Reactions of unsaturated hydrocarbons catalysed by transition metal compounds

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Reactions of Unsaturated Hydrocarbons Catalysed by Transition Metal Compounds

Volume Two : Appendices

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Appendix 2.1: Preliminary Work on Xylene Isomerisation

A2.1.1 Sulphated Zirconia Catalyst prepared from "Zirconium Hydroxide"

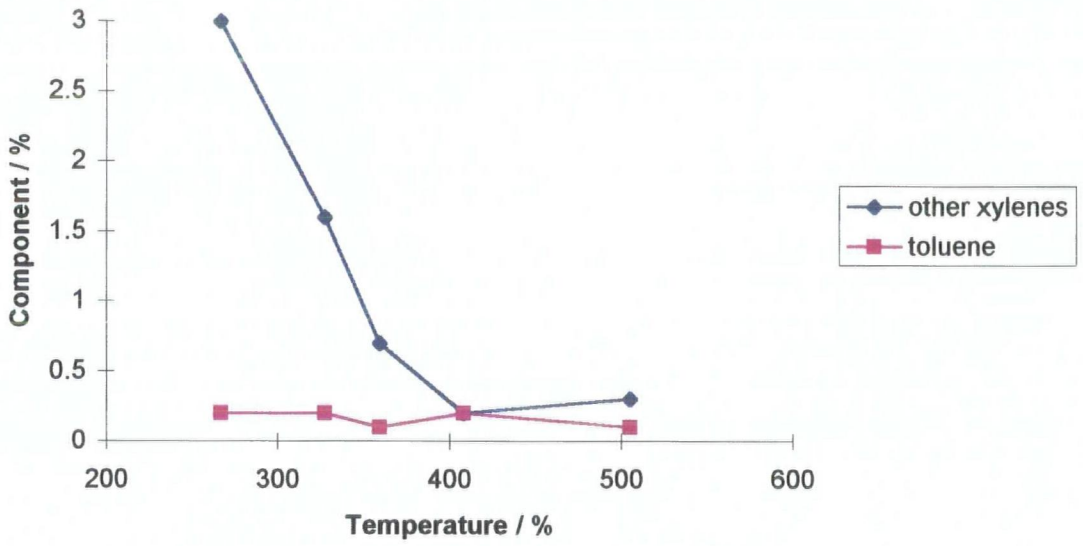

Fig. A2.1: Reaction of *Ortho*-Xylene over Sulphated Zirconia

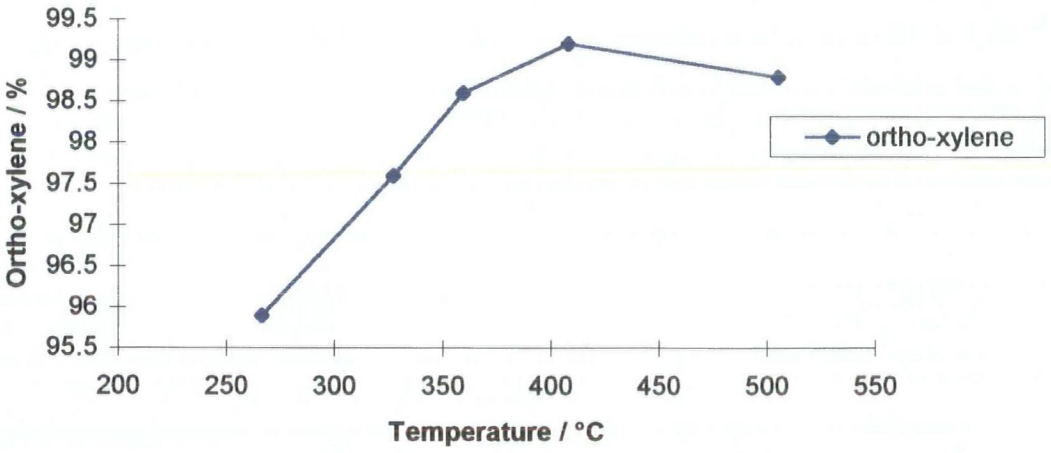

Fig. A2.2: Conversion of *Ortho*-Xylene over Sulphated Zirconia

A2.1.2 Platinum-doped Sulphated Zirconia

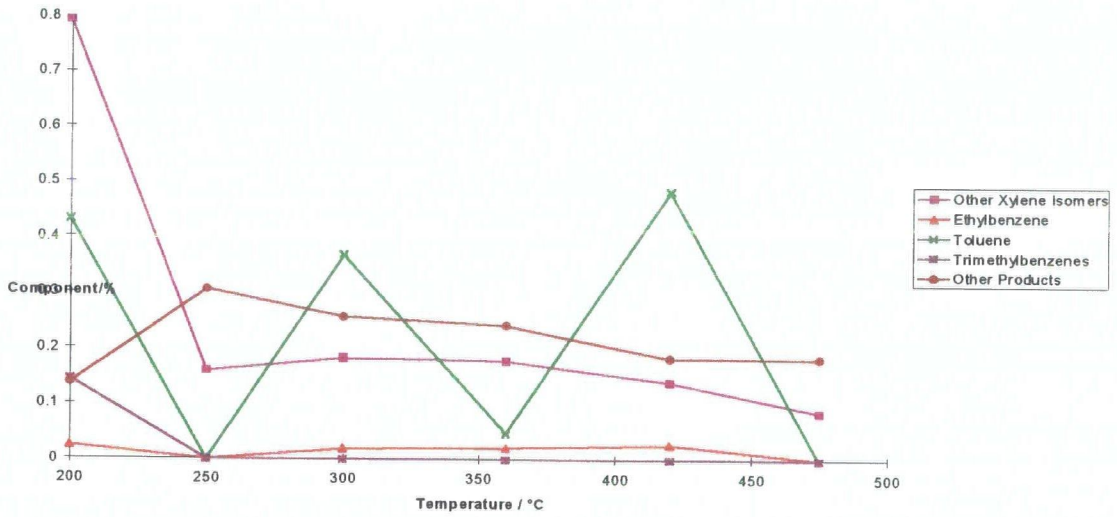

Fig A2.3: Product Distribution in the Isomerisation of *Ortho*-Xylene over Platinum-doped Sulphated Zirconia

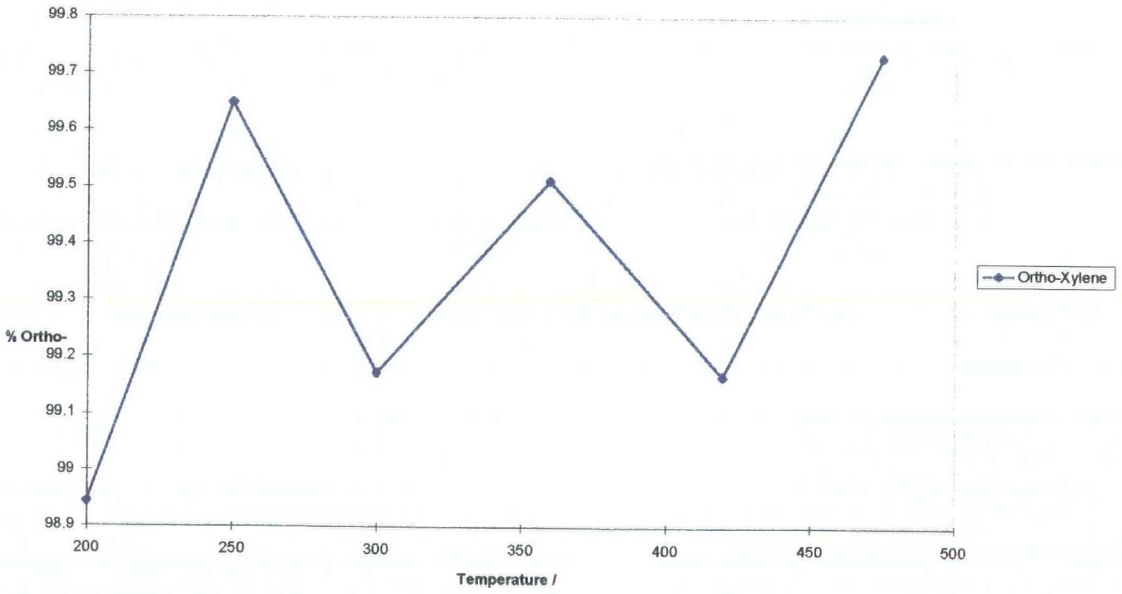

Fig A2.4: *Ortho*-Xylene Conversion over Platinum-doped Sulphated Zirconia

A2.1.3 Aluminium-doped Zirconia

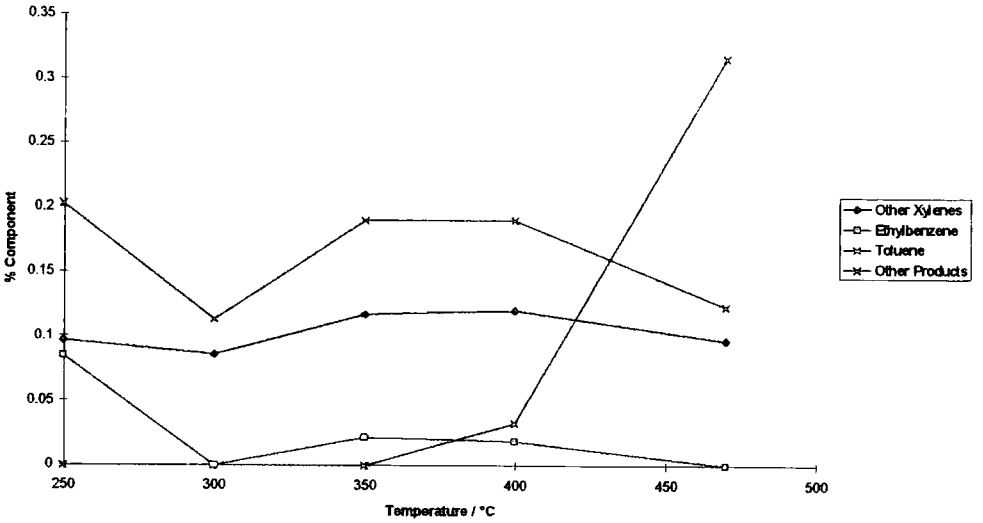

Fig. A2.5: Product Distribution for the Isomerisation of *Ortho*-Xylene over Aluminium-doped Zirconia

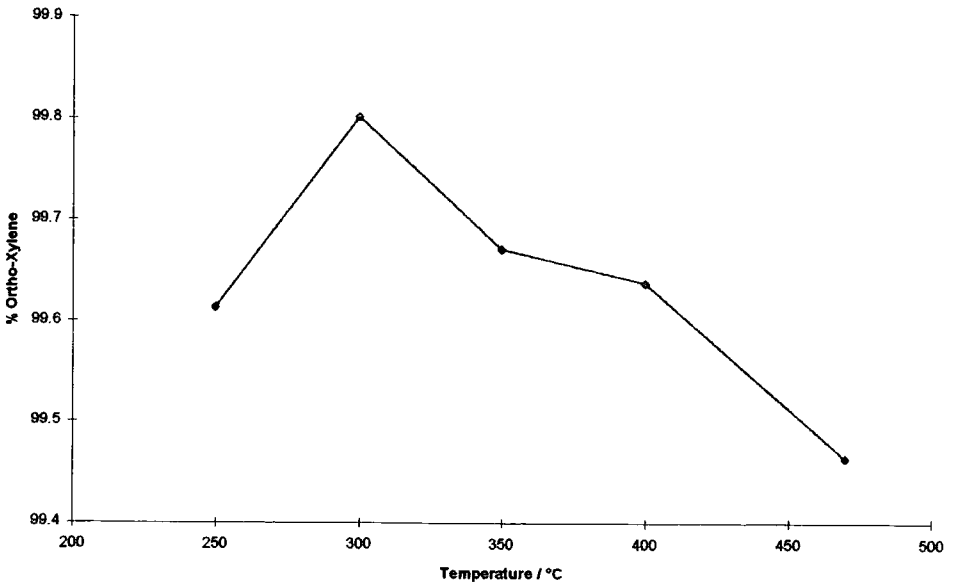

Fig. A2.6: Ortho-Xylene Conversion over Aluminium-doped Zirconia

A2.1.4 Aluminium-doped Sulphated Zirconia

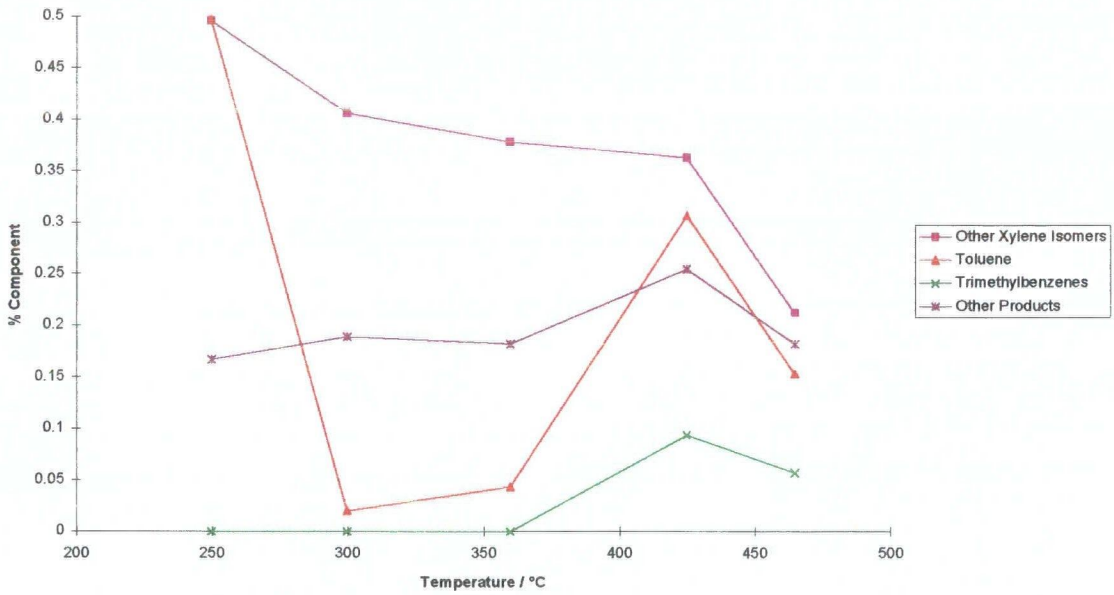

Fig. A2.7: Distribution of Products for the Isomerisation of *Ortho*-Xylene over Aluminium-doped Sulphated Zirconia

(sample prepared from $[Zr(OPr)_4]$)

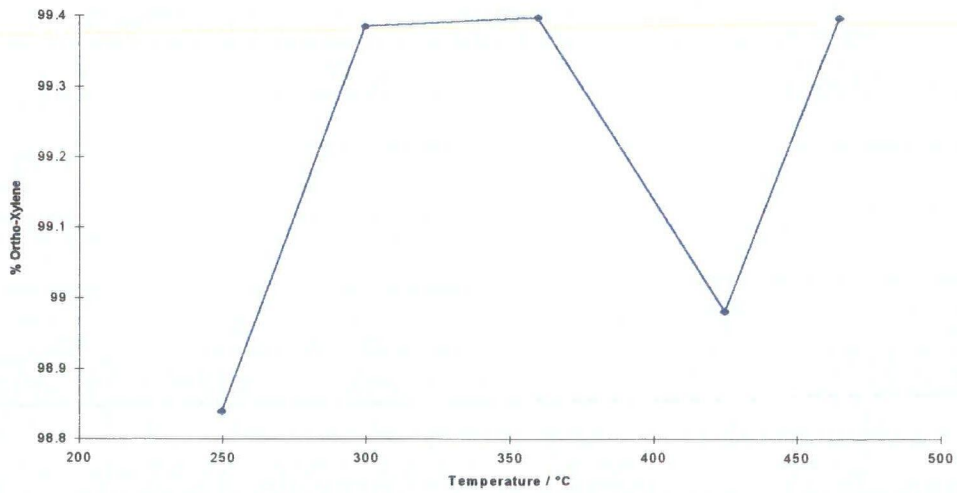

Fig. A2.8: Conversion of *Ortho*-Xylene over Aluminium-doped Sulphated Zirconia

(sample prepared from $[Zr(OPr)_4]$

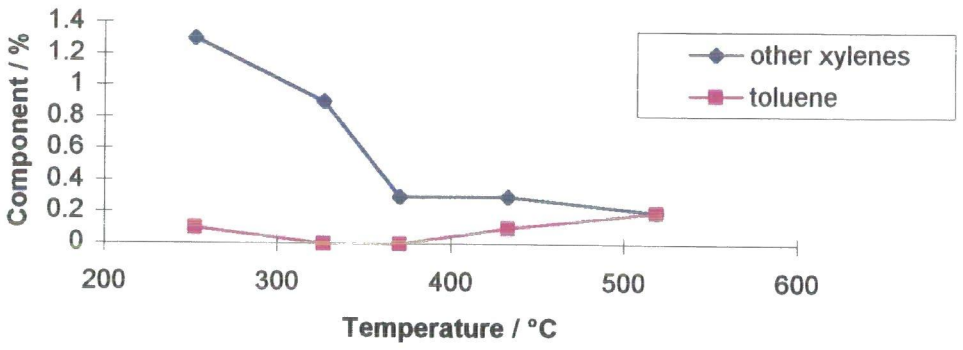

Fig. A2.9: Isomerisation of *Ortho*-Xylene over Aluminium Sulphate-doped "Zirconium Hydroxide"

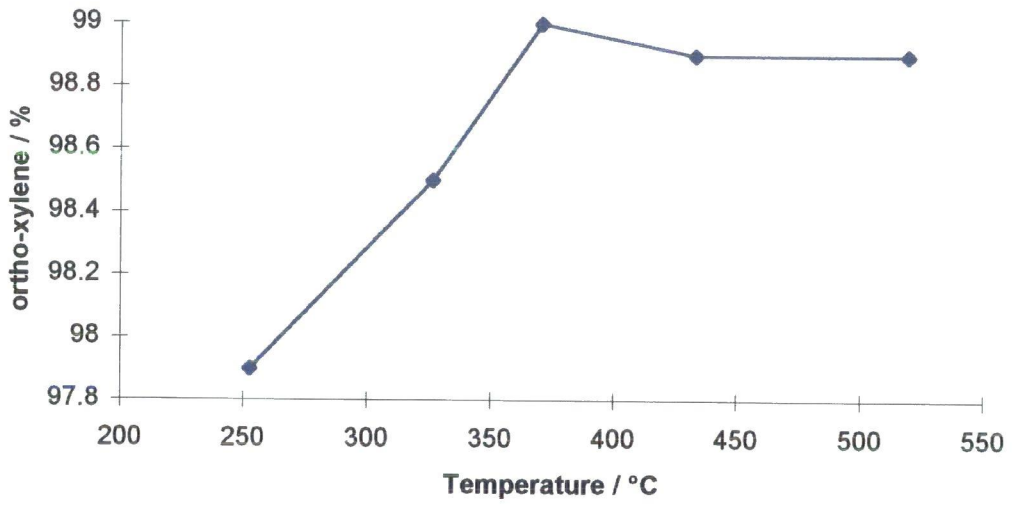

Fig. A2.10: *Ortho*-Xylene conversion over Aluminium Sulphate-doped "Zirconium Hydroxide"

A2.1.5 Nickel-doped Zirconia

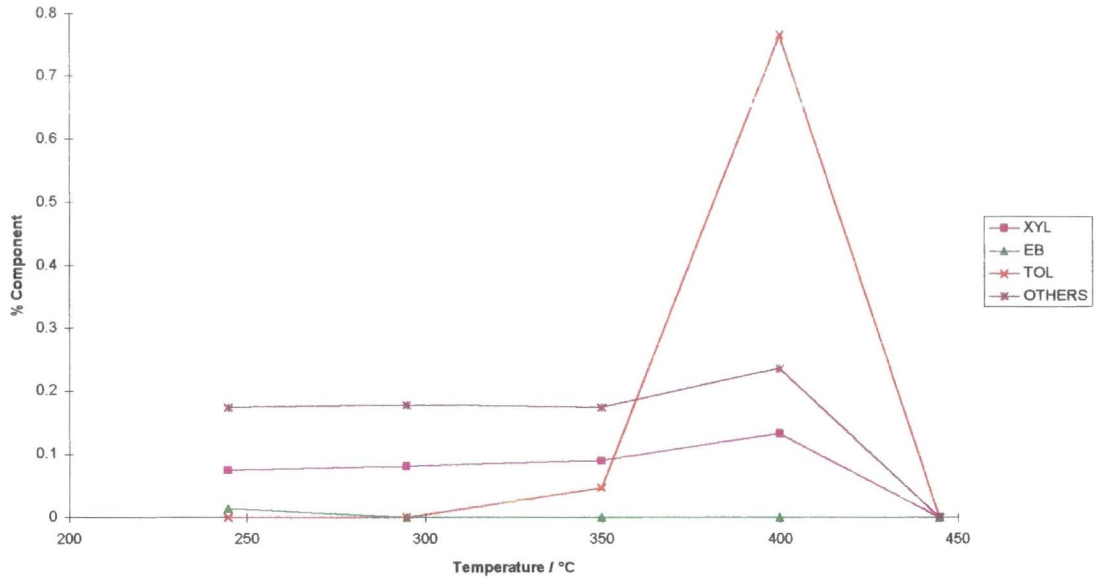

Fig. A2.11: Product Distribution for the Isomerisation of *Ortho*-Xylene over Nickel-doped Zirconia

(sample prepared using nickel dichloride)

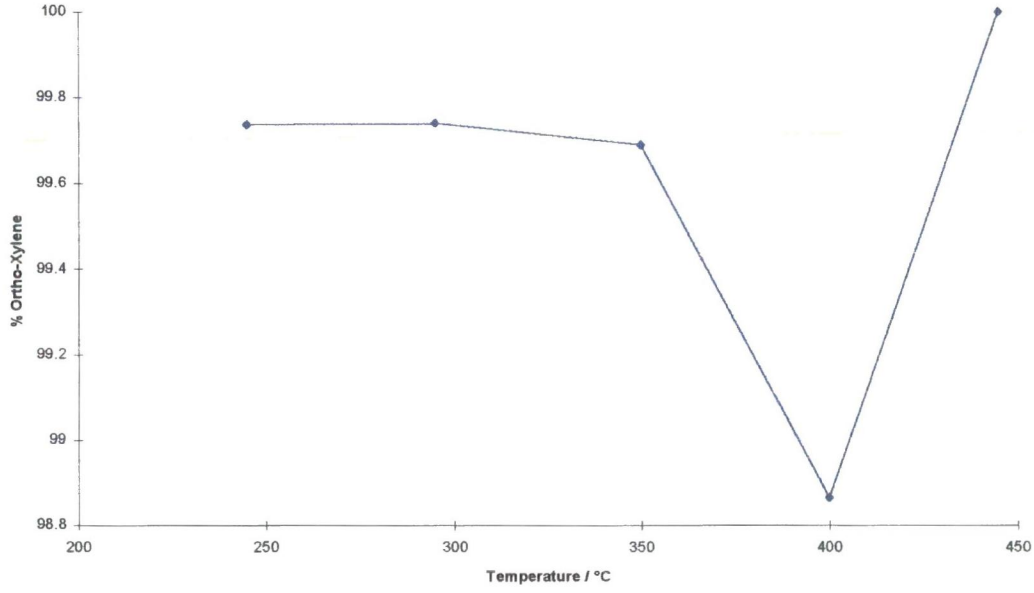

Fig. A2.12: Conversion of *Ortho*-Xylene over Nickel-doped Zirconia

(sample prepared using nickel dichloride)

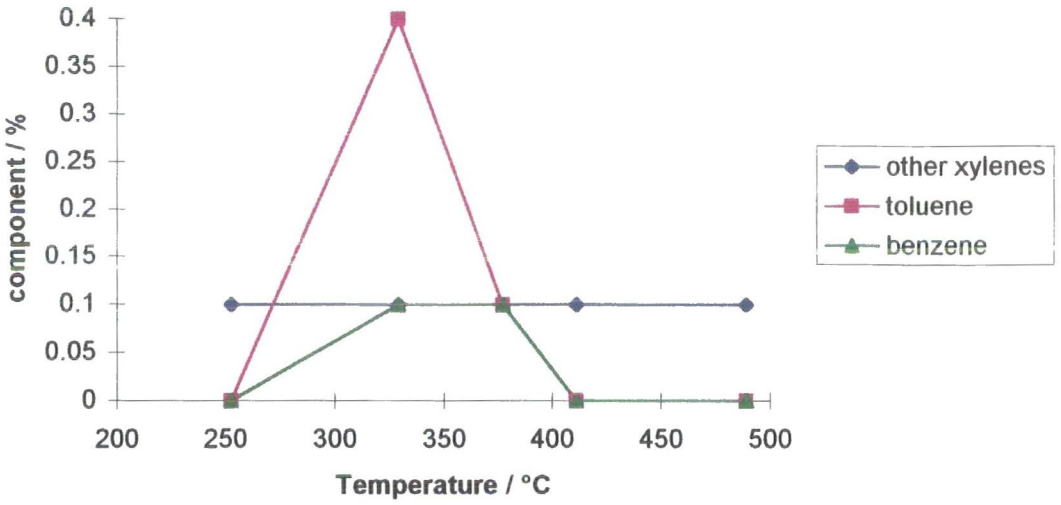

Fig. A2.13: Reaction of *Ortho*-Xylene over Nickel Hydroxide-doped Zirconia

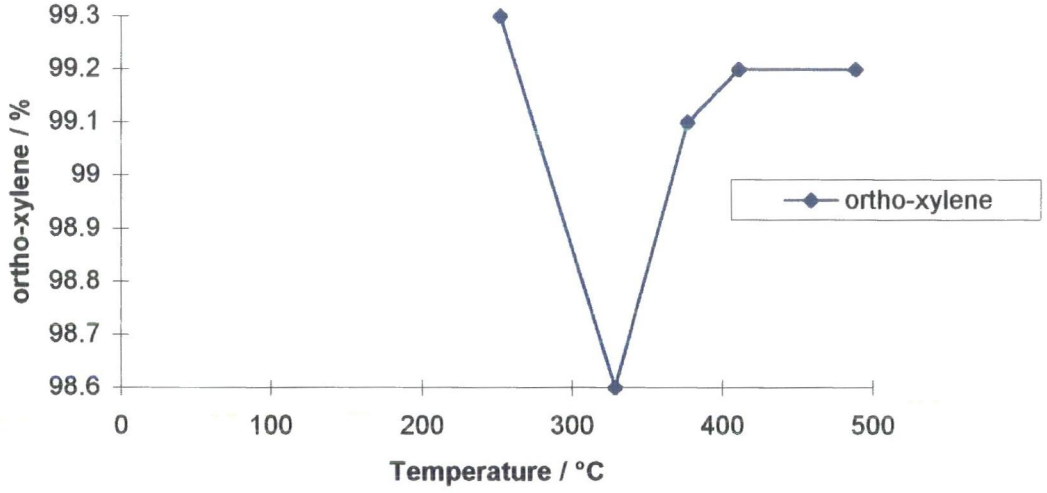

Fig. A2.14: Conversion of *Ortho*-Xylene over Nickel Hydroxide-doped Zirconia

A2.1.6 Nickel-doped Sulphated Zirconia

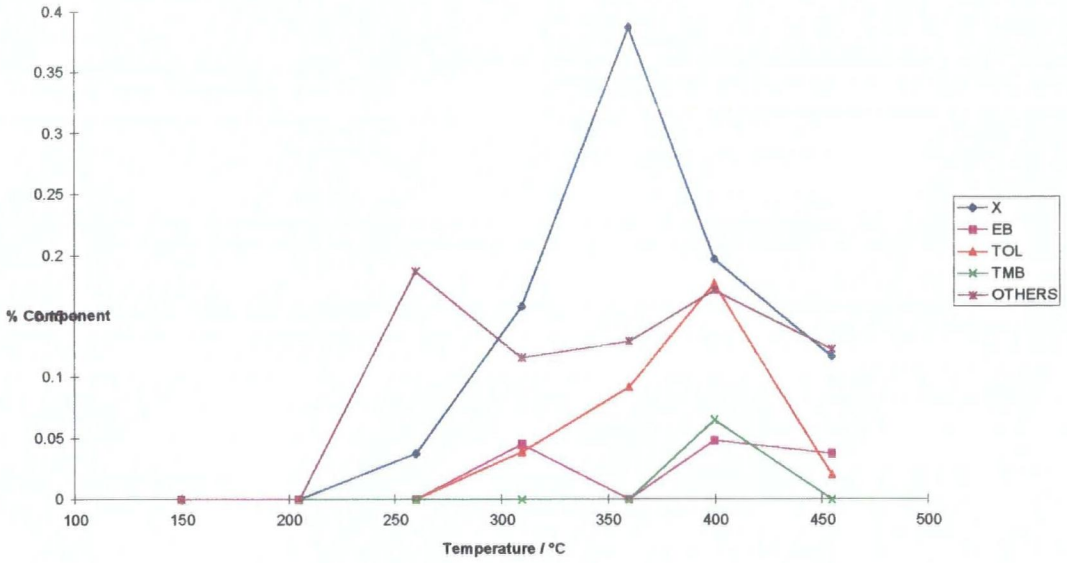

Fig. A2.15: Product Distribution for the Isomerisation of *Ortho*-Xylene over Nickel-doped Sulphated Zirconia

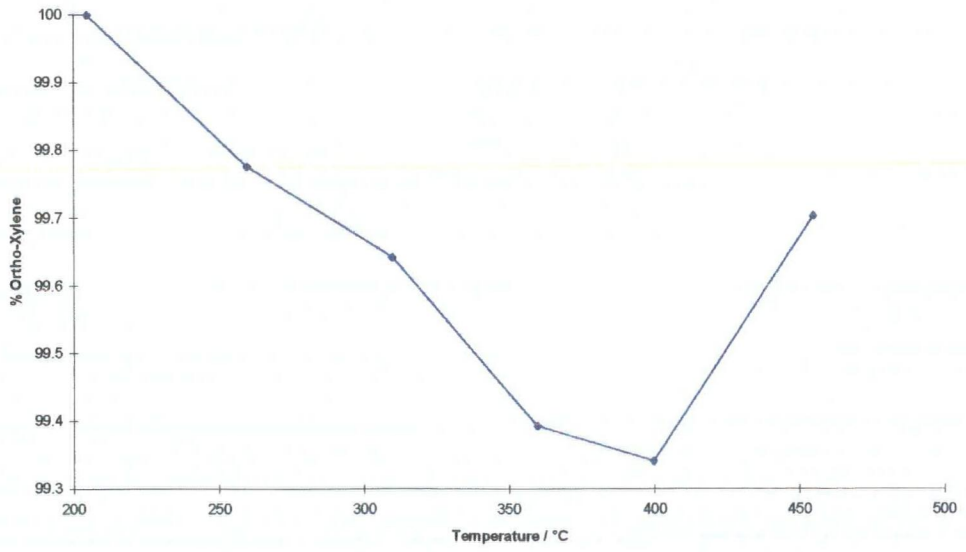

Fig. A2.16: Conversion of *Ortho*-Xylene over Nickel-doped Sulphated Zirconia

A2.1.7 Chromium-doped Sulphated Zirconia

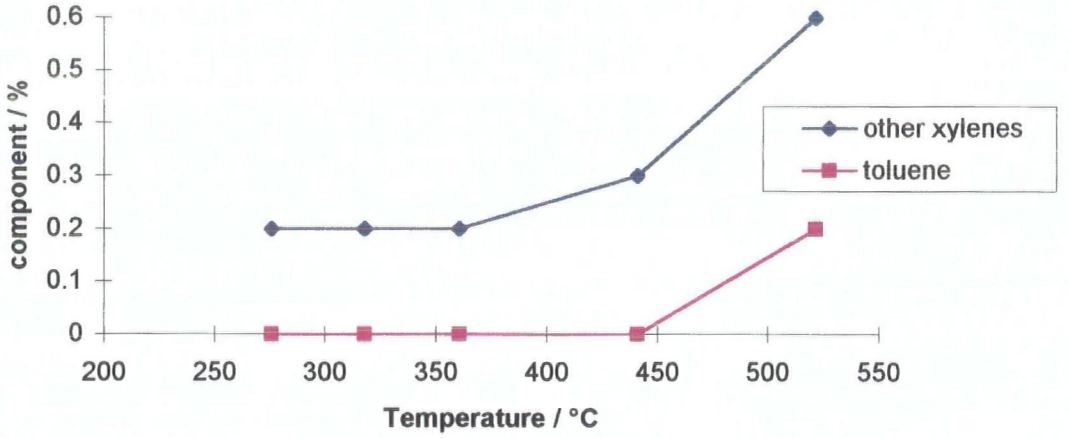

Fig. A2.17: Reaction of *Ortho*-Xylene over Chromium-doped Sulphated Zirconia

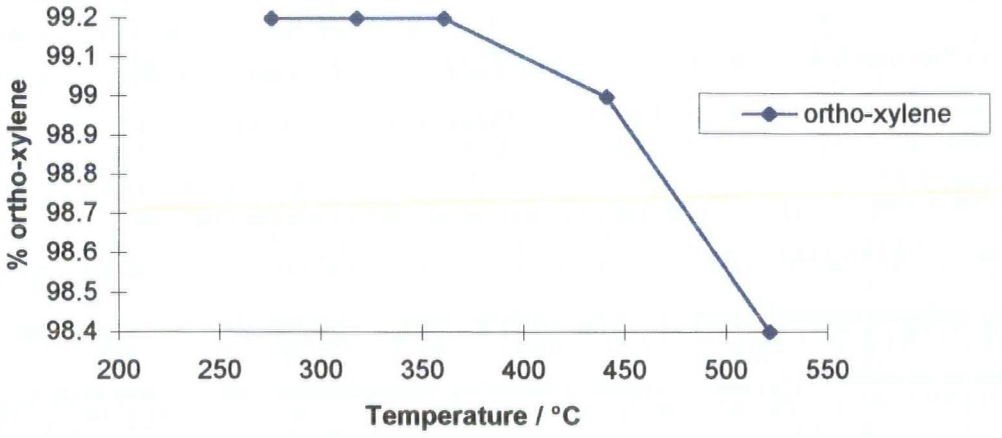

Fig. A2.18: Conversion of *Ortho*-Xylene over Chromium-doped Sulphated Zirconia

A2.1.8 Commercial Samples

A2.1.8.1 Catalyst EX-1720 in *Ortho*-Xylene Isomerisation

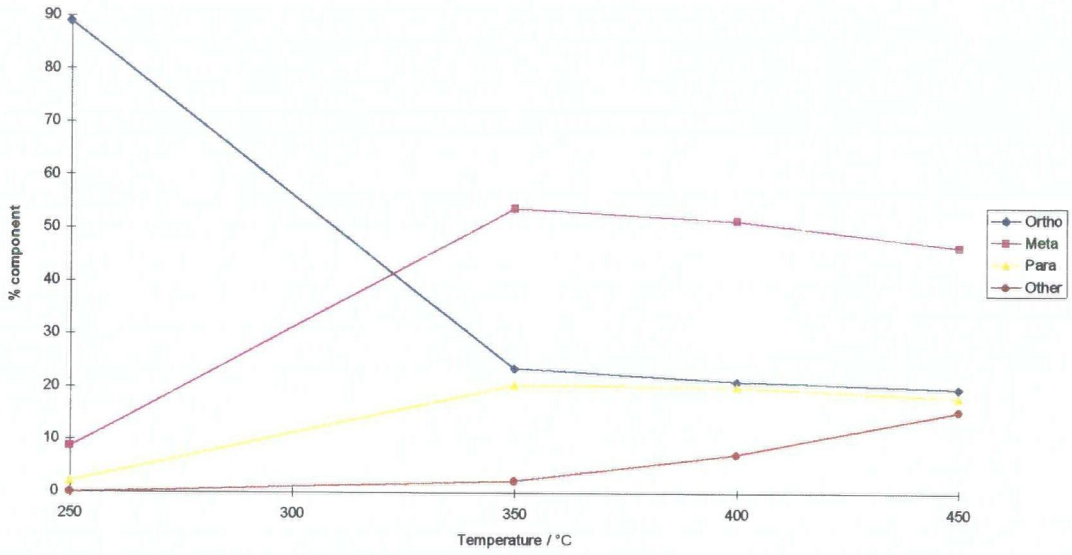

Fig. A2.19: Performance of Catalyst EX-1720 in *ortho*-xylene isomerisation

A2.1.8.2 Catalyst T-2581 in *Ortho*-Xylene Isomerisation

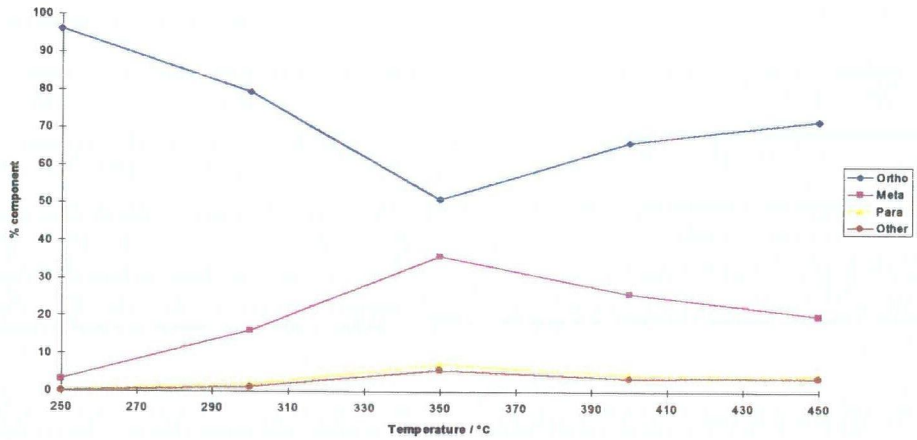

Fig A2.20: Performance of Catalyst T-2581 in *ortho*-xylene isomerisation

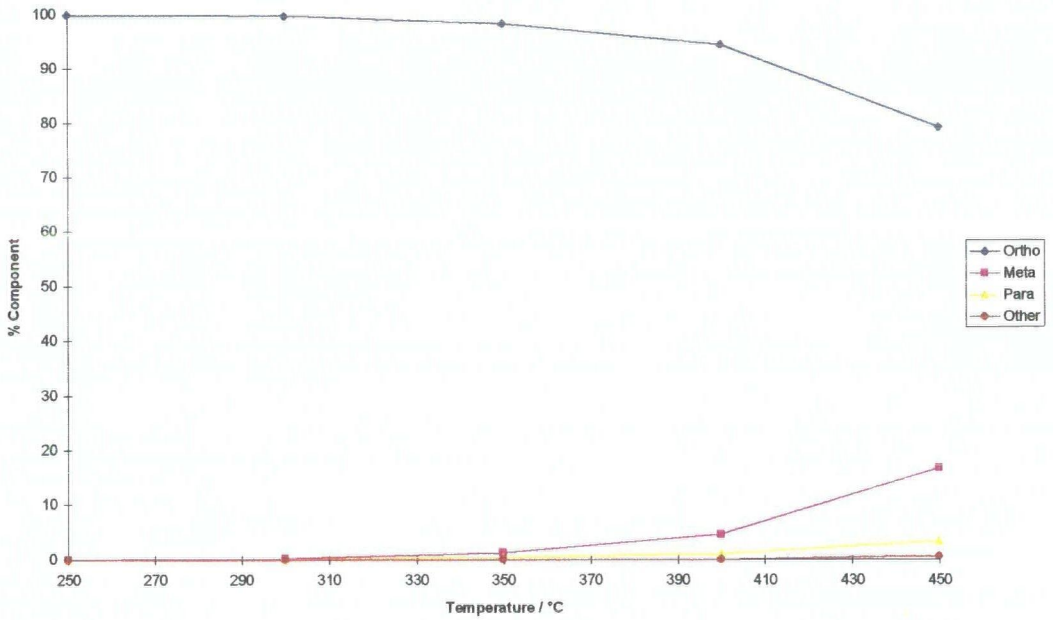

Fig. A2.21: Performance of re-used Catalyst T-2581 in *ortho*-xylene isomerisation

