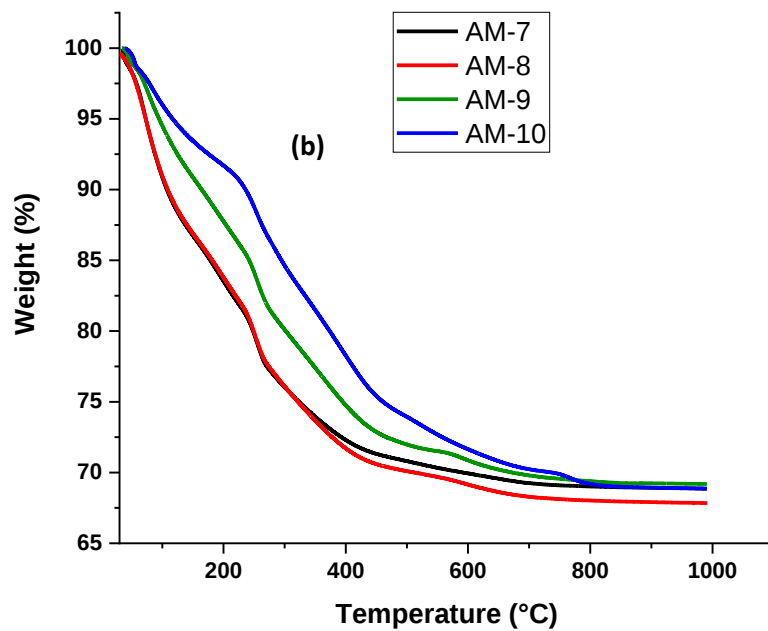
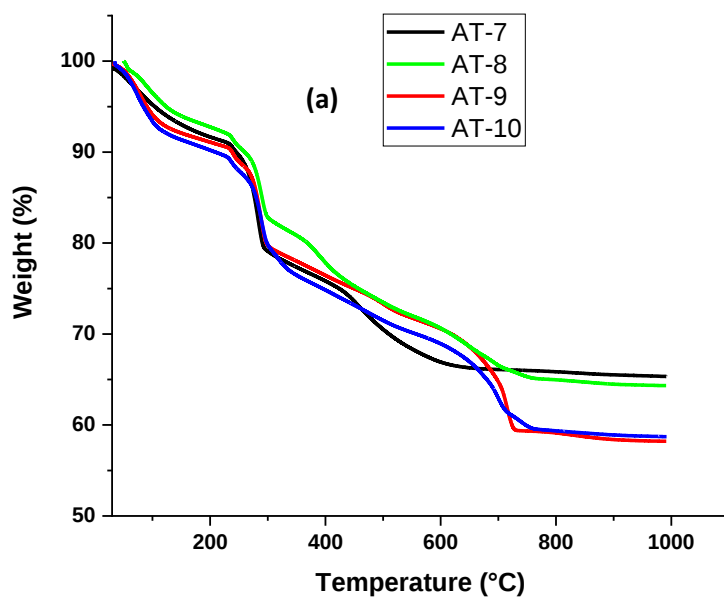
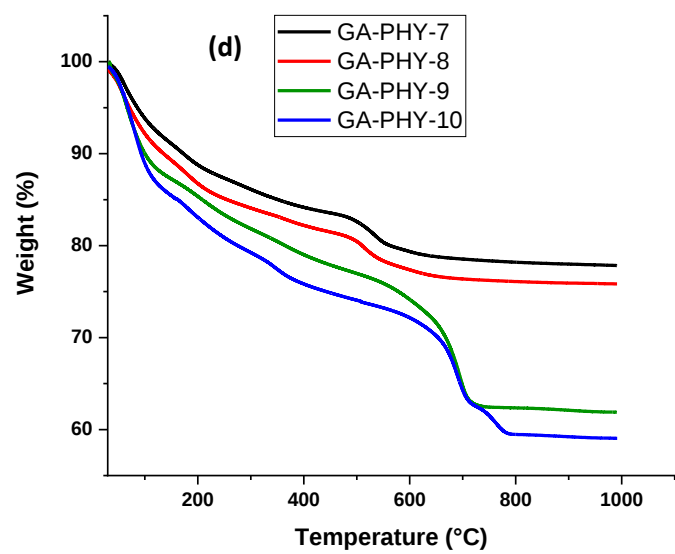
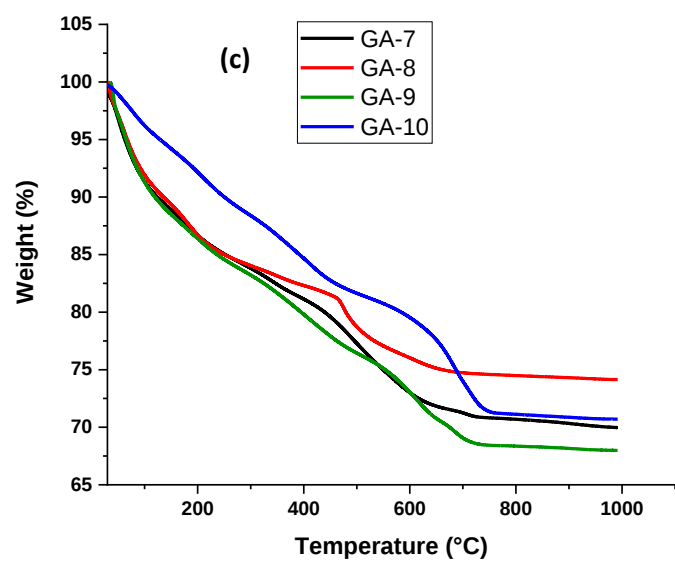
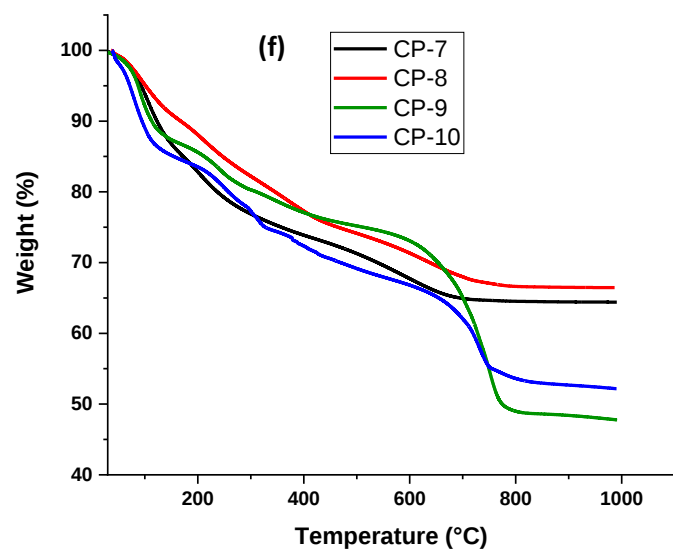
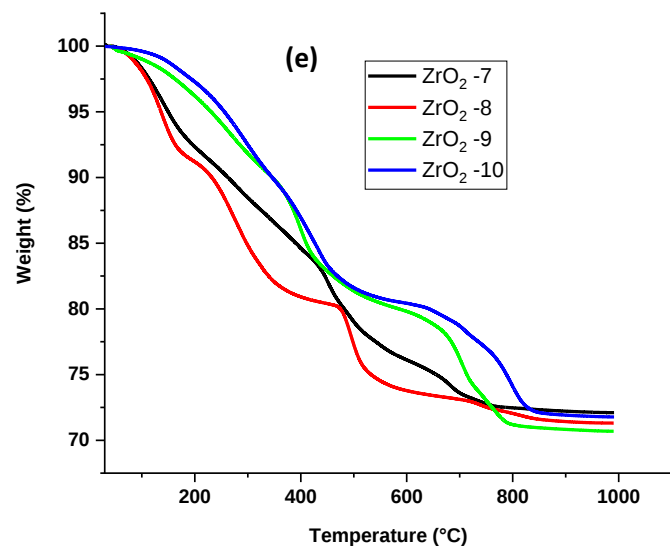


