

**COMPARISON STUDY OF THE GAS-PHASE OXIDATION OF
ALKYLBENZENES AND ALKYL CYCLOHEXANES**

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**Supplementary
Material**

Table S1: Comparison of carbon selectivities (in %) of most important products in the oxidation of ethyl-cyclohexane at low-temperature (625 K) for the three studied equivalence ratios.

	$\varphi = 0.25$	$\varphi = 1$	$\varphi = 2$
Fuel conversion (%)	68	50	31
Hydrocarbons			
ethylene	1.20	1.34	1.05
propene	0.116	0.225	0.206
1-butene	0.059	0.168	0.194
benzene	0.171	0.159	0.191
cyclohexene	0.264	0.198	0.330
styrene	0.168	0.180	1.23
ethyl-benzene	0.116	0.133	0.0817
C ₈ H ₁₄ isomers	1.15	2.72	4.81
Carbon oxides			
CO	25.7	13.9	7.36
CO ₂	8.48	3.04	0 ^a
Oxygenated molecules			
oxirane	0.767	0.962	0.86
acetaldehyde	1.25	1.34	1.04
acetic acid	1.16	0.942	0.210
acrolein	0.0992	0.132	0.101
propanal	0.139	0.203	0.143
acetone	0.0712	0.0967	0.0900
butanal	0.0345	0.0645	0.0365
butanone	0.106	0.158	0.0599
C ₈ H ₁₄ O isomers	3.40	3.33	5.19

^a CO₂ was not detected because the mole fraction was below the detection limit.

Table S2: Comparison of carbon selectivities (in %) of most important products in the oxidation of ethyl-cyclohexane at high-temperature (950 K) for the three studied equivalence ratios.

	$\varphi = 0.25$	$\varphi = 1$	$\varphi = 2$
Fuel conversion (%)	99	96	91
Hydrocarbons			
acetylene	0.078	0.393	0.541
ethylene	2.9	15.3	23.5
propene	0.256	1.18	2.80
1-butene	0.061	0.161	0.441
1,3-butadiene	0.199	0.633	1.674
benzene	0.396	1.43	2.15
cyclohexene	0.141	0.346	0.524
styrene	0.010	0.026	0.028
ethyl-benzene	0.011	0.017	0.031
C ₈ H ₁₄ isomers	0.064	0.091	0.109
Carbon oxides			
CO	45.4	55.6	34.7
CO ₂	49.4	12.9	3.7
Oxygenated molecules			
oxirane	0.017	0.075	0.078
acetaldehyde	0.103	0.261	0.361
oxetane	0.007	0.012	0.017
acrolein	0.034	0.095	0.153
propanal	0.008	0.019	0.036
acetone	0.022	0.054	0.098
C ₈ H ₁₄ O isomers	0.155	0.232	0.276

Table S3: Comparison of carbon product selectivities (in %) in the oxidation of ethyl-benzene at 1 and 6 bars for experiments providing the same fuel conversion (around 50 %).

Species	1.067 bar, 875 K (X=48.4%)	6 bars, 825 K (X=50.0%)	s(6 bars) / s(1.067 bar)
hydrocarbons			
methane	0.739	0.282	0.38
ethylene	2.34	1.04	0.44
acetylene	0.167	0.079	0.47
ethane	0.054	0	0.00
propene	0.143	0.043	0.30
allene	0.037	0.013	0.37
propyne	0.062	0.036	0.58
1-butene	0.026	0	0.00
1,3-butadiene	0.101	0.033	0.33
1,3-cyclopentadiene	0.173	0.018	0.10
benzene	2.96	1.15	0.39
toluene	0.445	0.215	0.48
styrene	36.5	28.2	0.77
cumene ^a	0.247	0.285	1.15
α -methyl-styrene ^a	0.056	1.28	22.94
2-propenyl-benzene ^a	0.079	0.179	2.28
total hydrocarbons	44.1	32.9	0.75
carbon oxides			
CO	15.3	14.8	0.97
CO ₂	3.00	3.52	1.18
Total CO + CO ₂	18.3	18.3	1.0
oxygenated species			
acetaldehyde	0.470	0.557	1.18
acrolein	0.423	1.18	2.80
benzofuran	7.231	12.2	1.68
phenol	3.347	7.83	2.34
benzaldehyde	10.486	20.8	1.98
2-phenyl-acetaldehyde ^a	4.339	6.6	1.53
2-methyl-phenol ^a	0.618	0.810	1.31
acetophenone ^a	0.950	1.29	1.35
total oxygenated species	27.9	51.2	1.84

^a The structures of this molecule is given in Figure S1.