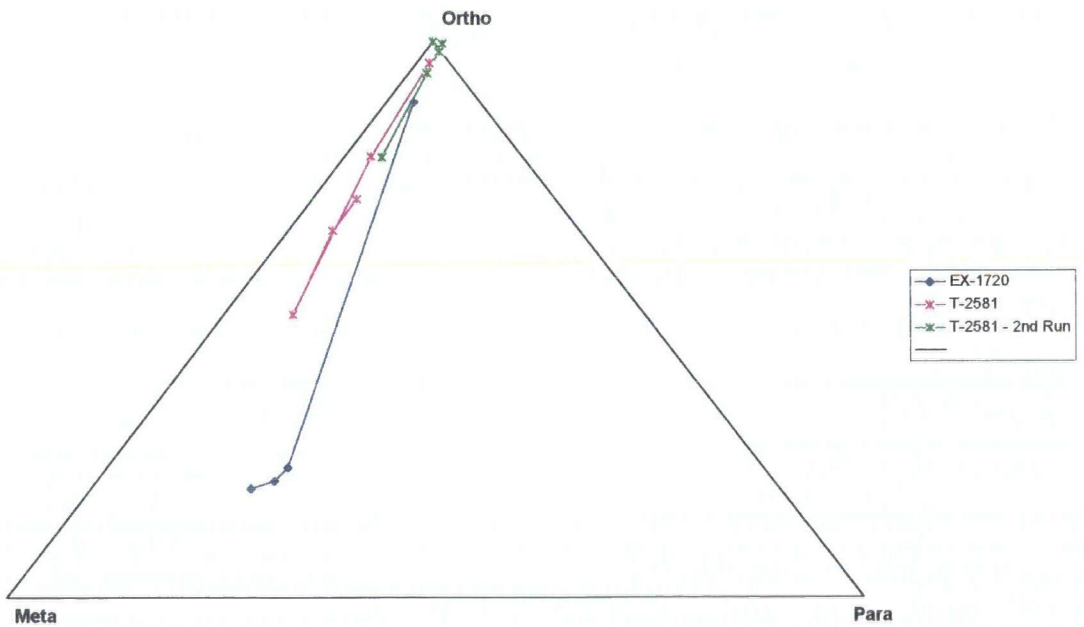

Fig A2.22: Isomer Distribution in the Isomerisation of *ortho*-xylene over catalysts EX-1720 and T-2581

A2.1.8.3 Catalyst EX-1720 in Mixed Xylene Isomerisation

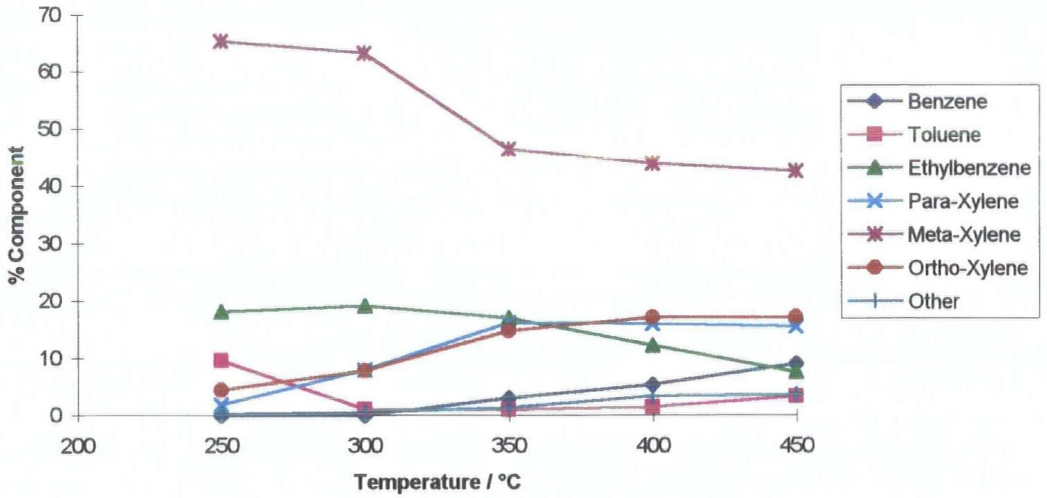

Fig. A2.23: Reactions of Mixed Xylenes over Catalyst EX-1720

A2.1.8.4 Catalyst EX-1720 in Toluene Disproportionation

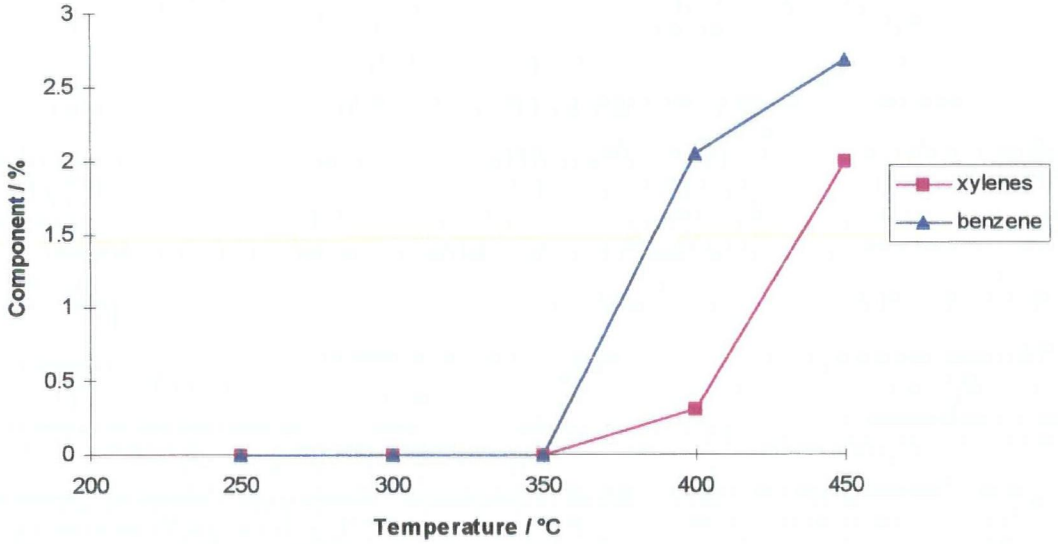

Fig. A2.24: Reactions of Toluene over Catalyst EX-1720

A2.1.8.5 Catalyst EX-1720 in Reactions of Toluene and Methanol

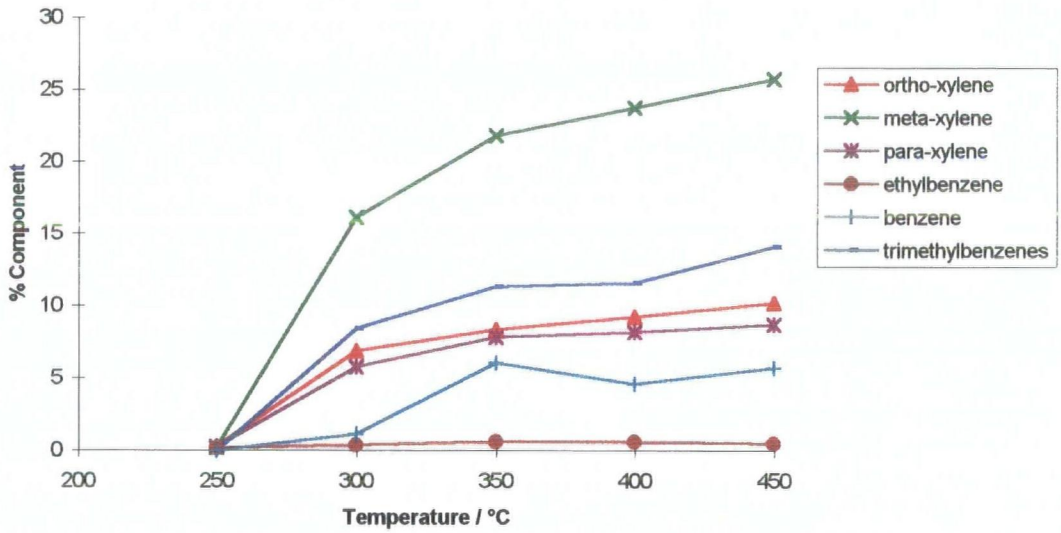

Fig. A2.25: Reactions of Toluene and Methanol over Catalyst EX-1720

A2.1.8.6 Catalyst EX-1720 in Reactions of Ethylbenzene

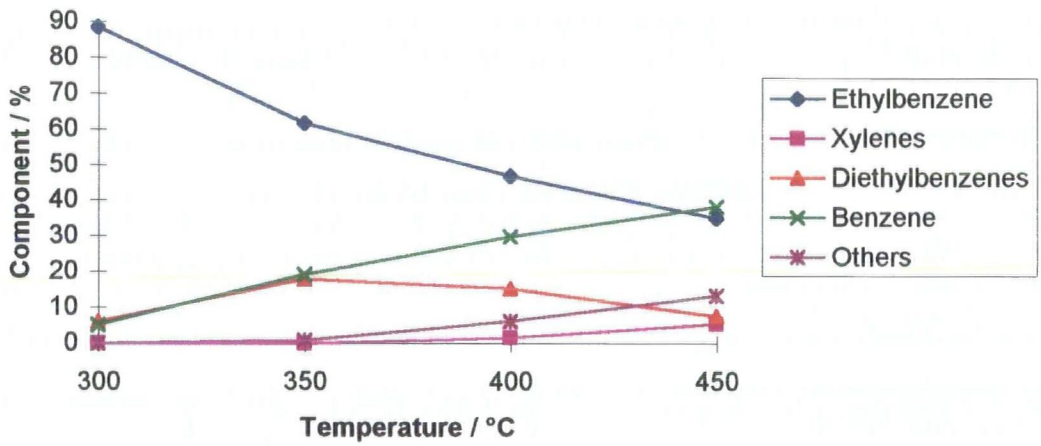

Fig. A2.26: Reactions of Ethylbenzene over Catalyst EX-1720

Appendix 2.2: Raw Data From Catalyst Testing

A2.2.1 Key to Abbreviations Used

Benz	benzene
Comm	commercial
EB	ethylbenzene
Expt	experiment
MeOH	methanol
MX	*meta*-xylene
OX	*ortho*-xylene
PRE	"P.R. Ellis" sample number
PX	*para*-xylene
T1	initial reaction temperature
T2	final reaction temperature
Tol	toluene
"ZrOH"	amorphous "zirconium hydroxide"

A2.2.2 Key To Catalyst Samples

A2.2.2.1 Commercial Samples

Glass Beads	2mm Glass Beads
Comm A	Commercial Ion-Exchange Resin
Comm B	Molecular Sieve 13X (BDH)
Comm C	Alumina Spheres (United Catalysts Inc.)
Comm D	Synthetic Aluminosilicate Zeolite Catalyst EX-1720 (Süd-Chemie)
Comm E	Aluminium Oxide on a Mordenite Carrier, Catalyst T-2581 (Süd-Chemie)

A2.2.2.2 Non-Commercial Samples

PRE18	Sulphated Zirconia
PRE22	Precipitated Zirconia, used to make PRE23-31
PRE23	Platinum-Zirconia
PRE24	Aluminium-Sulphated Zirconia
PRE25	Sulphated Zirconia
PRE26	Nickel-Sulphated Zirconia
PRE27	Platinum-Sulphated Zirconia
PRE28	Aluminium-Zirconia
PRE29	Phosphated Zirconia
PRE30	Platinum-Phosphated Zirconia
PRE31	Nickel-Zirconia
PRE67	Nickel Chloride - "ZrOH"
PRE68	Ammonium Sulphate - "ZrOH"
PRE69	Aluminium Sulphate - "ZrOH"
PRE70	Nickel Hydroxide - "ZrOH"

PRE72	Platinum Hydroxide - "ZrOH"
PRE73	Chromium Trioxide - "ZrOH"
PRE74	Ammonium Sulphate - Platinum/"ZrOH"
PRE75	Phosphoric Acid - Platinum/"ZrOH"
PRE79	Ammonium Sulphate - Chromium/"ZrOH"
PRE76/M	Chromium - Silver - MgO
PRE76/S	Chromium - Silver - SiO_2
PRE76/T	Chromium - Silver - TiO_2
PRE76/Z	Chromium - Silver - ZrO_2
PRE77/M	Palladium - Silver - MgO
PRE77/S	Palladium - Silver - SiO_2
PRE77/T	Palladium - Silver - TiO_2
PRE77/Z	Palladium - Silver - ZrO_2
PRE78/M	0.01% Palladium - Silver - MgO
PRE78/S	0.01% Palladium - Silver - SiO_2
PRE78/T	0.01% Palladium - Silver - TiO_2
PRE78/Z	0.01% Palladium - Silver - ZrO_2
PRE80/A	Al_2O_3
PRE80/M	MgO
PRE80/S	SiO_2
PRE80/T	TiO_2
PRE80/Z	"ZrOH"
PRE81	Silver - Al_2O_2
PRE82/M	Silver - MgO
PRE82/S	Silver - SiO_2
PRE82/T	Silver - TiO_2
PRE82/Z	Silver - ZrO_2
PRE83	0.01% Palladium - Silver - Al_2O_3
PRE84	Chromium - Silver - Al_2O_3
PRE85	Palladium - Silver - Al_2O_3
PRE86/A	Chromium - Al_2O_3
PRE86/M	Chromium - MgO
PRE86/S	Chromium - SiO_2
PRE86/T	Chromium - TiO_2
PRE86/Z	Chromium - ZrO_2
PRE87/A	Palladium - Al_2O_3
PRE87/M	Palladium - MgO
PRE87/S	Palladium - SiO_2
PRE87/T	Palladium - TiO_2
PRE87/Z	Palladium - ZrO_2

A2.2.3 Experimental Data

Data presented are in percentage peak area as determined by GC analysis. A dash represents zero.

Expt	Catalyst *Feedstock*	Run	Benz	Tol	EB	OX	MX	PX	T1	T2
1/96	Comm A	1	-	-	-	-	-	-	200	200
	Feed: OX	2	-	-	-	-	-	-	200	200
2/96	Glass Beads	1	-	-	-	100	-	-	319	325
	Feed: OX	2	-	-	-	100	-	-	329	332
		3	-	-	-	100	-	-	332	385
3/96	Comm B	1	-	-	-	100	-	-	385	385
	Feed: OX	2	-	-	-	100	-	-	376	397
		3	-	-	-	100	-	-	397	396
		4	-	-	-	100	-	-	399	401
4/96	Comm C	1	-	-	-	100	-	-	231	232
	Feed: OX	2	-	-	-	100	-	-	246	249
		3	-	-	-	100	-	-	378	379
		4	-	-	-	100	-	-	406	406
5/96	PRE18-SiO_2	1	-	-	-	-	-	-	190	196
	Feed: OX	2	-	-	-	-	-	-	316	321
		3	-	0.1	-	99.8	-	0.1	421	424
		4	-	-	-	-	-	-	415	409
6/96	PRE18X-SiO_2	1	-	-	-	-	-	-	418	421
	Feed:OX	2	-	-	-	-	-	-	413	401
7/96	Comm D	1	-	-	-	89.1	8.7	2.1	228	230
	Feed:OX	2	-	2.1	-	23.6	53.7	20.4	351	361
		3	-	4.7	-	21.1	51.5	20.1	409	411
		4	-	8.8	-	19.6	47.6	17.0	460	460
8/96	Comm E	1	-	0.2	-	96.2	3.2	0.4	209	232
	Feed: OX	2	-	1.1	-	79.5	16.2	2.1	271	282
		3	-	3.3	-	51.1	36.0	7.3	352	352
		4	-	2.2	-	66.1	26.0	4.4	400	401
		5	-	2.5	-	71.2	20.2	2.5	470	481
9/96	as 8/96	1	-	-	-	100	-	-	227	232
	Feed: OX	2	-	-	-	99.7	0.2	-	309	313
		3	-	-	-	98.2	1.3	0.5	362	362
		4	-	-	-	94.4	4.6	1.0	399	402
		5	-	0.7	-	79.2	16.7	3.4	482	482

10/96	Comm D	1	-	-	-	78.0	15.8	6.1	224	236
	Feed: OX	2	-	0.4	-	32.9	47.6	18.7	291	296
		3	-	3.5	-	22.0	52.3	19.3	406	411
11/96	as 10/96	1	-	-	-	89.4	8.2	2.3	218	212
	Feed: OX	2	-	0.1	-	45.2	38.8	15.5	273	285
		3	-	1.2	-	23.0	54.5	20.1	347	355
		4	-	3.2	-	22.1	52.2	19.7	408	412
		5	3.4	6.9	-	20.0	46.3	17.5	466	465
	Feed: EB	6	3.7	1.5	4.7	20.4	48.8	18.6	368	358
	Feed: EB	7	40.2	5.3	34.6	1.6	2.7	1.8	456	467
12/96	PRE29	1	-	-	4.0	95.6	-	-	244	247
	Feed: OX	2	-	-	0.1	99.6	0.1	-	305	304
		3	-	-	-	99.6	0.1	-	358	360
		4	-	-	-	99.6	0.1	-	414	419
		5	-	-	-	99.5	0.2		463	477
14/96	PRE30	1	-	-	0.1	99.6	0.1	-	252	249
	Feed: OX	2	-	-	-	99.6	0.1	-	308	317
		3	-	-	-	99.8	0.1	-	376	383
		4	-	-	-	99.7	0.1	-	433	435
		5	-	-	-	99.7	0.1	-	482	485
15/96	PRE23	1	-	-	-	99.7	0.1	-	236	236
	Feed: OX	2	-	-	-	99.7	0.1	-	330	325
		3	-	-	-	99.7	0.1	-	380	380
		4	-	-	-	99.7	0.1	-	372	377
		5	-	-	-	99.7	0.1	-	481	487
16/96	PRE27	1	-	-	-	99.7	0.2	-	261	263
	Feed: OX	2	-	0.4	-	99.2	0.2	-	316	327
		3	-	-	-	99.5	0.2	-	390	389
		4	-	0.5	-	99.2	0.1	-	442	444
		5	-	-	-	99.7	0.1	-	506	505
	Feed: EB	6	-	-	45.1	55.8	-	-	448	449
17/96	PRE25	1	-	-	-	99.6	0.2	-	254	250
	Feed: OX	2	-	-	0.1	99.5	0.1	-	348	349
		3	-	-	-	99.7	0.2	-	415	416
		4	-	-	0.1	99.5	0.1	-	487	487

18/96	PRE28	1	-	-	0.1	99.6	0.1	-	261	263
	Feed: OX	2	-	-	-	99.8	0.1	-	294	299
		3	-	-	-	99.7	0.1	-	356	357
		4	-	-	-	99.6	0.1	-	412	412
		5	-	0.3	-	99.5	-	-	484	487
19/96	PRE24	1	-	0.5	-	98.8	0.5	-	254	249
	Feed: OX	2	-	-	-	99.3	0.4	-	310	313
		3	-	-	-	99.4	0.4	-	381	380
		4	-	0.3	-	99.0	0.4	-	441	444
		5	-	0.2	-	99.4	0.2	-	491	497
20/96	PRE31	1	-	-	-	99.7	0.1	-	279	274
	Feed: OX	2	-	-	-	99.7	0.1	-	323	326
		3	-	-	-	99.7	0.1	-	389	393
		4	-	0.8	-	98.9	0.1	-	443	444
		5	-	-	-	100	-	-	495	495
21/96	PRE26	1	-	-	-	100	-	-	158	160
	Feed: OX	2	15.4	-	-	85.3	-	-	186	207
		3	-	-	-	99.8	-	-	263	277
		4	-	-	-	99.6	0.2	-	329	335
		5	-	0.1	-	99.4	0.4	-	388	389
		6	-	0.2	-	99.3	0.2	-	433	442
		7	-	-	-	99.7	0.1	-	488	492
22/96	PRE22	1	-	-	-	99.7	0.1	0.1	157	158
	Feed: OX	2	-	-	-	99.7	0.1	0.1	197	207
		3	-	-	-	100	-	-	261	272
		4	-	-	-	99.7	0.1	-	320	330
		5	-	-	-	99.6	0.2	0.1	382	385
		6	-	-	-	99.8	-	-	422	439
		7	-	-	-	99.6	0.1	-	463	496
23/96	Comm D	1	-	-	68.8	20.5	5.4	5.4	257	259
	Feed: EB	2	5.2	-	88.6	0.2	-	-	343	344
		3	19.3	0.4	61.2	-	-	-	389	396
		4	29.8	2.3	46.9	0.3	1.4	-	442	445
		5	38.3	6.7	37.1	0.5	0.8	-	486	490
24/96	as 23/96	1	-	53.3	46.6	0.1	-	-	250	263
	Feed: Tol	2	-	99.3	0.7	-	-	-	333	344
		3	-	99.8	0.1	-	-	-	391	398
		4	2.1	97.5	-	0.1	0.2	0.1	439	440
		5	2.7	95.3	-	0.4	1.1	0.4	497	501

25/96	as 23/96	1	-	92.8	0.2	0.3	0.2	0.3	283	279
	Feed: Tol/MeOH, 1:1	2	1.1	33.9	0.4	6.9	16.2	5.8	360	378
		3	6.1	30.7	0.6	8.4	21.8	7.8	440	440
		4	4.6	30.3	0.6	9.3	23.8	8.2	476	476
		5	5.7	27.3	0.5	10.2	25.7	8.7	529	529
26/96	as 23/96	1	-	9.6	18.1	4.5	65.4	1.8	247	262
	Feed: mixed xyl	2	-	1.1	19.1	7.8	63.3	7.9	325	328
		3	3.0	1.1	17.0	14.8	46.4	16.2	367	387
		4	5.4	1.5	12.2	17.1	44.0	16.0	436	439
		5	9.0	3.3	7.6	17.2	42.6	15.5	496	499

Expt	**Catalyst** *Feedstock*	**Run**	**Benz**	**Tol**	**EB**	**OX**	**MX**	**PX**	**T1**	**T2**
1/97	PRE80/S	1	-	-	-	99.0	-	-	255	260
	Feed: OX	2	-	-	-	99.0	-	-	300	344
		3	-	-	-	99.0	-	-	352	374
		4	-	-	-	99.0	-	-	401	415
		5	-	-	-	99.0	-	-	455	474
2/97	PRE86/M	1	-	-	-	99.0	-	-	228	267
	Feed:OX	2	-	-	-	99.0	-	-	261	301
		3	-	-	-	99.0	-	-	360	368
3/97	PRE78/M	1	-	-	-	99.0	-	-	251	264
	Feed:OX	2	-	-	-	99.0	-	-	300	327
		3	-	-	-	99.0	-	-	350	373
		4	-	-	-	99.0	-	-	403	421
		5	-	-	-	99.0	-	-	447	500
4/97	PRE78/S	1	-	-	-	99.0	-	-	120	205
	Feed:OX	2	-	-	-	99.0	-	-	238	259
		3	-	-	-	99.0	-	-	280	295
		4	-	-	-	99.0	-	-	312	359
		5	-	-	-	99.0	-	-	359	386
		6	-	-	-	99.0	-	-	430	488
5/97	PRE86/S	1	-	-	-	99.0	-	-	163	239
	Feed:OX	2	-	-	-	99.0	-	-	253	275
		3	-	-	-	99.0	-	-	306	333
		4	-	-	-	99.0	-	-	345	385
		5	-	-	-	99.0	-	-	391	457
		6	-	-	-	98.9	-	-	458	505

6/97	PRE76/M	1	-	-	-	99.0	-	-	129	247
	Feed: OX	2	-	-	-	99.0	-	-	265	298
		3	-	-	-	99.0	-	-	312	333
		4	-	-	-	99.0	-	-	360	386
		5	-	-	-	99.0	-	-	434	427
		6	-	-	-	99.0	-	-	425	529
		7	-	-	-	99.0	-	-	538	581
7/97	PRE77/S	1	-	-	-	99.0	-	-	250	299
	Feed: OX	2	-	-	-	99.0	-	-	302	313
		3	-	-	-	99.0	-	-	353	417
		4	-	-	-	99.0	-	-	409	423
		5	-	-	-	99.0	-	-	441	482
8/97	PRE85	1	-	-	-	99.1	-	-	168	219
	Feed: OX	2	-	-	-	99.1	-	-	229	271
		3	-	-	-	99.1	-	-	271	311
		4	-	-	-	99.1	-	-	355	370
		5	-	-	-	99.1	-	-	370	380
		6	-	-	-	99.1	-	-	403	443
		7	-	-	-	99.1	-	-	453	464
9/97	PRE87/S	1	-	-	-	99.1	-	-	242	277
	Feed: OX	2	-	-	-	99.1	-	-	299	339
		3	-	-	-	99.1	-	-	352	378
		4	-	-	-	99.1	-	-	401	428
		5	-	-	-	99.1	-	-	460	515
		6	-	-	-	99.1	-	-	515	529
10/97	PRE82/M	1	-	-	-	99.1	-	-	286	329
	Feed: OX	2	-	-	-	99.1	-	-	327	338
		3	-	-	-	99.1	-	-	358	408
		4	-	-	-	99.1	-	-	412	443
		5	-	-	-	99.1	-	-	458	484
		6	-	-	-	99.1	-	-	504	523
11/97	PRE86/Z	1	-	-	-	99.0	-	-	147	298
	Feed: OX	2	-	-	-	99.2	-	-	306	328
		3	-	-	-	99.1	-	-	343	406
		4	-	-	-	99.1	-	-	414	424
		5	-	-	-	99.1	-	-	449	470
		6	-	-	-	99.1	-	-	456	536
12/97	PRE77/Z	1	-	-	-	99.1	-	-	238	297
	Feed: OX	2	-	-	-	99.1	-	-	297	316
		3	-	-	-	99.0	-	-	348	389
		4	-	-	-	99.1	-	-	400	441
		5	-	-	-	99.1	-	-	452	480

14/97	PRE81	1	-	-	-	99.0	-	-	124	249
	Feed: OX	2	-	-	-	99.1	-	-	249	302
		3	-	-	-	99.1	-	-	302	331
		4	-	-	-	99.2	-	-	350	395
		5	-	-	-	99.0	-	-	403	454
		6	-	-	-	99.0	-	-	454	521
15/97	PRE82/S	1	-	-	-	99.0	-	-	210	253
	Feed: OX	2	-	-	-	99.0	-	-	308	337
		3	-	-	-	99.0	-	-	355	417
		4	-	-	-	99.1	-	-	421	450
		5	-	-	-	99.1	-	-	450	462
16/97	PRE84	1	-	-	-	99.0	-	-	213	264
	Feed: OX	2							297	323
		3							350	369
		4	-	-	-	99.1	-	-	402	448
		5	-	-	-	99.1	-	-	448	481
17/97	PRE87/T	1	-	-	-	99.1	-	-	206	289
	Feed: OX	2	-	-	-	99.1	-	-	289	328
		3	-	-	-	99.0	-	-	328	344
		4	-	-	-	99.1	-	-	413	466
		5	-	-	-	99.1	-	-	466	501
18/97	PRE76/S	1	-	-	-	99.0	-	-	186	269
	Feed: OX	2	-	-	-	99.1	-	-	296	334
		3	-	-	-	99.1	-	-	353	390
		4	-	-	-	99.1	-	-	397	455
		5	-	-	-	99.1	-	-	455	470
19/97	PRE77/M	1	-	-	-	99.1	-	-	230	253
	Feed: OX	2	-	-	-	99.1	-	-	305	353
		3	-	-	-	99.0	-	-	353	389
		4	-	-	-	99.0	-	-	400	449
		5	-	-	-	99.0	-	-	449	495
20/97	PRE86/T	1	-	-	-	99.0	-	-	225	278
	Feed: OX	2	-	-	-	99.1	-	-	300	343
		3	-	-	-	99.1	-	-	348	389
		4	-	-	-	99.1	-	-	406	428
		5	-	-	-	99.1	-	-	448	500
21/97	PRE80/T	1	-	-	-	99.1	-	-	200	285
	Feed: OX	2	-	-	-	99.1	-	-	303	350
		3	-	-	-	99.1	-	-	350	384
		4	-	-	-	99.1	-	-	402	449
		5	-	-	-	99.1	-	-	449	474

22/97	PRE82/T Feed: OX	1	-	-	-	99.1	-	-	208	266
23/97	PRE82/T	1	-	-	-	99.1	-	-	250	296
	Feed: OX	2	-	-	-	99.1	-	-	301	331
		3	-	-	-	99.0	-	-	352	397
		4	-	-	-	99.1	-	-	400	408
		5	-	-	-	99.1	-	-	450	470
24/97	PRE84/A	1	-	-	-	99.1	-	-	202	307
	Feed: OX	2	-	-	-	99.1	-	-	307	350
		3	-	-	-	99.1	-	-	350	369
		4	-	-	-	99.0	-	-	401	430
		5	-	-	-	98.9	-	-	451	525
25/97	PRE77/T	1	-	-	-	99.0	-	-	217	304
	Feed: OX	2	-	-	-	99.2	-	-	304	369
		3	-	-	-	99.1	-	-	369	388
		4	-	-	-	99.1	-	-	404	454
		5	-	-	-	99.1	-	-	454	480
26/97	PRE80/Z	1	-	-	-	99.0	-	-	229	313
	Feed: OX	2	-	-	-	99.1	-	-	313	353
		3	-	-	-	99.1	-	-	353	388
		4	-	-	-	99.1	-	-	408	457
		5	-	-	-	99.1	-	-	457	490
27/97	PRE82/Z	1	-	-	-	99.1	-	-	174	234
	Feed: OX	2	-	-	-	99.1	-	-	254	318
		3	-	-	-	99.1	-	-	318	352
		4	-	-	-	99.1	-	-	352	406
		5	-	-	-	99.1	-	-	406	435
		6	-	-	-	99.1	-	-	454	536
28/97	PRE76/Z	1	-	-	-	99.1	-	-	165	264
	Feed: OX	2	-	-	-	99.1	-	-	264	329
		3	-	-	-	99.0	-	-	329	391
		4	-	-	-	99.0	-	-	403	449
		5	-	-	-	99.1	-	-	449	491
29/97	PRE86/A	1	-	-	-	98.8	-	-	191	312
	Feed: OX	2	-	-	-	99.1	-	-	312	360
		3	-	-	-	99.1	-	-	360	407
		4	-	-	-	99.1	-	-	407	429
		5	-	-	-	99.1	-	-	453	490

30/97	PRE87/Z	1	-	-	-	99.1	-	-	153	216
	Feed: OX	2	-	-	-	99.1	-	-	216	303
		3	-	-	-	99.1	-	-	303	328
		4	-	-	-	99.1	-	-	356	466
31/97	PRE78/T	1	-	-	-	99.1	-	-	243	325
	Feed: OX	2	-	-	-	99.1	-	-	325	383
		3	-	-	-	99.0	-	-	383	413
		4	-	-	-	99.1	-	-	413	450
		5	-	-	-	99.1	-	-	450	551
32/97	PRE78/Z	1	-	-	-	99.1	-	-	230	295
	Feed: OX	2	-	-	-	99.1	-	-	295	355
		3	-	-	-	99.1	-	-	355	398
		4	-	-	-	99.1	-	-	398	435
		5	-	-	-	99.0	-	-	457	543
33/97	PRE87/M	1	-	-	-	99.1	-	-	203	251
	Feed: OX	2	-	-	-	99.2	-	-	251	304
		3	-	-	-	99.2	-	-	304	337
		4	-	-	-	99.3	-	-	337	397
		5	-	-	-	99.3	-	-	400	455
		6	-	-	-	99.3	-	-	455	489
34/97	PRE76/T	1	-	-	-	99.2	-	-	185	300
	Feed: OX	2	-	-	-	99.3	-	-	300	358
		3	-	-	-	99.2	-	-	358	401
		4	-	-	-	99.2	-	-	401	439
		5	-	-	-	99.3	-	-	489	594
35/97	PRE80/M	1	-	-	-	99.3	-	-	225	301
	Feed: OX	2	-	-	-	99.3	-	-	301	347
		3	-	-	-	99.3	-	-	351	388
		4	-	-	-	99.3	-	-	404	455
		5	-	-	-	99.3	-	-	455	515
36/97	PRE80/A	1	-	-	-	99.3	-	-	249	318
	Feed: OX	2	-	-	-	99.3	-	-	318	374
		3	-	-	-	99.3	-	-	374	419
		4	-	-	-	99.3	-	-	419	456
		5	-	-	-	99.3	-	-	456	521