APPENDIX

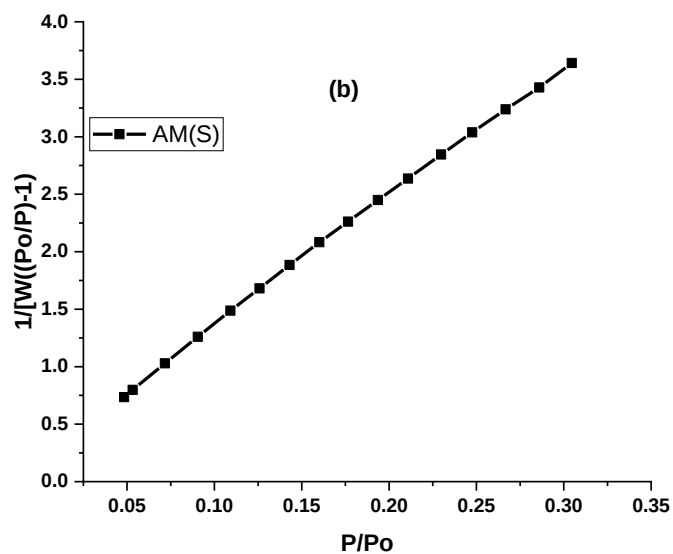
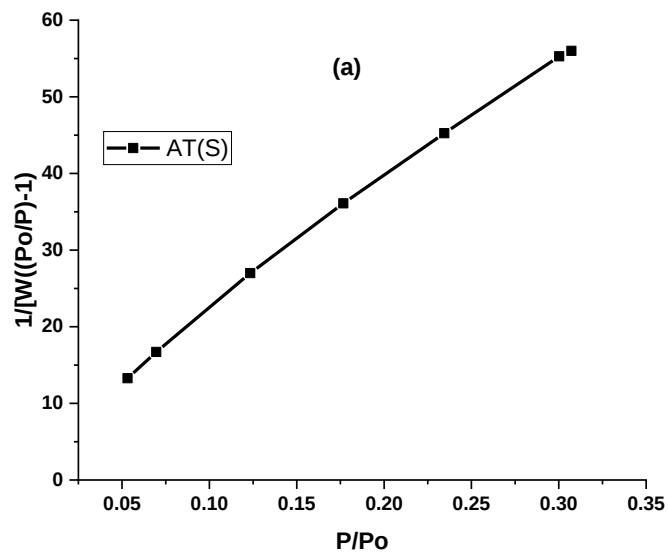
Appendix 1: TGA curves of bicomponent supports: (a) AT-series (b) AM-series (c) GA-series (d) GA(PHY)-series (e) ZrO₂-series (f) CP-series

