PHICL	PHICL
C	C	C	C
C,1,r21	C,1,r21	C,1,r21	C,1,r21
C,2,r32,1,a321	C,2,r32,1,a321	C,2,r32,1,a321	C,2,r32,1,a321
C,3,r43,2,a432,1,d4321,0	C,3,r43,2,a432,1,d4321,0	C,3,r43,2,a432,1,d4321,0	C,3,r43,2,a432,1,d4321,0
C,4,r54,3,a543,2,d5432,0	C,4,r54,3,a543,2,d5432,0	C,4,r54,3,a543,2,d5432,0	C,4,r54,3,a543,2,d5432,0
C,5,r65,4,a654,3,d6543,0	C,5,r65,4,a654,3,d6543,0	C,5,r65,4,a654,3,d6543,0	C,5,r65,4,a654,3,d6543,0
H,1,r71,2,a712,3,d7123,0	H,1,r71,2,a712,3,d7123,0	H,1,r71,2,a712,3,d7123,0	H,1,r71,2,a712,3,d7123,0
H,2,r82,1,a821,6,d8216,0	H,2,r82,1,a821,6,d8216,0	H,2,r82,1,a821,6,d8216,0	H,2,r82,1,a821,6,d8216,0
H,3,r93,2,a932,1,d9321,0	H,3,r93,2,a932,1,d9321,0	H,4,r94,3,a943,2,d9432,0	H,3,r93,2,a932,1,d9321,0
H,4,r104,3,a1043,2,d10432,0	H,5,r105,4,a1054,3,d10543,0	H,5,r105,4,a1054,3,d10543,0	H,4,r104,3,a1043,2,d10432,0
Cl,6,r116,5,a1165,4,d11654,0	Cl,6,r116,5,a1165,4,d11654,0	Cl,6,r116,5,a1165,4,d11654,0	H,5,r115,4,a1154,3,d11543,0
Variables:	Variables:	Variables:	Variables:
r21=1.39474813	r21=1.39401247	r21=1.40112414	r21=1.39337528
r32=1.39428497	r32=1.40127213	r32=1.37380111	r32=1.39312328
r43=1.4024431	r43=1.37343364	r43=1.37391124	r43=1.39322724
r54=1.37205615	r54=1.37289676	r54=1.40081653	r54=1.39321195
r65=1.36991226	r65=1.39939476	r65=1.3925924	r65=1.39080723
r71=1.08361092	r71=1.08188918	r71=1.08290668	r71=1.08228798
r82=1.08365567	r82=1.08474622	r82=1.08389226	r82=1.08397335
r93=1.08420182	r93=1.08340976	r94=1.08391311	r93=1.0835778
r104=1.0840935	r105=1.08272655	r105=1.08296612	r104=1.08398816
r116=1.7581833	r116=1.76099449	r116=1.76170343	r115=1.08236064
a321=121.11591387	a321=120.64613765	a321=117.03991785	r126=1.76195189
a432=119.98601426	a432=116.14068425	a432=125.59379064	a321=120.44963805
a543=116.73367071	a543=126.61012075	a543=117.05025594	a432=119.76661999
a654=125.16494453	a654=115.44737706	a654=119.15595476	a543=120.45523337
a712=121.12047002	a712=120.61353688	a712=120.66862086	a543=120.45523337
a821=119.07700166	a821=119.50370984	a821=120.3952607	a654=118.93575063
a932=120.33725688	a932=121.26871663	a943=122.52547649	a712=120.99090264
a1043=121.22928228	a1054=123.43945321	a1054=120.70227611	a821=119.32232295
a1165=121.32670887	a1165=119.17057578	a1165=119.01129141	a932=120.14211391
d4321=0.00379179	d4321=0.03138578	d4321=0.03613983	a1043=120.20067026
d5432=0.01982206	d5432=0.01054635	d5432=0.00323755	a1154=121.01935127
d6543=-0.02653308	d6543=-0.04605281	d6543=-0.03540698	a1265=119.29128455
d7123=179.99665209	d7123=179.9628513	d7123=179.96918597	d4321=0.01274773
d8216=179.99151249	d8216=-179.98892422	d8216=-179.98409859	d5432=0.01443669
d9321=-179.98989881	d9321=-179.96257134	d9432=179.99144532	d6543=-0.03243615
d10432=179.99198899	d10543=-179.97632897	d10543=179.99984888	d7123=179.98219553
d11654=-179.99472527	d11654=-179.95783199	d11654=-179.97687295	d8216=-179.99217508
			d9321=-179.98180983
			d10432=179.99884612
			d11543=179.99419032
			d12654=-179.98189901