37/97	PRE83	1	-	-	-	99.3	-	-	281	291
	Feed: OX	2	-	-	-	99.3	-	-	302	365
		3	-	-	-	99.3	-	-	365	380
		4	-	-	-	99.3	-	-	404	455
		5	-	-	-	99.2	-	-	455	519
38/97	PRE86/M - ex 2/97	1	-	-	-	99.3	-	-	232	314
	Feed: OX	2	-	-	-	99.3	-	-	314	375
		3	-	-	-	99.3	-	-	375	413
		4	-	-	-	99.2	-	-	413	423
		5	-	-	-	99.2	-	-	423	480
39/97	Zirconia, dried	1	-	-	-	99.3	-	-	247	321
	Feed: OX	2	-	-	-	99.3	-	-	321	377
		3	-	-	-	99.3	-	-	377	407
		4	-	-	-	99.2	-	-	407	437
		5	-	-	-	99.2	-	-	437	561
40/97	PRE80/T	1	-	-	-	99.3	-	-	242	305
	Feed: OX	2	-	-	-	99.3	-	-	305	337
		3	-	-	-	99.3	-	-	350	401
		4	-	-	-	99.3	-	-	401	436
		5	-	-	-	99.3	-	-	436	533
41/97	PRE87/Z	1	-	-	-	99.3	-	-	215	302
	Feed: OX	2	-	-	-	99.3	-	-	302	350
		3	-	-	-	99.3	-	-	350	390
		4	-	-	-	99.1	-	-	408	451
		5	-	-	-	99.2	-	-	451	521
42/97	Zirconia, dried	1	-	-	-	99.3	-	-	293	305
	Feed: OX	2	-	-	-	99.3	-	-	305	387
		3	-	-	-	99.3	-	-	387	513
		4	-	-	-	99.3	-	-	513	603
43/97	PRE72	1	-	-	-	99.3	-	-	228	314
	Feed: OX	2	-	-	-	99.3	-	-	314	352
		3	-	-	-	99.3	-	-	352	390
		4	-	-	-	99.3	-	-	403	451
		5	-	-	-	99.3	-	-	451	529

44/97	Zirconia, dried	1	-	-	-	99.3	-	-	216	305
	Feed: OX	2	-	-	-	99.2	-	-	305	350
		3	-	-	-	99.3	-	-	350	390
		4	-	-	-	99.3	-	-	404	460
		5	-	-	-	99.2	-	-	460	499
45/97	PRE75	1	-	-	-	99.1	-	-	246	301
	Feed: OX	2	-	-	-	99.3	-	-	301	358
		3	-	-	-	99.3	-	-	358	390
		4	-	-	-	99.3	-	-	390	436
		5	-	-	-	99.3	-	-	436	542
46/97	Zirconia, dried	1	-	-	-	99.3	-	-	216	303
	Feed: OX	2	-	-	-	99.3	-	-	303	356
		3	-	-	-	99.3	-	-	356	406
		4	-	-	-	99.3	-	-	406	454
		5	-	0.1	-	99.2	-	-	454	543
47/97	PRE82/Z	1	-	-	-	99.3	-	-	220	319
	Feed: OX	2	-	-	-	99.3	-	-	319	354
		3	-	-	-	99.3	-	-	354	400
		4	-	-	-	99.3	-	-	400	469
		5	-	-	-	99.3	-	-	469	547
48/97	PRE73	1	-	-	-	99.3	-	-	256	308
	Feed: OX	2	-	-	-	99.3	-	-	308	341
		3	-	-	-	99.3	-	-	341	388
		4	-	-	-	99.3	-	-	388	458
		5	-	0.1	-	99.2	-	-	458	553
49/97	PRE76/Z	1	-	-	-	99.2	-	-	249	303
	Feed: OX	2	-	-	-	99.2	-	-	303	333
		3	-	-	-	99.2	-	-	333	389
		4	-	-	-	99.0	-	-	389	494
		5	-	0.2	-	98.4		0.6	494	550
50/97	PRE79	1	-	-	-	99.2	-	-	227	312
	Feed: OX	2	-	-	-	99.3	-	-	312	352
		3	-	-	-	99.3	-	-	352	383
		4	-	-	-	99.3	-	-	383	428
		5	-	-	-	99.3	-	-	428	528

51/97	PRE68	1	-	0.2	-	95.9	3.0	231	303
	Feed: OX	2	-	0.2	-	97.6	1.6	303	353
		3	-	0.1	-	98.6	0.7	353	367
		4	-	-	-	99.2	- -	367	450
		5	-	0.1	-	98.8	0.3	450	561
52/97	PRE67	1	-	-	-	99.3	- -	200	313
	Feed: OX	2	-	-	-	99.3	- -	313	351
		3	-	-	-	99.2	- -	351	406
		4	-	0.1	-	99.1	0.2	406	450
		5	-	0.3	-	98.3	0.4	450	536
53/97	PRE70	1	-	-	-	99.3	- -	200	306
	Feed: OX	2	-	0.4	-	98.6	- -	306	353
		3	-	0.1	-	99.1	- -	353	402
		4	-	-	-	99.2	- -	402	421
		5	-	-	-	99.2	- -	421	558
54/97	PRE69	1	-	0.1	-	97.9	1.3	206	300
	Feed: OX	2	-	-	-	98.5	0.9	300	354
		3	-	-	-	99.0	0.3	354	388
		4	-	0.1	-	98.9	0.3	388	479
		5	-	0.2	-	98.9	0.2	479	560
55/97	PRE76/Z	1	-	-	-	99.2	- -	222	307
	Feed: OX	2	-	-	-	99.3	- -	307	350
		3	-	-	-	99.3	- -	350	397
		4	-	-	-	99.3	- -	397	455
		5	-	-	-	99.3	- -	455	615
56/97	PRE76/S	1	-	-	-	99.2	- -	216	320
	Feed: OX	2	-	-	-	99.2	- -	320	354
		3	-	-	-	99.3	- -	354	388
		4	-	-	-	99.3	- -	388	450
		5	-	-	-	99.3	- -	450	591
57/97	PRE82/S	1	-	-	-	99.3	- -	246	309
	Feed: OX	2	-	-	-	99.3	- -	309	369
		3	-	-	-	99.3	- -	369	411
		4	-	-	-	99.3	- -	411	450
		5	-	-	-	99.3	- -	450	576

58/97	PRE77/T	1	-	-	-	99.3	-	-	220	300
	Feed: OX	2	-	-	-	99.2	-	-	300	359
		3	-	0.2	-	98..9		0.1	359	417
		4	-	0.3	-	98.5		0.2	417	443
		5	-	0.2	-	98.9		0.1	443	531
59/97	PRE84/M	1	-	-	-	99.3	-	-	242	310
	Feed: OX	2	-	-	-	99.3	-	-	310	359
		3	-	-	-	99.3	-	-	359	383
		4	-	-	-	99.3	-	-	383	450
		5	-	-	-	99.3	-	-	450	552
60/97	PRE77/M	1	-	-	-	99.2	-	-	268	313
	Feed: OX	2	-	-	-	99.3	-	-	313	351
		3	-	-	-	99.3	-	-	351	398
		4	-	-	-	99.3	-	-	398	453
		5	-	-	-	99.3	-	-	453	555
61/97	PRE80/S	1	-	0.1	-	99.3	-	-	199	291
	Feed: OX	2	-	-	-	99.3	-	-	291	353
		3	-	-	-	99.3	-	-	353	403
		4	-	-	-	99.3	-	-	403	469
		5	-	-	-	99.3	-	-	469	545
62/97	PRE87/A	1	-	-	-	99.2	-	-	202	301
	Feed: OX	2	-	-	-	99.3	-	-	301	351
		3	-	-	-	99.2	-	-	351	405
		4	-	-	-	99.2	-	-	405	474
		5	0.1	0.8	-	98.4	-	-	474	580
63/97	PRE78/Z	1	-	-	-	99.2	-	-	214	303
	Feed: OX	2	-	-	-	99.2	-	-	303	350
		3	-	-	-	99.2	-	-	350	403
		4	-	-	-	99.2	-	-	403	459
		5	-	-	-	99.2	-	-	459	557
64/97	PRE76/M	1	-	-	-	99.2	-	-	202	303
	Feed: OX	2	-	-	-	99.2	-	-	303	347
		3	-	-	-	99.2	-	-	347	397
		4	-	-	-	99.2	-	-	397	457
		5	-	-	-	99.2	-	-	457	545
65/97	PRE76/T	1	-	-	-	99.2	-	-	205	306
	Feed: OX	2	-	-	-	99.2	-	-	306	350
		3	-	-	-	99.2	-	-	350	407
		4	-	-	-	99.1	-	-	407	476
		5	-	-	-	99.2	-	-	476	545

66/97	PRE77/Z	1	-	-	-	99.2	-	-	201	323
	Feed: OX	2	-	-	-	-	-	-	323	369
		3	-	-	-	99.2	-	-	369	410
		4	-	-	-	99.2	-	-	410	443
		5	-	-	-	99.2	-	-	443	519
67/97	PRE82/T	1	-	-	-	99.2	-	-	246	305
	Feed: OX	2	-	-	-	99.2	-	-	305	351
		3	-	-	-	99.2	-	-	351	398
		4	-	-	-	99.2	-	-	398	443
		5	-	-	-	99.2	-	-	443	529
68/97	PRE78/M	1	-	-	-	99.2	-	-	251	298
	Feed: OX	2	-	-	-	99.2	-	-	298	347
		3	-	-	-	99.2	-	-	347	399
		4	-	-	-	99.2	-	-	399	471
		5	-	-	-	99.2	-	-	471	536
69/97	PRE78/T	1	-	-	-	99.2	-	-	201	275
	Feed: OX	2	-	-	-	99.2	-	-	275	373
		3	-	-	-	99.2	-	-	373	411
		4	-	-	-	99.1	-	-	411	457
		5	-	-	-	99.1	-	-	457	570

Appendix 3.1: Developmental Work on Sulphated Zirconia Catalysts

A3.1.1 Catalysts Prepared with Different Heating Rates

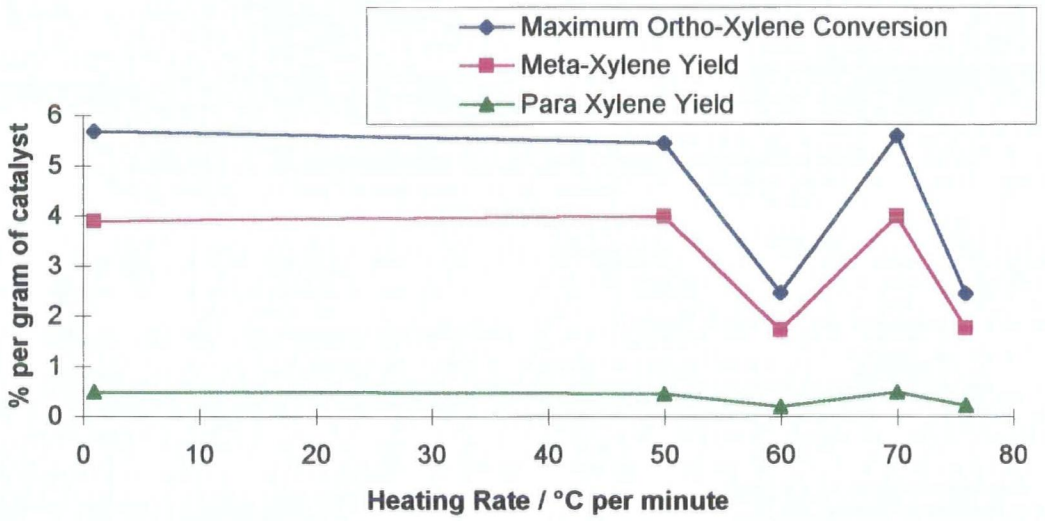

Fig. A3.1: Dependence of Catalyst Activity on Heating Rate

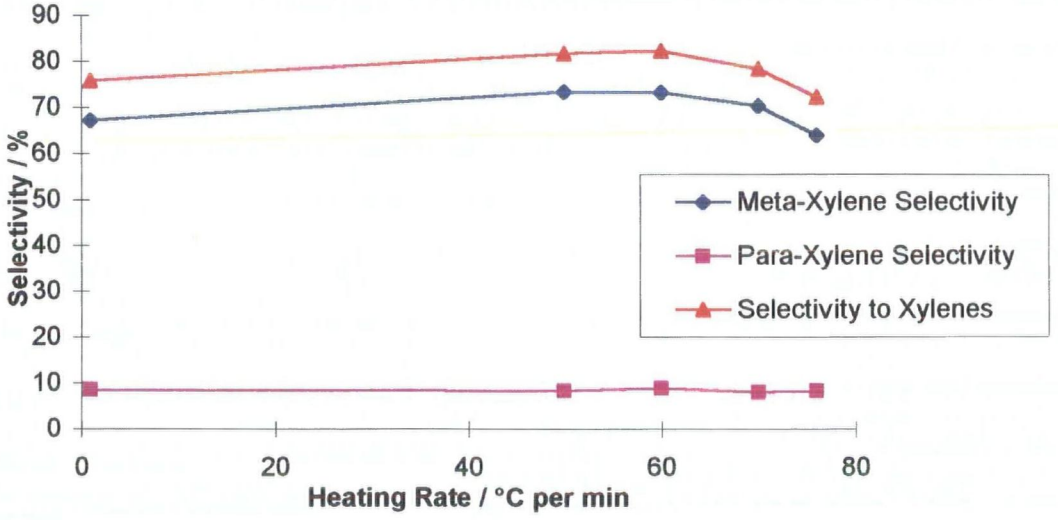

Fig. A3.2: Dependence of Catalyst Selectivity on Heating Rate

A3.1.2 Catalysts Prepared with Different Cooling Rates

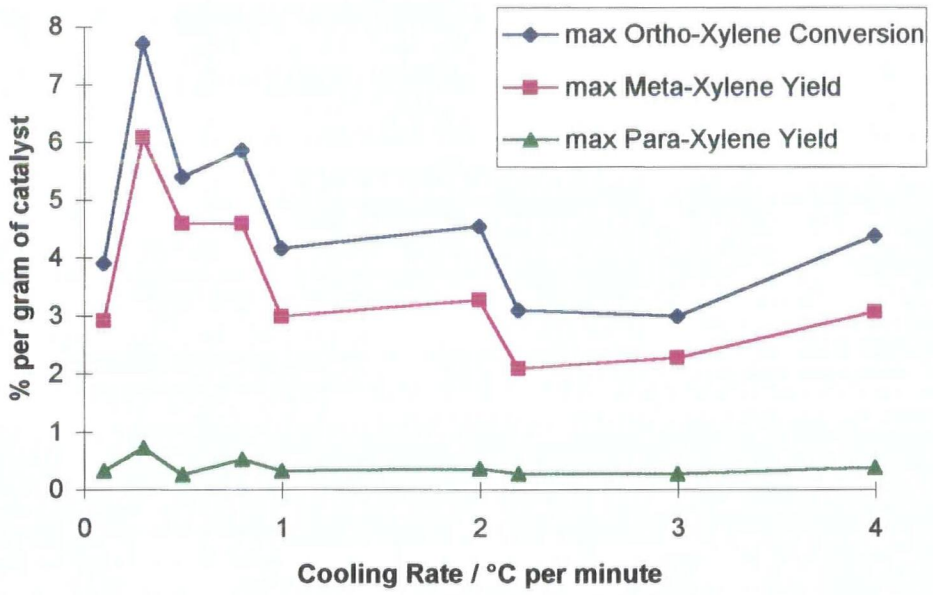

Fig. A3.3: Dependence of Catalyst Activity on Cooling Rate

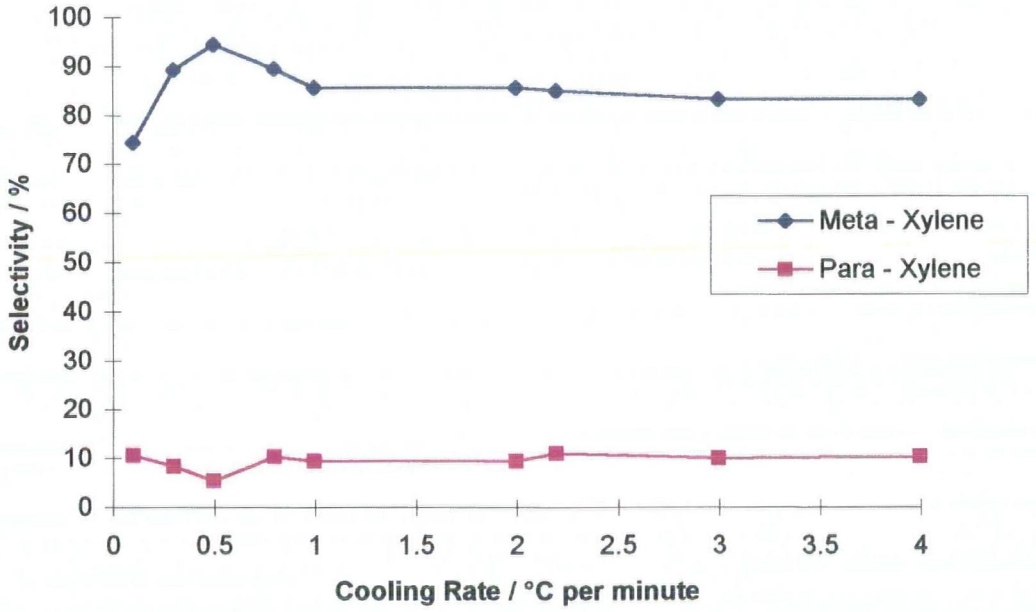

Fig. A3.4: Dependence of Catalyst Selectivity on Cooling Rate

A3.1.3 Catalysts Calcined at Different Temperatures

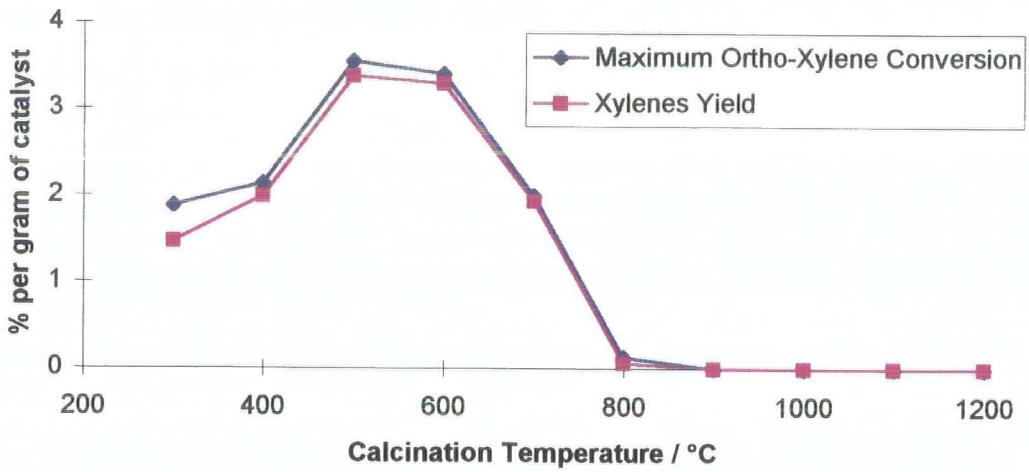

Fig. A3.5: Effect of Calcination Temperature on the Activity of Sulphated Zirconia Catalysts

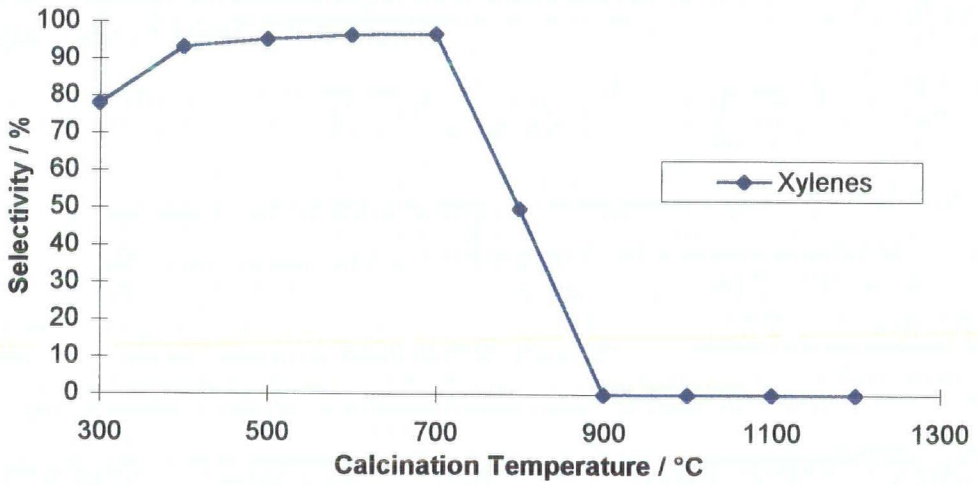

Fig. A3.6: Effect of Calcination Temperature on Selectivity of Sulphated Zirconia Catalysts

A3.1.4 Catalysts Calcined for Different Lengths of Time

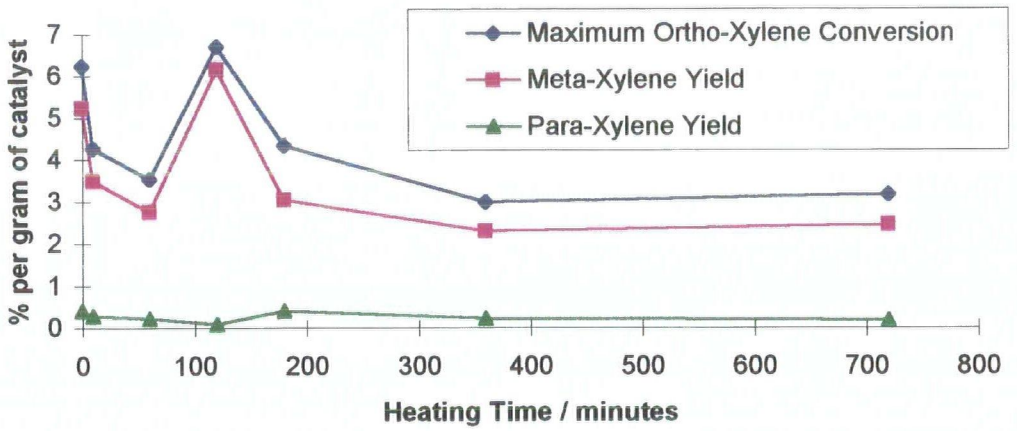

Fig. A3.7: Changes in Catalyst Activity with Calcination Period

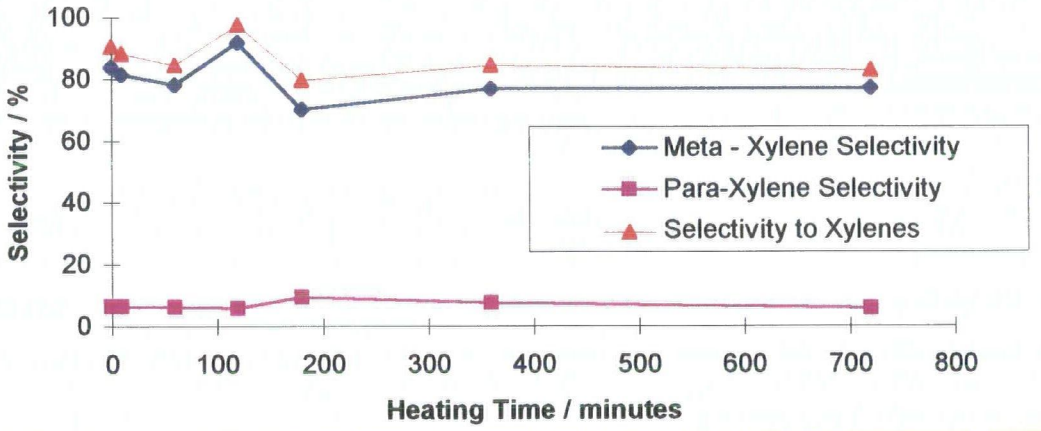

Fig. A3.8: Dependence of Catalyst Selectivity on Calcination Period

A3.1.5 Catalysts Stored and Activated in Different Ways

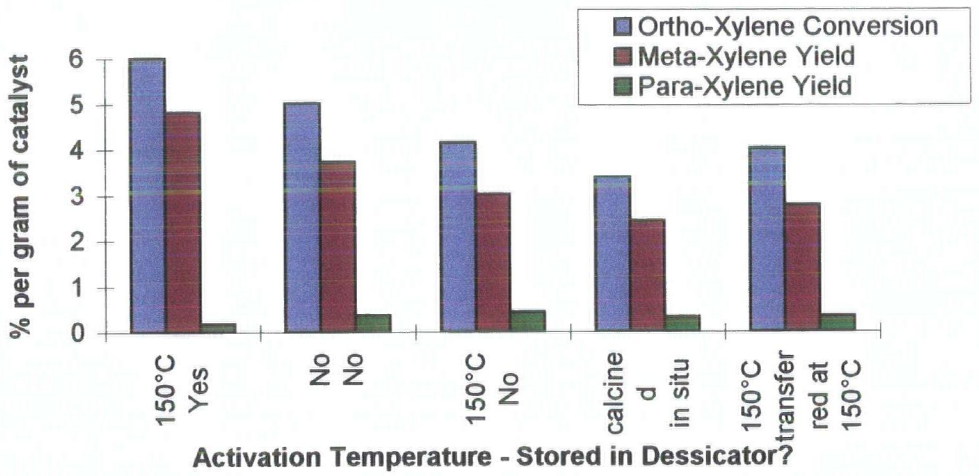

Fig. A3.9: Dependence of Catalyst Activity on Storage and Activation Procedures

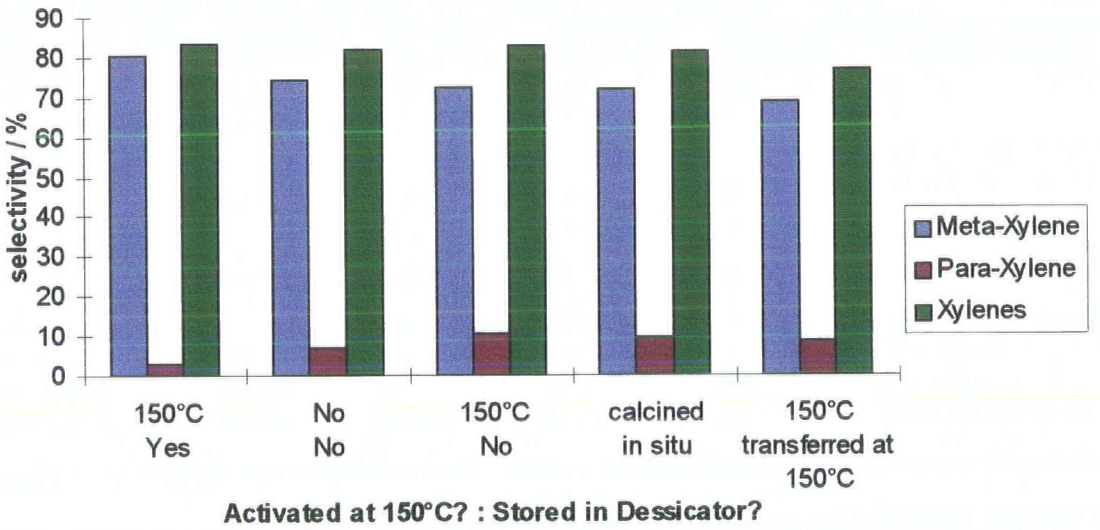

Fig. A3.10: Dependence of Catalyst Selectivity on Activation and Storage Procedures

A3.1.6 Catalysts Prepared with Different Sources of Sulphur and Zirconium

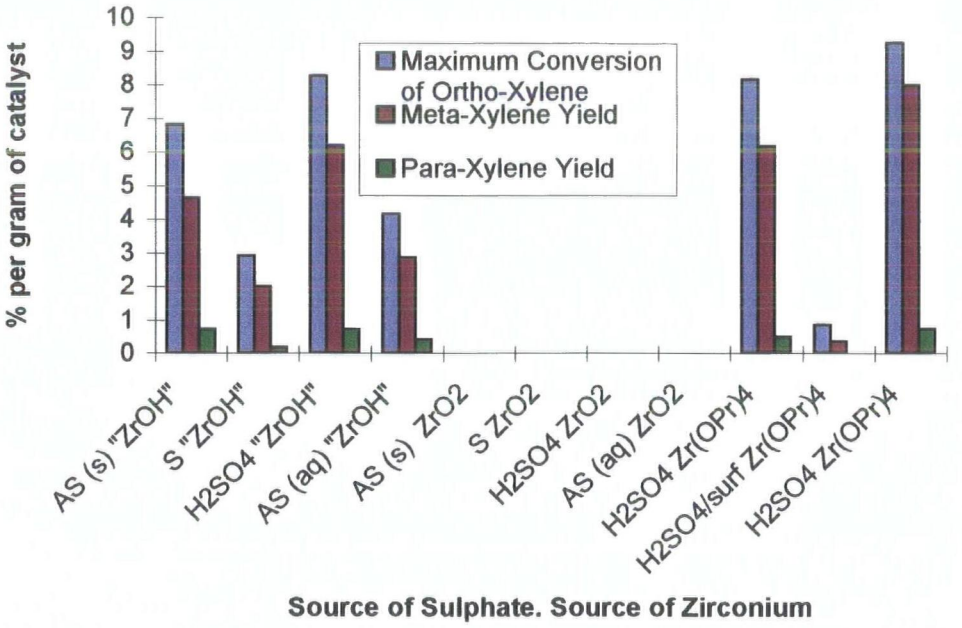

Fig. A3.11: Changes in Catalyst Activity using Different Sources of Sulphate and Zirconium

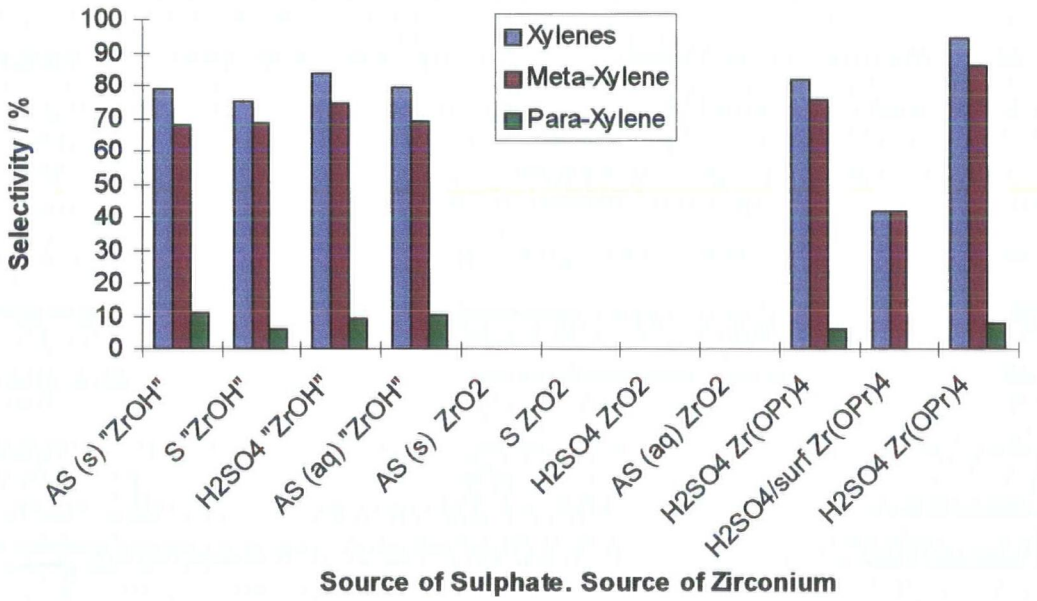

Fig. A3.12: Changes in Catalyst Selectivity using Different Sources of Sulphate and Zirconium