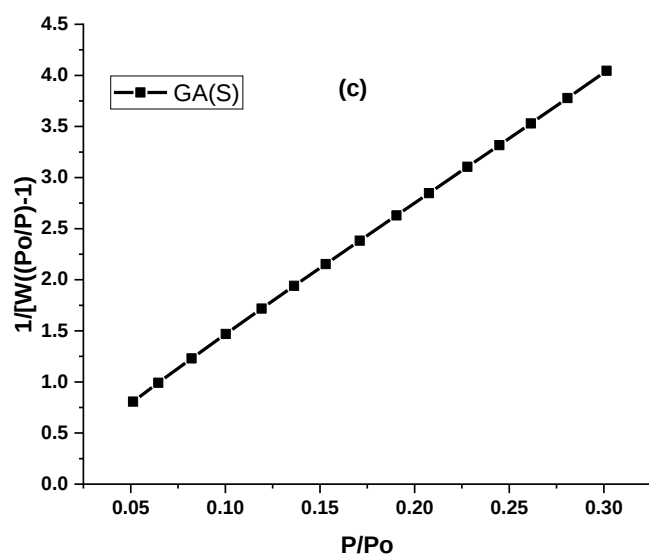




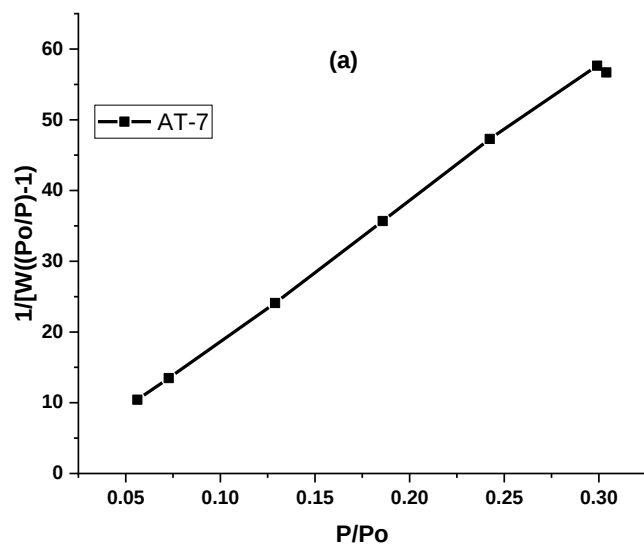


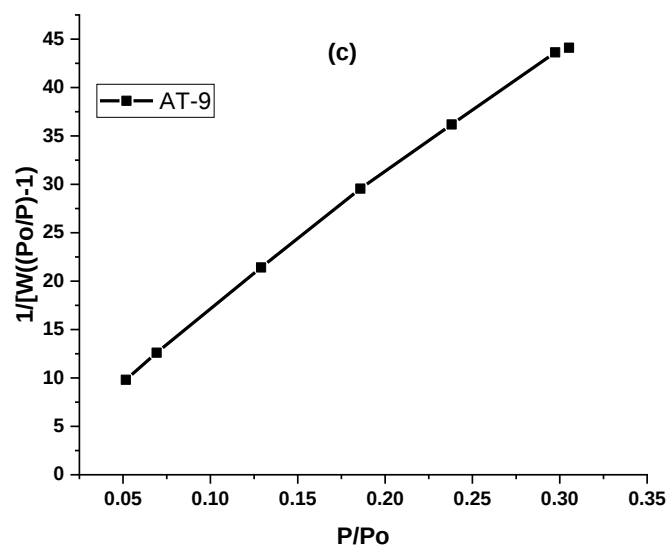
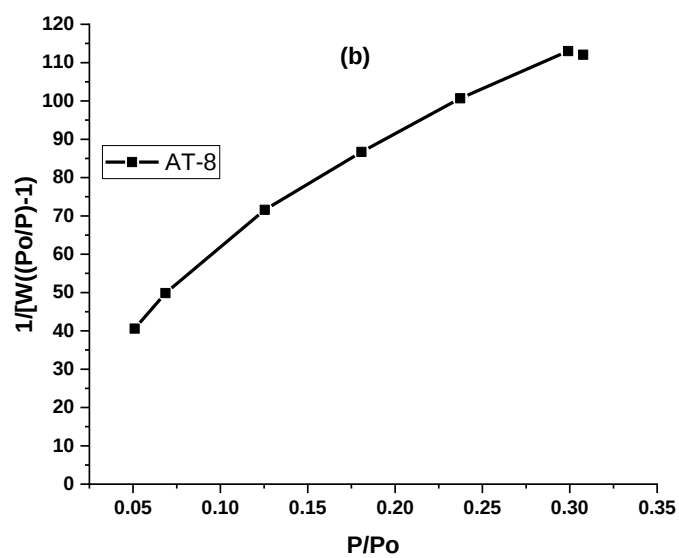
Appendix 2: BET plots of substrates used for deposition precipitation : (a) AT(S), (b) AM(S) and (c) GA(S)

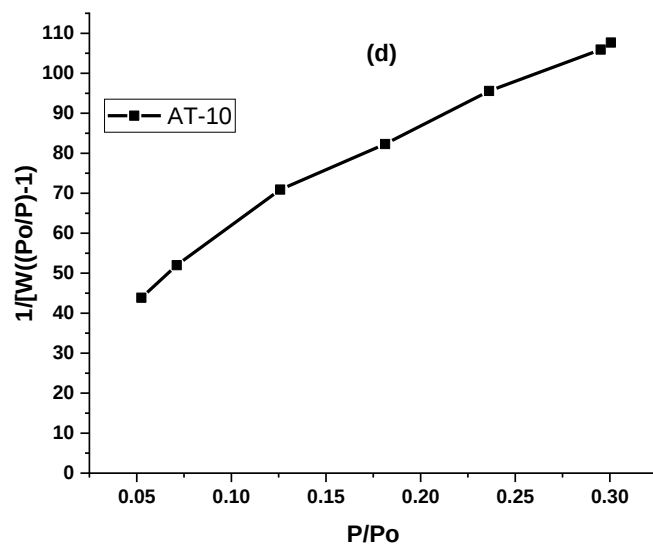




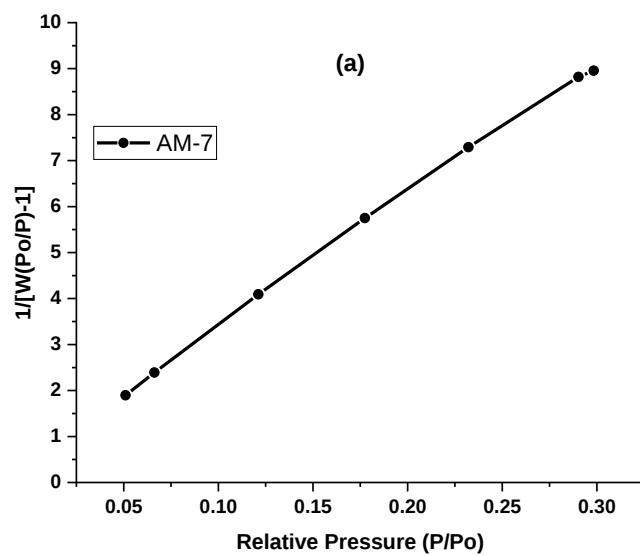
Appendix 3: BET plots of AT-series : (a) AT-7 (b) AT-8 (c) AT-9 (d) AT-10

