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APPENDICES

Appendix A MCH Conversion and Products Distribution

Table A.1 The catalytic activity and selectivity of MCH over bare acidic catalysts

Sample		MFI	BEA	FAU	WZ
MCH Conversion (%)		6.8	26.0	28.9	37.2
MCH (wt%)		93.2	74.0	71.1	62.8
Products	(RON)	Selectivity to (wt%)			
Cracking Product		-	-	-	10.9
RC Products					
1,1-DMCP	(92.3)	5.2	4.2	2.5	1.5
<i>cis</i> -1,3-DMCP	(79.2)	31.1	42.1	25.8	23.0
<i>trans</i> -1,3-DMCP	(80.6)	21.7	29.6	24.5	24.6
<i>trans</i> -1,2-DMCP	(86.5)	20.0	7.2	28.1	33.1
ECP	(67.2)	21.7	16.9	19.1	6.9
RO Products					
3,3-DMP	(80.8)	-	-	-	-
2,2-DMP	(92.8)	-	-	-	-
2,4-DMP	(83.1)	-	-	-	-
2,3-DMP	(91.1)	-	-	-	-
<i>n</i> -heptane	(0.0)	-	-	-	-
2-MH	(42.4)	-	-	-	-
3-MH	(52.0)	-	-	-	-
3-EP	(65.0)	-	-	-	-
Heavy products		-	-	-	-

Reaction conditions: Total pressure = 2MPa; Temperature = 533 K; H₂/feed molar ratio = 40; TOS = 120 min, W/F = 0.65 h.

Table A.2 The catalytic conversion of MCH over acidic and bifunctional catalysts

Sample		CBV400	CBV720	Pt/CBV400	Pt/CBV720
MCH Conversion (%)		25.3	10.5	36.0	21.7
MCH (wt%)		74.7	89.5	64	78.3
Products	(RON)	Selectivity to (wt%)			
Cracking Product		0.8	0.9	0.8	0.9
RC Products					
1,1-DMCP	(92.3)	1.6	0.9	15.0	11.5
<i>cis</i> -1,3-DMCP	(79.2)	26.8	26.5	17.2	12.9
<i>trans</i> -1,3-DMCP	(80.6)	24.8	22.2	16.9	12.4
<i>trans</i> -1,2-DMCP	(86.5)	24.8	25.6	26.3	24.4
ECP	(67.2)	20.1	23.1	20.2	35.0
RO Products					
3,3-DMP	(80.8)	-	-	0.3	-
2,2-DMP	(92.8)	-	-	0.3	-
2,4-DMP	(83.1)	0.4	-	0.8	0.9
2,3-DMP	(91.1)	-	-	0.3	-
<i>n</i> -heptane	(0.0)	-	-	0.8	0.5
2-MH	(42.4)	0.8	0.9	1.1	1.4
3-MH	(52.0)	-	-	-	-
3-EP	(65.0)	-	-	-	-
Heavy products		-	-	-	-

Reaction conditions: Total pressure = 2MPa; Temperature = 533 K; H₂/feed molar ratio = 40; TOS = 60 min, W/F = 0.65 h.

Appendix B MCH Conversion Plotted vs. Time on Steam (TOS)