PHI12CL2	PHI13CL2	PHI14CL2
C	C	C
C,1,r21	C,1,r21	C,1,r21
C,2,r32,1,a321	C,2,r32,1,a321	C,2,r32,1,a321
C,3,r43,2,a432,1,d4321,0	C,3,r43,2,a432,1,d4321,0	C,3,r43,2,a432,1,d4321,0
C,4,r54,3,a543,2,d5432,0	C,4,r54,3,a543,2,d5432,0	C,4,r54,3,a543,2,d5432,0
C,5,r65,4,a654,3,d6543,0	C,5,r65,4,a654,3,d6543,0	C,5,r65,4,a654,3,d6543,0
H,1,r71,2,a712,3,d7123,0	H,1,r71,2,a712,3,d7123,0	H,1,r71,2,a712,3,d7123,0
H,2,r82,1,a821,6,d8216,0	H,2,r82,1,a821,6,d8216,0	H,2,r82,1,a821,6,d8216,0
H,3,r93,2,a932,1,d9321,0	H,3,r93,2,a932,1,d9321,0	Cl,3,r93,2,a932,1,d9321,0
H,4,r104,3,a1043,2,d10432,0	Cl,4,r104,3,a1043,2,d10432,0	H,4,r104,3,a1043,2,d10432,0
Cl,5,r115,4,a1154,3,d11543,0	H,5,r115,4,a1154,3,d11543,0	H,5,r115,4,a1154,3,d11543,0
Cl,6,r126,5,a1265,4,d12654,0	Cl,6,r126,5,a1265,4,d12654,0	Cl,6,r126,5,a1265,4,d12654,0
Variables:	Variables:	Variables:
r21=1.39027992	r21=1.392418	r21=1.39209013
r32=1.39258974	r32=1.39229973	r32=1.39087165
r43=1.39024486	r43=1.39077114	r43=1.39090702
r54=1.39365803	r54=1.39108073	r54=1.39205781
r65=1.39765319	r65=1.39090955	r65=1.39073537
r71=1.08228982	r71=1.08170472	r71=1.08209819
r82=1.08330147	r82=1.08357258	r82=1.08222522
r93=1.08336423	r93=1.08176485	r93=1.7563944
r104=1.08226126	r104=1.7562936	r104=1.0820553
r115=1.74832216	r115=1.08059247	r115=1.0819142
r126=1.74922485	r126=1.75744096	r126=1.7583181
a321=119.98170041	a321=120.96803417	a321=119.49242137
a432=120.00816979	a432=118.79511899	a432=121.03377509
a543=120.21385448	a543=121.63751029	a543=119.4924752
a654=119.76372262	a654=118.16302202	a654=119.44307173
a712=120.87592819	a712=121.09277548	a712=120.33728224
a821=119.54813888	a821=119.518281	a821=120.29503325
a932=120.4665356	a932=121.04312633	a932=119.48334139
a1043=120.86676212	a1043=119.48350106	a1043=120.20775833
a1154=118.76571865	a1154=120.94313495	a1154=120.34215034
a1265=121.42634093	a1265=118.84574621	a1265=119.45367322
d4321=-0.0011578	d4321=0.00205729	d4321=0.00113819
d5432=-0.00041054	d5432=0.00056658	d5432=0.00127334
d6543=0.00152972	d6543=-0.00218558	d6543=-0.00255431
d7123=-179.99889867	d7123=179.99851314	d7123=179.99916229
d8216=-179.99991796	d8216=179.99937352	d8216=179.9995505
d9321=179.99890057	d9321=-179.99883019	d9321=-179.99845279
d10432=180.	d10432=179.99804021	d10432=180.
d11543=179.99890796	d11543=179.99904885	d11543=179.99942592
d12654=179.99842919	d12654=-179.99900343	d12654=-179.99881398

TS1	TS2
C,0,-0.2891667779,1.2309682769,0.3088745606	C,0,0.2012205904,0.4819158471,0.1837792689
C,0,-1.6231720738,1.2059688065,-0.102004432	C,0,0.0520484908,-0.0435424237,1.4727582793
C,0,-2.2914787759,0.0001024609,-0.3068118468	C,0,1.1771998281,-0.3361124828,2.2432285855
C,0,-1.6232674466,-1.2058137408,-0.1019912074	C,0,2.4579165353,-0.1086490718,1.7409066695
C,0,-0.2892637903,-1.2309137071,0.3088892883	C,0,2.6246400572,0.4163341887,0.4548568194
C,0,0.3167139695,0.0000042631,0.4551053292	C,0,1.4852009384,0.6906139657,-0.2741219573
H,0,0.2509768981,2.1545127502,0.4578142466	H,0,-0.6646869829,0.7145375848,-0.4264015533
H,0,-2.1307374395,2.1502264637,-0.2622872653	H,0,-0.941398388,-0.2222212553,1.8701288964
H,0,-3.3270804201,0.0001415837,-0.6223973891	H,0,1.0552886856,-0.7433649666,3.2406496395
H,0,-2.1309066576,-2.150033332,-0.2622644688	H,0,3.3289949114,-0.3382611248,2.3458130845
H,0,0.250806291,-2.1544989435,0.4578422985	H,0,3.6150338345,0.5959759763,0.0508328156
Cl,0,2.493892207,-0.0001030954,-0.5144503669	H,0,1.6543799064,1.2553630912,-1.64778859
H,0,1.6992034869,-0.000024178,1.2696810768	H,0,1.7507349395,1.5770001997,-2.4301351762
H,0,1.0791985292,-0.0000193684,1.8086351763	