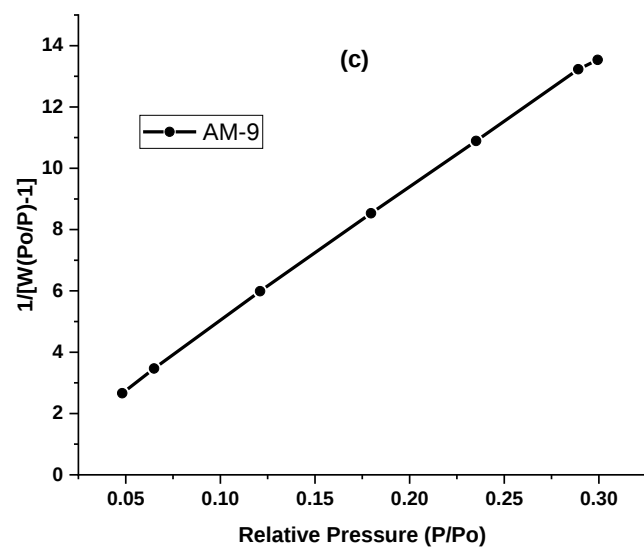
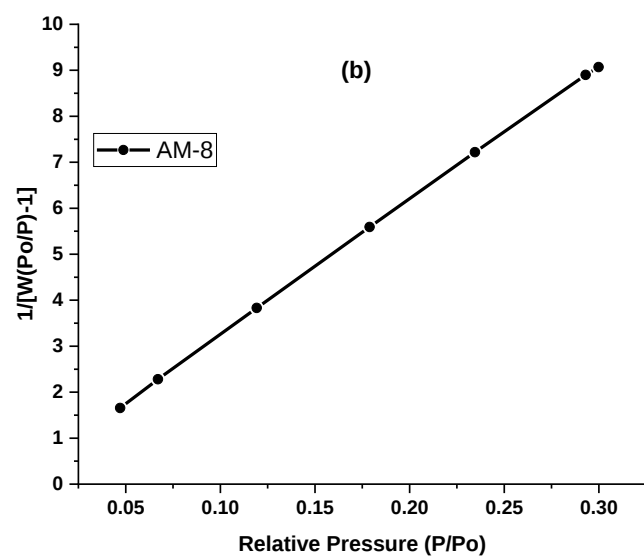


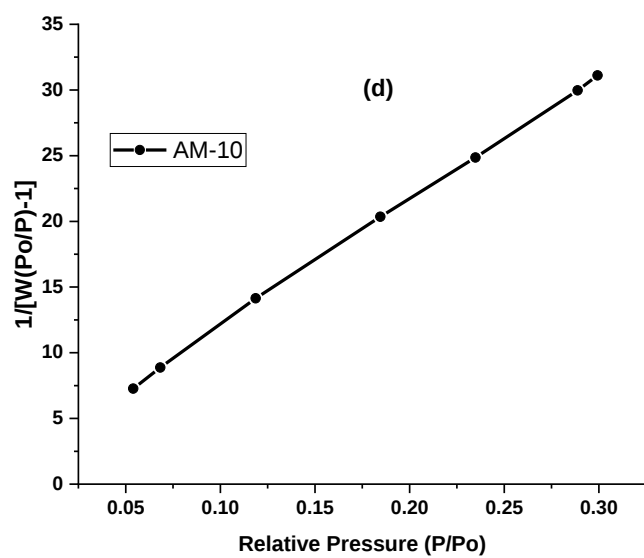




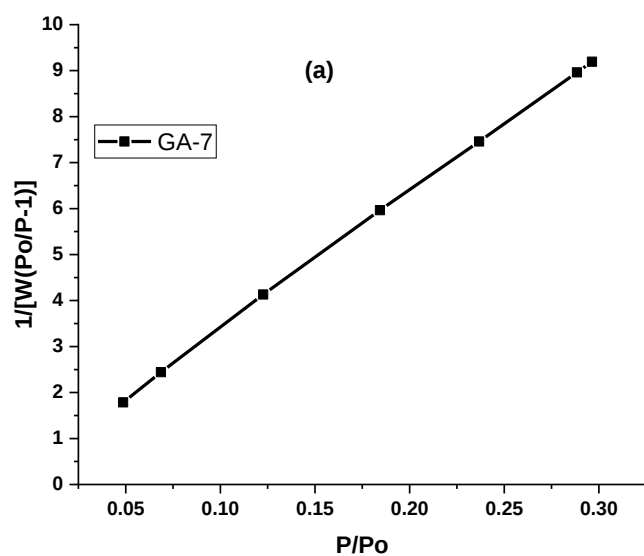
Appendix 4: BET plots of AM-series: (a) AM-7 (b) AM-8 (c) AM-9 (d) AM-10