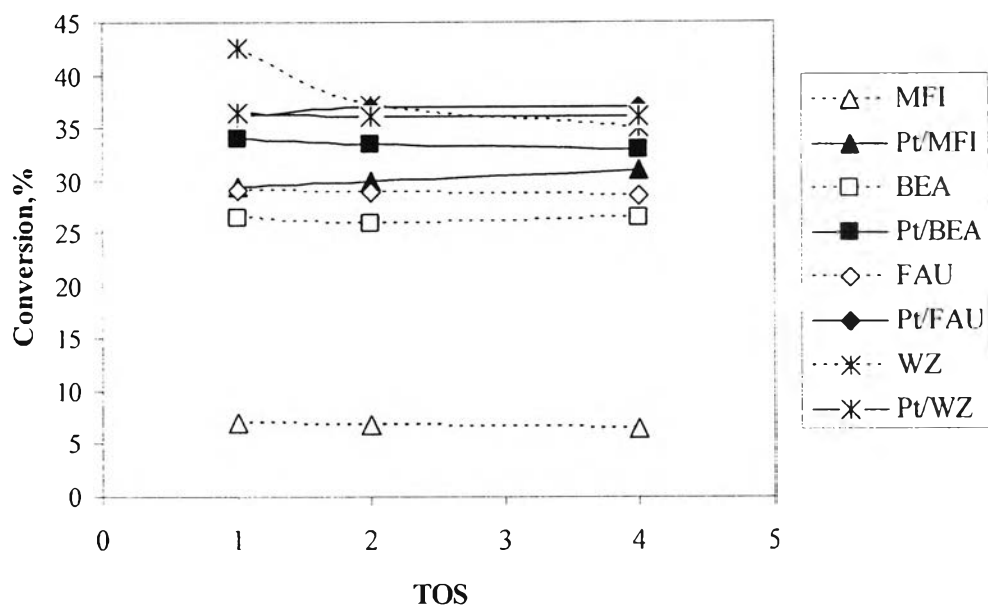


Figure B.1 MCH Conversion (%) plotted vs. Time on Steam (TOS) for both bare and Pt-supported catalysts.

Appendix C Selectivity to RC products plotted vs. W/F at 2 MPa and 533 K

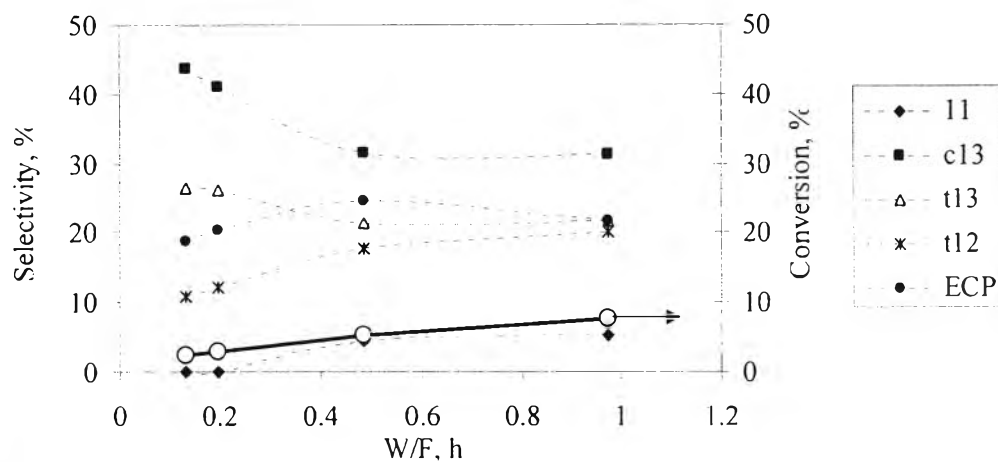


Figure C.1 Selectivity to RC products plotted vs. W/F over MFI.

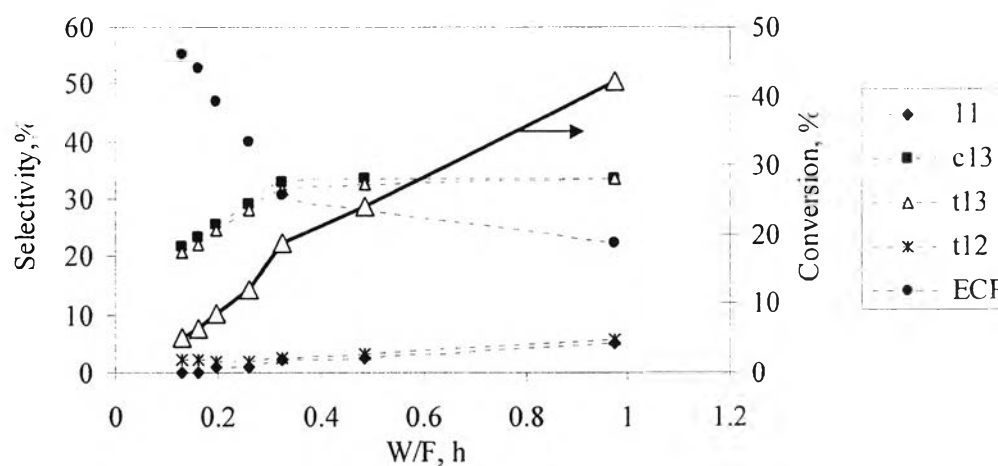


Figure C.2 Selectivity to RC products plotted vs. W/F over Pt/MFI.