A3.1.7 Catalysts Containing Different Amounts of Sulphate

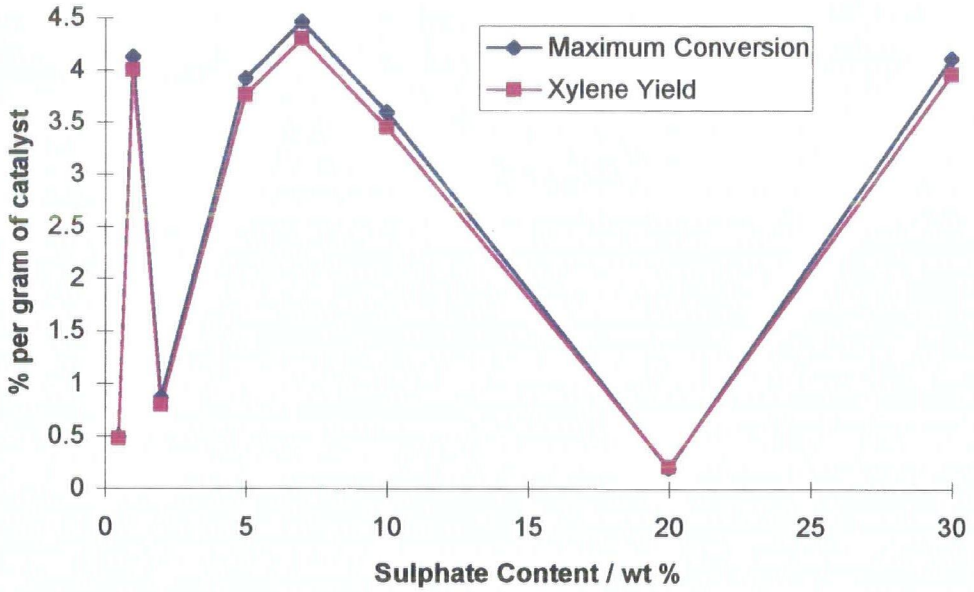

Fig. A3.13: Effect of Sulphate Content on Catalyst Activity

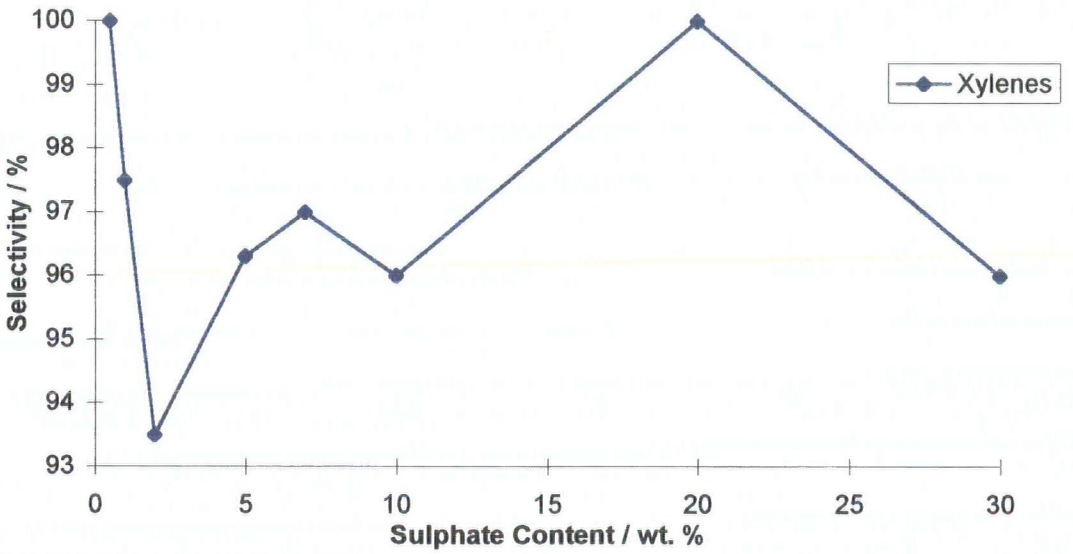

Fig. A3.14: Changes in Catalyst Selectivity with Sulphate Content

A3.1.8 Catalysts Prepared using Other Dopants in place of Sulphate

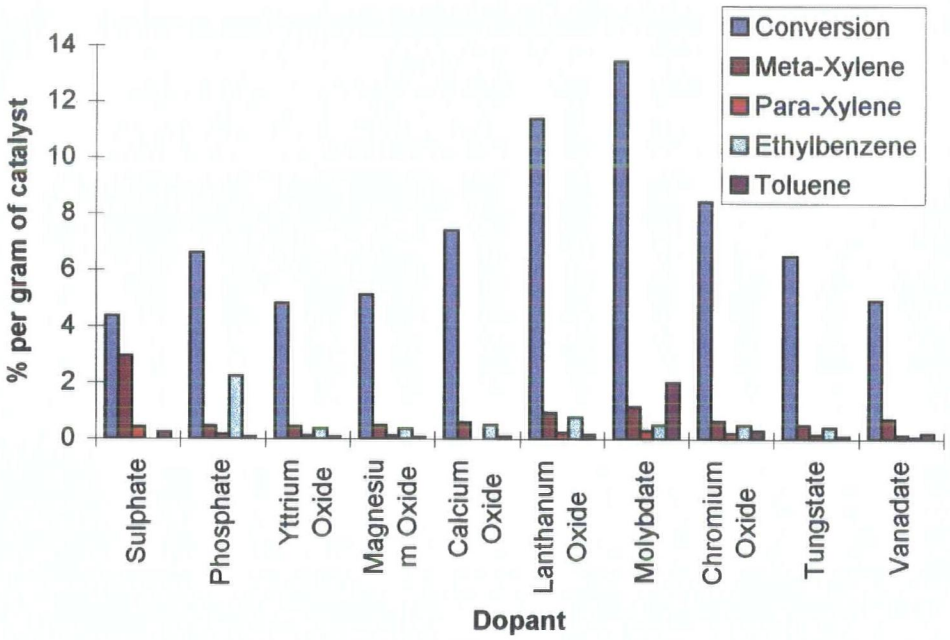

Fig. A3.15: Changes in Catalyst Activity using Different Dopants

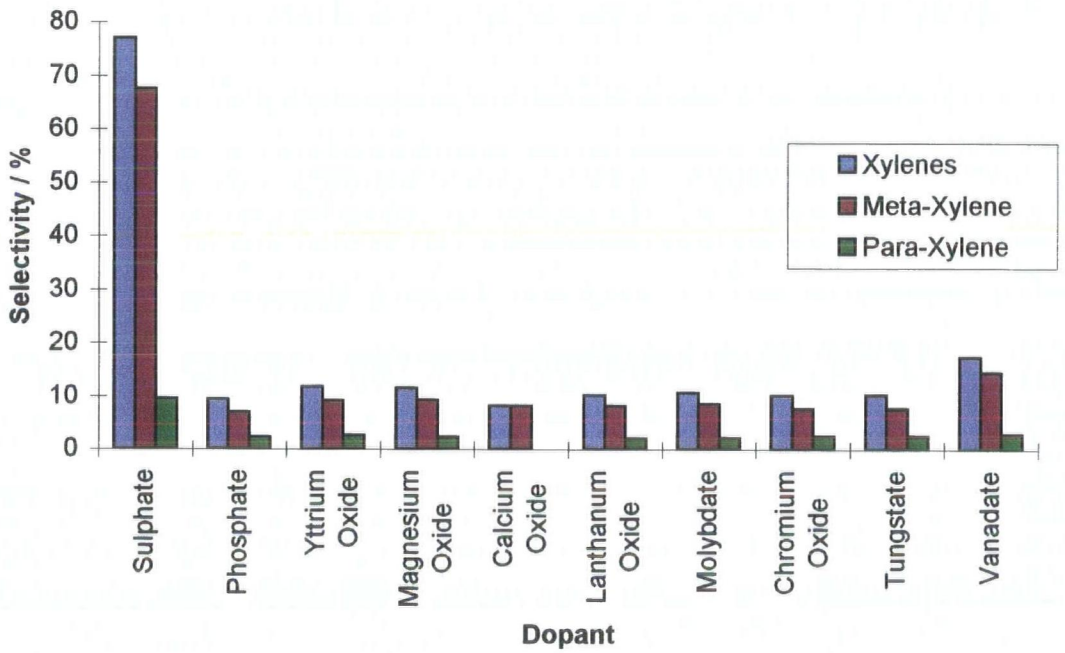

Fig A3.16: Dependence of Catalyst Selectivity on Dopant

A3.1.9 Catalysts Prepared with Different Grinding Times

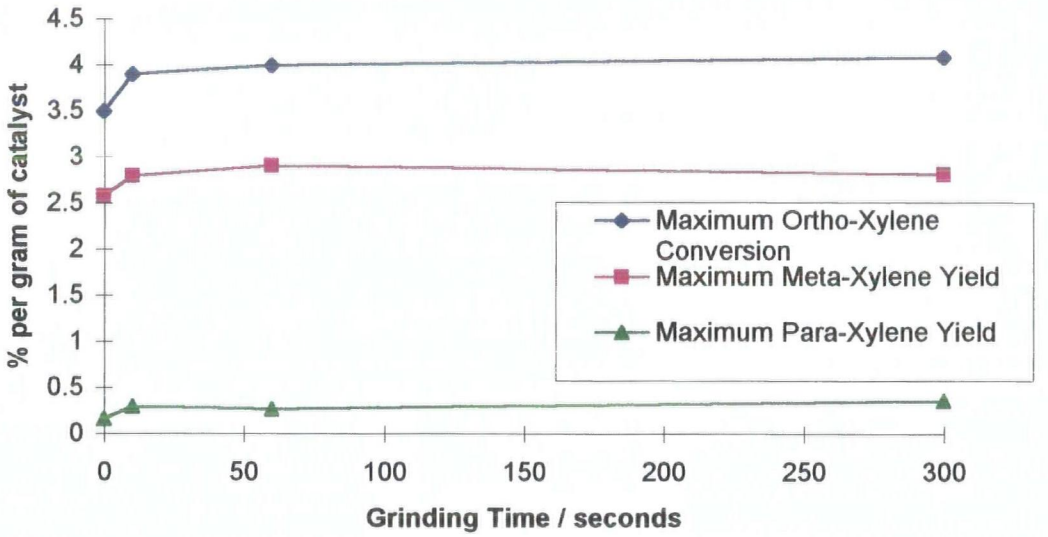

Fig. A3.17: Dependence of Activity on Grinding Time

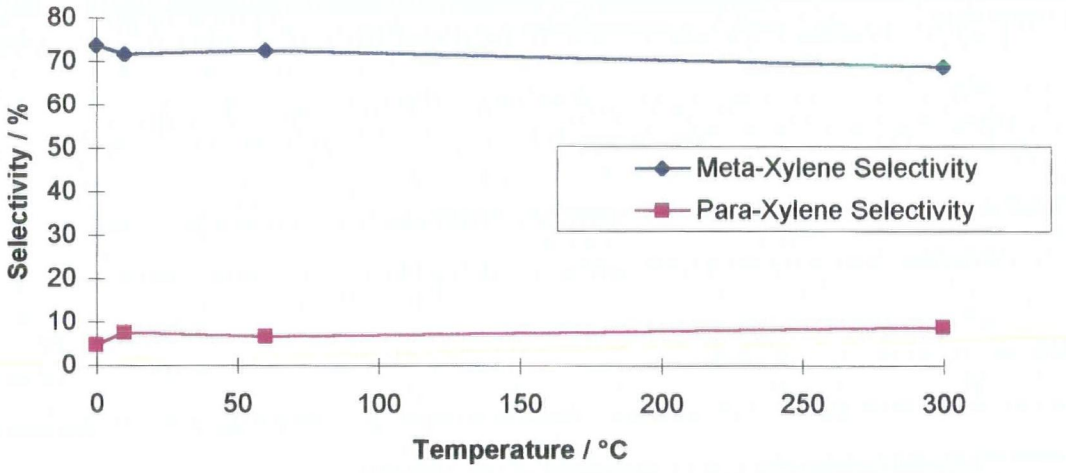

Fig. A3.18: Dependence of Catalyst Selectivity on Grinding Time

Appendix 3.2: Raw Data from Catalyst Testwork

A3.2.1 Key to Abbreviations Used

Benz	benzene
EB	ethylbenzene
Expt	experiment
MeOH	methanol
MX	*meta*-xylene
OX	*ortho*-xylene
PRE	"P.R. Ellis" sample number
PX	*para*-xylene
T1	initial reaction temperature
T2	final reaction temperature
Tol	toluene
'ZrOH'	amorphous "zirconium hydroxide"

A3.2.2 Key to Catalysts Used

PRE93/A	Ammonium Sulphate - "ZrOH" with 0.5wt% Sulphate
PRE93/B	Ammonium Sulphate - "ZrOH" with 1wt% Sulphate
PRE93/C	Ammonium Sulphate - "ZrOH" with 2wt% Sulphate
PRE93/D	Ammonium Sulphate - "ZrOH" with 5wt% Sulphate
PRE93/E	Ammonium Sulphate - "ZrOH" with 7wt% Sulphate
PRE93/F	Ammonium Sulphate - "ZrOH" with 10wt% Sulphate
PRE93/G	Ammonium Sulphate - "ZrOH" with 20wt% Sulphate
PRE93/H	Ammonium Sulphate - "ZrOH" with 30wt% Sulphate
PRE94/A	Ammonium Sulphate - "ZrOH" calcined at 600°C
PRE94/B	Ammonium Sulphate - "ZrOH" calcined at 300°C
PRE94/C	Ammonium Sulphate - "ZrOH" calcined at 400°C
PRE94/D	Ammonium Sulphate - "ZrOH" calcined at 500°C
PRE94/E	Ammonium Sulphate - "ZrOH" calcined at 700°C
PRE94/F	Ammonium Sulphate - "ZrOH" calcined at 800°C
PRE94/G	Ammonium Sulphate - "ZrOH" calcined at 900°C
PRE94/H	Ammonium Sulphate - "ZrOH" calcined at 1000°C
PRE94/I	Ammonium Sulphate - "ZrOH" calcined at 1100°C
PRE94/J	Ammonium Sulphate - "ZrOH" calcined at 1200°C
PRE100/A	Ammonium Sulphate - Al_2O_3
PRE100/B	Ammonium Sulphate - Cr_2O_3
PRE100/C	Ammonium Sulphate - MgO
PRE100/D	Ammonium Sulphate - $Ni(OH)_2$
PRE100/E	Ammonium Sulphate - $NiSO_4$
PRE100/F	Ammonium Sulphate - SiO_2
PRE100/G	Ammonium Sulphate - SnO_2
PRE100/H	Ammonium Sulphate - TiO_2
PRE100/I	Ammonium Sulphate - "ZrOH"
PRE100/J	Ammonium Sulphate - Y_2O_3

PRE100/K	Ammonium Sulphate - Nb_2O_5
PRE100/L	Ammonium Sulphate - Pr_2O_3
PRE100/M	Ammonium Sulphate - RuO_2
PRE100/N	Ammonium Sulphate - OsO_2
PRE100/O	Ammonium Sulphate - Fe_2O_3
PRE100/P	$FeSO_4$
PRE116/A	Ammonium Sulphate - "ZrOH". Heated to 600°C at 1°C/min
PRE116/B	Ammonium Sulphate - "ZrOH". Heated to 600°C at 50°C/min
PRE116/C	Ammonium Sulphate - "ZrOH". Heated to 600°C at 70°C/min
PRE116/D	Ammonium Sulphate - "ZrOH". Heated to 600°C at 66°C/min
PRE116/E	Ammonium Sulphate - "ZrOH". Heated to 600°C at 76°C/min
PRE116/F	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 1°C/min
PRE116/G	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 3°C/min
PRE116/H	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 4°C/min
PRE116/I	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 2.2°C/min
PRE116/J	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 2°C/min
PRE128/A	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 0.1°C/min
PRE128/B	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 0.3°C/min
PRE128/C	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 0.5°C/min
PRE128/D	Ammonium Sulphate - "ZrOH". Cooled from 600°C at 0.8°C/min
PRE117/A	Ammonium Sulphate - "ZrOH".
PRE117/B	Ammonium Sulphate - "ZrOH".
PRE117/C	Ammonium Sulphate - "ZrOH".
PRE117/D	Ammonium Sulphate - "ZrOH".
PRE117/E	Ammonium Sulphate - "ZrOH".
PRE117/F	Ammonium Sulphate - "ZrOH".
PRE117/G	Ammonium Sulphate - "ZrOH".
PRE118/A	Ammonium Sulphate - "ZrOH".
PRE118/B	Ammonium Hydrogen Phosphate - "ZrOH"
PRE118/C	Yttrium Trioxide - "ZrOH"
PRE118/D	Magnesium Oxide - "ZrOH"
PRE118/E	Calcium Oxide - "ZrOH"
PRE118/F	Lanthanum Trioxide - "ZrOH"
PRE118/G	Ammonium Molybdate - "ZrOH"
PRE118/H	Chromium Trioxide - "ZrOH"
PRE118/I	Ammonium *meta*-tungstate - "ZrOH"
PRE118/J	Ammonium Vanadate - "ZrOH"
PRE119/A	Ammonium Sulphate (solid) - "ZrOH".
PRE119/B	Sulphur (solid) - "ZrOH"
PRE119/C	Sulphuric Acid - "ZrOH"

PRE119/D	Ammonium Sulphate (solution) - "ZrOH"
PRE119/E	Ammonium Sulphate (solution) - monoclinic ZrO_2
PRE119/F	Sulphur (solid) - monoclinic ZrO_2
PRE119/G	Sulphuric Acid - monoclinic ZrO_2
PRE119/H	Ammonium Sulphate (solution) - monoclinic ZrO_2
PRE120	Precipitated Sulphated Zirconia prepared from Sulphuric Acid and Zirconium Propoxide
PRE121	Precipitated Sulphated Zirconia prepared from Sulphuric Acid and Zirconium Propoxide in the presence of Aerosol-OT, a surfactant
PRE124	Precipitated Sulphated Zirconia prepared from Sulphuric Acid and Zirconium Propoxide. Precipitated slowly.
PRE122/A	Ammonium Sulphate (solid) - "ZrOH". Not ground together, but mixed well.
PRE122/B	Ammonium Sulphate (solid) - "ZrOH". Ground together for 10s
PRE122/C	Ammonium Sulphate (solid) - "ZrOH". Ground together for 60s
PRE122/D	Ammonium Sulphate (solid) - "ZrOH". Ground together for 5 minutes
PRE123/A	Ammonium Sulphate - "ZrOH". Stored in a desiccator and activated at 150°C before use.
PRE123/B	Ammonium Sulphate - "ZrOH". Not stored in a desiccator nor activated at 150°C before use.
PRE123/C	Ammonium Sulphate - "ZrOH". Stored in a desiccator but not activated at 150°C.
PRE123/D	Ammonium Sulphate - "ZrOH". Transferred to desiccator at 150°C. Activated at 150°C prior to use.
PRE123/E	Ammonium Sulphate - "ZrOH". Calcined immediately prior to use.
PRE129/A	Ammonium Sulphate - "ZrOH". Heated to 600°C, cooled immediately.
PRE129/B	Ammonium Sulphate - "ZrOH". Heated at 600°C for 10 mins.
PRE129/C	Ammonium Sulphate - "ZrOH". Heated at 600°C for 1h.
PRE129/D	Ammonium Sulphate - "ZrOH". Heated at 600°C for 2h.
PRE129/E	Ammonium Sulphate - "ZrOH". Heated at 600°C for 6h.
PRE129/F	Ammonium Sulphate - "ZrOH". Heated at 600°C for 12h.

A3.2.2 Raw Data

Data presented as percentage of total peak area. A dash represents zero.

Expt	Catalyst *Feedstock*	Run	Benz	Tol	EB	OX	MX	PX	T1	T2
70/97	PRE94/M	1	-	0.1	-	96.0		1.5	252	225
	Feed: OX	2	-	-	-	99.3	-	-	251	314
		3	-	-	-	99.3	-	-	314	404
		4	-	-	-	99.1		0.3	404	457
		5	-	0.1	-	98.6		0.8	457	557
71/97	PRE93/A	1	-	-	-	99.4	-	-	250	287
	Feed: OX	2	-	-	-	99.3		0.2	287	399
		3	-	-	-	99.2		0.3	399	434
		4	-	-	-	99.1		0.4	434	459
		5	-	-	-	98.7		0.7	459	530
72/97	PRE93/B	1	0.1	0.1	-	95.0		4.2	264	364
	Feed: OX	2	0.1	0.1	-	93.2		6.0	364	416
		3	-	0.1	-	95.2		4.1	416	450
		4	-	0.2	-	96.1		2.9	450	530
73/97	PRE93/C	1	-	0.1	-	97.9		1.3	208	299
	Feed: OX	2	-	0.1	-	98.4		0.9	299	348
		3	-	-	-	99.1		0.2	348	390
		4	-	-	-	98.9		0.3	390	470
		5	-	-	-	99.2	-	-	470	553
74/97	PRE93/D	1	0.1	0.1	-	93.8		5.3	231	292
	Feed: OX	2	-	-	-	98.6		0.8	292	351
		3	-	0.1	-	98.9		0.5	351	400
		4	-	0.2	-	98.8		0.4	400	465
		5	-	0.1	-	99.2	-	-	465	518
75/97	PRE93/E	1	0.1	0.2	-	92.5		6.5	234	298
	Feed: OX	2	-	-	-	98.1		1.2	298	355
		3	-	0.1	-	97.9		1.1	355	416
		4	-	0.3	-	97.8		1.0	416	453
		5	-	0.3	-	98.6		0.4	453	518
76/97	PRE93/F	1	0.1	0.2	-	93.8		5.2	201	295
	Feed: OX	2	-	-	-	98.4		1.0	295	351
		3	-	-	-	98.5		0.8	351	401
		4	-	-	-	99.2		0.3	401	450
		5	-	0.1	-	98.5		0.8	450	515

77/97	PRE93/G	1	-	-	-	99.2	0.3	206	295
	Feed: OX	2	-	-	-	99.3	0.2	295	351
		3	-	-	-	99.4	- -	351	398
		4	-	-	-	99.4	- -	398	452
		5	-	-	-	99.4	- -	452	523
78/97	PRE93/H	1	0.1	0.2	-	99.2	6.7	252	309
	Feed: OX	2	-	-	-	98.6	0.8	309	361
		3	-	0.1	-	98.6	0.7	361	425
		4	-	0.4	-	98.0	0.8	425	488
		5	-	0.1	-	99.1	- -	488	526
79/97	PRE94/A	1	0.1	0.2	-	93.4	5.6	203	281
	Feed: OX	2	-	-	-	98.8	0.7	281	351
		3	-	-	-	98.8	0.5	351	401
		4	-	-	-	98.9	0.5	401	453
		5	-	0.2	-	98.6	0.5	453	530
80/97	PRE94/B	1	-	-	-	99.4	- -	233	299
	Feed: OX	2	-	-	-	99.2	0.2	299	348
		3	-	0.1	-	96.6	2.5	348	397
		4	-	0.7	-	95.5	2.4	397	463
		5	-	-	-	99.4	- -	463	525
81/97	PRE94/C	1	-	-	-	98.5	0.9	209	306
	Feed: OX	2	-	0.1	-	96.4	2.8	306	350
		3	-	0.1	-	96.9	2.2	350	404
		4	-	0.3	-	98.2	0.7	404	456
		5	-	0.1	-	99.2	0.1	456	535
82/97	PRE94/D	1	0.1	0.2	-	92.8	6.1	200	300
	Feed: OX	2	-	-	-	98.6	0.8	300	353
		3	-	0.1	-	98.8	0.5	353	403
		4	-	0.1	-	99.1	0.2	403	460
		5	-	-	-	99.4	- -	460	544
83/97	PRE94/E	1	-	0.1	-	96.2	3.1	210	314
	Feed: OX	2	-	0.1	-	98.2	1.1	314	353
		3	-	0.1	-	98.7	0.6	353	402
		4	-	0.2	-	98.4	0.6	402	466
		5	-	0.1	-	99.3	- -	466	614
84/97	PRE94/F	1	-	-	-	99.4	- -	240	298
	Feed: OX	2	-	-	-	99.4	0.1	298	351
		3	-	-	-	99.3	0.1	351	418
		4	-	-	-	99.4	0.1	418	452
		5	-	-	-	99.4	- -	452	531

85/97	PRE94/G	1	-	-	-	99.4	-	-	171	301
	Feed: OX	2	-	-	-	99.4	-	-	301	367
		3	-	-	-	99.4	-	-	367	405
		4	-	-	-	99.4	-	-	405	452
		5	-	-	-	99.4	-	-	452	514
86/97	PRE94/H	1	-	-	-	99.4	-	-	206	304
	Feed: OX	2	-	-	-	99.4	-	-	304	351
		3	-	-	-	99.4	-	-	351	400
		4	-	-	-	99.4	-	-	400	455
		5	-	-	-	99.4	-	-	455	526
87/97	PRE94/I	1	-	-	-	99.4	-	-	190	306
	Feed: OX	2	-	-	-	99.4	-	-	306	356
		3	-	-	-	99.4	-	-	356	401
		4	-	-	-	99.4	-	-	401	473
		5	-	-	-	99.4	-	-	473	553
88/97	PRE94/J	1	-	-	-	99.4	-	-	197	299
	Feed: OX	2	-	-	-	99.4	-	-	299	356
		3	-	-	-	99.4	-	-	356	423
		4	-	-	-	99.4	-	-	423	465
		5	-	-	-	99.4	-	-	465	525
89/97	PRE100/A	1	-	-	-	99.4	-	-	179	298
	Feed: OX	2	-	-	-	99.4	-	-	298	363
		3	-	-	-	99.4	-	-	363	436
		4	-	-	-	99.4	-	-	436	484
		5	-	-	-	99.4	-	-	484	545
90/97	PRE100/B	1	-	-	-	99.4	-	-	167	304
	Feed: OX	2	-	-	-	99.4	-	-	304	352
		3	-	-	-	99.4	-	-	352	407
		4	-	-	-	99.4	-	-	407	454
		5	-	-	-	99.4	-	-	454	516
91/97	PRE100/C	1	-	-	-	99.4	-	-	237	310
	Feed: OX	2	-	-	-	99.4	-	-	310	353
		3	-	-	-	99.4	-	-	353	408
		4	-	-	-	99.4	-	-	408	450
		5	-	-	-	99.4	-	-	450	537
92/97	PRE100/D	1	-	-	-	99.4	-	-	258	322
	Feed: OX	2	-	-	-	99.4	-	-	322	357
		3	-	-	-	99.4	-	-	357	423
		4	-	-	-	99.4	-	-	423	460
		5	-	-	-	99.4	-	-	460	523

93/97	PRE100/E	1	-	-	-	99.4	-	-	174	316
	Feed: OX	2	-	-	-	99.4	-	-	316	359
		3	-	-	-	99.4	-	-	359	403
		4	-	-	-	99.4	-	-	403	452
		5	-	-	-	99.4	-	-	452	520
94/97	PRE100/F	1	-	-	-	99.4	-	-	265	302
	Feed: OX	2	-	-	-	99.4	-	-	302	366
		3	-	-	-	99.4	-	-	366	399
		4	-	-	-	99.4	-	-	399	462
		5	-	-	-	99.4	-	-	462	538
95/97	PRE100/G	1	-	-	-	99.4	-	-	184	301
	Feed: OX	2	-	-	-	99.4	-	-	301	351
		3	-	-	-	99.4	-	-	351	402
		4	-	-	-	99.4	-	-	402	452
		5	-	-	-	99.4	-	-	452	508
96/97	PRE100/H	1	-	-	-	99.4	-	-	248	309
	Feed: OX	2	-	-	-	99.4	-	-	309	359
		3	-	-	-	99.4	-	-	359	404
		4	-	-	-	99.4	-	-	404	453
		5	-	-	-	99.4	-	-	453	520
97/97	PRE100/I	1	0.1	0.1	-	97.4		2.0	169	202
	Feed: OX	2	0.1	0.1	-	96.7		2.6	202	236
		3	0.1	0.1	-	95.0		4.2	236	302
		4	-	0.1	-	96.7		2.6	302	352
		5	-	0.1	-	98.2		1.1	352	403
		6	-	0.2	-	98.4		0.7	403	460
		7	-	0.4	-	98.4		0.4	460	537
98/97	PRE100/J	1	-	-	-	99.4	-	-	232	306
	Feed: OX	2	-	-	-	99.5	-	-	306	363
		3	-	-	-	99.3	-	-	363	412
		4	-	-	-	99.3	-	-	412	450
		5	-	-	-	99.4	-	-	450	512
99/97	PRE100/K	1	-	-	-	99.4	-	-	214	310
	Feed: OX	2	-	-	-	99.4	-	-	310	388
		3	-	-	-	99.4	-	-	388	426
		4	-	-	-	99.4	-	-	426	474
		5	-	-	-	99.4	-	-	474	575
100/97	PRE100/L	1	-	-	-	99.4	-	-	215	302
	Feed: OX	2	-	-	-	99.4	-	-	302	355
		3	-	-	-	99.4	-	-	355	400
		4	-	-	-	99.4	-	-	400	459
		5	-	-	-	99.4	-	-	459	526

101/97	PRE100/M	1	-	-	-	99.4	-	-	238	305
	Feed: OX	2	-	-	-	99.4	-	-	305	359
		3	-	-	-	99.4	-	-	359	408
		4	-	-	-	99.4	-	-	408	454
		5	-	-	-	99.3	-	-	454	508
102/97	PRE100/N	1	-	-	-	99.4	-	-	230	301
	Feed: OX	2	-	-	-	99.4	-	-	301	359
		3	-	-	-	99.4	-	-	359	410
		4	-	-	-	99.4	-	-	410	491
		5	-	-	-	99.4	-	-	491	537
103/97	PRE100/O	1	-	-	-	99.4	-	-	230	305
	Feed: OX	2	-	-	-	99.4	-	-	305	352
		3	-	-	-	99.4	-	-	352	411
		4	-	-	-	99.4	-	-	411	449
		5	-	-	-	99.4	-	-	449	548
104/97	PRE100/P	1	-	-	-	99.4	-	-	220	318
	Feed: OX	2	-	-	-	99.4	-	-	318	375
		3	-	-	-	99.4	-	-	375	412
		4	-	-	-	99.3	-	-	412	483
		5	-	-	-	99.4	-	-	483	587
105/97	PRE117/A	1	0.3	0.4	-	92.6	5.0	0.7	250	300
	Feed: OX	2	0.3	0.3	-	94.2	3.9	0.5	300	354
		3	0.3	0.1	-	97.8	1.3	0.1	354	425
		4	0.3	0.2	-	97.9	0.8	0.1	425	493
		5	0.3	0.2	-	98.4	0.4	-	493	581
106/97	PRE117/A	1	2.9	0.6	-	76.5	16.2	0.4	176	214
	Feed: MX	2	0.1	0.2	*	41.1	58.8	*	214	262
	*=peak hidden	3	-	0.2	*	5.2	92.0	*	262	350
	under MX peak	4	-	-	-	-	-	-	350	415
		5	-	0.3	*	97.8	1.5	*	415	474
107/97	PRE117/B	1	-	1.7	1.3	1.9	94.9	*	197	234
	Feed: TOL	2	-	69.1	0.7	0.8	29.3	*	234	289
		3	-	97.0	-	0.2	2.7	0.1	289	359
		4	-	99.0	-	0.1	0.8	-	359	413
		5	-	99.2	-	0.1	0.5	-	413	484
108/97	PRE117/C	1	-	98.8	-	0.3	0.7	0.2	243	292
	Feed: TOL/MeOH	2	-	96.3	-	0.9	0.9	0.5	292	424
		3	-	93.8	-	1.1	0.7	0.7	424	455
		4	-	95.1	-	0.8	0.5	0.5	455	338

109/97	PRE117/C	1	-	40.9	-	0.5	0.2	52.5	219	271
	Feed: PX	2	-	4.0	-	0.2	*	92.5	271	341
		3	-	1.2	-	0.2	0.5	97.7	341	408
		4	-	1.4	-	0.2	0.4	97.8	408	492
		5	-	0.5	-	0.2	*	99.3	492	565
110/97	PRE117/B	1	-	1.3	9.2	2.8	52.2	34.1	234	299
	Feed: mixed xylenes	2	-	1.0	20.1	5.3	73.2	*	299	351
		3	-	0.9	20.5	5.4	72.8	*	351	401
		4	-	1.0	20.5	5.4	72.9	*	401	459
		5	-	1.1	20.4	5.3	72.8	*	459	544
111/97	PRE117/D	1	-	1.2	27.1	5.1	64.3	*	183	273
	Feed: EB	2	-	0.2	91.1	-	7.1	-	273	342
		3	-	0.1	99.2	0.1	0.5	-	342	400
		4	-	-	99.3	-	0.3	-	400	456
		5	-	0.1	99.4	-	0.2	-	456	525
112/97	PRE118/A	1	-	0.2	89.0	3.9	0.6	-	222	297
	Feed: OX	2	0.6	0.6	63.3	28.4	4.9	-	297	365
		3	1.9	2.0	13.2	73.5	6.0	0.9	365	434
		4	1.7	1.6	4.0	88.1	2.2	0.5	434	476
		5	0.2	0.1	0.1	98.5	0.2	-	476	582
113/97	PRE118/B	1	0.3	0.1	0.5	98.5	0.1	0.1	171	260
	Feed: OX	2	0.3	-	0.6	98.5	0.1	-	260	300
		3	0.1	0.1	2.9	91.4	0.6	0.2	300	350
		4	0.3	-	0.4	98.8	0.1	-	350	416
		5	0.3	-	0.3	98.6	0.2	-	416	465
		6	0.3	0.1	0.3	98.4	0.4	-	465	564
114/97	PRE118/C	1	0.3	-	0.2	98.9	0.1	-	181	250
	Feed: OX	2	0.3	-	0.1	99.1	0.1	-	250	300
		3	2.9	0.1	0.6	92.3	0.7	0.2	300	352
		4	0.3	-	0.1	99.1	0.1	-	352	413
		5	0.3	-	0.1	99.1	0.1	-	413	506
115/97	PRE118/D	1	0.3	-	0.1	99.1	0.1	-	225	303
	Feed: OX	2	0.2	0.1	0.6	91.3	0.8	0.2	303	353
		3	0.3	-	0.1	99.1	0.1	-	353	406
		4	0.3	-	0.1	99.1	0.1	-	406	466
		5	0.3	-	0.1	99.1	0.1	-	466	530

116/97	PRE118/E	1	0.3	-	0.1	99.1	0.1	-	220	300
	Feed: OX	2	0.3	-	0.1	99.0	0.1	-	300	356
		3	0.2	0.1	0.5	92.6	0.6	-	356	401
		4	0.3	-	0.1	99.1	0.1	-	401	494
		5	0.3	-	0.1	99.1	0.1	-	494	570
117/97	PRE118/F	1	0.3	-	0.1	99.1	0.1	-	174	254
	Feed: OX	2	0.3	-	0.1	99.0	0.1	-	254	309
		3	0.3	0.2	1.0	85.2	1.2	0.3	309	368
		4	0.3	-	0.1	99.1	0.1	-	368	434
		5	0.3	0.2	0.6	91.0	0.7	0.2	434	521
118/97	PRE118/G	1	0.3	-	0.1	99.1	0.1	-	247	300
	Feed: OX	2	0.1	0.2	0.3	94.2	0.5	0.1	300	352
		3	0.3	0.1	0.1	98.9	0.1	-	352	404
		4	0.2	2.8	0.7	81.2	1.6	0.4	404	463
		5	0.3	0.3	0.1	98.6	0.1	-	463	534
119/97	PRE118/H	1	0.3	-	0.1	99.1	0.1	-	222	303
	Feed: OX	2	0.2	0.1	0.7	88.2	0.9	0.3	303	353
		3	0.3	0.4	0.7	88.2	0.9	0.3	353	398
		4	0.3	0.1	0.1	99.0	0.1	-	398	460
		5	0.2	0.2	0.1	99.0	0.1	-	460	533
120/97	PRE118/I	1	0.3	-	0.1	99.2	0.1	-	245	310
	Feed: OX	2	0.2	0.1	0.5	92.2	0.6	0.2	310	365
		3	0.3	-	0.1	99.1	0.1	-	365	408
		4	0.3	0.1	0.1	99.0	0.1	-	408	480
		5	0.2	0.2	0.1	98.7	0.3	-	480	550
121/97	PRE118/J	1	0.3	0.1	0.1	99.0	0.1	-	203	263
	Feed: OX	2	0.2	-	-	99.2	0.1	-	263	318
		3	0.3	0.3	0.1	93.1	1.0	0.2	318	408
		4	0.3	-	-	99.3	0.1	-	408	466
		5	0.3	0.1	-	99.2	0.1	-	466	543
122/97	PRE119/A	1	0.2	0.5	-	92.5	5.1	0.8	215	231
	Feed: OX	2	0.3	0.3	-	95.4	3.4	0.4	231	251
		3	0.2	0.1	-	96.9	2.2	0.2	251	298
		4	0.2	0.1	-	97.7	1.4	0.1	298	377
		5	0.1	0.3	-	98.3	1.0	0.1	377	439
		6	0.3	0.4	-	98.3	0.4	0.1	439	521
123/97	PRE119/B	1	0.2	0.1	-	98.1	1.2	0.1	185	252
	Feed: OX	2	0.2	0.1	-	96.8	2.2	0.2	252	301
		3	0.2	0.1	-	96.7	1.2	0.1	301	353
		4	0.3	0.1	-	98.0	1.2	0.1	353	414
		5	0.2	0.2	-	98.6	0.4	-	414	511