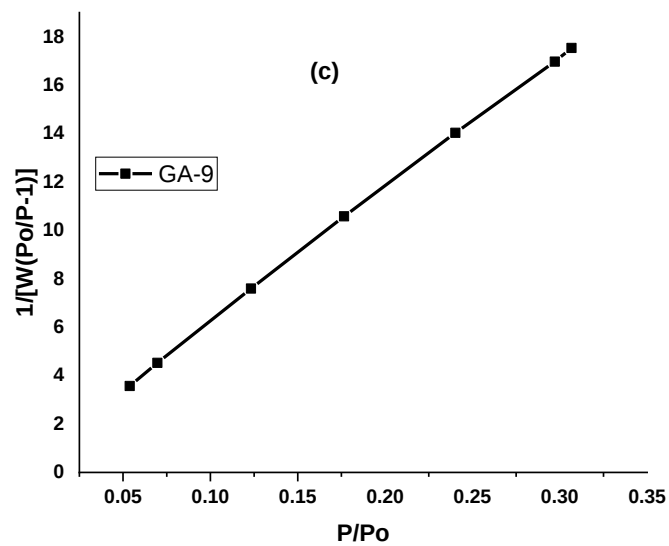
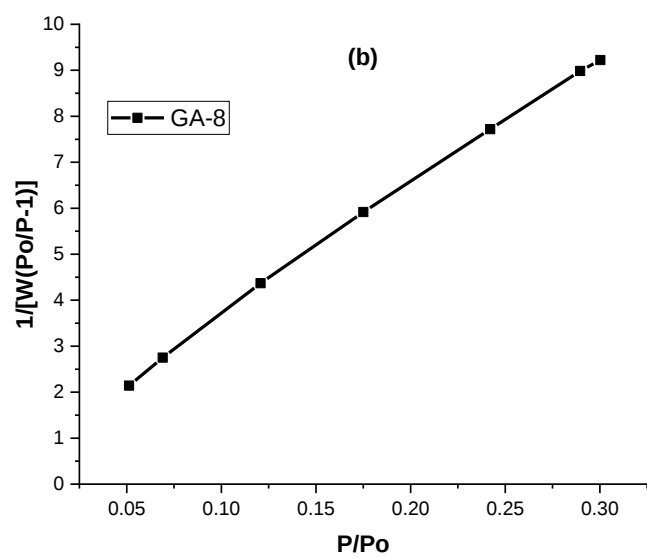


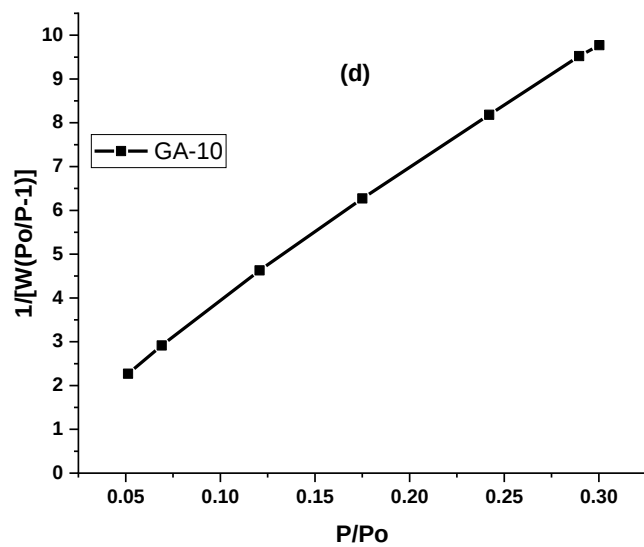




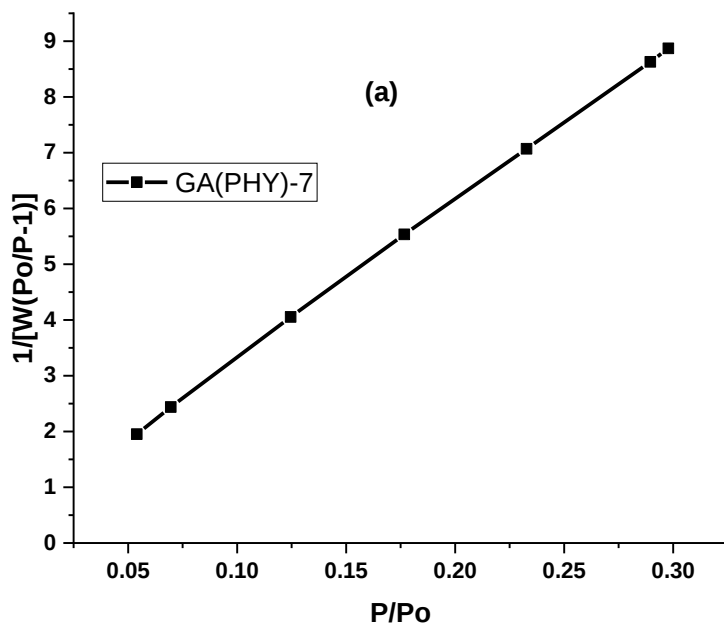
Appendix 5: BET plots of GA-series : (a) GA-7 (b) GA-8 (c) GA-9 (d) GA-10

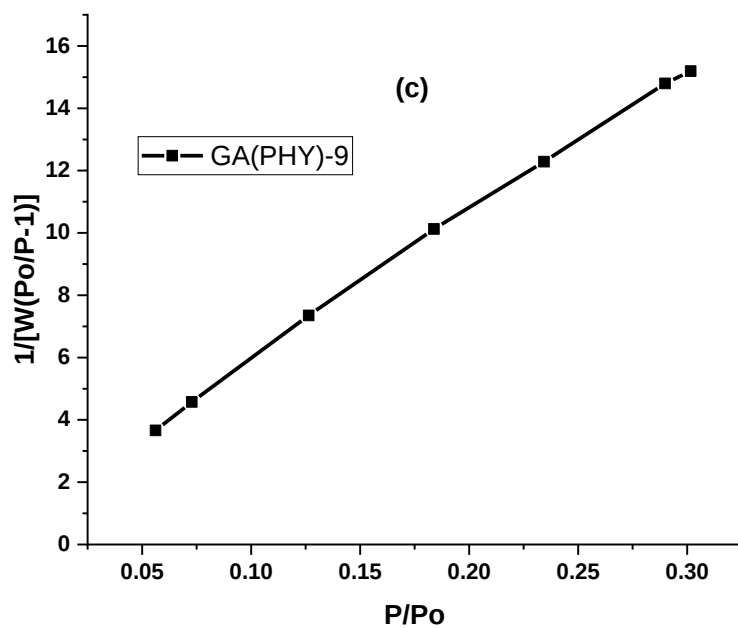
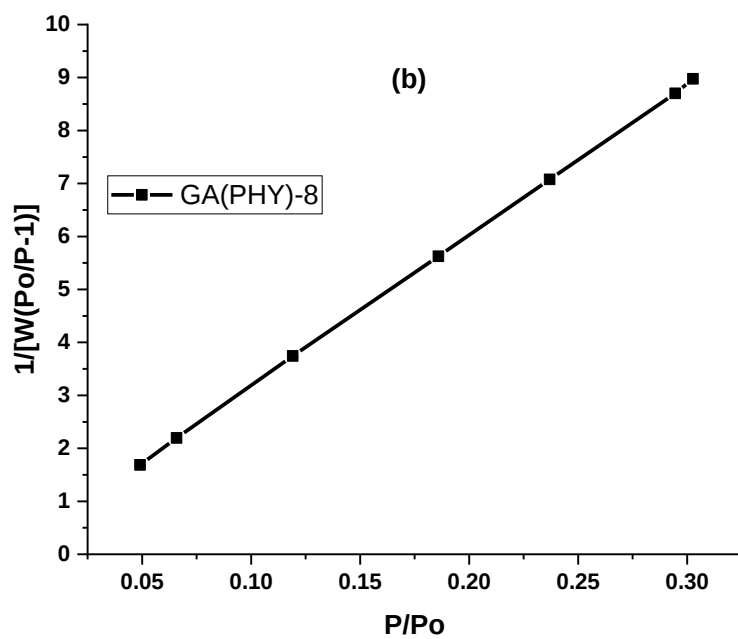