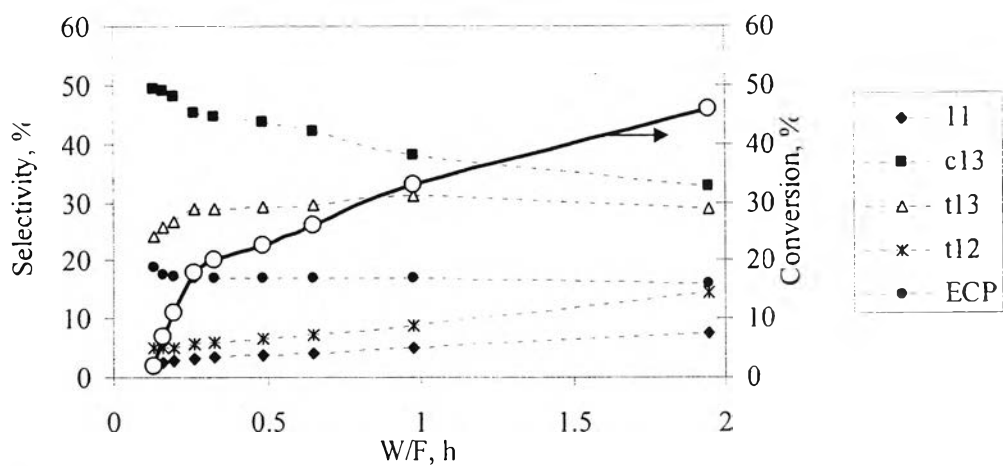


Figure C.3 Selectivity to RC products plotted vs. W/F over BEA.

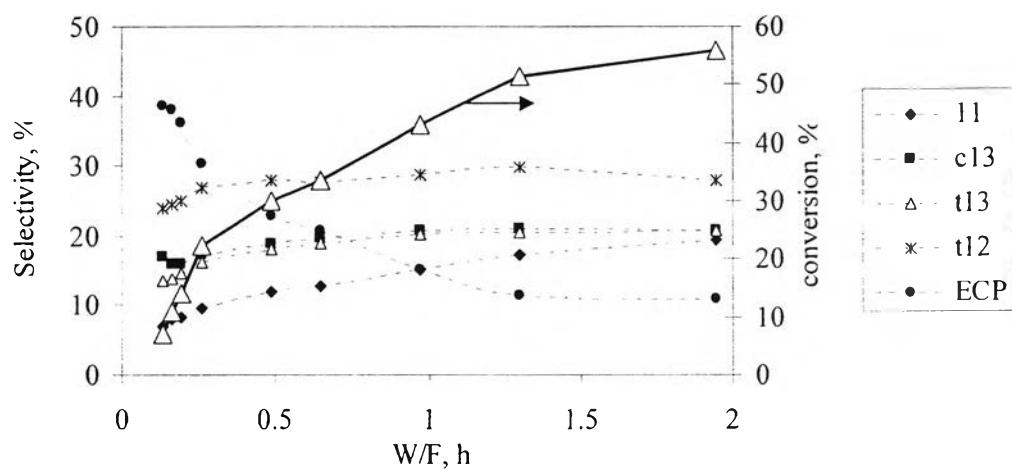


Figure C.4 Selectivity to RC products plotted vs. W/F over Pt/BEA.