124/97	PRE119/C	1	0.2	0.4	-	90.9	6.8	0.8	226	273
	Feed: OX	2	0.3	0.1	-	95.9	3.0	0.2	273	327
		3	0.2	0.1	-	97.6	1.4	0.1	327	392
		4	0.2	0.4	-	98.2	0.7	0.1	392	462
		5	0.2	0.2	-	99.0	0.2	-	462	542
125/97	PRE119/D	1	0.3	0.3	-	94.2	4.0	0.6	210	278
	Feed: OX	2	0.3	0.1	-	97.3	1.9	0.2	278	337
		3	0.2	0.1	-	97.5	1.5	0.1	337	390
		4	0.2	0.4	-	97.4	1.1	0.1	390	460
		5	0.2	0.4	-	98.4	0.3	-	460	570
126/97	PRE119/E	1	0.3	-	-	99.3	0.1	-	180	237
	Feed: OX	2	0.2	-	-	99.3	0.1	-	237	303
		3	0.2	-	-	99.3	0.1	-	303	353
		4	0.2	-	-	99.3	0.1	-	353	433
		5	0.3	-	-	99.2	0.1	-	433	513
127/97	PRE119/F	1	0.2	-	-	99.3	0.1	-	212	284
	Feed: OX	2	0.2	-	-	99.3	0.1	-	284	350
		3	0.2	-	-	99.3	0.1	-	350	406
		4	0.2	-	-	99.3	0.1	-	406	469
		5	0.2	-	-	99.3	0.1	-	469	552
128/97	PRE119/G	1	0.2	-	-	99.3	0.1	-	225	287
	Feed: OX	2	0.2	-	-	99.3	0.1	-	287	344
		3	0.2	-	-	99.3	0.1	-	344	395
		4	0.3	-	-	99.3	0.1	-	395	445
		5	0.3	-	-	99.3	0.1	-	445	529
129/97	PRE119/H	1	0.3	-	-	99.3	0.1	-	228	280
	Feed: OX	2	0.2	-	-	99.2	0.2	-	280	343
		3	0.2	-	-	99.2	0.1	-	343	553
130/97	PRE120	1	0.2	0.1	-	94.9	4.1	0.2	171	206
	Feed: OX	2	0.2	0.2	-	92.0	6.6	0.4	206	254
		3	0.2	0.2	-	91.2	7.4	0.6	254	312
		4	0.2	0.1	-	95.6	3.3	0.2	312	418
		5	0.2	0.4	-	97.5	1.4	0.1	418	472
131/97	PRE121	1	0.2	-	-	99.3	0.1	-	152	182
	Feed: OX	2	0.3	-	-	99.3	0.1	-	182	234
		3	0.2	-	-	99.2	0.2	-	234	306
		4	0.2	-	-	98.9	0.5	-	306	386
		5	0.2	0.2	-	98.8	0.3	-	386	494

132/97	PRE124	1	0.2	0.4	-	82.4	15.2	1.4	229	265
	Feed: OX	2	0.2	0.3	-	85.6	12.5	0.8	265	313
		3	0.2	0.2	-	90.7	8.1	0.4	313	393
		4	0.3	0.5	-	94.7	3.5	0.1	393	443
		5	0.3	1.2	-	94.0	2.8	0.1	443	492
133/97	PRE122/A	1	0.2	0.1	-	95.6	3.1	0.2	221	235
	Feed: OX	2	0.2	0.1	-	96.2	2.8	0.2	235	300
		3	0.2	0.1	-	96.8	2.4	0.2	300	360
		4	0.2	0.2	-	98.1	1.1	0.1	360	447
		5	0.2	0.3	-	98.4	0.6	0.1	447	560
134/97	PRE122/B	1	0.2	0.1	-	96.1	2.8	0.3	219	295
	Feed: OX	2	0.2	0.1	-	98.6	1.2	0.1	295	360
		3	0.2	0.2	-	98.6	0.6	-	360	435
		4	0.3	0.3	-	98.4	0.4	-	435	471
		5	0.3	0.3	-	98.6	0.3	-	471	498
135/97	PRE122/C	1	0.2	0.2	-	95.6	3.2	0.3	198	263
	Feed: OX	2	0.2	0.1	-	96.4	2.6	0.2	263	305
		3	0.2	0.1	-	97.7	1.8	0.1	305	356
		4	0.3	0.2	-	98.1	1.1	0.1	356	434
		5	0.2	0.3	-	98.4	0.5	0.1	434	515
136/97	PRE122/D	1	0.2	0.2	-	95.5	3.1	0.4	195	279
	Feed: OX	2	0.3	0.1	-	97.6	1.6	0.1	279	333
		3	0.2	0.1	-	98.3	0.9	0.1	333	386
		4	0.2	0.2	-	98.3	0.7	0.1	386	437
		5	0.2	0.2	-	98.8	0.3	-	437	553
137/97	PRE123/A	1	0.2	0.2	-	93.4	5.3	0.2	195	253
	Feed: OX	2	0.3	0.1	-	97.0	2.3	0.1	253	311
		3	0.3	0.1	-	97.5	1.7	0.1	311	364
		4	0.2	0.1	-	98.1	1.0	-	364	427
		5	0.2	0.2	-	98.3	0.7	-	427	523
138/97	PRE123/B	1	0.3	0.2	-	94.5	4.1	0.4	178	235
	Feed: OX	2	0.2	0.2	-	94.7	3.9	0.4	235	304
		3	0.3	0.1	-	97.5	1.6	0.1	304	376
		4	0.2	0.1	-	98.2	0.9	0.1	376	446
		5	0.3	0.2	-	98.4	0.3	-	446	591
139/97	PRE123/C	1	0.2	0.2	-	94.2	4.2	0.6	190	223
	Feed: OX	2	0.2	0.2	-	95.3	3.6	0.3	237	297
		3	0.2	0.2	-	97.6	1.6	0.1	297	431
		4	0.2	0.2	-	98.2	0.9	0.1	431	494
		5	0.2	0.1	-	99.2	0.1	-	494	555

140/97	PRE123/D	1	0.2	0.4	-	93.6	4.6	0.6	231	304
	Feed: OX	2	0.2	0.1	-	97.7	1.5	0.1	304	371
		3	0.2	0.3	-	97.2	1.6	0.1	371	429
		4	0.2	0.7	-	96.8	1.2	0.1	429	505
		5	0.2	0.3	-	98.9	0.2	-	505	564
141/97	PRE123/D	1	0.2	0.1	-	98.2	1.1	0.1	177	230
	Feed: OX	2	0.3	0.2	-	95.2	3.3	0.4	230	314
		3	0.3	0.1	-	96.9	1.9	0.2	314	388
		4	0.3	0.2	-	97.8	1.0	0.1	388	460
		5	0.3	0.3	-	98.4	0.3	-	460	542
142/97	PRE116/A	1	0.3	0.3	-	94.2	3.9	0.5	222	270
	Feed: OX	2	0.3	0.1	-	96.8	2.2	0.2	270	322
		3	0.3	0.1	-	98.0	1.2	0.1	322	378
		4	0.3	0.2	-	98.4	0.7	-	378	449
		5	0.3	0.3	-	98.5	0.3	-	449	537
143/97	PRE128/B	1	0.3	0.3	-	94.0	4.4	0.5	231	272
	Feed: OX	2	0.3	0.1	-	96.3	2.6	0.2	272	330
		3	1.3	1.7	-	71.9	15.3	1.0	330	404
		4	0.3	0.3	-	97.7	0.9	0.1	404	472
		5	0.3	0.3	-	98.5	0.3	-	472	577
144/97	PRE116/B	1	0.3	0.3	-	94.0	4.4	0.5	197	266
	Feed: OX	2	0.3	0.1	-	97.0	2.3	0.2	266	313
		3	0.3	0.1	-	98.1	1.1	0.1	313	385
		4	0.3	0.2	-	98.4	0.7	-	385	456
		5	0.3	0.2	-	98.8	0.3	-	456	528
145/97	PRE116/C	1	0.3	0.2	-	96.3	2.6	0.3	170	241
	Feed: OX	2	0.3	0.1	-	96.9	2.1	0.2	241	306
		3	0.3	0.1	-	97.9	1.2	0.1	306	377
		4	0.3	0.2	-	98.2	0.6	-	377	450
		5	0.3	0.2	-	98.9	0.2	-	450	535
146/97	PRE116/D	1	0.3	0.3	-	94.4	4.0	0.5	187	252
	Feed: OX	2	0.3	0.2	-	94.4	4.1	0.4	252	307
		3	0.3	0.1	-	96.5	2.3	0.2	307	375
		4	0.3	0.3	-	97.6	1.0	0.1	375	476
		5	0.3	0.2	-	98.9	0.2	-	476	579
147/97	PRE116/E	1	0.3	0.2	-	96.8	2.0	0.3	211	259
	Feed: OX	2	0.3	0.2	-	96.4	2.3	0.3	259	333
		3	0.3	0.1	-	98.0	1.4	0.1	333	395
		4	0.3	0.1	-	98.3	0.9	0.1	395	445
		5	0.3	0.3	-	98.2	0.6	0.1	445	539

148/97	PRE116/F	1	0.3	0.1	-	96.9	2.1	0.2	184	262
	Feed: OX	2	0.3	0.1	-	95.0	3.6	0.4	262	318
		3	0.3	0.1	-	96.1	2.7	0.3	318	389
		4	0.3	0.1	-	97.9	1.3	0.1	389	462
		5	0.3	0.3	-	98.5	0.5	-	462	559
149/97	PRE116/G	1	0.2	0.2	-	96.7	2.5	0.3	264	274
	Feed: OX	2	0.3	0.1	-	96.8	2.1	0.2	274	333
		3	0.3	0.2	-	97.9	1.2	0.1	333	398
		4	0.3	0.2	-	98.2	0.7	-	398	476
		5	0.3	0.2	-	98.8	0.2	-	476	558
150/97	PRE116/H	1	0.3	0.3	-	94.3	4.0	0.5	183	255
	Feed: OX	2	0.3	0.2	-	94.2	4.1	0.4	255	305
		3	0.3	0.1	-	96.5	2.3	0.2	305	372
		4	0.3	0.3	-	97.7	1.0	0.1	372	450
		5	0.3	0.2	-	98.8	0.2	-	450	549
151/97	PRE116/I	1	0.3	0.2	-	96.8	2.0	0.3	194	246
	Feed: OX	2	0.3	0.2	-	96.6	2.3	0.3	246	328
		3	0.3	0.1	-	97.8	1.4	0.1	328	402
		4	0.3	0.1	-	98.1	0.9	0.1	402	471
		5	0.3	0.3	-	98.1	0.6	0.1	471	576
152/97	PRE116/J	1	0.3	0.1	-	96.9	2.1	0.2	181	240
	Feed: OX	2	0.3	0.2	-	95.0	3.6	0.4	240	321
		3	0.3	0.1	-	96.2	2.7	0.1	321	378
		4	0.3	0.1	-	98.2	1.1	0.1	378	454
		5	0.3	0.3	-	98.2	0.5	-	454	529
153/97	PRE128/A	1	0.3	0.2	-	95.3	3.5	0.4	195	233
	Feed: OX	2	0.3	0.2	-	96.2	3.0	0.3	233	293
		3	0.3	0.1	-	96.9	2.2	0.2	293	375
		4	0.3	0.3	-	97.9	1.2	0.1	375	463
		5	0.3	0.3	-	98.8	0.4	-	463	533
154/97	PRE128/B	1	0.3	0.4	-	91.5	6.7	0.8	220	285
	Feed: OX	2	0.3	0.1	-	96.2	3.0	0.2	285	351
		3	0.3	0.1	-	98.2	1.0	0.1	351	407
		4	0.3	0.3	-	98.6	0.5	-	407	483
		5	0.2	0.1	-	99.2	0.2	-	483	660
1/98	PRE128/C	1	0.3	0.3	-	91.9	6.9	0.4	224	262
	Feed: OX	2	0.3	0.1	-	95.3	4.0	0.1	262	322
		3	0.3	0.2	-	97.1	2.1	0.1	322	291
		4	0.3	0.4	-	97.9	1.1	0.1	391	466
		5	0.3	0.5	-	98.4	0.5	0.1	466	515

2/98	PRE128/D	1	0.3	0.4	-	91.2	6.9	0.8	221	263
	Feed: OX	2	0.2	0.4	-	94.4	4.5	0.4	263	309
		3	0.3	0.2	-	95.9	3.2	0.2	309	363
		4	0.3	0.2	-	97.4	1.7	0.1	363	435
		5	0.3	0.5	-	97.9	0.8	0.1	435	523
3/98	PRE129/A	1	0.3	0.2	-	92.5	6.3	0.5	208	237
	Feed: OX	2	0.3	0.1	-	95.4	4.1	0.1	237	311
		3	0.2	0.1	-	97.7	1.8	-	311	366
		4	0.3	0.1	-	98.6	0.7	-	366	418
		5	0.3	0.4	-	98.7	0.4	-	418	528
4/98	PRE129/B	1	0.2	0.2	-	94.0	4.9	0.2	212	269
	Feed: OX	2	0.2	0.3	-	94.6	4.4	0.3	269	340
		3	0.2	0.1	-	97.4	1.9	0.1	340	399
		4	0.3	0.2	-	98.4	0.9	0.1	399	479
		5	0.3	0.3	-	98.7	0.4	-	479	532
5/98	PRE129/C	1	0.2	0.3	-	95.4	3.6	0.3	170	218
	Feed: OX	2	0.2	0.3	-	95.1	3.9	0.3	218	282
		3	0.3	0.1	-	97.3	2.0	0.1	282	353
		4	0.2	0.2	-	98.5	0.8	-	353	423
		5	0.3	0.3	-	98.9	0.3	-	423	528
6/98	PRE129/D	1	0.2	0.2	-	92.6	6.8	0.2	217	261
	Feed: OX	2	0.2	0.1	-	95.5	4.0	0.1	261	325
		3	0.2	0.1	-	98.3	1.0	0.1	325	403
		4	0.2	0.3	-	98.7	0.5	-	403	463
		5	0.2	0.2	-	99.0	0.2	-	463	551
7/98	PRE129/E	1	0.2	0.1	-	97.1	2.2	0.1	184	225
	Feed: OX	2	0.2	0.2	-	96.2	2.9	0.2	225	289
		3	0.2	0.1	-	96.1	3.0	0.3	289	343
		4	0.3	0.2	-	97.9	1.3	0.1	343	421
		5	0.2	0.4	-	98.5	0.6	-	421	520
8/98	PRE129/F	1	0.2	0.1	-	96.5	2.7	0.2	235	256
	Feed: OX	2	0.2	0.1	-	97.6	1.8	0.1	256	295
		3	0.2	0.1	-	97.5	1.8	0.1	295	378
		4	0.2	0.2	-	98.5	0.8	-	378	455
		5	0.2	0.3	-	98.8	0.4	-	455	545

Appendix 4.1: Raw Data from Catalyst Testwork

A4.1.1 Key to Abbreviations Used

ABG	anti-bumping granules
acetal	1,1-diethoxyethane
Benz	benzene
EB	ethylbenzene
Exp't	experiment
MEL	MEL Chemicals sample number
MeOH	methanol
MX	*meta*-xylene
OX	*ortho*-xylene
PRE	"P.R. Ellis" sample number
PX	*para*-xylene
T	reaction temperature at sampling (for gas samples)
T1	initial reaction temperature (for liquid samples)
T2	final reaction temperature (for liquid samples)
Tol	toluene

A4.1.2 Key to Catalysts Used

PRE182	Sulphated Zirconia Catalyst
PRE189	Sulphated Zirconia Catalyst
PRE196	Sulphated Zirconia Catalyst
PRE207	Sulphated Zirconia Catalyst
PRE230	'Averaged' Sulphated Zirconia Catalyst
MEL X20631/01	Sulphated Zirconia Catalyst, 0.01μm particle size
MEL X20632/03	Sulphated Zirconia Catalyst, 0.03μm particle size
MEL X20645/01	Silicic Acid-doped Zirconia
MEL X20680/01	Lanthanum Hydroxide-doped Zirconia
ABG	Alumina Anti-Bumping Granules

A4.1.3 Raw Data

Data presented as percentage of total peak area. A dash represents zero.

Exp't	Catalyst *Feedstock*	Run	Benz	Tol	EB	OX	MX	PX	T1	T2
9/98	PRE230	1	-	-	-	99.6	-	-	145	141
	Feed: OX	2	-	0.2	-	99.6	-	-	144	171
		3	-	0.4	-	99.5	-	-	171	193
		4	-	0.4	-	99.4	-	-	193	207
		5	-	0.3	-	99.5	-	-	207	237
		6	-	0.2	-	99.6	-	-	237	237
		7	-	0.2	-	99.5	-	-	237	266
		8	-	0.3	-	99.3	0.1	-	266	301
		9	-	0.2	-	99.0	0.1	-	301	350
		10	-	0.2	-	99.1	0.2	-	350	396
		11	-	0.2	-	99.0	0.2	-	469	544
10/98	PRE230	1	nd[†]	nd	nd	nd	nd	nd	161	183
	Feed: MX	2	-	0.4	-	0.8	98.7	[‡]	183	195
		3	-	0.3	-	0.6	99.0	[‡]	195	248
		4	-	0.3	-	0.5	99.2	[‡]	248	362
		5	-	0.4	-	0.5	99.0	[‡]	362	516
11/98	PRE230	1	-	0.2	-	0.1	[§]	99.7	141	180
	Feed: PX	2	-	0.2	-	0.1	[§]	99.8	180	197
		3	-	0.1	-	-	[§]	99.8	197	236
		4	-	0.1	-	-	[§]	99.8	236	300
		5	-	0.1	-	-	[§]	99.8	300	435
		6	-	0.2	0.1	-	[§]	99.7	435	542
12/98	PRE230	1	-	1.0	20.3	5.2	73.4 [**]	[**]	174	203
	Feed: Mixed Xylenes	2	-	1.1	20.4	5.3	73.0	[**]	203	244
		3	-	1.0	20.6	5.3	73.0	[**]	244	324
		4	-	1.0	20.5	5.3	72.9	[**]	324	461
		5	-	1.0	20.1	5.4	72.8	[**]	461	505

[†] Not determined.
[‡] Peak not separated from *meta*-xylene peak, which is much larger.
[§] Peak not separated from *para*-xylene peak, which is much larger.
[**] *Meta*- and *para*-xylene peaks not resolved.

14/98	PRE230	1	-	0.1	99.0	0.1	-	-	173	191
	Feed: EB	2	-	0.2	99.5	0.1	-	-	191	217
		3	-	0.1	99.8	-	-	-	217	353
		4	-	0.2	99.5	0.1	-	-	353	434
		5	-	0.3	98.8	0.1	-	-	434	524

Exp't	**Catalyst** ***Feedstock***	**Run**	**Benz**	**Tol**	**EB**	**OX**	**MX**	**PX**	**T1**	**T2**
15/98	PRE230	1	-	99.6	-	0.1	0.2	0.1	127	158
	Feed: Toluene	2	-	99.6	-	0.1	0.1	-	158	173
		3	-	99.8	-	0.1	0.1	-	173	239
		4	-	99.7	-	0.1	0.1	-	239	322
		5	-	99.5	0.1	0.2	0.2	-	322	440
		6	-	99.4	0.2	0.1	0.2	0.1	440	560

Exp't	**Catalyst** ***Feedstock***	**Run**	**MeOH**	**Tol**	**EB**	**OX**	**MX**	**PX**	**T1**	**T2**
16/98	PRE230	1	10.8	89.0	0.1	0.1	-	-	160	176
	Feed 1:1	2	12.3	87.2	0.1	0.1	0.1	0.1	176	203
	Toluene : Methanol	3	4.5	93.7	0.1	0.4	0.3	0.3	203	332
		4	71.5	26.2	-	0.3	0.3	-	332	426
		5	1.4	96.0	0.2	0.9	0.6	0.6	426	539
		6	0.1	97.0	0.5	1.1	0.6	0.6	539	692

Exp't	**Catalyst** ***Feedstock***	**Run**	**Me_2O**	**MeOH**	**HCO_2Me**	**CO**	**T**
18/98	PRE230	1	-	0.68	98.1	Small amount	64
	Feed:	2	-	0.65	96.9	Small amount	80
	Methyl Methanoate	3	-	0.61	97.7	Small amount	97
		4	-	0.61	98.0	Yes	106
		5	0.15	0.65	96.9	Yes	149
		6	0.70	0.95	97.7	Yes	188
		7	1.17	1.27	97.2	Yes	206
		8	1.35	1.59	96.9	Yes	220
		9	2.54	2.71	94.6	Yes	247

Exp't Run	Catalyst *Feedstock*	etha -nol	acetone	ethyl acetate	buta -nol	butyl acetate	acetal	T1	T2
19/98 1	PRE230 ethyl acetate	0.04	-	99.96	-	-	-	114	130
2		0.01	-	99.99	-	-	-	130	148
3		0.03	-	99.93	0.04	-	-	148	184
4		0.13	0.04	99.79	0.04	-	-	184	218
5		0.10	0.02	99.83	0.03	-	0.02	218	254
6		0.16	0.03	99.71	0.06	-	0.04	254	292
7		0.18	0.05	99.65	0.07	0.01	0.04	292	318
8		0.18	0.07	99.61	0.07	0.01	0.06	318	338
9		0.21	0.07	99.57	0.08	0.01	0.06	338	371
10		0.41	0.13	99.26	0.12	0.01	0.07	371	425

Exp't	Catalyst *Feedstock*	Run	Tol	OX	MX	PX	EB	T1	T2
20/98	PRE182	1	-	99.3	0.1	-	-	152	159
	Feed: OX	2	-	99.3	0.1	-	-	159	211
		3	-	99.3	0.1	-	-	211	249
		4	-	99.3	0.1	-	-	249	311
		5	-	99.5	0.1	-	-	311	374
		6	-	99.4	0.1	-	-	374	460
21/98	PRE207	1	-	99.3	0.1	-	-	165	175
	Feed: OX	2	-	99.4	0.1	-	-	175	194
		3	-	99.4	0.1	-	-	194	247
		4	-	99.3	0.1	-	-	247	308
		5	-	99.4	0.1	-	-	308	380
		6	-	99.3	0.1	-	-	380	469
22/98	PRE189	1	-	99.2	0.1	-	-	164	174
	Feed: OX	2	-	99.3	0.1	-	-	174	198
		3	-	99.5	0.1	-	-	198	222
		4	-	99.3	0.1	-	-	222	288
		5	-	99.2	0.2	-	-	288	351
		6	-	99.2	0.1	-	-	351	438
		7	-	99.1	0.3	-	-	438	541
23/98	PRE196	1	-	98.8	0.6	0.1	-	186	206
	Feed: OX	2	-	99.3	0.1	-	-	206	247
24/98	PRE196	1	-	99.3	0.1	-	-	199	208
	Feed: OX	2	-	99.3	0.2	-	-	208	247
		3	-	99.3	0.2	-	-	247	319
		4	-	99.3	0.1	-	-	319	371
		5	-	99.3	0.1	-	-	371	451
		6	-	99.3	0.1	-	-	451	537

25/98	MEL X20645/01 *Feed: OX*	1	-	99.4	0.1	-	-	168	187
		2	-	99.3	0.1	-	-	187	202
		3	-	99.3	0.1	-	-	202	264
		4	-	99.3	0.1	-	-	264	342
		5	-	99.3	0.1	-	-	342	396
		6	-	99.3	0.1	-	-	396	494
26/98	MEL X20631/01 *Feed: OX*	1	0.1	96.3	2.9	0.1	0.1	176	199
		2	0.1	97.2	2.2	0.1	0.1	199	217
		3	0.1	97.5	1.9	0.1	0.1	217	281
		4	0.1	98.1	1.3	0.1	-	281	331
		5	0.1	98.7	0.6	-	-	331	418
		6	0.1	98.6	0.4	-	-	418	489
27/98	MEL X20632/03 *Feed: OX*	1	0.1	97.6	1.7	0.1	-	160	177
		2	0.1	96.7	1.7	0.1	-	177	222
		3	0.1	96.5	2.5	0.3	-	222	277
		4	0.1	97.2	1.9	0.2	-	277	331
		5	0.1	98.0	1.1	0.1	-	331	424
		6	0.5	97.9	0.7	0.1	-	424	497
28/98	MEL X20680/01 *Feed: OX*	1	-	99.3	0.1	-	-	158	202
		2	-	99.3	0.1	-	-	202	267
		3	-	99.3	0.1	-	-	267	304
		4	-	99.3	0.1	-	-	304	361
		5	-	99.3	0.1	-	-	361	420
		6	-	99.3	0.1	-	-	420	520

29/98	PRE230	1	-	98.6	0.8	0.1	-	170	188
	Feed: OX	2	-	98.7	0.7	-	-	188	195
		3	-	98.9	0.5	-	-	195	198
		4	-	98.9	0.5	-	-	198	199
		5	-	99.0	0.4	-	-	199	201
		6	-	99.1	0.3	-	-	201	201
		7	-	99.2	0.3	-	-	201	203
		8	-	99.2	0.3	-	-	203	203
		9	-	99.2	0.2	-	-	203	204
		10	-	99.3	0.2	-	-	204	204
		11	-	99.3	0.2	-	-	204	204
		12	-	99.3	0.2	-	-	204	204
		13	-	99.3	0.2	-	-	204	205
		14	-	99.3	0.1	-	-	205	204
		15	-	99.3	0.1	-	-	204	204
		16	-	99.3	0.1	-	-	204	203
		17	-	99.3	0.1	-	-	203	203
		18	-	99.3	0.1	-	-	203	203
		19	-	99.4	0.1	-	-	203	203
		20	-	99.3	0.1	-	-	203	203
30/98	ABG	1	-	99.4	0.1	-	-	158	202
	Feed: OX	2	-	99.4	0.1	-	-	202	267
		3	-	99.3	0.1	-	-	267	304
		4	-	99.3	0.1	-	-	304	361
		5	-	99.4	0.1	-	-	361	420
		6	-	99.3	0.1	-	-	420	520

Appendix 7.1: Supplementary Crystal Structure Data for N,N' - bis (diphenylphosphino) - N,N' - di - *tert* - butylethylenediamine (dpptben)

X-ray crystallographic work on this compound was performed by Dr. A.S. Batsanov.

Empirical formula	$C_{34}H_{42}N_2P_2$
Formula Weight	540.64
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal System	Monoclinic
Space Group	P2(1)/c
Unit Cell Dimensions	a = 10.278 Å
	b = 11.385 Å
	c = 12.750 Å
	$\alpha = 90°$
	$\beta = 92.39(1)°$
	$\gamma = 90°$
Volume	1490.6(2) $Å^3$
Z	2
Density (Calculated)	1.205 g cm^{-3}
Absorption Coefficient	0.171 mm^{-1}
F(000)	580
Crystal Size	0.3 x 0.25 x 0.2 mm
θ Range for Data Collection	2.0° to 27.5°
Index Ranges	$-13 \leq h \leq 14$
	$-15 \leq k \leq 15$
	$-14 \leq l \leq 17$
Reflections Collected	10531
Independent Reflections	3423 (R_{int} = 0.0421)
Observed Reflections ($I > 2\Sigma(I)$)	2860

Absorption Correction	None
Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	3372 / 0 / 256
Goodness of Fit on F^2	1.071
Final R Indices ($I > 2\Sigma(I)$)	R1 = 0.0372, wR2 = 0.0810
R Indices (all data)	R1 = 0.0507, wR2 = 0.0939
Largest Diffraction Peak and Hole	0.372 and -0.253 e A^{-3}

Bond Length Data

Bond	Length / Å	Bond	Length / Å
P-N	1.710(1)	C(1)-C(1')	1.546(3)
P-C(11)	1.850(2)	C(2)-C(3)	1.532(2)
P-C(21)	1.841(2)	C(2)-C(4)	1.532(2)
N-C(1)	1.488(2)	C(2)-C(5)	1.539(2)
N-C(2)	1.511(2)	C(11)-C(12)	1.396(2)
C(11)-C(16)	1.410(2)	C(12)-C(13)	1.396(2)
C(13)-C(14)	1.394(2)	C(14)-C(15)	1.388(3)
C(15)-C(16)	1.392(2)	C(21)-C(26)	1.397(2)
C(21)-C(22)	1.405(2)	C(22)-C(23)	1.384(2)
C(23)-C(24)	1.392(2)	C(24)-C(25)	1.384(2)
C(25)-C(26)	1.397(2)		

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
N-P-C(21)	101.37(6)	N-C(2)-C(3)	110.79(11)
N-P-C(11)	110.09(6)	N-C(2)-C(4)	110.54(13)
C(21)-P-C(11)	101.22(7)	N-C(2)-C(5)	109.88(12)
C(1)-N-P	120.05(10)	C(3)-C(2)-C(5)	107.22(13)
C(2)-N-P	116.24(9)	C(4)-C(2)-C(3)	108.44(13)
C(1)-N-C(2)	117.11(11)	C(4)-C(2)-C(5)	109.90(13)
N-C(1)-C(1')	113.3(2)	C(12)-C(11)-C(16)	117.68(14)

C(12)-C(11)-P	126.50(12)	C(16)-C(11)-P	115.63(12)
C(11)-C(12)-C(13)	121.3(2)	C(14)-C(13)-C(12)	119.9(2)
C(15)-C(14)-C(13)	119.9(2)	C(14)-C(15)-C(16)	119.8(2)
C(15)-C(16)-C(11)	121.3(2)	C(26)-C(21)-C(22)	117.83(14)
C(26)-C(21)-P	125.44(12)	C(22)-C(21)-P	116.54(11)
C(23)-C(22)-C(21)	121.3(2)	C(22)-C(23)-C(24)	120.2(2)
C(25)-C(24)-C(23)	119.4(2)	C(24)-C(25)-C(26)	120.5(2)
C(25)-C(26)-C(21)	120.8(2)		

Appendix 7.2: Supplementary Crystal Structure Data for Dichloro-P,P'-(N,N'-bis(diphenylphosphino)-N,N'-dimethylethylenediamine)palladium(II) dichloromethane solvate [(dppmen)$PdCl_2$. CH_2Cl_2]

X-ray crystallographic work on this compound was performed by Dr. D.S. Yufit.

Empirical Formula	$C_{29}H_{32}Cl_4N_2P_2Pd$
Formula Weight	718.71
Temperature	120.0 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space Group	P21/n
Unit Cell Dimensions	a = 10.7017(1) Å
	b = 16.8761(2) Å
	c = 16.9923(1) Å
	$\alpha = 90°$
	$\beta = 94.726°$
	$\gamma = 90°$
Volume	3058.43(5) $Å^3$
Z	4
Density (calculated)	1.561 Mg m^{-3}
Absorption Coefficient	1.084 mm^{-1}
F(000)	1456
Crystal Size	0.24 x 0.20 x 0.06mm
θ Range for Data Collection	1.70° to 30.45°
Index Ranges	$-14 \leq h \leq 14$
	$-23 \leq k \leq 23$
	$-23 \leq l \leq 23$
Reflections Collected	36646
Independent Reflections	8605 (R_{int} = 0.0565)

Absorption Correction	Multi-Scan
Min. and Max. Transmission	0.887 and 1.000
Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	8581 / 0 / 471
Goodness of Fit on F^2	1.111
Final R Indices	R1 = 0.0377, wR2 = 0.0650
R Indices (all data)	R1 = 0.0676, wR2 = 0.0793
Largest Diffraction Peak and Hole	0.610 and -0.803 e $Å^{-3}$

Bond Length Data

Bond	Length / Å	Bond	Length / Å
Pd(1)-P(1)	2.2518(7)	P(1)-N(1)	1.655(2)
Pd(1)-P(2)	2.2807(7)	P(1)-C(5)	1.829(3)
Pd(1)-Cl(1)	2.3715(7)	P(1)-C(11)	1.824(3)
Pd(1)-Cl(2)	2.3734(7)	P(2)-N(2)	1.691(2)
N(1)-C(2)	1.467(3)	P(2)-C(17)	1.824(3)
N(1)-C(1)	1.469(3)	P(2)-C(23)	1.828(3)
N(2)-C(3)	1.481(3)	C(2)-C(3)	1.518(4)
N(2)-C(4)	1.474(4)	Cl(1S)-C(1S)	1.773(4)
Cl(2S)-C(1S)	1.775(4)	C(5)-C(10)	1.387(4)
C(5)-C(6)	1.395(4)	C(6)-C(7)	1.386(4)
C(7)-C(8)	1.392(5)	C(8)-C(9)	1.386(5)
C(9)-C(10)	1.403(4)	C(11)-C(16)	1.389(4)
C(11)-C(12)	1.406(4)	C(12)-C(13)	1.386(4)
C(13)-C(14)	1.392(5)	C(14)-C(15)	1.388(5)
C(15)-C(16)	1.395(4)	C(17)-C(22)	1.386(4)
C(17)-C(18)	1.407(4)	C(18)-C(19)	1.390(4)
C(19)C(20)	1.387(4)	C(20)-C(21)	1.387(5)
C(21)-C(22)	1.397(4)	C(23)-C(24)	1.401(4)
C(23)-C(28)	1.402(4)	C(24)-C(25)	1.404(4)
C(25)-C(26)	1.385(4)	C(26)-C(27)	1.385(4)
C(27)-C(28)	1.393(4)		

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
P(1)-Pd(1)-P(2)	94.87(3)	N(1)-P(1)-C(5)	101.06(12)
P(2)-Pd(1)-Cl(1)	85.14(2)	N(1)-P(1)-C(11)	110.27(12)
P(1)-Pd(1)-Cl(2)	88.47(2)	C(11)-P(1)-C(5)	106.58(12)
Cl(1)-Pd(1)-Cl(2)	91.03(2)	N(1)-P(1)-Pd(1)	115.03(8)
P(1)-Pd(1)-Cl(1)	175.93(3)	C(5)-P(1)-Pd(1)	118.75(9)
P(2)-Pd(1)-Cl(2)	172.34(3)	C(11)-P(1)-Pd(1)	104.86(9)
C(1)-N(1)-P(1)	120.7(2)	N(2)-P(2)-C(17)	102.77(12)
C(2)-N(1)-P(1)	122.9(2)	N(2)-P(2)-C(23)	105.38(11)
C(2)-N(1)-C(1)	116.4(2)	C(17)-P(2)-C(23)	108.47(13)
C(3)-N(2)-P(2)	117.0(2)	N(2)-P(2)-Pd(1)	118.47(8)
C(4)-N(2)-P(2)	121.9(2)	C(17)-P(2)-Pd(1)	106.26(9)
C(4)-N(2)-C(3)	109.5(2)	C(23)-P(2)-Pd(1)	114.56(9)
N(1)-C(2)-C(3)	111.4(2)	N(2)-C(3)-C(2)	113.0(2)
C(10)-C(5)-C(6)	119.2(3)	C(10)-C(5)-P(1)	124.6(2)
C(6)-C(5)-P(1)	115.8(2)	C(7)-C(6)-C(5)	120.5(3)
C(6)-C(7)-C(8)	120.6(3)	C(9)-C(8)-C(7)	119.2(3)
C(8)-C(9)-C(10)	120.4(3)	C(5)-C(10)-C(9)	120.1(3)
C(16)-C(11)-C(12)	119.5(3)	C(16)-C(11)-P(1)	122.6(2)
C(12)-C(11)-P(1)	117.3(2)	C(13)-C(12)-C(11)	120.0(3)
C(12)-C(13)-C(14)	120.2(3)	C(15)-C(14)-C(13)	120.0(3)
C(14)-C(15)-C(16)	120.2(3)	C(11)-C(16)-C(15)	120.1(3)
C(22)-C(17)-C(18)	119.2(3)	C(22)-C(17)-P(2)	124.1(2)
C(18)-C(17)-P(2)	116.7(2)	C(19)-C(18)-C(17)	120.5(3)
C(20)-C(19)-C(18)	119.7(3)	C(19)-C(20)-C(21)	120.2(3)
C(20)-C(21)-C(22)	120.4(3)	C(17)-C(22)-C(21)	120.0(3)
C(24)-C(23)-C(28)	119.2(3)	C(24)-C(23)-P(2)	120.4(2)
C(28)-C(23)-P(2)	120.1(2)	C(23)-C(24)-C(25)	119.9(3)
C(26)-C(25)-C(24)	120.1(3)	C(25)-C(26)-C(27)	120.3(3)
C(26)-C(27)-C(28)	120.2(3)	C(27)-C(28)-C(23)	120.2(3)
Cl(2S)-C(1S)-Cl(1S)	111.7(2)		

Appendix 7.3: Supplementary Crystal Structure Data for Dichloro-P,P'-(N,N'-bis(diphenylphosphino)-N,N'-diphenylethylenediamine)palladium(II) chloroform solvate [(dpppen)$PdCl_2$. $CHCl_3$]

X-ray crystallographic work on this compound was performed by Mr. S. Borwick.