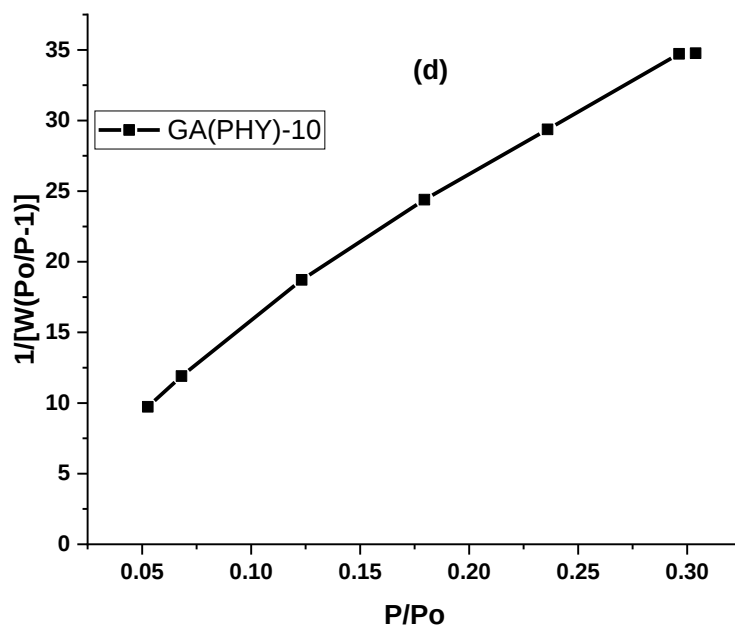




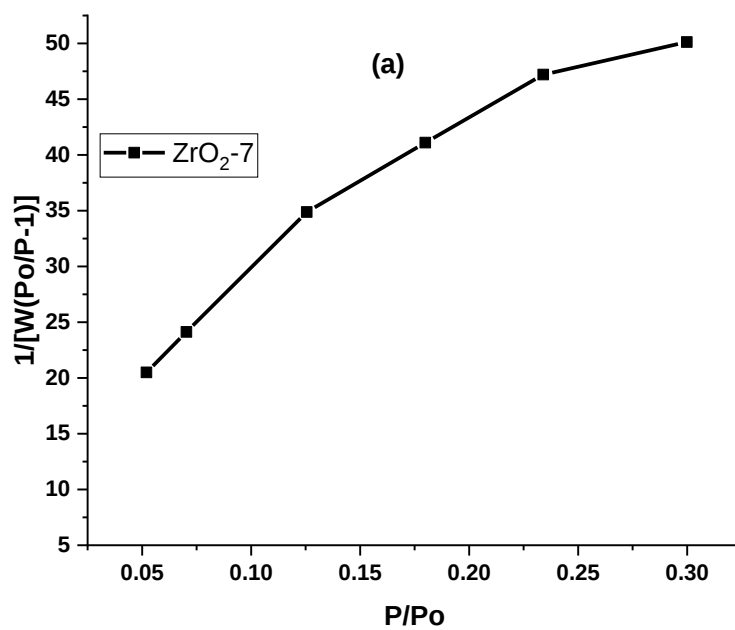
Appendix 6: BET plots of GA(PHY)-series : (a) GA(PHY)-7 (b) GA(PHY)-8 (c) GA(PHY)-9 (d) GA(PHY)-10