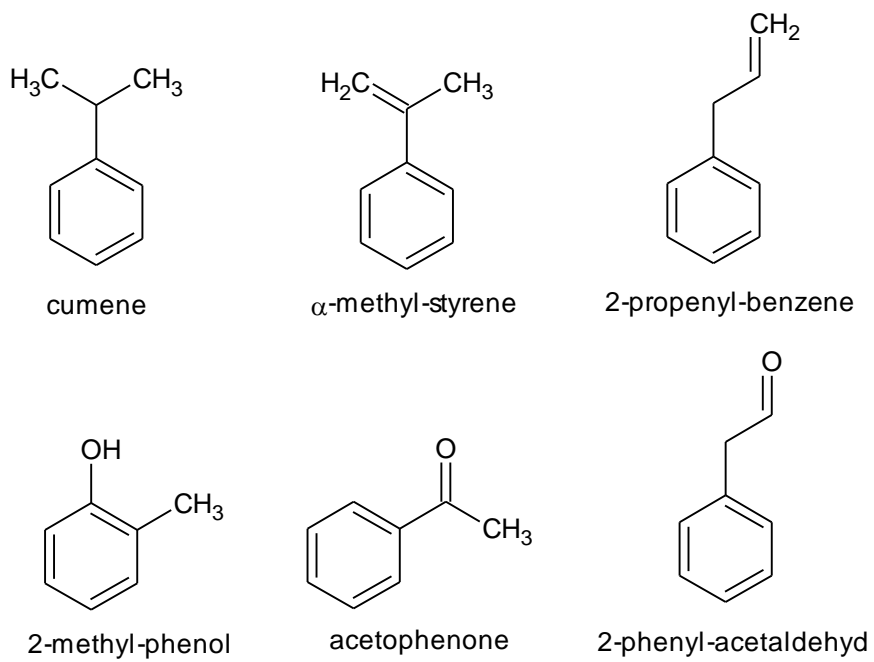


Figure S1: Structure of some large species of Table S3.

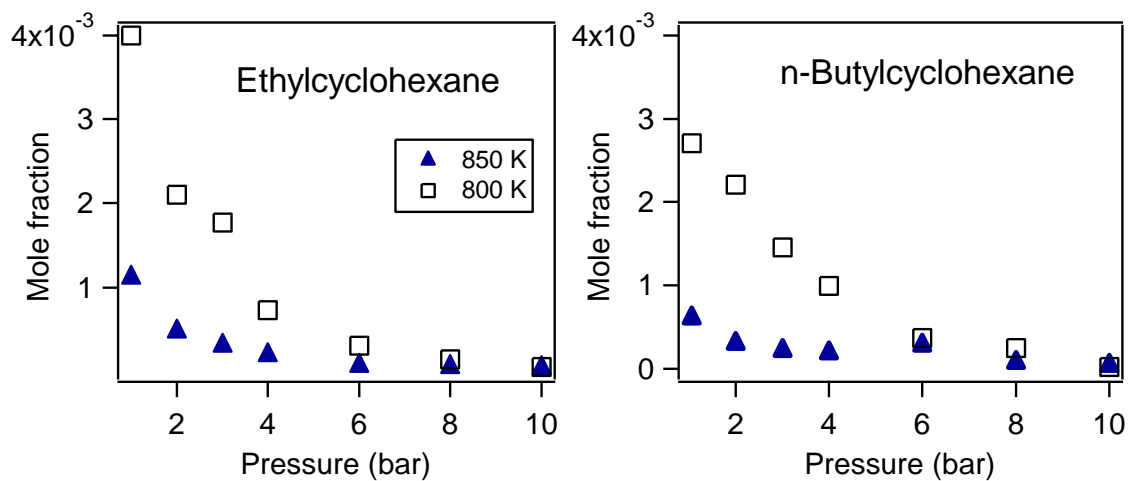


Figure S2: Oxidation of ethylcyclohexane and *n*-butylcyclohexane in a jet-stirred reactor. Influence of a variation of pressure from 1 to 10 bars on the evolution of the conversion ($x_{\varphi C_2H_5} = 0.005$, $x_{\varphi C_4H_9} = 0.004$, $\tau = 2$ s, $\varphi = 1$).