Empirical Formula	$C_{39}H_{35}Cl_5N_2P_2Pd$
Formula Weight	877.28
Temperature	150K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space Group	P2 (1)/n
Unit Cell Dimensions	a = 8.9145(2) Å
	b = 19.9703(4) Å
	c = 21.4936(3) Å
	$\alpha = 90°$
	$\beta = 97.361(1)°$
	$\gamma = 90°$
Volume	3794.87(13) $Å^3$
Z	4
Density (calculated)	1.536 g cm^{-3}
Absorption Coefficient	0.957 mm^{-1}
Crystal Size	0.25 x 0.09 x 0.07mm
θ Range for Data Collection	1.91° to 27.50°
Index Ranges	$-12 \leq h \leq 12$
	$-25 \leq k \leq 26$
	$-29 \leq l \leq 30$
Reflections Collected	26939
Independent Reflections	8700 (R_{int} = 0.0566)
Absorption Correction	Integration

Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	8516 / 0 / 582
Final R Indices ($I > 2\Sigma(I)$)	R1 = 0.0436, w(R2) = 0.0826
R Indices (All Data)	R1 = 0.0723, w(R2) = 0.1042
Largest Diffraction Peak and Hole	0.510 and -0.582 e $Å^{-3}$

Bond Length Data

Bond	Length / Å	Bond	Length / Å
Pd(1) - P(2)	2.262(1)	P(1)-N(1)	1.692(3)
Pd(1)-P(2)	2.288(1)	P(2)-N(2)	1.681(3)
Pd(1)-Cl(1)	2.369(1)	P(1)-C(1A)	1.821(4)
Pd(1)-Cl(2)	2.368(1)	P(1)-C(1B)	1.829(4)
N(1)-C(1)	1.488(4)	P(2)-C(1E)	1.840(4)
N(2)-C(2)	1.479(4)	P(2)-C(1F)	1.809(4)
N(1)-C(1C)	1.435(4)	C(1)-C(2)	1.509(5)
N(2)-C(1D)	1.438(4)	C(1A)-C(2A)	1.399(5)
C(1B)-C(2B)	1.399(5)	C(2A)-C(3A)	1.396(5)
C(2B)-C(3B)	1.388(5)	C(3A)-C(4A)	1.382(6)
C(3B)-C(4B)	1.382(6)	C(4A)-C(5A)	1.388(6)
C(4B)-C(5B)	1.385(6)	C(5A)-C(6A)	1.386(6)
C(5B)-C(6B)	1.394(6)	C(6A)-C(1A)	1.401(5)
C(6B)-C(1B)	1.398(5)	C(1C)-C(2C)	1.392(5)
C(1D)-C(2D)	1.389(5)	C(2C)-C(3C)	1.394(6)
C(2D)-C(3D)	1.389(5)	C(3C)-C(4C)	1.371(7)
C(3D)-C(4D)	1.387(6)	C(4C)-C(5C)	1.378(7)
C(4D)-C(5D)	1.379(6)	C(5C)-C(6C)	1.386(6)
C(5D)-C(6D)	1.396(5)	C(6C)-C(1C)	1.392(5)
C(6D)-C(1D)	1.395(5)	C(1E)-C(2E)	1.393(5)
C(1F)-C(2F)	1.394(5)	C(2E)-C(3E)	1.388(5)
C(2F)-C(3F)	1.391(6)	C(3E)-C(4E)	1.379(6)
C(3F)-C(4F)	1.381(6)	C(4E)-C(5E)	1.389(6)
C(4F)-C(5F)	1.375(6)	C(5E)-C(6E)	1.385(5)
C(5F)-C(6F)	1.396(5)	C(6E)-C(1E)	1.404(5)

C(6F)-C(1F)	1.392(5)	C(1S)-Cl(1S)	1.756(5)
C(1S)-Cl(2S)	1.755(4)	C(1S)-Cl(3S)	1.766(4)

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
P(1)-Pd(1)-P(2)	98.19(3)	N(1)-P(1)-C(1A)	101.7(2)
P(1)-Pd(1)-Cl(1)	94.94(3)	N(1)-P(1)-C(1B)	102.2(2)
P(2)-Pd(1)-Cl(2)	88.32(3)	C(1A)-P(1)-C(1B)	108.8(2)
Cl(1)-Pd(1)-Cl(2)	88.87(3)	N(1)-P(1)-Pd(1)	123.33(11)
C(1)-N(1)-P(1)	120.1(2)	C(1A)-P(1)-Pd(1)	109.90(12)
C(1)-N(1)-C(1C)	116.0(3)	C(1B)-P(1)-Pd(1)	109.94(12)
C(1C)-N(1)-P(1)	123.8(2)	N(2)-P(2)-C(1F)	105.0(2)
C(2)-N(2)-P(2)	113.6(2)	N(2)-P(2)-C(1E)	101.6(2)
C(2)-N(2)-C(1D)	117.1(3)	C(1E)-P(2)-C(1F)	106.3(2)
C(1D)-N(2)-P(2)	129.3(2)	N(2)-P(2)-Pd(1)	116.51(11)
N(1)-C(1)-C(2)	112.1(3)	C(1E)-P(2)-Pd(1)	112.02(12)
C(1)-C(2)-N(2)	111.0(3)	C(1F)-P(2)-Pd(1)	114.18(12)

Appendix 7.4: Supplementary Crystal Structure Data for Dichloro-P,P'-(N,N'-bis(diphenylphosphino)-N,N'-di-*tert*-butylethylenediamine)palladium(II) bis(tetrahydrofuran) solvate [(dpptben)$PdCl_2$. 2 THF]

X-ray crystallographic work on this compound was performed by Mr. M. Leech.

Empirical Formula	$C_{42}H_{58}Cl_2N_2P_2PdO_2$
Formula Weight	830.19
Temperature	120.0 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space Group	P1 bar
Unit Cell Dimensions	a = 11.292(1) Å
	b = 12.005(2) Å
	c = 15.629(1) Å
	α = 87.311(4)°
	β = 86.235(4)°
	γ = 79.190(4)°
Volume	2075.29 $Å^3$
Z	2
Density (calculated)	1.33 Mg m^{-3}
Absorption Coefficient	0.68 mm^{-1}
Crystal Size	0.25 x 0.20 x 0.10mm
θ Range for Data Collection	13.63° to 21.32°
Index Ranges	$-13 \leq h \leq 13$
	$-13 \leq k \leq 14$
	$0 \leq l \leq 19$
Reflections Collected	16365
Independent Reflections	7176 (R_{int} = 0.045)
Absorption Correction	Multi-Scan (SADABS [1])

Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	5586 / 0 / 460
r(F)	0.0346
$wR(F^2)$	0.0400
Largest Diffraction Peak and Hole	0.95 and -0.71 e $Å^{-3}$

Bond Length Data

Bond	Length / Å	Bond	Length / Å
Pd(1)-P(1)	2.2904(7)	P(1)-N(1)	1.698(3)
Pd(1)-P(2)	2.2758(8)	P(2)-N(2)	1.676(3)
Pd(1)-Cl(1)	2.3504(7)	N(1)-C(1)	1.554(4)
Pd(1)-Cl(2)	2.3653(8)	N(1)-C(2)	1.491(4)
C(2)-C(3)	1.520(4)	N(2)-C(3)	1.482(4)
C(1)-C(5)	1.530(5)	N(2)-C(4)	1.533(4)
C(1)-C(6)	1.525(5)	C(4)-C(8)	1.526(5)
C(1)-C(7)	1.542(4)	C(4)-C(9)	1.527(5)
C(4)-C(10)	1.529(5)	P(1)-C(11)	1.833(3)
C(11)-C(12)	1.396(4)	C(12)-C(13)	1.395(4)
C(13)-C(14)	1.383(5)	C(14)-C(15)	1.384(5)
C(15)-C(16)	1.389(5)	C(16)-C(11)	1.405(4)
P(1)-C(17)	1.823(3)	C(17)-C(18)	1.391(5)
C(18)-C(19)	1.389(5)	C(19)-C(20)	1.386(6)
C(20)-C(21)	1.390(6)	C(21)-C(22)	1.379(5)
C(22)-C(17)	1.404(4)	P(2)-C(23)	1.834(3)
C(23)-C(24)	1.400(6)	C(24)-C(25)	1.412(6)
C(25)-C(26)	1.40(1)	C(26)-C(27)	1.36(1)
C(27)-C(28)	1.380(7)	C(28)-C(23)	1.398(6)
P(2)-C(29)	1.819(3)	C(29)-C(30)	1.405(5)
C(30)-C(31)	1.394(5)	C(31)-C(32)	1.390(6)
C(32)-C(33)	1.391(6)	C(33)-C(34)	1.400(5)
C(34)-C(29)	1.385(5)	O(100)-C(102)	2.342(5)
O(200)-C(201)	1.412(8)	O(100)-C(101)	1.413(6)
O(200)-C(202)	2.100(13)	O(100)-C(103)	2.396(7)

O(200)-C(203)	2.337(11)	O(100)-C(104)	1.451(9)
O(200)-C(204)	1.428(16)	C(101)-C(102)	1.527(6)
C(201)-C(202)	1.200(13)	C(102)-C(103)	1.509(7)
C(202)-C(203)	1.466(19)	C(103)-C(104)	1.490(8)
C(203)-C(204)	1.374(17)		

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
P(1)-Pd(1)-P(2)	98.54(3)	Pd(1)-P(1)-N(1)	120.03(9)
P(1)-Pd(1)-Cl(2)	83.62(3)	Pd(1)-P(1)-C(17)	101.4(1)
P(2)-Pd(1)-Cl(1)	89.31(3)	N(1)-P(1)-C(17)	108.45(13)
Cl(1)-Pd(1)-Cl(2)	87.95(3)	Pd(1)-P(1)-C(11)	110.5(1)
P(1)-Pd(1)-Cl(1)	169.93(3)	N(1)-P(1)-C(11)	105.82(13)
P(2)-Pd(1)-Cl(2)	173.79(3)	C(17)-P(1)-C(11)	110.47(14)
Pd(1)-P(2)-C(23)	113.39(12)	P(1)-N(1)-C(1)	127.8(2)
Pd(1)-P(2)-C(29)	103.57(11)	P(1)-N(1)-C(2)	111.91(19)
C(23)-P(2)-C(29)	106.02(17)	C(1)-N(1)-C(2)	109.3(2)
Pd(1)-P(2)-N(2)	115.5(1)	P(2)-N(2)-C(3)	115.3(2)
C(23)-P(2)-N(2)	106.94(15)	P(2)-N(2)-C(4)	127.3(2)
C(29)-P(2)-N(2)	111.04(14)	C(3)-N(2)-C(4)	114.9(2)
N(1)-C(2)-C(3)	118.7(2)	N(2)-C(3)-C(2)	115.4(2)
N(1)-C(1)-C(5)	106.9(3)	N(2)-C(4)-C(8)	109.0(3)
N(1)-C(1)-C(6)	115.0(3)	N(2)-C(4)-C(9)	111.7(3)
N(1)-C(1)-C(7)	110.9(2)	N(2)-C(4)-C(10)	110.6(3)
C(5)-C(1)-C(6)	106.7(3)	C(8)-C(4)-C(9)	107.4(3)
C(5)-C(1)-C(7)	109.9(3)	C(8)-C(4)-C(10)	109.4(3)
C(6)-C(1)-C(7)	107.3(3)	C(9)-C(4)-C(10)	108.7(3)
P(1)-C(11)-C(12)	118.0(2)	P(1)-C(11)-C(16)	123.1(2)
C(11)-C(12)-C(13)	121.1(3)	C(12)-C(13)-C(14)	119.6(3)
C(13)-C(14)-C(15)	120.2(3)	C(14)-C(15)-C(16)	120.7(3)
C(15)-C(16)-C(11)	120.0(3)	C(16)-C(11)-C(12)	118.6(3)
P(1)-C(17)-C(18)	122.9(2)	P(1)-C(17)-C(22)	117.5(2)

C(17)-C(18)-C(19)	119.5(3)	C(18)-C(19)-C(20)	120.6(4)
C(19)-C(20)-C(21)	120.0(3)	C(20)-C(21)-C(22)	119.4(3)
C(21)-C(22)-C(17)	120.7(3)	C(22)-C(17)-C(18)	119.4(3)
P(2)-C(23)-C(24)	116.6(3)	P(2)-C(23)-C(28)	123.7(3)
C(23)-C(24)-C(25)	119.1(5)	C(24)-C(25)-C(26)	119.2(6)
C(25)-C(26)-C(27)	121.2(4)	C(26)-C(27)-C(28)	119.9(6)
C(27)-C(28)-C(23)	120.8(5)	C(28)-C(23)-C(24)	119.6(4)
P(2)-C(29)-C(30)	117.7(3)	P(2)-C(29)-C(34)	122.1(2)
C(29)-C(30)-C(31)	120.2(3)	C(30)-C(31)-C(32)	120.1(3)
C(31)-C(32)-C(33)	119.8(3)	C(32)-C(33)-C(34)	120.2(3)
C(33)-C(34)-C(29)	120.3(3)	C(34)-C(29)-C(30)	119.4(3)
O(100)-C(101)-C(102)	105.6(4)	C(101)-C(102)-C(103)	103.1(4)
C(102)-C(103)-C(104)	104.4(5)	C(103)-C(104)-O(100)	109.1(4)
C(104)-O(100)-C(101)	105.6(4)	O(200)-C(201)-C(202)	106.8(8)
C(201)-C(202)-C(203)	118.0(15)	C(202)-C(203)-C(204)	94.9(9)
C(203)-C(204)-O(200)	113.0(8)	C(204)-O(200)-C(201)	102.8(7)

Reference

1. G.M. Sheldrick, SADABS, University of Gottingen, Germany, 1997.

Appendix 7.5: Supplementary Crystal Structure Data for Dichloro-P,P'-(N,N'-bis(diphenylphosphino)-N,N'-dimethylpropylenediamine)palladium(II) [(dppmpn)$PdCl_2$]

X-ray crystallographic work on this compound was performed by Dr. D.S. Yufit.

Empirical Formula	$C_{29}H_{32}N_2P_2PdCl_2$
Formula Weight	647.81
Temperature	120(1)K
Wavelength	0.71073Å
Crystal system	Monoclinic
Space Group	P 21/c
Unit Cell Dimensions	a = 10.852(1)Å
	b = 14.956(1)Å
	c = 17.244(1)Å
	$\alpha = 90°$
	$\beta = 97.45(1)°$
	$\gamma = 90°$
Volume	2775.2(4)$Å^3$
Z	4
Density (calculated)	1.550Mg m^{-3}
Absorption Coefficient	0.999mm^{-1}
F(000)	1320
Crystal Size	0.20 x 0.18 x 0.04mm
θ Range for Data Collection	1.81 to 27.50°
Index Ranges	$-15 \leq h \leq 14$
	$-20 \leq k \leq 20$
	$-24 \leq l \leq 24$
Reflections Collected	26141
Independent Reflections	6351
Absorption Correction	Multi - Scan

Max. and Min. Transmission	1.000 and 0.817
Refinement Method	Full - Matrix Least Squares on F^2
Data / Restraints / Parameters	6195 / 0 / 453
Goodness of Fit on F^2	1.062
Final R Indices	$R_1 = 0.0359$, $w(R^2) = 0.0648$
R Indices (all data)	$R_1 = 0.0592$, $w(R^2) = 0.0756$
Largest Diffraction Peak and Hole	0.658 and -0.904 e A^{-3}

Bond Length Data

Bond	Length / Å	Bond	Length / Å
Pd(1) - P(1)	2.2593(9)	P(1) - N(1)	1.683(2)
Pd(1) - P(2)	2.2693(8)	P(1) - C(6)	1.812(3)
Pd(1) - Cl(1)	2.3757(9)	P(1) - C(12)	1.839(3)
Pd(1) - Cl(2)	2.3861(8)	P(2) - N(2)	1.670(2)
N(1) - C(1)	1.474(4)	P(2) - C(18)	1.835(3)
N(1) - C(2)	1.477(4)	P(2) - C(24)	1.828(3)
N(2) - C(4)	1.471(4)	C(2) - C(3)	1.526(4)
N(2) - C(5)	1.470(4)	C(3) - C(4)	1.530(4)
C(6) - C(7)	1.392(4)	C(7) - C(8)	1.387(5)
C(8) - C(9)	1.377(5)	C(9) - C(10)	1.382(5)
C(10) - C(11)	1.388(4)	C(6) - C(11)	1.394(4)
C(12) - C(13)	1.401(4)	C(13) - C(14)	1.394(4)
C(14) - C(15)	1.381(4)	C(15) - C(16)	1.390(5)
C(16) - C(17)	1.391(4)	C(12) - C(17)	1.402(4)
C(18) - C(19)	1.400(4)	C(19) - C(20)	1.396(4)
C(20) - C(21)	1.389(4)	C(21) - C(22)	1.388(4)
C(22) - C(23)	1.385(4)	C(18) - C(23)	1.400(4)
C(24) - C(25)	1.399(4)	C(25) - C(26)	1.392(4)
C(26) - C(27)	1.385(4)	C(27) - C(28)	1.387(5)
C(28) - C(29)	1.390(5)	C(24) - C(29)	1.394(4)

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
P(1) - Pd - P(2)	99.74(3)	N(1) - P(1) - C(6)	102.83(13)
P(1) - Pd - Cl(2)	84.88(3)	N(1) - P(1) - C(12)	104.28(13)
P(2) - Pd - Cl(1)	86.73(3)	C(6) - P(1) - C(12)	109.06(14)
Cl(1) - Pd(1) - Cl(2)	90.19(3)	N(1) - P(1) - Pd(1)	109.11(9)
P(1) - Pd(1) - Cl(1)	169.63(3)	C(6) - P(1) - Pd(1)	111.57(10)
P(2) - Pd(1) - Cl(2)	169.10(3)	C(12) - P(1) - Pd(1)	109.38(10)
C(1) - N(1) - P(1)	122.7(2)	N(2) - P(2) - C(18)	100.67(13)
C(2) - N(1) - P(1)	115.7(2)	N(2) - P(2) - C(24)	102.57(13)
C(1) - N(1) - C(2)	113.0(3)	C(18) - P(2) - C(24)	110.45(13)
C(4) - N(2) - P(2)	124.5(2)	N(2) - P(2) - Pd(1)	124.92(10)
C(5) - N(2) - P(2)	120.4(2)	C(18) - P(2) - Pd(1)	107.51(10)
C(4) - N(2) - C(5)	114.5(2)	C(24) - P(2) - Pd(1)	110.02(10)
N(1) - C(2) - C(3)	113.0(3)	C(2) - C(3) - C(4)	112.9(3)
C(3) - C(4) - N(2)	115.3(3)	C(7) - C(6) - P(1)	123.7(2)
C(11) - C(6) - P(1)	116.8(2)	C(7) - C(6) - C(11)	119.3(3)
C(6) - C(7) - C(8)	119.8(3)	C(7) - C(8) - C(9)	120.5(3)
C(8) - C(9) - C(10)	120.2(3)	C(9) - C(10) - C(11)	119.7(3)
C(10) - C(11) - C(6)	120.5(3)	C(13) - C(12) - P(1)	121.5(3)
C(17) - C(12) - P(1)	119.6(2)	C(17) - C(12) - C(13)	118.6(3)
C(12) - C(13) - C(14)	120.6(3)	C(13) - C(14) - C(15)	120.3(3)
C(14) - C(15) - C(16)	119.7(3)	C(15) - C(16) - C(17)	120.5(3)
C(16) - C(17) - C(12)	120.2(3)	C(19) - C(18) - P(2)	120.1(2)
C(23) - C(18) - P(2)	120.8(2)	C(23) - C(18) - C(19)	119.0(3)
C(18) - C(19) - C(20)	120.0(3)	C(19) - C(20) - C(21)	120.4(3)
C(20) - C(21) - C(22)	119.6(3)	C(21) - C(22) - C(23)	120.4(3)
C(22) - C(23) - C(18)	120.5(3)	C(25) - C(24) - P(2)	119.0(2)
C(29) - C(24) - P(2)	119.0(2)	C(29) - C(24) - C(25)	119.1(3)
C(24) - C(25) - C(26)	120.1(3)	C(25) - C(26) - C(27)	120.5(3)
C(26) - C(27) - C(28)	119.7(3)	C(27) - C(28) - C(29)	120.3(3)
C(28) - C(29) - C(24)	120.3(3)		

Appendix 7.6: Supplementary Crystal Structure Data for Diacetato-P,P'-(N,N'-bis(diphenylphosphino)-N,N'-dimethylethylenediamine) palladium(II) [(dppmen)Pd(OCOCH$_3$)$_2$]

X-ray crystallographic work on this compound was performed by Mr. A. Mackinnon.

Empirical formula	$C_{32}H_{36}N_2O_4P_2Pd$
Formula Weight	680.96
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal System	triclinic
Space Group	P-1
Unit Cell Dimensions	a = 10.004 Å
	b = 11.775 Å
	c = 14.415 Å
	α = 81.89(3)°
	β = 86.22(3)°
	γ = 66.22(3)°
Unit Cell Volume	1538.3(5) Å^3
Z	4
Density (Calculated)	1.470 g cm^{-3}
Absorption Coefficient	0.746 mm^{-1}
F(000)	700
Crystal Size	0.5 x 0.5 x 0.3mm
θ Range for Data Collection	1.43° to 27.48°
Index Ranges	$-12 \leq h \leq 12$
	$-15 \leq k \leq 15$
	$-16 \leq l \leq 18$
Reflections Collected	11328
Independent Reflections	6979

Observed Reflections (I > 2Σ(I))	5175
Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	6967 / 0 / 371
Goodness of Fit on F^2	1.024
Final R Indices (I > 2Σ(I))	R = 0.0541, wR = 0.1232
R Indices (all data)	R = 0.0816, wR = 0.1455

Bond Length Data

Bond	Length / Å	Bond	Length / Å
Pd(1)-O(8)	2.088(3)	P(2)-N(3)	1.654(4)
Pd(1)-O(12)	2.091(3)	P(2)-C(16)	1.824(5)
Pd(1)-P(2)	2.2348(13)	P(2)-C(22)	1.826(5)
Pd(1)-P(7)	2.2494(15)	P(7)-N(6)	1.691(4)
O(8)-C(9)	1.275(6)	P(7)-C(28)	1.820(4)
O(12)-C(13)	1.285(5)	P(7)-C(34)	1.811(5)
C(4)-N(3)	1.460(6)	C(9)-O(10)	1.222(6)
C(40)-N(3)	1.471(6)	C(13)-O(15)	1.236(6)
C(5)-N(6)	1.485(6)	C(9)-C(11)	1.513(7)
C(41)-N(6)	1.468(6)	C(13)-C(14)	1.528(7)
C(4)-C(5)	1.515(6)	C(16)-C(17)	1.392(7)
C(17)-C(18)	1.391(7)	C(18)-C(19)	1.392(8)
C(19)-C(20)	1.382(8)	C(20)-C(21)	1.390(7)
C(21)-C(16)	1.394(7)	C(22)-C(23)	1.407(7)
C(23)-C(24)	1.393(7)	C(24)-C(25)	1.369(8)
C(25)-C(26)	1.398(8)	C(26)-C(27)	1.389(8)
C(27)-C(22)	1.400(7)	C(28)-C(29)	1.396(6)
C(29)-C(30)	1.385(7)	C(30)-C(31)	1.394(7)
C(31)-C(32)	1.385(7)	C(32)-C(33)	1.393(6)
C(33)-C(28)	1.389(7)	C(34)-C(35)	1.398(6)
C(35)-C(36)	1.400(7)	C(36)-C(37)	1.374(7)
C(37)-C(38)	1.388(7)	C(38)-C(39)	1.401(7)
C(39)-C(34)	1.404(6)		

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
P(2)-Pd(1)-P(7)	95.65(5)	C(4)-N(3)-C(40)	116.2(4)
P(2)-Pd(1)-O(8)	88.70(10)	C(4)-N(3)-P(2)	121.5(3)
O(8)-Pd(1)-O(12)	90.37(13)	P(2)-N(3)-C(40)	112.3(3)
O(12)-Pd(1)-P(7)	84.82(10)	C(5)-N(6)-C(41)	107.7(4)
P(2)-Pd(1)-O(12)	176.31(9)	C(5)-N(6)-P(7)	118.5(3)
P(7)-Pd(1)-O(8)	171.35(9)	P(7)-N(6)-C(41)	117.9(3)
N(6)-C(5)-C(4)	115.4(4)	N(6)-P(7)-Pd(1)	120.21(14)
N(3)-C(4)-C(5)	114.2(4)	C(28)-P(7)-Pd(1)	104.8(2)
N(3)-P(2)-Pd(1)	114.9(2)	C(34)-P(7)-Pd(1)	112.0(2)
C(22)-P(2)-Pd(1)	107.7(2)	N(6)-P(7)-C(28)	103.7(2)
C(16)-P(2)-Pd(1)	113.9(2)	N(6)-P(7)-C(34)	107.5(2)
N(3)-P(2)-C(16)	103.8(2)	C(28)-P(7)-C(34)	107.7(2)
N(3)-P(2)-C(22)	109.9(2)	Pd(1)-O(12)-C(13)	122.4(3)
C(16)-P(2)-C(22)	106.3(2)	O(12)-C(13)-O(15)	122.3(4)
Pd(1)-O(8)-C(9)	112.1(3)	O(12)-C(13)-C(14)	118.6(4)
O(8)-C(9)-C(11)	114.6(5)	C(14)-C(13)-O(15)	119.1(4)
O(8)-C(9)-O(10)	124.7(5)	C(35)-C(34)-C(39)	119.3(4)
C(11)-C(9)-O(10)	120.7(5)	C(35)-C(34)-P(7)	119.1(4)
C(39)-C(34)-P(7)	121.4(3)	C(34)-C(35)-C(36)	119.9(4)
C(35)-C(36)-C(37)	120.5(5)	C(36)-C(37)-C(38)	120.5(5)
C(37)-C(38)-C(39)	119.8(5)	C(38)-C(39)-C(34)	120.0(4)
C(33)-C(28)-C(29)	119.4(4)	C(33)-C(28)-P(7)	121.5(3)
C(29)-C(28)-P(7)	118.6(4)	C(28)-C(29)-C(30)	120.0(4)
C(29)-C(30)-C(31)	120.5(5)	C(30)-C(31)-C(32)	119.5(4)
C(31)-C(32)-C(33)	120.2(5)	C(32)-C(33)-C(28)	120.3(4)
C(23)-C(22)-C(27)	119.3(5)	C(23)-C(22)-P(2)	118.7(4)
C(27)-C(22)-P(2)	121.8(4)	C(22)-C(23)-C(24)	120.0(5)
C(23)-C(24)-C(25)	120.3(5)	C(24)-C(25)-C(26)	120.3(5)
C(25)-C(26)-C(27)	120.3(5)	C(26)-C(27)-C(22)	119.7(5)
C(17)-C(16)-C(21)	119.2(5)	C(17)-C(16)-P(2)	124.2(4)

C(21)-C(16)-P(2)	116.6(4)	C(16)-C(17)-C(18)	120.5(5)
C(17)-C(18)-C(19)	120.0(5)	C(18)-C(19)-C(20)	119.6(5)
C(19)-C(20)-C(21)	120.6(5)	C(20)-C(21)-C(16)	120.1(5)

Appendix 7.7: Supplementary Crystal Structure Data for Dichloro-P,P'-(N,N'-bis(diphenylphosphino)-N,N'-dimethylethylenediamine)platinum(II) dichloromethane solvate [(dppmen)$PtCl_2$. CH_2Cl_2]

X-ray crystallographic work on this compound was performed by Dr. J.W. Yao.

Empirical Formula	$C_{29}H_{32}Cl_4N_2P_2Pt$
Formula Weight	807.40
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal System	Monoclinic
Space Group	P2(1)/n
Unit Cell Dimensions	a = 10.6635(1) Å
	b = 16.8728(2) Å
	c = 17.0720(2) Å
	$\alpha = 90°$
	$\beta = 95.10(1)°$
	$\gamma = 90°$
Volume	3059.5(1) $Å^3$
Z	4
Number of Reflections Used	379
Crystal Description	block
Crystal Colour	colourless
Density (calculated)	1.753 Mg m^{-3}
Absorption Coefficient	5.063 mm^{-1}
F(000)	1584
Crystal Size	0.26 x 0.30 x 0.44 mm
θ Range for Data Collection	1.70° to 27.47°

Index Ranges	$-13 \leq h \leq 13$
	$-21 \leq k \leq 21$
	$-22 \leq l \leq 15$
Experiment Device	Siemens Smart CCD
Experiment Methods	Omega
Reflections Collected	21902
Independent Reflections	6987 (R_{int} = 0.0215)
Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	6987 / 0 / 371
Goodness of Fit on F^2	1.200
Final R indices ($I > 2\Sigma(I)$)	R1 = 0.0209, wR2 = 0.0496
R Indices (all data)	R1 = 0.0269, wR2 = 0.0544
Largest Diffraction Peak and Hole	0.597 and -1.942 e A^{-3}

Bond Length Data

Bond	Length / Å	Bond	Length / Å
Pt(1)-P(1)	2.2498(7)	P(1)-N(1)	1.693(2)
Pt(1)-P(2)	2.2302(6)	P(1)-C(11)	1.823(3)
Pt(1)-Cl(1)	2.3707(6)	P(1)-C(21)	1.824(3)
Pt(1)-Cl(2)	2.3674(7)	P(2)-N(2)	1.649(2)
N(1)-C(1)	1.473(3)	P(2)-C(31)	1.825(3)
N(1)-C(01)	1.476(3)	P(2)-C(41)	1.813(3)
N(2)-C(2)	1.463(3)	C(1)-C(2)	1.519(4)
N(2)-C(02)	1.468(3)	C(11)-C(12)	1.388(4)
C(11)-C(16)	1.394(4)	C(12)-C(13)	1.397(4)
C(13)-C(14)	1.379(5)	C(14)-C(15)	1.382(5)
C(15)-C(16)	1.384(4)	C(21)-C(26)	1.395(4)
C(21)-C(22)	1.398(4)	C(22)-C(23)	1.389(4)
C(23)-C(24)	1.386(4)	C(24)-C(25)	1.385(4)
C(25)-C(26)	1.392(4)	C(31)-C(36)	1.388(4)
C(31)-C(32)	1.396(4)	C(32)-C(33)	1.388(4)
C(33)-C(34)	1.388(5)	C(34)-C(35)	1.371(5)

C(35)-C(36)	1.398(4)	C(41)-C(46)	1.394(4)
C(41)-C(42)	1.401(4)	C(42)-C(43)	1.384(4)
C(43)-C(44)	1.383(5)	C(44)-C(45)	1.385(5)
C(45)-C(46)	1.390(4)	C(1A)-Cl(3)	1.764(4)
C(1A)-Cl(4)	1.769(4)		

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
P(1)-Pt(1)-P(2)	95.46(2)	N(1)-P(1)-C(11)	102.6(1)
P(1)-Pt(1)-Cl(1)	85.97(2)	N(1)-P(1)-C(21)	105.0(1)
P(2)-Pt(1)-Cl(2)	89.60(2)	C(11)-P(1)-C(21)	108.5(1)
Cl(1)-Pt(1)-Cl(2)	88.54(2)	N(1)-P(1)-Pt(1)	117.8(1)
P(1)-Pt(1)-Cl(2)	171.95(2)	C(11)-P(1)-Pt(1)	107.1(1)
P(2)-Pt(1)-Cl(1)	175.70(2)	C(21)-P(1)-Pt(1)	114.8(1)
C(1)-N(1)-C(01)	109.6(2)	N(2)-P(2)-C(41)	109.9(1)
C(1)-N(1)-P(1)	117.1(2)	N(2)-P(2)-C(31)	101.1(1)
C(01)-N(1)-P(1)	121.2(2)	C(41)-P(2)-C(31)	106.4(1)
C(2)-N(2)-C(02)	116.6(2)	N(2)-P(2)-Pt(1)	115.1(1)
C(2)-N(2)-P(2)	122.8(2)	C(41)-P(2)-Pt(1)	106.1(1)
C(02)-N(2)-P(2)	120.5(2)	C(31)-P(2)-Pt(1)	117.9(1)
N(1)-C(1)-C(2)	112.9(2)	N(2)-C(2)-C(1)	111.4(2)
C(12)-C(11)-C(16)	119.3(3)	C(12)-C(11)-P(1)	124.1(2)
C(16)-C(11)-P(1)	116.7(2)	C(11)-C(12)-C(13)	119.5(3)
C(14)-C(13)-C(12)	120.8(3)	C(13)-C(14)-C(15)	119.6(3)
C(14)-C(15)-C(16)	120.1(3)	C(15)-C(16)-C(11)	120.6(3)
C(26)-C(21)-C(22)	119.2(3)	C(26)-C(21)-P(1)	120.3(2)
C(22)-C(21)-P(1)	120.2(2)	C(23)-C(22)-C(21)	120.1(3)
C(24)-C(23)-C(22)	120.1(3)	C(23)-C(24)-C(25)	120.4(3)
C(24)-C(25)-C(26)	119.8(3)	C(25)-C(26)-C(21)	120.3(3)
C(36)-C(31)-C(32)	119.1(3)	C(36)-C(31)-P(2)	125.0(2)
C(32)-C(31)-P(2)	115.6(2)	C(33)-C(32)-C(31)	120.7(3)
C(34)-C(33)-C(32)	119.9(3)	C(35)-C(34)-C(33)	119.5(3)

C(34)-C(35)-C(36)	121.2(3)	C(31)-C(36)-C(35)	119.5(3)
C(46)-C(41)-C(42)	119.0(3)	C(46)-C(41)-P(2)	122.7(2)
C(42)-C(41)-P(2)	117.6(2)	C(43)-C(42)-C(41)	120.6(3)
C(44)-C(43)-C(42)	120.0(3)	C(45)-C(44)-C(43)	120.0(3)
C(44)-C(45)-C(46)	120.4(3)	C(45)-C(46)-C(41)	120.1(3)
Cl(3)-C(1A)-Cl(4)	111.9(2)		

Appendix 7.8: Analysis of ^{31}P nmr Data

Change in ^{31}P nmr Chemical Shift of Ligands on Complexation to Palladium Dichloride

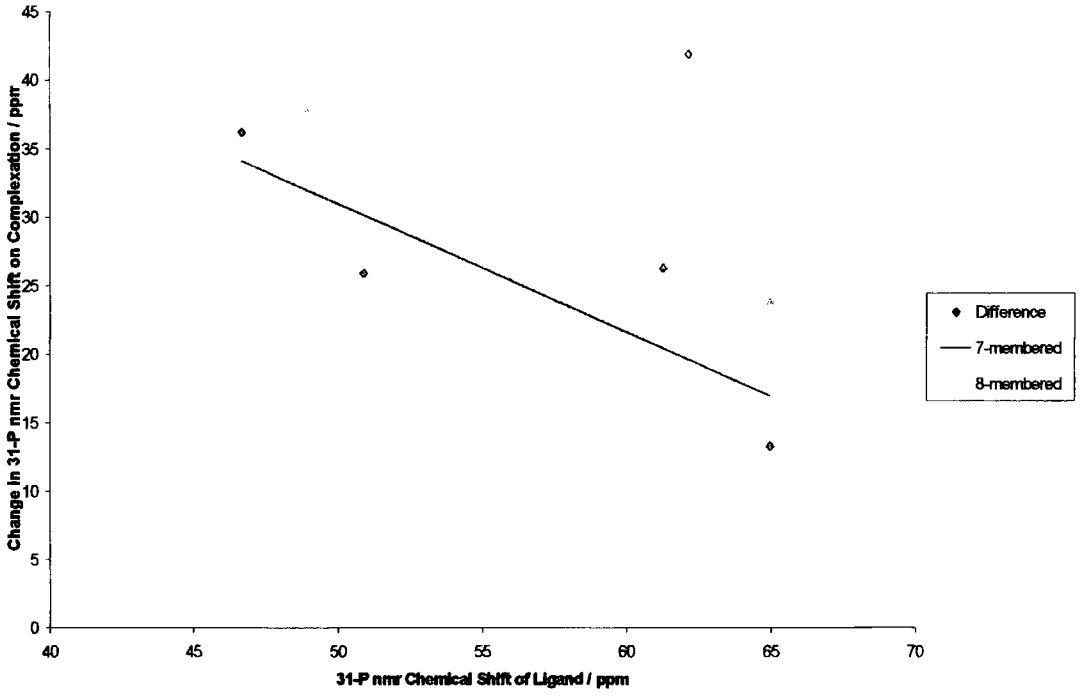

Fig. A7.1: Change in 31-P nmr Chemical Shift on Complexation to Palladium Dichloride

The blue points represent the compounds with two-carbon backbones, and hence seven-membered chelate rings (dppmen, dpppen, dppipen, dpptben). The blue line is a line of best fit considering only these data (gradient –0.93, intercept 77.7 ppm). The green points represent the compounds with three-carbon backbones and hence eight-membered chelate rings (dppmpn and dppippn). The green line is a line of best fit considering these compounds and the two-carbon backbone ligands (gradient –0.89, intercept 77.1ppm). The red data point is for dpppip, which does not fit the trend (see Discussion, Chapter Seven).