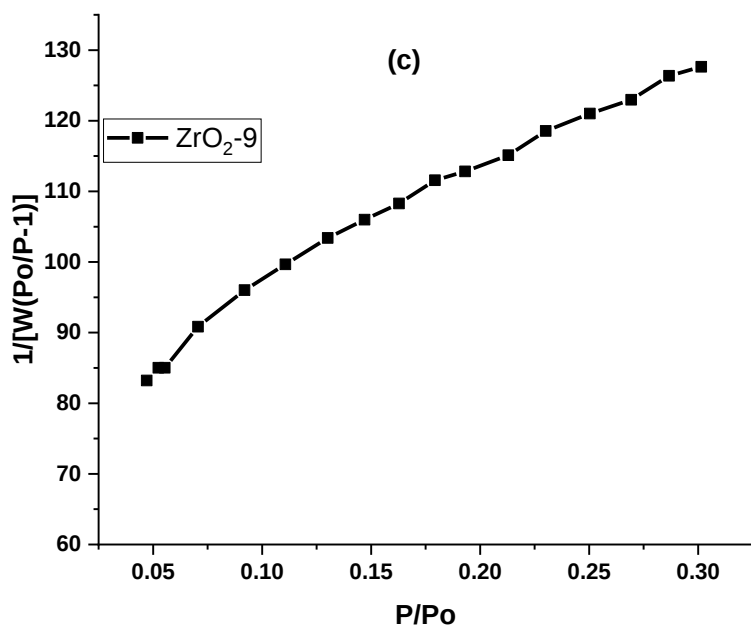
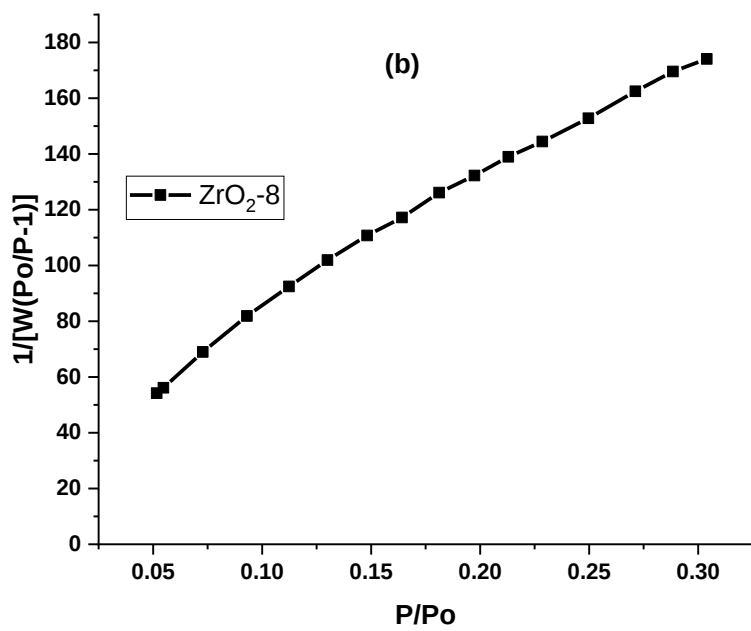


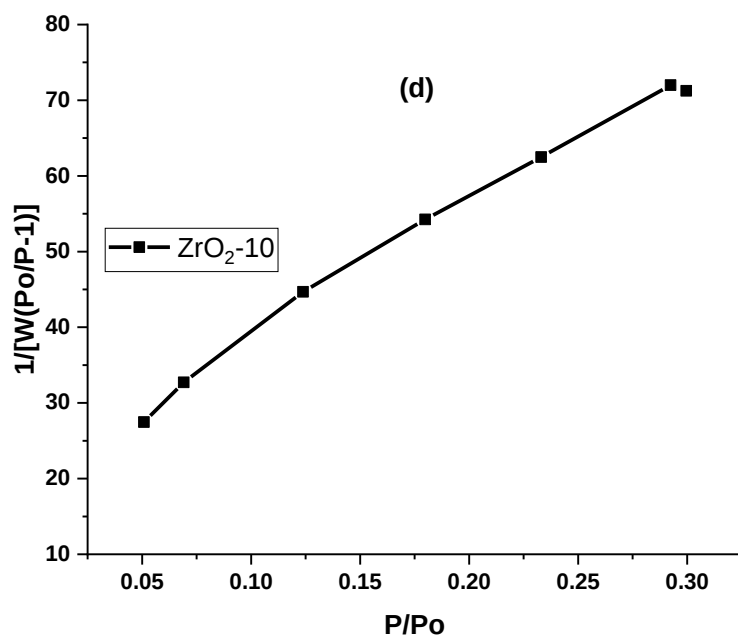




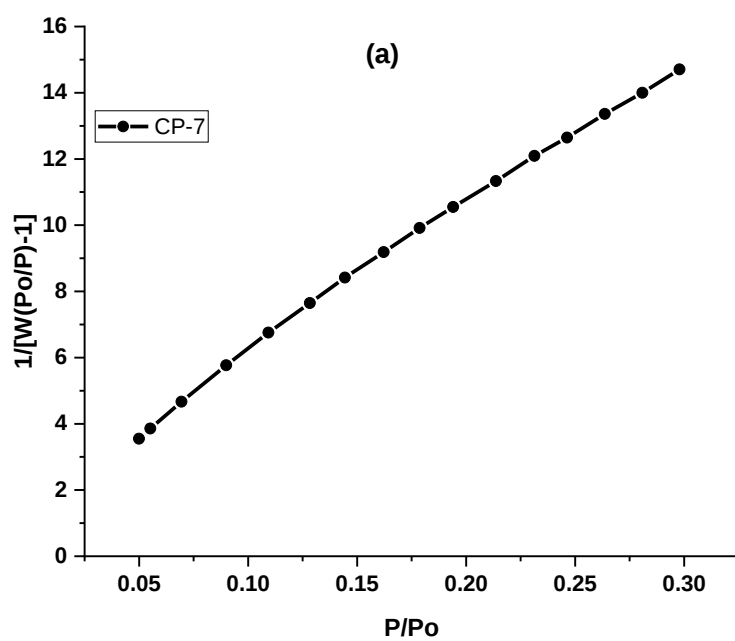
Appendix 7: BET plots of ZrO_2 -series : (a) ZrO_2 -7 (b) ZrO_2 -8 (c) ZrO_2 -9 (d) ZrO_2 -10