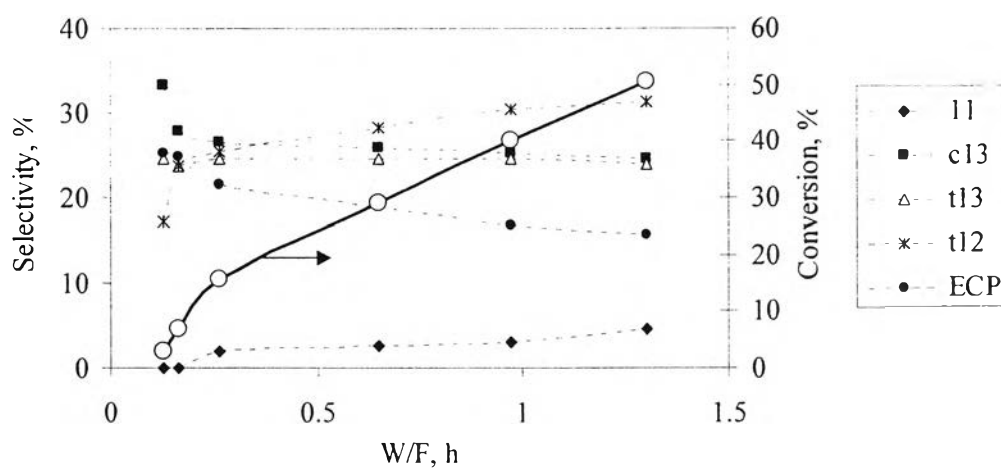


Figure C.5 Selectivity to RC products plotted vs. W/F over FAU.

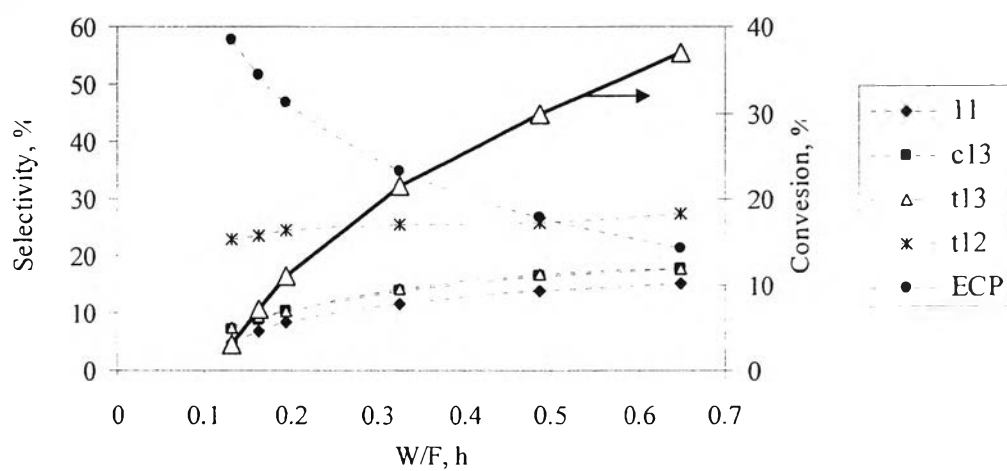


Figure C.6 Selectivity to RC products plotted vs. W/F over Pt/FAU.

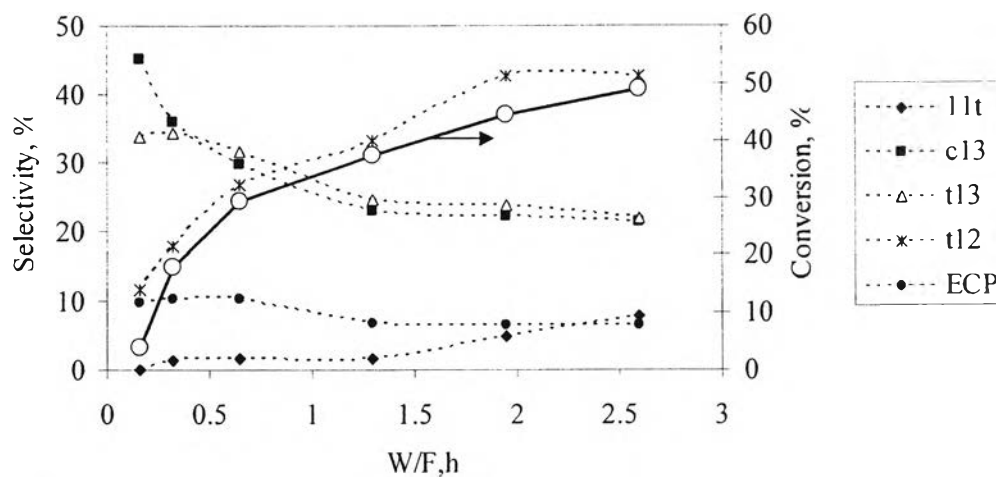


Figure C.7 Selectivity to RC products plotted vs. W/F over WZ.