Change in ^{31}P nmr Chemical Shift of Ligands on Complexation to Platinum Dichloride

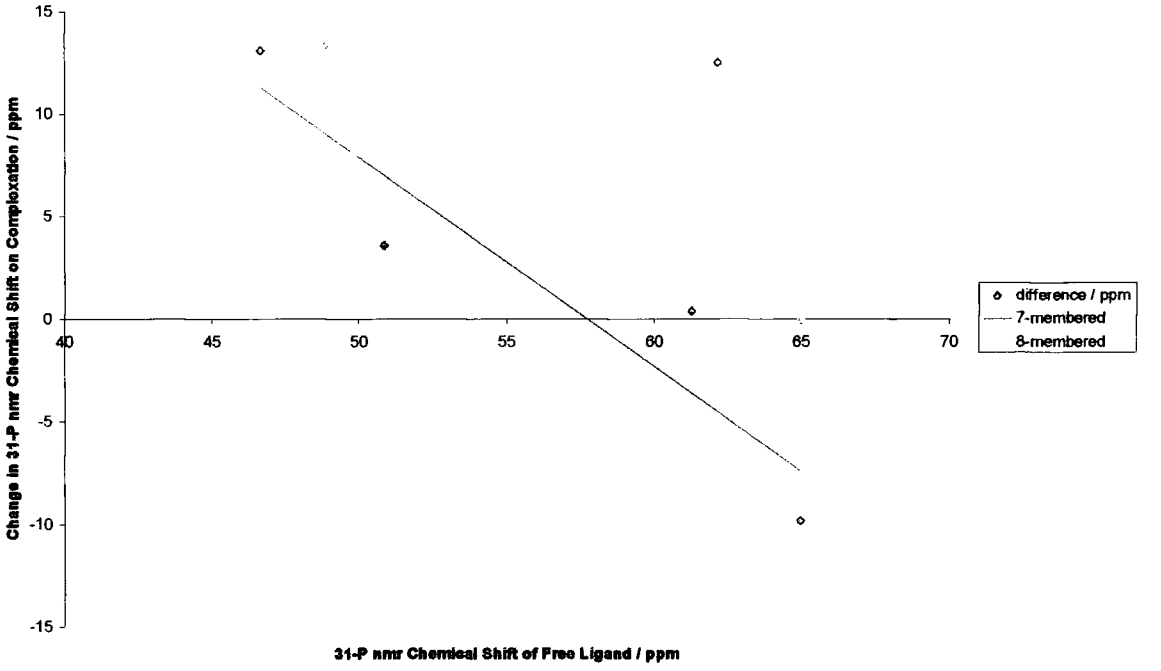

Fig A7.2: Change in 31-P nmr Chemical Shift on Complexation to Platinum Dichloride

The blue points represent the compounds with two-carbon backbones, and hence seven-membered chelate rings (dppmen, dpppen, dppipen, dpptben). The blue line is a line of best fit considering only these data (gradient –1.02, intercept 58.9 ppm). The green points represent the compounds with three-carbon backbones and hence eight-membered chelate rings (dppmpn and dppippn). The green line is a line of best fit considering these compounds and the two-carbon backbone ligands (gradient –0.93, intercept 55.6 ppm). The red data point is for dpppip, which does not fit the trend (see Discussion, Chapter Seven).

Appendix 8.1: Raw Data from Manganese Pentacarbonyl Bromide Reactions

A8.1.1 Key to Compounds Described in this Appendix

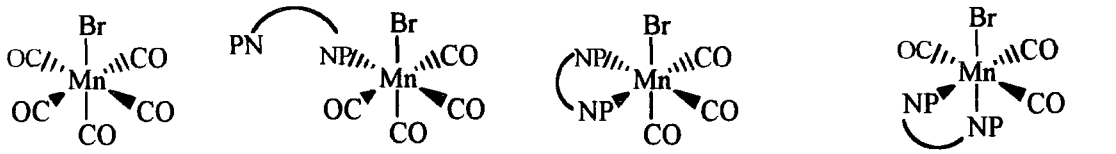

Fig. A8.1: Manganese Complexes of Chelating Aminophosphine Ligands

A8.1.2 Reaction of $[Mn(CO)_5Br]$ with dppb

A8.1.2.1 Room Temperature Reaction in CH_2Cl_2

Reaction Time / minutes	IR Peaks / cm^{-1}	Peak Intensity / arbitrary units
5	2137 (m) 2089 (w) 2052 (vs) 2007 (s) 1958 (br)	 35.4 4.9
14	2137 (m) 2089 (m) 2052 (vs) 2006 (br, s) 1957 (m)	 33.4 15.1
22	2155 (w) 2137 (w) 2126 (w) 2090 (s) 2052 (s) ~2020 (sh) 2006 (vs) 1957 (s)	 21.3 17.4
37	2155 (w) 2137 (vw) 2126 (w) 2090 (s) 2052 (s) 2014 (sh) 2006 (vs) 1957 (s)	 18.8 21.1

44	2155 (w) 2126 (w) 2090 (m) 2053 (m) 2014 (sh) 2006 (vs) 1957 (s)	 8.0 19.6
53	2155 (w) 2126 (w) 2090 (m) 2053 (w) 2020 (sh) 2006 (vs) 1957 (s)	 6.1 22.4
59	2155 (w) 2126 (w) 2090 (s) 2053 (w) 2020 (sh) 2006 (vs) 1957 (vs)	 4.8 25.3
70	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2020 (sh) 2006 (vs) 1957 (s)	 3.9 21.5
100	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2020 (sh) 2006 (vs) 1957 (s)	 3.5 20.3
135	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2019 (sh) 2006 (vs) 1956 (vs)	 4.6 29.6

24 hours	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2023 (vs) 2006 (vs) 1956 (vs) 1908 (s)	 3.1 26.5
∞	2155 (w) 2126 (w) 2090 (m) 2054 (w) 2024 (vs) 2006 (vs) 1956 (vs) 1908 (s)	 3.7 27.7

A8.1.2.2 Assignment of Peaks

Peak at / cm^{-1}	Assignment	Peak at / cm^{-1}	Assignment
2155	Solvent	2020	*fac*-[$(L_2)Mn(CO)_3Br$] and *cis*-[$LMn(CO)_4Br$]
2137	[$Mn(CO)_5Br$]	2006	*cis*-[$LMn(CO)_4Br$] and [$Mn(CO)_5Br$]
2126	Solvent	1956	*fac*-[$(L_2)Mn(CO)_3Br$]
2090	*cis*-[$LMn(CO)_4Br$]	1908	*fac*-[$(L_2)Mn(CO)_3Br$]
2052	[$Mn(CO)_5Br$]		

A8.1.2.3 Reaction in Refluxing $CHCl_3$

Reaction Time	IR Peaks / cm^{-1}	Assignment
10	2137 (vw)	[$Mn(CO)_5Br$]
	2090 (w)	*cis*-[$LMn(CO)_5Br$]
	2053 (w)	[$Mn(CO)_5Br$]
	2028 (vs)	*fac*-[$(L_2)Mn(CO)_3Br$] and *cis*-[$LMn(CO)_4Br$]
	2008 (sh)	*cis*-[$LMn(CO)_4Br$]
	1962 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]
	1910 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]
20	2029 (vs)	*fac*-[$(L_2)Mn(CO)_3Br$]
	1961 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]
	1909 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]

A8.1.3 Reaction of $[Mn(CO)_5Br]$ with dppmen

A8.1.3.1 Room Temperature Reaction in CH_2Cl_2

Reaction Time / minutes	IR Peaks / cm^{-1}	Peak Intensity / arbitrary units
3	2155 (vw) 2138 (m) 2051 (vs) 2007 (s) 1970 (vw)	 35.6 1.2
13	2155 (w) 2138 (w) 2087 (sh) 2052 (vs) 2007 (s) 1969 (w)	 38.0 1.6
21	2155 (w) 2137 (w) 2090 (w) 2052 (vs) 2006 (s) 1964 (w)	 36.9 4.9
33	2155 (w) 2137 (w) 2090 (w) 2052 (vs) 2022 (sh) 2006 (s) 1962 (m)	 34.6 9.8
44	2155 (w) 2137 (w) 2090 (m) 2052 (vs) 2020 (sh) 2006 (vs) 1961 (s)	 29.3 16.4
58	2155 (w) 2137 (w) 2127 (w) 2090 (m) 2052 (vs) 2022 (sh) 2006 (vs) 1961 (s)	 33.2 15.2

70	2155 (w) 2137 (vw) 2126 (w) 2090 (m) 2052 (vs) 2021 (sh) 2006 (s) 1961 (s)	 25.5 10.5
85	2155 (w) 2137 (vw) 2126 (w) 2090 (m) 2052 (vs) 2022 (sh) 2005 (vs) 1960 (s) 1925 (vw)	 26.3 15.0
101	2155 (w) 2137 (w) 2126 (w) 2090 (m) 2052 (s) 2023 (s) 2005 (vs) 1960 (s) 1925 (w)	 22.2 18.6
120	2155 (w) 2126 (w) 2090 (m) 2052 (m) 2023 (s) 2005 (vs) 1960 (s) 1924 (w)	 12.2 15.4
140	2155 (w) 2126 (w) 2090 (m) 2052 (m) 2024 (s) 2005 (vs) 1960 (s) 1924 (w)	 11.7 16.1

∞	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2025 (vs) 2005 (vs) 1960 (vs) 1922 (m)	 2.6 20.0

A8.1.3.2 Assignment of Peaks

Peak at / cm^{-1}	Assignment	Peak at / cm^{-1}	Assignment
2155	Solvent	2024	*cis*-[$LMn(CO)_4Br$] and *fac*-[$(L_2)Mn(CO)_3Br$]
2137	[$Mn(CO)_5Br$]	2006	[$Mn(CO)_5Br$] and *cis*-[$LMn(CO)_4Br$]
2126	Solvent	1960	*cis*-[$LMn(CO)_4Br$] and *fac*-[$(L_2)Mn(CO)_3Br$]
2090 2052	*cis*-[$LMn(CO)_4Br$] [$Mn(CO)_5Br$]	1922	*fac*-[$(L_2)Mn(CO)_3Br$]

A8.1.3.3 Reaction in Refluxing $CHCl_3$

Reaction Time / minutes	IR Peaks / cm^{-1}	Assignment
5	2138 (w) 2093 (m) 2053 (vs) 2029 (vs) 2010 (s) 1965 (s) 1923 (m)	[$Mn(CO)_5Br$] *cis*-[$LMn(CO)_4Br$] [$Mn(CO)_5Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *cis*-[$LMn(CO)_4Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$]
10	2138 (vw) 2093 (m) 2053 (m) 2029 (vs) 2011 (sh) 1965 (s) 1923 (m)	[$Mn(CO)_5Br$] *cis*-[$LMn(CO)_4Br$] [$Mn(CO)_5Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *cis*-[$LMn(CO)_4Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$]
15	2138 (vw) 2093 (m) 2053 (m) 2029 (s) 2011 (sh) 1965 (s) 1923 (m)	[$Mn(CO)_5Br$] *cis*-[$LMn(CO)_4Br$] [$Mn(CO)_5Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *cis*-[$LMn(CO)_4Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$]

20	2091 (vw) 2029 (vs) 1962 (s) 1920 (s)	*cis*-[$LMn(CO)_4Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$]
30	2029 (s) 1961 (vs) 1919 (s)	*fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
40	2029 (s) 1961 (vs) 1920 (s)	*fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
50	2029 (s) 1960 (vs) 1919 (s)	*fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
60	~2045 (sh) 2029 (m) 1960 (vs) 1921 (m, br)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
70	~2045 (w) 2030 (m) 1960 (vs) 1927 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
80	2045 (w) 2029 (m) 1960 (vs) 1919 (m, br)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
90	2046 (w) 2029 (m) 1960 (vs) 1920 (m, br)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
100	2046 (w, br) 2029 (w) 1960 (vs) 1924 (m, br)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
110	2047 (w, br) 2029 (w, br) 1960 (vs) 1924 (m, br)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
120	2048 (w, br) 2029 (w, br) 1960 (vs) 1924 (m, br)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers

A8.1.4 Reaction of $[Mn(CO)_5Br]$ with dpppen

A8.1.4.1 Room Temperature Reaction in CH_2Cl_2

Reaction Time / minutes	IR Peaks / cm^{-1}	Peak Intensity / arbitrary units
6	2155 (w) 2137 (w) 2052 (vs) 2007 (s) 1970 (vw)	 38.5 1.2
14	2155 (w) 2137 (w) 2088 (sh) 2052 (vs) 2007 (s) 1969 (w)	 37.7 1.7
21	2155 (w) 2137 (w) 2090 (sh) 2052 (vs) 2007 (s) 1968(br)	 36.9 2.2
40	2155 (w) 2137 (w) 2127 (w) 2090 (w) 2052 (vs) 2007 (s) 1966 (br) 1919 (vw)	 37.2 3.1
62	2155 (w) 2137 (w) 2127 (w) 2090 (w) 2052 (vs) 2021 (sh) 2007 (s) 1959 (m) 1919 (w)	 35.9 5.6
82	2155 (w) 2137 (w) 2127 (w) 2091 (w) 2052 (vs) 2021 (sh) 2008 (s) 1959 (m) 1919 (w)	 35.1 7.8

102	2155 (w) 2137 (w) 2127 (w) 2091 (w) 2052 (vs) 2023 (sh) 2008 (s) 1959 (m) 1919 (w)	 33.9 7.0
∞	2156 (w) 2126 (w) 2091 (m) 2054 (w) 2027 (vs) ~2010 (sh) 1957 (s) 1918 (m)	 6.2 12.8

A8.1.4.2 Assignment of Peaks

Peak At / cm^{-1}	Assignment	Peak At / cm^{-1}	Assignment
2155	Solvent	2027	*fac*-[$(L_2)Mn(CO)_3Br$] and *cis*-[$LMn(CO)_4Br$]
2137	[$Mn(CO)_5Br$]	2007	*cis*-[$LMn(CO)_4Br$] and [$Mn(CO)_5Br$]
2126	Solvent	1957	[$(L_2)Mn(CO)_3Br$] isomers
2091	*cis*-[$LMn(CO)_4Br$]	1918	[$(L_2)Mn(CO)_3Br$] isomers
2052	[$Mn(CO)_5Br$]		

A8.1.4.3 Reaction in Refluxing $CHCl_3$

Reaction Time / minutes	IR Peaks / minutes	Assignment
5	2093 (vw) 2053 (w) 2028 (vs) 1957(s) 1919 (s)	*cis*-[$LMn(CO)_4Br$] [$Mn(CO)_5Br$] *fac*-[$(L_2)Mn(CO)_3Br$] and *cis*-[$LMn(CO)_4Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$]
10	2093 (vw) 2028 (vs) 1958 (s) 1919 (s)	*cis*-[$LMn(CO)_4Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$]

15	2093 (vw) 2029 (vs) 1959 (vs) 1919 (s)	*cis*-[$LMn(CO)_4Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers $(L_2)Mn(CO)_5Br$ isomers
20	2030 (s) 1959 (vs) 1919 (s)	*fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
25	2050 (sh) 2032 (s) 1959 (vs) 1919 (s)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
30	2050 (sh) 2035 (m) 1959 (vs) 1919 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
35	2050 (sh) 2036 (m) 1960 (vs) 1919 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
40	2050 (sh) 2036 (w) 1960 (vs) 1919 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
45	2045 (w, br) 2037 (w) 1960 (vs) 1919 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
50	2045 (w, br) 2037 (w) 1960 (s) 1920 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
55	2045 (w, br) 2037 (w) 1960 (vs) 1920 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
60	2045 (w, br) 2037 (w) 1960 (vs) 1920 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers
65	2044 (w, br) 1960 (vs) 1920 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$]
70	2045 (w, br) 1960 (vs) 1920 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$]

A8.1.5 Reaction of $[Mn(CO)_5Br]$ with dppipen

A8.1.5.1 Room Temperature Reaction in CH_2Cl_2

Reaction Time / minutes	IR Peaks / cm^{-1}	Peak Intensity / arbitrary units
4	2155 (w) 2137 (w) 2126 (w) 2086 (sh) 2052 (vs) 2007 (s) 1971 (vw)	 37.0 1.4
13	2155 (w) 2137 (w) 2126 (w) 2088 (sh) 2052 (vs) 2007 (s) 1969 (br)	 37.9 2.0
22	2155 (w) 2137 (w) 2126 (w) 2088 (w) 2052 (vs) 2007 (s) 1968 (br)	 37.1 2.2
31	2155 (w) 2137 (w) 2126 (w) 2089 (w) 2052 (vs) 2022 (sh) 2007 (s) 1960 (w)	 36.7 3.9
49	2155 (w) 2137 (w) 2127 (w) 2089 (w) 2052 (vs) 2022 (sh) 2006 (s) 1959 (w) 1923 (vw)	 35.7 4.8

62	2155 (w) 2137 (w) 2127 (w) 2089 (w) 2052 (vs) 2023 (sh) 2006 (s) 1958 (m) 1924 (vw)	 35.1 5.5
81	2155 (w) 2137 (w) 2127 (w) 2089 (w) 2052 (vs) 2024 (m) 2006 (s) 1958 (m) 1923 (w)	 34.1 6.5
97	2155 (w) 2137 (w) 2127 (w) 2089 (w) 2052 (vs) 2024 (m) 2007 (s) 1957 (m) 1924 (w)	 33.6 8.0
110	2155 (w) 2137 (w) 2127 (w) 2089 (w) 2052 (vs) 2024 (m) 2006 (s) 1957 (m) 1923 (w)	 32.2 7.5
141	2155 (w) 2137 (w) 2126 (w) 2089 (w) 2052 (vs) 2024 (m) 2006 (m) 1957 (m) 1923 (w)	 25.0 5.8

156	2155 (w) 2137 (w) 2127 (w) 2089 (w) 2052 (vs) 2025 (s) 2007 (s) 1957 (s) 1923 (w)	 31.9 12.3
176	2155 (w) 2137 (w) 2126 (w) 2089 (w) 2052 (vs) 2025 (s) 2007 (s) 1957 (s) 1923 (m)	 26.9 8.5
200	2155 (w) 2137 (vw) 2126 (w) 2089 (w) 2052 (vs) 2025 (s) 2007 (m) 1957 (s) 1923 (m)	 26.2 9.1
224	2155 (w) 2137 (vw) 2126 (w) 2090 (w) 2052 (vs) 2025 (s) 2007 (m) 1957 (s) 1923 (m)	 27.5 11.9
255	2155 (w) 2137 (vw) 2126 (w) 2090 (w) 2052 (vs) 2024 (s) 2008 (m) 1957 (s) 1923 (m)	 21.6 9.0

285	2155 (w) 2137 (vw) 2126 (w) 2090 (w) 2052 (vs) 2025 (s) 2008 (sh) 1956 (s) 1923 (m)	 23.6 11.4
340	2155 (w) 2137 (vw) 2126 (w) 2090 (vw) 2052 (vs) 2025 (vs) 2009 (sh) 1956 (s) 1923 (m)	 18.6 9.8
401	2155 (w) 2137 (vw) 2126 (w) 2052 (vs) 2025 (vs) 2010 (sh) 1956 (s) 1923 (m)	 20.9 13.5
∞	2155 (w) 2126 (w) 2091 (w) 2053 (w) 2024 (vs) ~2010 (sh) 1956 (s) 1923 (s)	 6.5 18.5

A8.1.5.2 Assignment of Peaks

Peak At / cm^{-1}	Assignment	Peak At / cm^{-1}	Assignment
2155	Solvent	2025	*cis*-[LMn(CO)$_4$Br]
2137	[Mn(CO)$_5$Br]	2006	*cis*-[LMn(CO)$_4$Br] and [Mn(CO)$_5$Br]
2126	Solvent	1956	*cis*-[LMn(CO)$_4$Br] and [(L$_2$)Mn(CO)$_3$Br] isomers
2090	*cis*-[LMn(CO)$_4$Br]	1923	[(L$_2$)Mn(CO)$_3$Br] isomers
2052	[Mn(CO)$_5$Br]		

A8.1.5.3 Reaction in Refluxing $CHCl_3$

Reaction time / minutes	IR Peaks / cm^{-1}	Assignment
5	2051 (vw, br)	$[Mn(CO)_5Br]$
	2028 (vs)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1961 (s)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1919 (s)	*fac*-$[(L_2)Mn(CO)_3Br]$
10	2028 (vs)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1961 (vs)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1920 (s)	*fac*-$[(L_2)Mn(CO)_3Br]$
15	2052 (sh)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2028 (s)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1961 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (s)	$[(L_2)Mn(CO)_3Br]$ isomers
20	2045 (sh)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2029 (s)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (m)	$[(L_2)Mn(CO)_3Br]$ isomers
25	2046 (sh)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2029 (s)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (s)	$[(L_2)Mn(CO)_3Br]$ isomers
30	2045 (sh)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2029 (s)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (s)	$[(L_2)Mn(CO)_3Br]$ isomers
40	2044 (w, br)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2029 (m)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (m)	$[(L_2)Mn(CO)_3Br]$ isomers
50	2045 (w, br)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2029 (m)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1924 (m)	$[(L_2)Mn(CO)_3Br]$ isomers
60	2045 (w, br)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2029 (w)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (m)	$[(L_2)Mn(CO)_3Br]$ isomers
70	2047 (w)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2030 (w)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (m)	$[(L_2)Mn(CO)_3Br]$ isomers
80	2047 (w)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2030 (w)	*fac*-$[(L_2)Mn(CO)_3Br]$
	1960 (vs)	$[(L_2)Mn(CO)_3Br]$ isomers
	1923 (m)	$[(L_2)Mn(CO)_3Br]$ isomers

90	2049 (w) 2031 (vw) 1960 (vs) 1924 (m, br)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers

A8.1.6 Reaction of $[Mn(CO)_5Br]$ with dpptben

A8.1.6.1 Room Temperature Reaction in CH_2Cl_2

Reaction time / minutes	IR Peaks / cm^{-1}	Peak Intensity / arbitrary units
6	2155 (vw) 2137 (w) 2052 (vs) 2007 (s) 1970 (vw)	 37.7 1.1
13	2155 (w) 2137 (w) 2051 (vs) 2007 (s) 1970 (vw)	 34.8 1.2
24	2155 (w) 2137 (w) 2052 (vs) 2007 (s) 1969 (vw)	 38.7 1.3
36	2155 (w) 2137 w) 2052 (vs) 2007 (s) 1969 (vw)	 38.4 1.4
63	2155 (w) 2137 (w) 2052 (vs) 2007 (s) 1969 (vw)	 38.6 1.4
92	2155 (w) 2137 (w) 2052 (vs) 2007 (s) 1969 (vw) 1941 (vw) 1912 (vw)	 37.1 1.4

125	2155 (w) 2137 (w) 2127 (w) 2052 (vs) 2007 (s) 1969 (vw) 1941 (vw) 1912 (vw)	 39.6 1.5
177	2155 (w) 2137 (w) 2126 (w) 2090 (sh) 2052 (vs) 2007 (s) 1968 (w) 1940 (w) 1912 (w)	 36.6 1.6
270	2155 (w) 2137 (w) 2126 (w) 2091 (sh) 2052 (vs) 2007 (s) 1968 (w) 1939 (w) 1912 (w)	 37.6 1.8
303	2155 (w) 2137 (w) 2127 (w) 2090 (sh) 2052 (vs) 2007 (s) 1968 (w) 1939 (w) 1912 (w)	 38.0 1.8
336	2155 (w) 2137 (w) 2126 (w) 2091 (sh) 2052 (vs) 2007 (s) 1967 (w) 1939 (w) 1912 (w)	 36.5 2.1

374	2155 (w) 2137 (w) 2126 (w) 2090 (sh) 2052 (vs) 2007 (s) 1967 (w) 1939 (w) 1912 (w)	 36.6 2.2
408	2155 (w) 2137 (w) 2127 (w) 2090 (w) 2052 (vs) 2007 (s) 1967 (w) 1939 (w) 1912 (w)	 37.5 2.1
443	2155 (w) 2137 (w) 2126 (w) 2091 (w) 2052 (vs) 2007 (s) 1967 (w) 1939 (w) 1912 (w)	 37.2 2.3
473	2155 (w) 2137 (w) 2127 (w) 2090 (w) 2052 (vs) 2016 (sh) 2007 (s) 1967 (w) 1939 (w) 1912 (w)	 37.1 2.3
1115	2155 (w) 2137 (w) 2126 (w) 2091 (w) 2052 (vs) 2017 (s) 2008 (s) 1962 (m) 1928 (m) 1911 (m)	 30.3 4.1

∞	2155 (m) 2126 (m) 2092 (m) 2054 (w) 2024 (s) 2008 (s) 1960 (vs) 1927 (m) ~1910 (sh)	 4.0 15.6

A8.1.6.2 Assignment of Peaks

Peak At / cm^{-1}	Assignment	Peak At / cm^{-1}	Assignment
2155	Solvent	2024	*cis*-[LMn(CO)$_4$Br]
2137	[Mn(CO)$_5$Br]	2008	[Mn(CO)$_5$Br] and *cis*-[LMn(CO)$_4$Br]
2126	Solvent	1967	[(L$_2$)Mn(CO)$_3$Br]
2090	*cis*-[LMn(CO)$_4$Br]	1939	[(L$_2$)Mn(CO)$_3$Br]
2052	[Mn(CO)$_5$Br]	1912	[(L$_2$)Mn(CO)$_3$Br]

A8.1.6.3 Reactions in Refluxing $CHCl_3$

Reaction Time / minutes	IR Peaks / cm^{-1}	Assignment
5	2138 (vw)	[Mn(CO)$_5$Br]
	2092 (w)	*cis*-[LMn(CO)$_4$Br]
	2053 (w)	[Mn(CO)$_5$Br]
	2020 (vs)	*cis*-[LMn(CO)$_4$Br]
	1964 (sh)	[(L$_2$)Mn(CO)$_3$Br] isomers
	1943 (s)	[(L$_2$)Mn(CO)$_3$Br] isomers
	1911 (s)	[(L$_2$)Mn(CO)$_3$Br] isomers
10	2092 (w)	*cis*-[LMn(CO)$_4$Br]
	2024 (vs)	*cis*-[LMn(CO)$_4$Br]
	1961 (s)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1936 (s)	[(L$_2$)Mn(CO)$_3$Br] isomers
	1910 (s)	[(L$_2$)Mn(CO)$_3$Br] isomers
15	2093 (vw)	*cis*-[LMn(CO)$_4$Br]
	2027 (s)	*cis*-[LMn(CO)$_4$Br] and *fac*-[(L$_2$)Mn(CO)$_3$Br]
	1960 (vs)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1933 (s)	[(L$_2$)Mn(CO)$_3$Br] isomers
	1911 (s)	[(L$_2$)Mn(CO)$_3$Br] isomers
20	~2045 (sh)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	2027 (s)	*cis*-[LMn(CO)$_4$Br]
	1960 (vs)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1931 (s)	[(L$_2$)Mn(CO)$_3$Br] isomers
	1911 (s)	(L$_2$)Mn(CO)$_3$Br isomers

25	~2045 (sh) 2027 (s) 1960 (vs) 1931 (s) 1912 (s)	*mer*-[$(L_2)Mn(CO)_3Br$] *fac*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$] [$(L_2)Mn(CO)_3Br$] isomers [$(L_2)Mn(CO)_3Br$] isomers

Reaction Time	IR Peaks / cm^{-1}	Assignment
5	2093 (w) 2050 (sh) 2027 (s) 1961 (vs) 1918 (m)	*cis*-[$LMn(CO)_4Br$] [$Mn(CO)_5Br$] *cis*-[$LMn(CO)_4Br$] *mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$]
15	2044 (w) 2028 (m) 1960 (vs) 1918 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *cis*-[$LMn(CO)_4Br$] *mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$]
25	2045 (w) 2028 (w) 1960 (vs) 1920 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *cis*-[$LMn(CO)_4Br$] *mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$]
40	2046 (w) 1960 (vs) 1920 (m)	*mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$] *mer*-[$(L_2)Mn(CO)_3Br$]

A8.1.7 Reaction of [$Mn(CO)_5Br$] with dppmpn

A8.1.7.1 Room Temperature Reaction in CH_2Cl_2

Reaction Time / minutes	IR Peaks / cm^{-1}	Peak Intensity / arbitrary units
6	2155 (w) 2137 (w) 2126 (w) 2090 (w) 2052 (vs) ~2020 (sh) 2006 (s) 1961 (m)	 34.6 12.3
14	2155 (w) 2126 (w) 2090 (s) 2052 (m) 2020 (s) 2005 (vs) 1960 (s) 1919 (vw)	 15.2 21.3

20	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2020 (vs) 2005 (vs) 1960 (vs) 1918 (vw)	 3.4 23.8
27	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2021 (vs) 2005 (vs) 1960 (vs) 1918 (w)	 3.3 23.1
33	2155 (w) 2126 (w) 2090 (s) 2054 (w) 2021 (vs) 2005 (vs) 1959 (vs) 1918 (w)	 3.1 24.6
∞	2155 (w) 2126 (w) 2054 (w) 2023 (vs) 1951 (vs) 1917 (vs)	 3.2 24.1

A8.1.7.2 Assignment of Peaks

Peak At / cm^{-1}	Assignment	Peak At / cm^{-1}	Assignment
2155	Solvent	2023	*cis*-[$LMn(CO)_4Br$] and *fac*-[$(L_2)Mn(CO)_3Br$]
2137	[$Mn(CO)_5Br$]	2005	[$Mn(CO)_5Br$] and *cis*-[$LMn(CO)_4Br$]
2126	Solvent	1960	*fac*-[$(L_2)Mn(CO)_3Br$]
2090	*cis*-[$LMn(CO)_4Br$]	1951	*cis*-[$LMn(CO)_4Br$]
2052	[$Mn(CO)_5Br$]	1918	*fac*-[$(L_2)Mn(CO)_3Br$]

A8.1.7.3 Reaction in Refluxing $CHCl_3$

Reaction Time / minutes	IR Peaks / cm^{-1}	Assignment
5	2091 (vw)	*cis*-[$LMn(CO)_4Br$]
	2052 (w)	[$Mn(CO)_5Br$]
	2026 (vs)	*fac*-[$(L_2)Mn(CO)_3Br$]
	1957 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]
	1918 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]
10	2026 (vs)	*fac*-[$(L_2)Mn(CO)_3Br$]
	1956 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]
	1918 (s)	*fac*-[$(L_2)Mn(CO)_3Br$]

A8.1.8 Reaction of $[Mn(CO)_5Br]$ with dppippn

A8.1.8.1 Room Temperature Reaction in CH_2Cl_2

Reaction Time / minutes	IR Peaks / cm^{-1}	Peak Intensity / arbitrary units
8	2155 (w)	
	2137 (m)	
	2052 (vs)	35.1
	2007 (s)	
	1970 (w)	1.3
16	2155 (w)	
	2137 (m)	
	2088 (sh)	
	2052 (vs)	34.6
	2007 (s)	
	1969 (w)	1.5
29	2155 (w)	
	2137 (m)	
	2088 (sh)	
	2052 (vs)	35.8
	2007 (s)	
	1969 (br)	2.0
42	2155 (w)	
	2137 (m)	
	2088 (w)	
	2052 (vs)	34.1
	2007 (s)	
	1967 (br)	3.1
	1911 (br)	

57	2155 (w) 2137 (w) 2089 (w) 2052 (vs) ~2020 (sh) 2007 (s) 1967 (br) 1911 (w)	 35.4 3.0
76	2155 (w) 2137 (w) 2089 (w) 2052 (vs) 2020 (sh) 2007 (s) 1963 (br) 1911 (w)	 34.2 4.3
116	2155 (w) 2137 (w) 2126 (w) 2089 (w) 2052 (vs) 2020 (sh) 2006 (s) 1961 (br) 1912 (w)	 35.6 4.7
152	2155 (w) 2137 (w) 2126 (w) 2089 (w) 2052 (vs) 2019 (sh) 2007 (s) 1949 (br) 1912 (m)	 33.6 8.1
192	2155 (w) 2137 (w) 2126 (w) 2089 (w) 2052 (vs) 2020 (s) 2007 (s) 1948 (m, br) 1912 (m)	 33.5 9.7

225	2155 (w) 2137 (w) 2128 (w) 2089 (w) 2052 (vs) 2020 (s) 2007 (s) 1948 (m, br) 1912 (m)	 34.0 10.2
318	2155 (w) 2137 (w) 2128 (w) 2089 (w) 2052 (vs) 2020 (s) 2007 (s) 1947 (s, br) 1912 (s)	 33.1 13.9
417	2155 (w) 2137 (w) 2126 (w) 2089 (w) 2052 (vs) 2021 (s) 2008 (s) 1960 (sh) 1950 (s) 1912 (s)	 32.8 10.2
∞	2155 (w) 2137 (vw) 2126 (w) 2089 (s) 2052 (s) 2021 (vs) 2005 (vs) 1960 (s, br) 1913 (m)	 15.8 12.9

A8.1.8.2 Assignment of Peaks

Peak At / cm^{-1}	Assignment	Peak At / cm^{-1}	Assignment
2155	Solvent	2020	*cis*-[LMn(CO)$_4$Br]
2137	[Mn(CO)$_5$Br]	2005	*cis*-[LMn(CO)$_4$Br] or [Mn(CO)$_5$Br]
2126	Solvent	1960	*cis*-[LMn(CO)$_4$Br] or [(L$_2$)Mn(CO)$_3$Br] isomers
2090	[LMn(CO)$_4$Br]	1948	[(L$_2$)Mn(CO)$_3$Br] isomers
2052	[Mn(CO)$_5$Br]	1913	[(L$_2$)Mn(CO)$_3$Br] isomers

A8.1.8.3 Reaction in Refluxing $CHCl_3$

Reaction Time / minutes	IR Peaks / cm^{-1}	Assignment
5	2093 (vw)	*cis*-[LMn(CO)$_4$Br]
	2045 (sh)	*mer*-[(L$_2$)Mn(CO)$_3$Br] and/or [Mn(CO)$_5$Br]
	2032 (m)	*cis*-[LMn(CO)$_4$Br]
	2010 (sh)	*cis*-[LMn(CO)$_4$Br] and/or [Mn(CO)$_5$Br]
	1961 (vs)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1919 (s)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
10	2044 (w)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	2031 (sh)	*cis*-[LMn(CO)$_4$Br]
	1960 (vs)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1920 (m)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
15	2045 (w)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1960 (vs)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1920 (m)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
20	2046 (w)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1960 (vs)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1920 (m)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
25	2046 (w)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1960 (vs)	*mer*-[(L$_2$)Mn(CO)$_3$Br]
	1920 (m)	*mer*-[(L$_2$)Mn(CO)$_3$Br]