TS3	TS4
C,0,-0.0157664224,0.0073158241,-0.0273805981 C,0,0.0042010029,-0.0010203295,1.369374632 C,0,1.2170258425,-0.0054178702,2.0561424121 C,0,2.4206623516,-0.0015269864,1.3533916264 C,0,2.422151853,0.0068042922,-0.0435059198 C,0,1.1988949343,0.0109292013,-0.68505676 H,0,-0.9485279576,0.0108275014,-0.576905366 H,0,-0.9326625693,-0.0040427149,1.915333701 H,0,1.2241922298,-0.0118799574,3.1398315449 H,0,3.3646651676,-0.0049433308,1.8869093764 H,0,3.3475614038,0.009926362,-0.6053259597 Cl,0,1.1860731342,0.0225419543,-2.6326453137 H,0,1.1751583354,0.0334596403,-4.2676482311	C,0,0.0341010385,-0.0008048124,-0.0266886645 C,0,0.0622810954,-0.0036348049,1.3669144911 C,0,1.2726622061,0.000624775,2.0587012569 C,0,2.4786938244,0.0078362134,1.3503913029 C,0,2.4206841692,0.0105264584,-0.0267081917 C,0,1.239037868,0.0064103943,-0.7314710317 H,0,-0.905028765,-0.0041011463,-0.5667383332 H,0,-0.8733124524,-0.0092412549,1.913868771 H,0,1.2827418063,-0.0016411532,3.1427546197 H,0,3.431088306,0.0111938528,1.8693284563 H,0,3.7376310671,0.0172195239,-0.7757490445 Cl,0,1.2299415456,0.0101440117,-2.4910584473 H,0,4.4833878093,0.0207600987,-1.158666557
TS5	TS6
C,0,0.064902752,-0.0031692412,0.0385588671 C,0,0.0729928975,0.000014027,1.4322640322 C,0,1.2813575104,0.0067963233,2.1361411506 C,0,2.4434294767,0.0101484216,1.3939127028 C,0,2.497374866,0.0072461539,0.016490672 C,0,1.2728284025,0.0004690266,-0.6541805176 H,0,-0.8684979002,-0.0084220163,-0.5088010699 H,0,-0.868142957,-0.0028173907,1.971336146 H,0,1.2966585944,0.0093058907,3.2198913484 H,0,3.7466936619,0.0183328291,2.1324122901 H,0,3.4321052349,0.0100340566,-0.5304877736 Cl,0,1.257168075,-0.003570803,-2.415464967 H,0,4.4836798719,0.0215567105,2.5512085066	C,0,0.0027983538,0.0005249418,0.0661363102 C,0,0.0090967836,0.0070649397,1.4643288336 C,0,1.2295787118,0.0101429467,2.1061563146 C,0,2.4438442992,0.0071581819,1.4526373879 C,0,2.4367130042,0.0006184118,0.05444815 C,0,1.2165072831,-0.0025919705,-0.616003034 H,0,-0.9298774462,-0.0021054237,-0.4840344031 H,0,-0.9253412136,0.0095810701,2.0143569946 H,0,1.2361840062,0.0172847632,3.6158561896 H,0,3.3835271127,0.0097454636,1.9936518215 H,0,3.3640610122,-0.0019404664,-0.5046560148 Cl,0,1.2080513066,-0.0108295019,-2.377077166 H,0,1.2397233959,0.0212706317,4.4597189669
TS7	TS8
C,0,-0.0411890276,0.6311822182,0.1244732962 C,0,1.1764663824,1.3431512286,0.0629152006 C,0,2.3794373224,0.6636714788,-0.0059000108 C,0,2.3938893487,-0.7303904919,-0.08930674 C,0,1.1966189855,-1.4402908448,-0.1267837771 C,0,-0.0187817424,-0.7715922146,-0.0643987392 Cl,0,-1.534374942,1.5432233674,-0.1049429784 H,0,1.1445153426,2.423425225,0.114039843 H,0,3.3082764763,1.2212332828,-0.0112079002 H,0,3.3335827618,-1.2660333139,-0.1465925496 H,0,1.1959336051,-2.5188500677,-0.2176650467 H,0,-0.2113547668,0.5755905622,1.9333670367 Cl,0,-1.4982487459,-1.69020743,-0.1193286344	C,0,0.0388457252,0.0558643983,-0.0318570987 C,0,0.0407408784,-0.1142203139,1.3522454171 C,0,1.2556571628,-0.0566227951,2.0369754006 C,0,2.4497603055,0.1376610502,1.3610627617 C,0,2.43246826,0.200306016,-0.0470322224 C,0,1.2088404063,0.2553921038,-0.7446563714 Cl,0,-1.4913103481,0.0475756207,-0.8951444267 H,0,-0.890792276,-0.2631543583,1.8812254708 H,0,1.2629456584,-0.1518361089,3.1163808557 H,0,3.3930757317,0.1931843212,1.886967589 H,0,2.7877599101,-1.5373828471,-0.338899384 H,0,1.1959543943,0.4014529055,-1.8151096949 Cl,0,3.8906557711,0.7593727369,-0.8866385266
TS9	TS10
C,0,0.0243585594,-0.1393103936,-0.0053352944 C,0,0.0342995331,0.0028244212,1.3822648547 C,0,1.2220071048,0.2949141497,2.032314846 C,0,2.4197892681,0.3680267681,1.2933448924 C,0,2.3781959602,0.3321074488,-0.1148930059 C,0,1.1859537676,0.0399653921,-0.7565254169 Cl,0,-1.4824090552,-0.5076069597,-0.823076894 H,0,-0.8853241311,-0.098268703,1.9438340158 H,0,1.2468597148,0.42176653,3.1064172576 H,0,2.9496425173,-1.3426024866,1.5487827929 H,0,3.2865302389,0.487428419,-0.6816540088 H,0,1.1498533474,-0.0327059336,-1.8357401899 Cl,0,3.855430696,1.050561533,2.0783253697	C,0,1.5825276542,1.2089296025,-0.0435953794 C,0,0.1973589655,1.2221957483,0.0163381271 C,0,-0.4943927269,-0.0000930307,0.1411330065 C,0,0.1974957743,-1.2222940119,0.0162493386 C,0,1.5826634029,-1.2088682445,-0.0436832674 C,0,2.2821965045,0.0000702731,-0.0591293448 H,0,2.1206288425,2.1483991663,-0.0964028169 H,0,-0.3581482753,2.1506840867,0.0147324260 H,0,-0.3579068002,-2.1508455160,0.0145831320 H,0,2.1208696901,-2.1482737908,-0.0965575265 H,0,3.3643013215,0.0001331705,-0.1115919289 Cl,0,-2.2519128105,-0.0001802478,-0.0994444363 H,0,-0.6279965427,-0.0001749859,1.9295076701