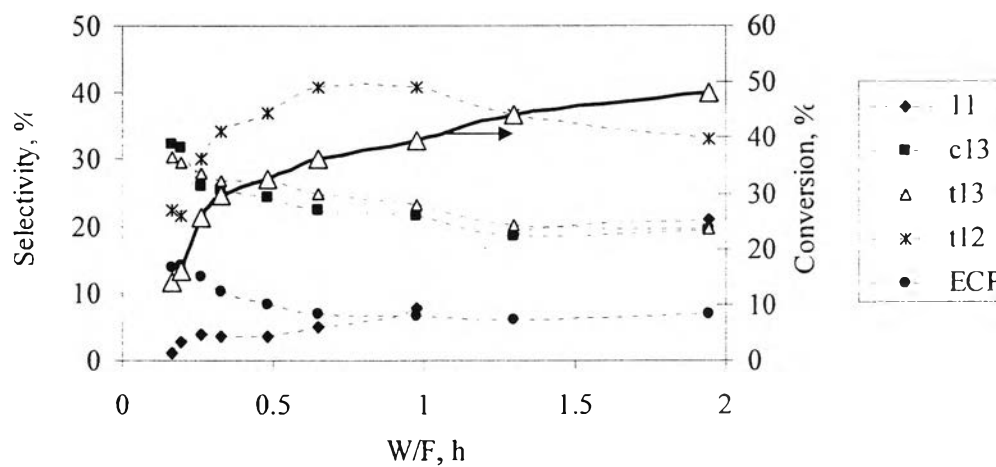
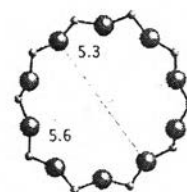
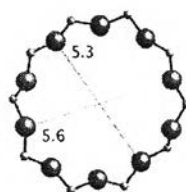
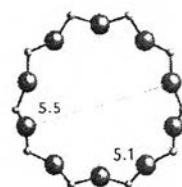
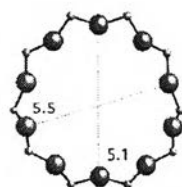
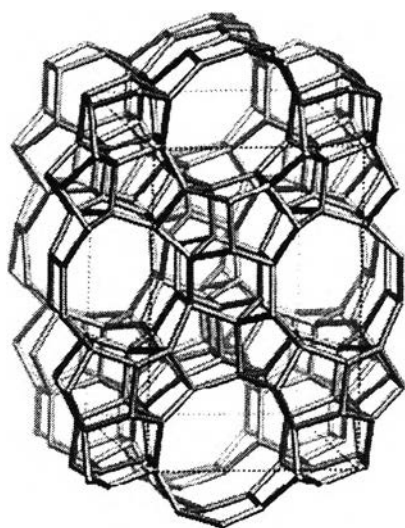


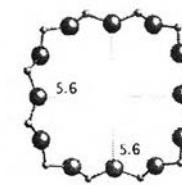
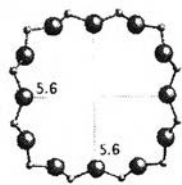
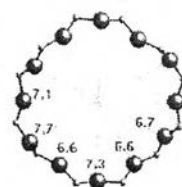
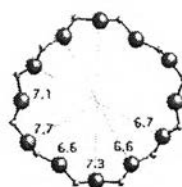
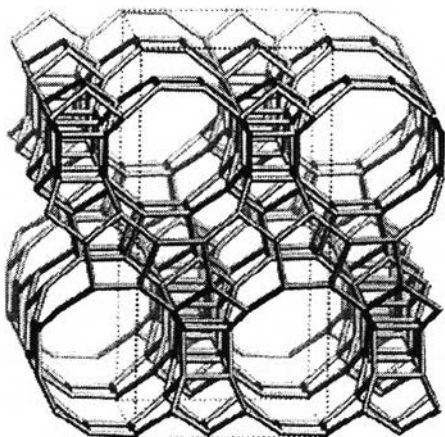
Figure C.8 Selectivity to RC products plotted vs. W/F over Pt/WZ.