A8.1.9 Reaction of $[Mn(CO)_5Br]$ and dpppip

A8.1.9.1 Room Temperature Reaction in CH_2Cl_2

Reaction Time / minutes	Peak At / cm^{-1}	Peak Intensity / arbitrary units
6	2155 (w)	
	2137 (w)	
	2126 (w)	
	2052 (vs)	46.4
	2007 (s)	
	1970 (br)	1.9
13	2155 (w)	
	2137 (w)	
	2126 (w)	
	2090 (w)	
	2052 (vs)	43.3
	2006 (s)	
	1963 (m)	8.2
22	2155 (w)	
	2137 (m)	
	2126 (w)	
	2090 (m)	
	2052 (vs)	39.3
	2021 (sh)	
	2006 (s)	
	1962 (m)	16.7
29	2155 (w)	
	2137 (w)	
	2126 (w)	
	2090 (m)	
	2052 (vs)	41.3
	2021 (sh)	
	2006 (s)	
	1961 (m)	17.3
42	2155 (w)	
	2137 (w)	
	2127 (w)	
	2090 (m)	
	2052 (vs)	42.6
	2021 (sh)	
	2006 (s)	
	1961 (m)	16.1

64	2155 (w) 2137 (w) 2126 (w) 2090 (s) 2052 (vs) 2022 (sh) 2005 (vs) 1961 (s)	 32.3 20.5
84	2155 (w) 2126 (w) 2091 (s) 2052 (s) 2022 (s) 2005 (vs) 1961 (s)	 18.3 24.3
106	2155 (w) 2126 (w) 2091 (s) 2054 (w) 2023 (vs) 2005 (vs) 1961 (vs) 1915 (vw)	 5.1 26.2
139	2155 (w) 2126 (w) 2091 (s) 2054 (w) 2023 (vs) 2005 (vs) 1960 (vs) 1915 (vw)	 4.1 27.4
168	2155 (w) 2126 (w) 2091 (s) 2054 (w) 2023 (vs) 2005 (vs) 1960 (vs) 1915 (w)	 3.9 27.9
∞	2155 (w) 2126 (w) 2091 (vs) 2052 (sh) 2022 (vs) 2005 (vs) 1954 (vs) 1920 (s)	 2.1 21.0

A8.1.9.2 Assignment of Peaks

Peak At / cm^{-1}	Assignment	Peak At / cm^{-1}	Assignment
2155	Solvent	2023	*cis*-[LMn(CO)$_4$Br]
2137	[Mn(CO)$_5$Br]	2005	[Mn(CO)$_5$Br] and *cis*-[LMn(CO)$_4$Br]
2126	Solvent	1960	*mer*-[(L$_2$)Mn(CO)$_3$Br]
2090	*cis*-[LMn(CO)$_4$Br]	1915	*mer*-[(L$_2$)Mn(CO)$_3$Br]
2052	[Mn(CO)$_5$Br]		

A8.1.9.3 Reaction in Refluxing $CHCl_3$

Reaction Time / minutes	IR Peaks / cm^{-1}	Assignment
5	2138 (vw)	$[Mn(CO)_5Br]$
	2091 (s)	*cis*-$[LMn(CO)_4Br]$
	2053 (m)	$[Mn(CO)_5Br]$
	2024 (sh)	*cis*-$[LMn(CO)_4Br]$
	2007 (vs)	$[Mn(CO)_5Br]$
	1960 (vs)	mer-$[(L_2)Mn(CO)_3Br]$
	1913 (m)	*mer*-$[(L_2)Mn(CO)_3Br]$
10	2091 (w)	*cis*-$[LMn(CO)_4Br]$
	2040 (vw)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2015 (m)	*cis*-$[LMn(CO)_4Br]$
	1954 (vs)	*mer*-$[(L_2)Mn(CO)_3Br]$
	1916 (m)	*mer*-$[(L_2)Mn(CO)_3Br]$
15	2042 (w)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2016 (w)	*cis*-$[LMn(CO)_4Br]$
	1954 (vs)	*mer*-$[(L_2)Mn(CO)_3Br]$
	1916 (m)	*mer*-$[(L_2)Mn(CO)_3Br]$
20	2043 (w)	*mer*-$[(L_2)Mn(CO)_3Br]$
	2017 (vw)	*cis*-$[LMn(CO)_4Br]$
	1955 (vs)	*mer*-$[(L_2)Mn(CO)_3Br$
	1916 (m)	*mer*-$(L_2)Mn(CO)_3Br]$

Appendix 8.2: Graphical Representations of Reactions of Ligands with $[Mn(CO)_5Br]$

A8.2.1 Reaction of dppb with $[Mn(CO)_5Br]$

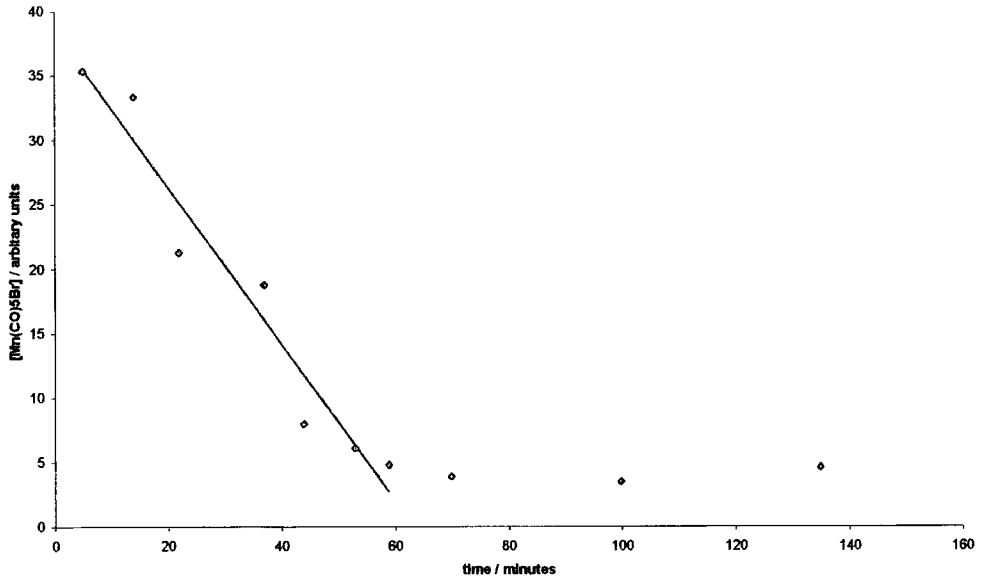

Fig A8.2: Reaction of dppb with $[Mn(CO)_5Br]$

A8.2.2 Reaction of dppmen with $[Mn(CO)_5Br]$

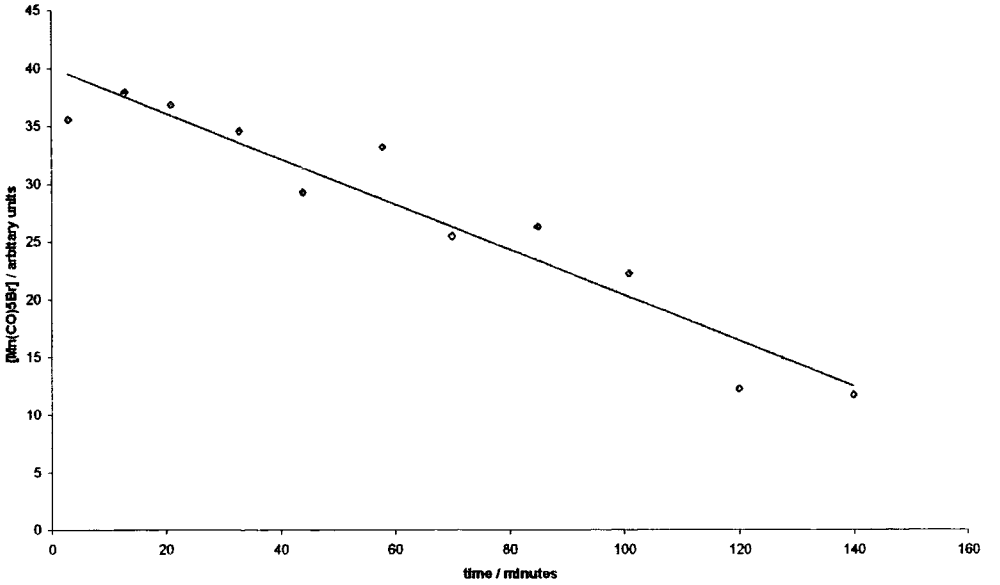

Fig A8.3: Reaction of dppmen with $[Mn(CO)_5Br]$

A8.2.3 Reaction of dpppen with [Mn(CO)$_5$Br]

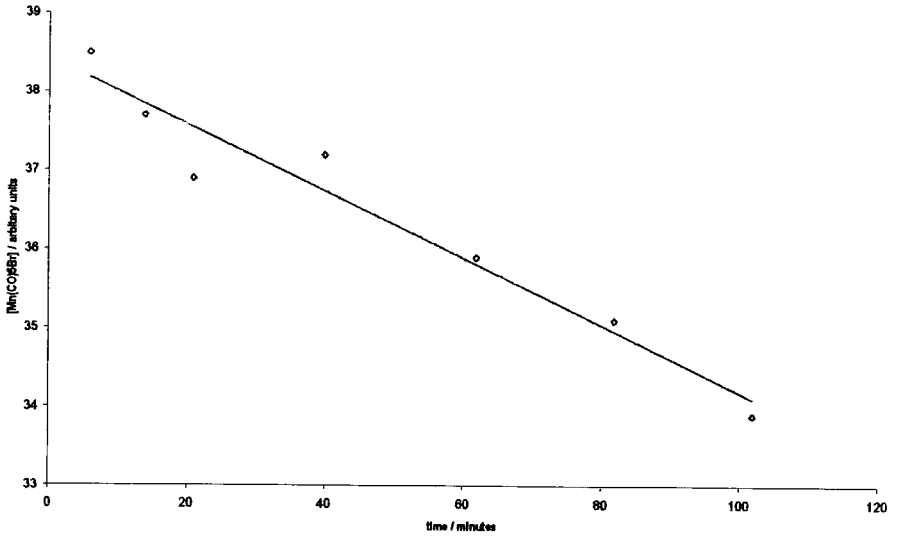

Fig A8.4: Reaction of dpppen with [Mn(CO)$_5$Br]

A8.2.4 Reaction of dppipen with [Mn(CO)$_5$Br]

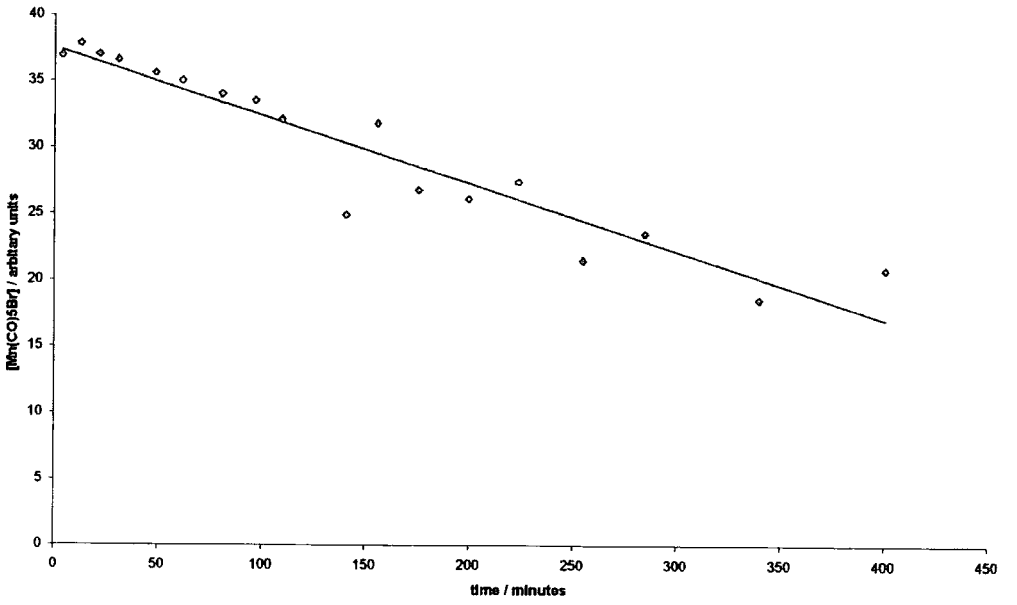

Fig A8.5: Reaction of dppipen with [Mn(CO)$_5$Br]

A8.2.5 Reaction of dpptben with $[Mn(CO)_5Br]$

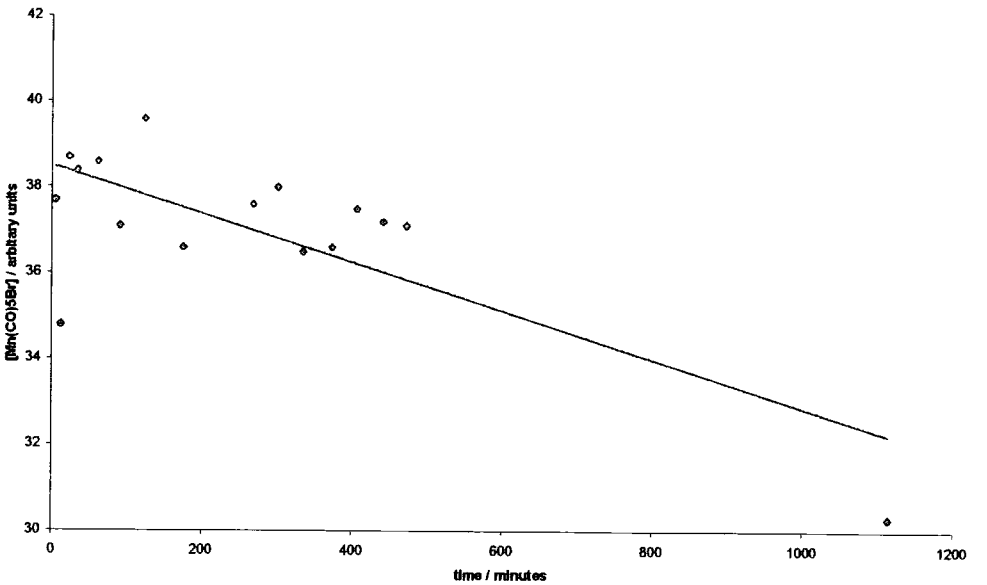

Fig. A8.6: Reaction of dpptben with $[Mn(CO)_5Br]$

A8.2.6 Reaction of dppmpn with $[Mn(CO)_5Br]$

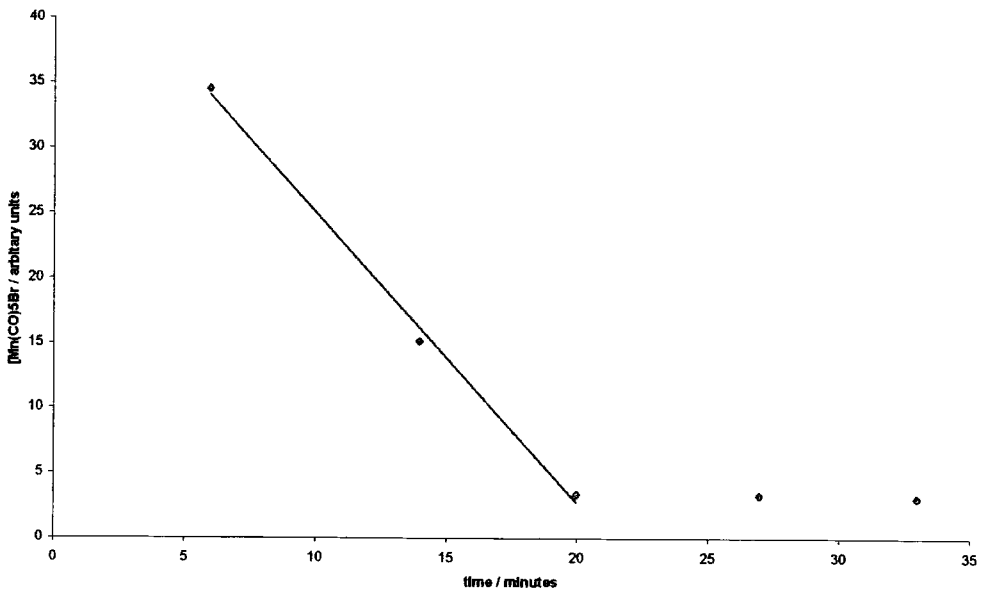

Fig. A8.7: Reaction of dppmpn with $[Mn(CO)_5Br]$

A8.2.7 Reaction of dppippn with [Mn(CO)$_5$Br]

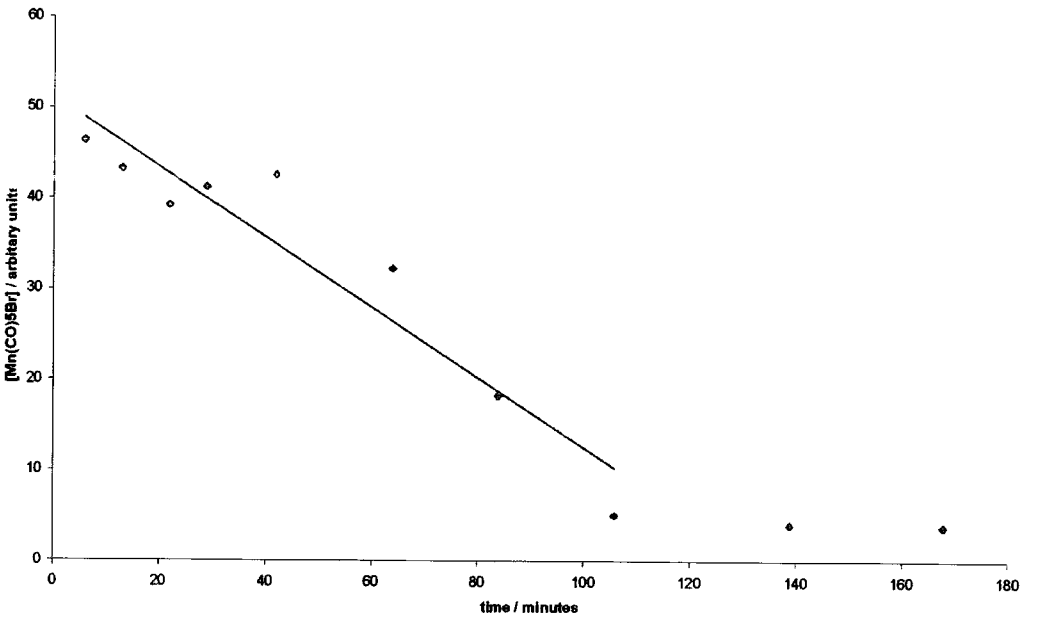

Fig. A8.8: Reaction of dppippn with [Mn(CO)$_5$Br]

A8.2.8 Reaction of dpppip with [Mn(CO)$_5$Br]

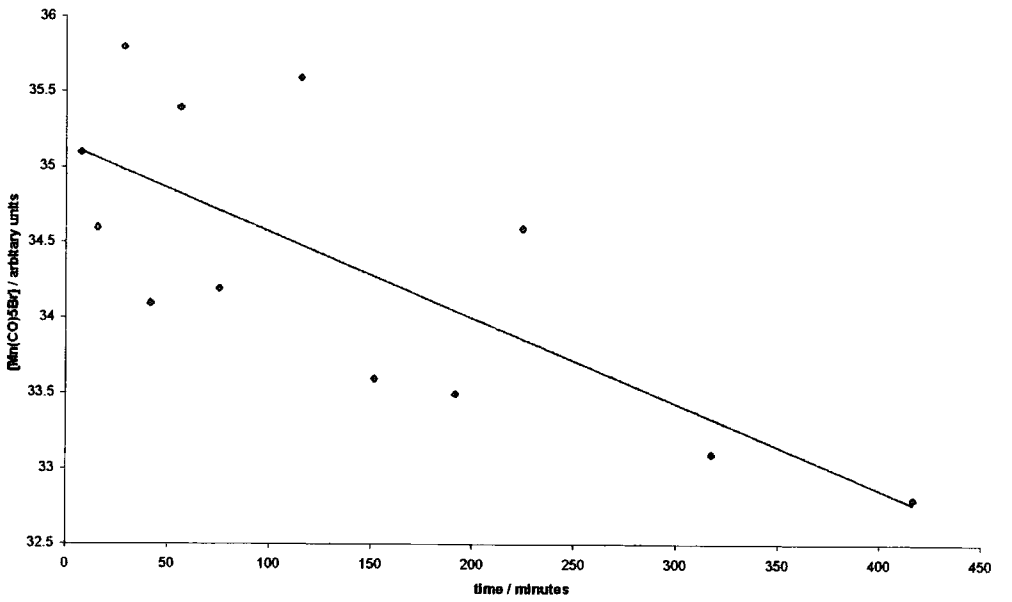

Fig. A8.9: Reaction of dpppip with [Mn(CO)$_5$Br]

A8.2.9 Gradients of Lines of Best Fit

Ligand Used	Gradient of Line of Best Fit
dppb	-0.61(15)
dppmen	-0.20(6)
dpppen	-0.042(10)
dppipen	-0.051(17)
dpptben	*
dppmpn	-2.24(13)
dppippn	-0.006(5)
dpppip	-0.39(13)

* No meaningful value was observed in this case. However, the reaction can be said to be much slower than all the others.

Appendix 8.3: Supplementary Crystal Structure Data for N,N'-di-*tert*-butylethyleneammonium dihydrohalide dihydrate (halide = chlorine or bromine in a ratio of 4:1)

X-ray crystallographic work on this compound was performed by Dr. A.S. Batsanov.

Empirical Formula	$C_{10}H_{30}Br_{0.4}Cl_{1.6}N_2O_2$
Formula Weight	299.0
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal System	Monoclinic
Space Group	P2(1)/c
Unit Cell Dimensions	a = 10.3002(6) Å
	b = 6.7913(4) Å
	c = 12.6402(9) Å
	$\alpha = 90°$
	$\beta = 107.117(4)°$
	$\gamma = 90°$
Unit Cell Volume	845.04(9) $Å^3$
Z	2
Density (calculated)	1.117 g cm^{-3}
Absorption Coefficient	1.269 mm^{-1}
F(000)	293
Crystal Size	0.46 x 0.44 x 0.10 mm
θ Range for Data Collection	2.07 to 30.02°
Index Range	$-13 \leq h \leq 14$
	$-9 \leq k \leq 9$
	$-14 \leq l \leq 16$
Reflections Collected	6254
Independent Reflections	2287
Absorption Correction	Integration

Max. and Min. Transmission	0.8820 and 0.5957
Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	2280 / 0 / 139
Goodness of Fit on F^2	1.104
Final R Indices ($I > 2\Sigma(I)$)	$R1 = 0.0280$, $wR^2 = 0.0668$
R Indices (all data)	$R1 = 0.0343$, $wR^2 = 0.0734$
Largest Diffraction Peak and Hole	0.333 and -0.236 e $Å^{-3}$

Bond Length Data

Bond	Length / Å	Bond	Length / Å
N - C(1)	1.489(2)	C(1) - C(1')	1.525(2)
N - C(2)	1.527(2)	C(2) - C(3)	1527(2)
C(2) - C(4)	1.521(2)	C(2) - C(5)	1.525(2)
N - H(1)	0.90(2)	N - H(2)	0.92(2)
O(1A) - H(01)	0.81(2)	O(1A) - H(02)	0.83(3)
O(1B) - H(01)	0.89(3)	O(1B) - H(02)	0.94(3)
C(1) - H(11)	0.96(2)	C(1) - H(12)	0.98(2)
C(3) - H(31)	0.98(2)	C(3) - H(32)	1.01(2)
C(3) - H(33)	0.98(2)	C(4) - H(41)	0.98(2)
C(4) - H(42)	1.01(2)	C(4) - H(43)	0.99(2)
C(5) - H(51)	1.04(3)	C(5) - H(52)	0.96(2)
C(5) - H(53)	1.06(3)		

Bond Angle Data

Bond	Angle / °	Bond	Angle / °
N - C(1) - C(1')	108.90(12)	C(1) - N - C(2)	117.66(10)
C(2) - N - H(1)	106.8(10)	C(1) - N - H(1)	108.9(11)
C(2) - N - H(2)	106.9(11)	C(1) - N - H(2)	110.2(12)
H(01) - O(1A) - H(02)	108(2)	H(1) - N - H(2)	106(2)
N - C(1) - H(11)	110.6(11)	H(01) - O(1B) - H(02)	94(2)
N - C(1) - H(12)	108.6(10)	C(1') - C(1) - H(11)	109.6(10)

H(11) - C(1) - H(12)	107.9(14)	C(1') - C(1) - H(12)	111.3(10)
C(4) - C(2) - N	108.73(12)	C(4) - C(2) - C(5)	112.5(2)
C(4) - C(2) - C(3)	110.46(12)	C(5) - C(2) - N	108.54(11)
N - C(2) - C(3)	105.05(11)	C(5) - C(2) - C(3)	111.3(2)
C(2) - C(3) - H(32)	110.0(11)	C(2) - C(3) - H(31)	110.9(11)
H(31) - C(3) - H(32)	108(2)	C(2) - C(3) - H(33)	108.7(11)
H(31) - C(3) - H(33)	109(2)	H(32) - C(3) - H(33)	110(2)
C(2) - C(4) - H(42)	110.9(11)	C(2) - C(4) - H(41)	107.4(13)
H(41) - C(4) - H(42)	110(2)	C(2) - C(4) - H(43)	111.9(12)
H(41) - C(4) - H(43)	109(2)	H(42) - C(4) - H(43)	108(2)
C(2) - C(5) - H(52)	107.1(14)	C(2) - C(5) - H(51)	111.2(13)
H(51) - C(5) - H(52)	110(2)	C(2) - C(5) - H(53)	110.7(14)
H(51) - C(5) - H(53)	111(2)	H(52) - C(5) - H(53)	107(2)

Appendix 8.4: Supplementary Crystal Structure Data for Dichloro-N,N'-(*trans*-N,N'-bis(benzyl)-cyclohexane-1,2-diamine)palladium(II)

X-ray crystallographic work on this compound was performed by Dr. C.W. Lehmann.

Empirical Formula	$C_{20}H_{24}Cl_2N_2Pd$
Formula Weight	467.71
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal System	Monoclinic
Space Group	P2(1)/n
Unit Cell Dimensions	a = 14.4833(14) Å
	b = 9.6694(8) Å
	c = 14.9700(14) Å
	$\alpha = 90°$
	$\beta = 99.755(4)°$
	$\gamma = 90°$
Unit Cell Volume	2066.2(3)
Z	4
Density (calculated)	1.510 Mg m^{-3}
Absorption Coefficient	1.162 mm^{-1}
F(000)	952
Crystal Size	0.1 x 0.15 x 0.4 mm
θ Range for Data Collection	1.81° to 27.50°
Index Range	$-18 \leq h \leq 18$
	$-12 \leq k \leq 12$
	$-19 \leq l \leq 15$
Reflections Collected	14714
Independent Reflections	4748 (R_{int} = 0.1281)
Absorption Correction	Semi-Empirical from Psi-Scans

Max. and Min. Transmission	0.8743 and 0.4621
Refinement Method	Full-Matrix Least Squares on F^2
Data / Restraints / Parameters	4692 / 0 / 226
Goodness of Fit on F^2	1.159
Final R Indices ($I > 2\Sigma(I)$)	R1 = 0.0558, wR2 = 0.1289
R Indices (all data)	R1 = 0.0969, wR2 = 0.1814
Largest Diffraction Peak and Hole	1.093 and -1.413 e $Å^{-3}$

Selected Bond Length Data

Bond	Length / Å	Bond	Length / Å
Pd(1) - N(1)	2.069(5)	Pd(1) - Cl(1)	2.322(2)
Pd(1) - N(2)	2.075(5)	Pd(1) - Cl(2)	2.314(2)
N(1) - C(1)	1.501(7)	N(1) - C(10)	1.490(8)
N(2) - C(6)	1.499(8)	N(2) - C(20)	1.500(8)
C(1) - C(6)	1.537(8)	C(1) - C(2)	1.522(8)
C(2) - C(3)	1.529(9)	C(3) - C(4)	1.505(10)
C(4) - C(5)	1.538(10)	C(5) - C(6)	1.519(8)

Selected Bond Angle Data

Bond	Angle / °	Bond	Angle / °
N(2) - Pd(1) - N(1)	83.2(2)	N(1) - Pd(1) - Cl(2)	93.61(14)
N(2) - Pd(1) - Cl(1)	94.39(14)	Cl(1) - Pd(1) - Cl(2)	88.86(6)
N(1) - Pd(1) - Cl(1)	176.32(13)	N(2) - Pd(1) - Cl(2)	176.69(14)
C(10) - N(1) - C(1)	114.3(5)	C(6) - N(2) - C(20)	113.5(5)
C(10) - N(1) - Pd(1)	120.5(4)	C(20) - N(2) - Pd(1)	120.3(4)
C(1) - N(1) - Pd(1)	109.3(4)	C(6) - N(2) - Pd(1)	108.0(4)
N(1) - C(1) - C(6)	106.9(4)	N(2) - C(6) - C(1)	106.5(5)
N(1) - C(1) - C(2)	113.3(5)	N(2) - C(6) - C(5)	113.2(5)
C(1) - C(2) - C(3)	110.7(6)	C(2) - C(3) - C(4)	110.6(5)
C(3) - C(4) - C(5)	111.0(6)	C(4) - C(5) - C(6)	109.8(6)
C(5) - C(6) - C(1)	111.5(5)	C(6) - C(1) - C(2)	110.1(5)

Appendix A: Lectures and Seminars Attended

Lectures and Seminars Attended in Durham

1995

October 13 Prof. R. Schmutzler, Univ Braunschweig, FRG.
Calixarene-Phosphorus Chemistry: A New Dimension in Phosphorus Chemistry

November 1 Prof. W. Motherwell, UCL London
New Reactions for Organic Synthesis

November 15 Dr Andrea Sella, UCL, London
Chemistry of Lanthanides with Polypyrazoylborate Ligands

November 29 Prof. Dennis Tuck, University of Windsor, Ontario, Canada
New Indium Coordination Chemistry

December 8 Professor M.T. Reetz, Max Planck Institut, Mulheim
Perkin Regional Meeting

1996

January 10 Dr Bill Henderson, Waikato University, NZ
Electrospray Mass Spectrometry - a new sporting technique

January 31 Dr J. Penfold, Rutherford Appleton Laboratory,
Soft Soap and Surfaces

February 21 Dr C R Pulham , Univ. Edinburgh
Heavy Metal Hydrides - an exploration of the chemistry of stannanes and plumbanes

March 6 Dr Richard Whitby, Univ of Southampton
New approaches to chiral catalysts: Induction of planar and metal centred asymmetry

March 12 RSC Endowed Lecture - Prof. V. Balzani, Univ of Bologna
Supramolecular Photochemistry

October 22 Professor Lutz Gade, Univ. Wurzburg, Germany
Organic transformations with Early-Late Heterobimetallics: Synergism and Selectivity

October 22 Professor B. J. Tighe, Department of Molecular Sciences and Chemistry, University of Aston
Making Polymers for Biomedical Application - can we meet Nature's Challenge?

October 23 Professor H. Ringsdorf, Johannes Gutenberg-Universitat, Mainz, Germany
Function Based on Organisation

October 29 Professor D. M. Knight, Department of Philosophy, University of Durham.
The Purpose of Experiment - A Look at Davy and Faraday

October 30 Dr Phillip Mountford, Nottingham University
Recent Developments in Group IV Imido Chemistry

November 12 Professor R. J. Young, Manchester Materials Centre, UMIST
New Materials - Fact or Fantasy?

November 18 Professor G. A. Olah, University of Southern California, USA
Crossing Conventional Lines in my Chemistry of the Elements

November 19 Professor R. E. Grigg, University of Leeds
Assembly of Complex Molecules by Palladium-Catalysed Queueing Processes

December 3 Professor D. Phillips, Imperial College, London
A Little Light Relief

December 11 Dr Chris Richards, Cardiff University
Sterochemical Games with Metallocenes

1997

January 15 Dr V. K. Aggarwal, University of Sheffield
Sulfur Mediated Asymmetric Synthesis

January 21 Mr D. Rudge, Zeneca Pharmaceuticals
High Speed Automation of Chemical Reactions

January 22 Dr Neil Cooley, BP Chemicals, Sunbury
Synthesis and Properties of Alternating Polyketones

February 4 Dr A. J. Banister, University of Durham
From Runways to Non-metallic Metals - A New Chemistry Based on Sulphur

February 18 Professor Sir James Black, Foundation/King's College London
My Dialogues with Medicinal Chemists

February 19 Professor Brian Hayden, University of Southampton
The Dynamics of Dissociation at Surfaces and Fuel Cell Catalysts

February 25 Professor A. G. Sykes, University of Newcastle
The Synthesis, Structures and Properties of Blue Copper Proteins

March 4 Professor C. W. Rees, Imperial College
Some Very Heterocyclic Chemistry

March 11 Dr A. D. Taylor, ISIS Facility, Rutherford Appleton Laboratory
Expanding the Frontiers of Neutron Scattering

October 15 Dr R M Ormerod, Department of Chemistry, Keele University
Studying catalysts in action

October 21 Professor A F Johnson, IRC, Leeds
Reactive processing of polymers: science and technology

October 22 Professor R J Puddephatt (RSC Endowed Lecture), University of Western Ontario
Organoplatinum chemistry and catalysis

October 23 Professor M R Bryce, University of Durham, Inaugural Lecture
New Tetrathiafulvalene Derivatives in Molecular, Supramolecular and Macromolecular Chemistry: controlling the electronic properties of organic solids

October 27 Professor W Roper FRS. University of Auckland, New Zealand
Silyl Complexes of Ruthenium and Osmium

October 28 Professor A P de Silva, The Queen's University, Belfast
Luminescent signalling systems

November 5 Dr M Hii, Oxford University
Studies of the Heck reaction

November 11 Professor V.C. Gibson, Imperial College, London
Metallocene polymerisation

November 25 Dr R Withnall, University of Greenwich
Illuminated molecules and manuscripts

November 26 Professor R W Richards, University of Durham, Inaugural Lecture
A random walk in polymer science

1998

January 20 Professor J Brooke, University of Lancaster
What's in a formula? Some chemical controversies of the 19th century

January 21 Professor D Cardin, University of Reading
Aspects of Metal and Cluster Chemistry

January 27 Professor R Jordan, Dept. of Chemistry, Univ. of Iowa, USA.
Cationic transition metal and main group metal alkyl complexes in olefin polymerisation

January 28 Dr S Rannard, Courtaulds Coatings (Coventry)
The synthesis of dendrimers using highly selective chemical reactions

February 3 Dr J Beacham, ICI Technology
The chemical industry in the 21st century

February 25 Dr C Jones, Swansea University
Low coordination arsenic and antimony chemistry

March 18 Dr J Evans, Oxford University
Materials which contract on heating (from shrinking ceramics to bulletproof vests)

Other Scientific Meetings

1996

September 1st Anglo-Dutch Symposium on Organometallic Chemistry (Sheffield)

1997

September XIIth FECHEM Conference on Organometallic Chemistry (Prague) - Poster Contribution

December Durham University Chemistry Department Poster Competition (Durham) - Poster Contribution

1998

June Departmental Reseach Colloquia (Durham) - Oral Contribution
"Aminophosphines: New Ligands for Homogeneous Catalysis"