5) Methane, ethylene, acetylene, biphenyl and biphenylene profiles during the pyrolysis of chlorobenzene in JSR and TR

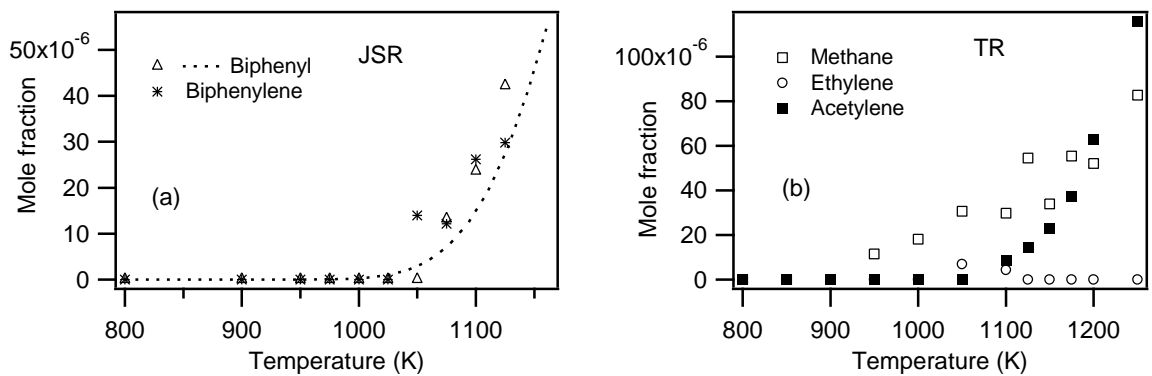


Figure S3: Evolution with temperature of (a) biphenyl and biphenylene in JSR, (b) methane, ethylene, acetylene in TR, (c) methane and ethylene in JSR mole fractions (Symbols are experiments and lines simulations, 0.5% chlorobenzene inlet mole fraction, $\tau = 2$ s, $P = 106.7$ kPa).

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