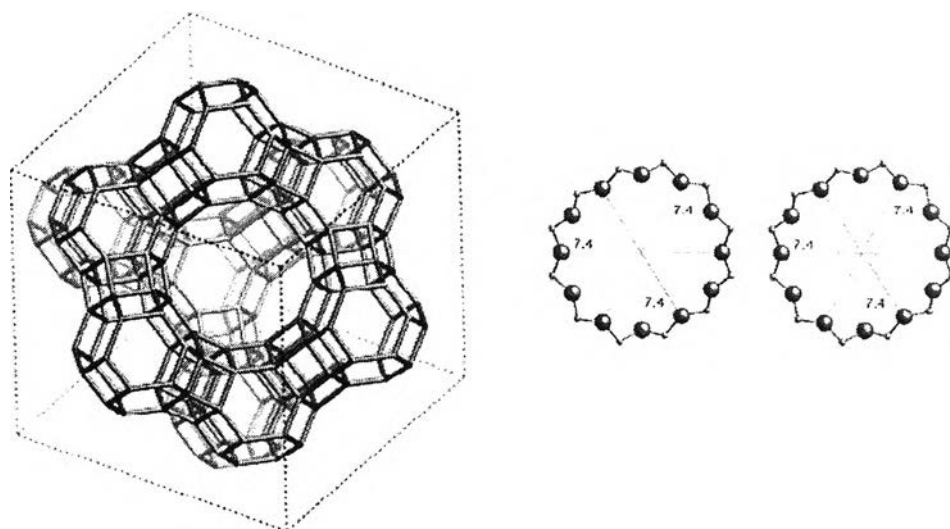
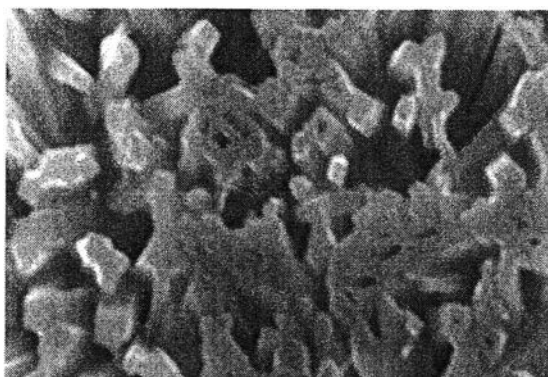
Appendix D Catalyst Structures and Molecule Sizes

MFI (ZSM-5 zeolite)



BEA (Beta zeolite)



FAU (Faujasite zeolite)WZ (Tungstated zirconia)**Table D.1** Critical diameters

Molecules	Diameter (Å)
Methylcyclohexane	6.9
Cyclopentane	6.4
1,1-Dimethylcyclopentane	6.6
<i>cis</i> -1,2-Dimethylcyclopentane	7.3
<i>trans</i> -1,2-Dimethylcyclopentane	6.7
<i>cis</i> -1,3-Dimethylcyclopentane	6.4
<i>trans</i> -1,3-Dimethylcyclopentane	6.4
Ethylcyclopentane	6.4

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International Proceedings and Presentations:

- Prasomsri, T., Santikunaporn, M., and Resasco, D.E., “Selectivity of Ring-Contraction Products in the Hydroisomerization of Methylcyclohexane”, 52nd Annual Oklahoma ACS Pentasectional Meeting, Ponca City, Oklahoma, USA, 10 March 2007.
- Prasomsri, T., Jongpatiwut, S., Santikunaporn, M., and Resasco, D.E., “Selectivity of Ring-Contraction Products in the Hydroisomerization of Methylcyclohexane”, Proceedings of the AIChE Spring National Meeting, Houston, Texas, USA, 22-27 April 2007.