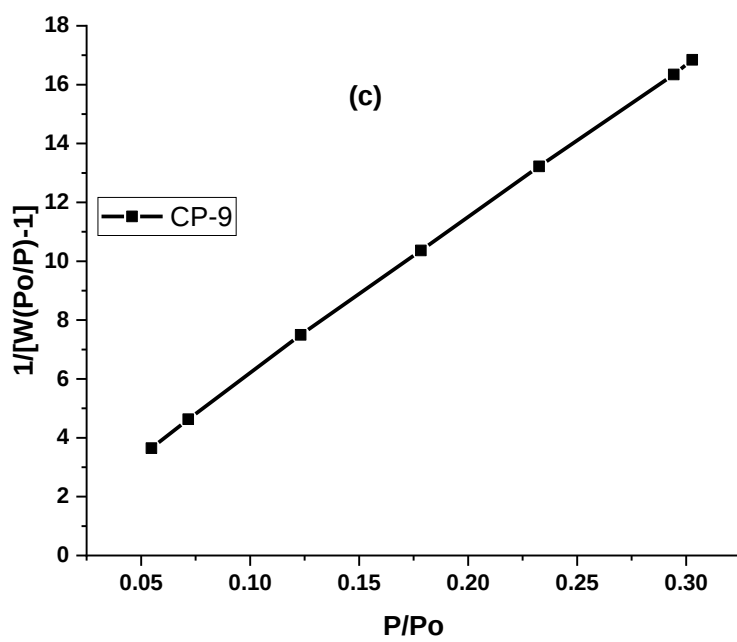
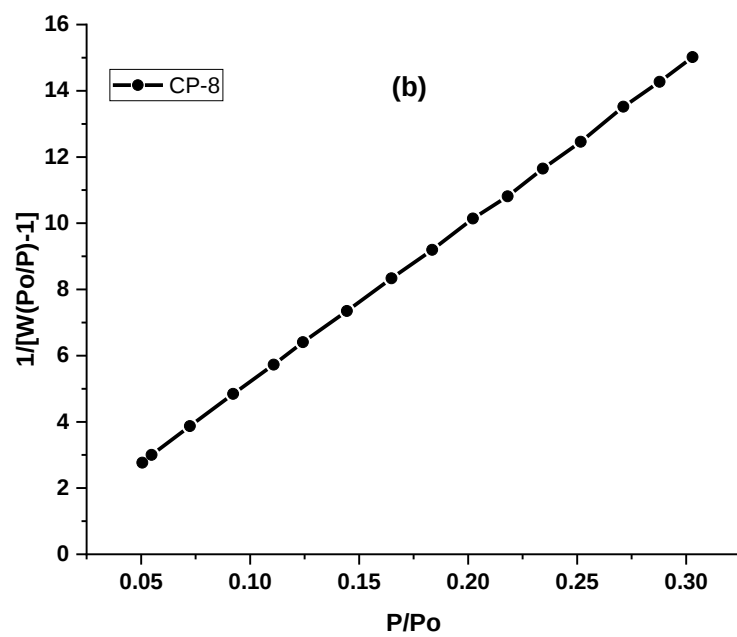


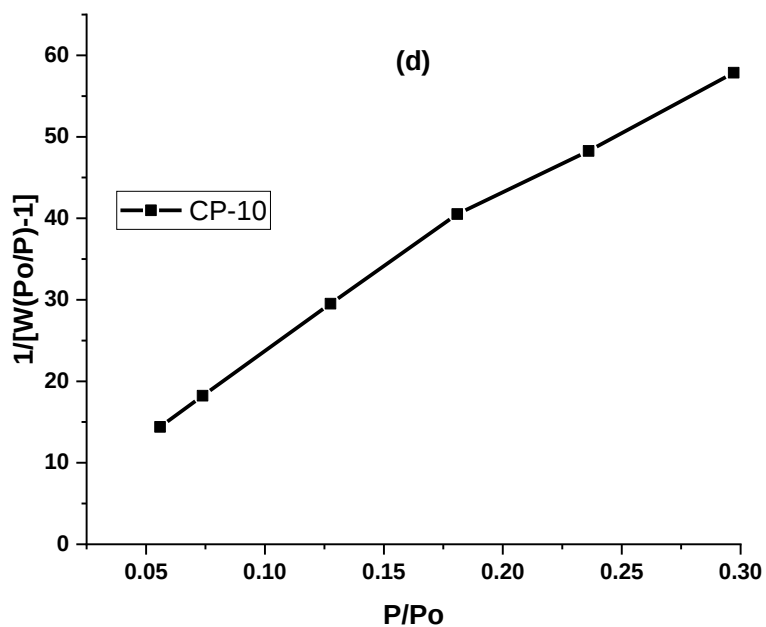




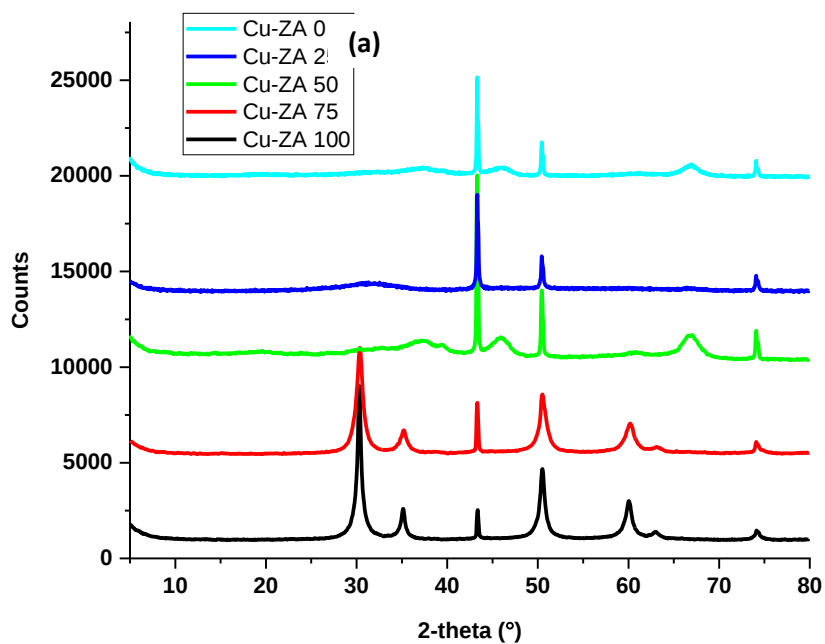
Appendix 8: BET plots of CP series : (a) CP-7 (b) CP-8 (c) CP-9 (d) CP-10

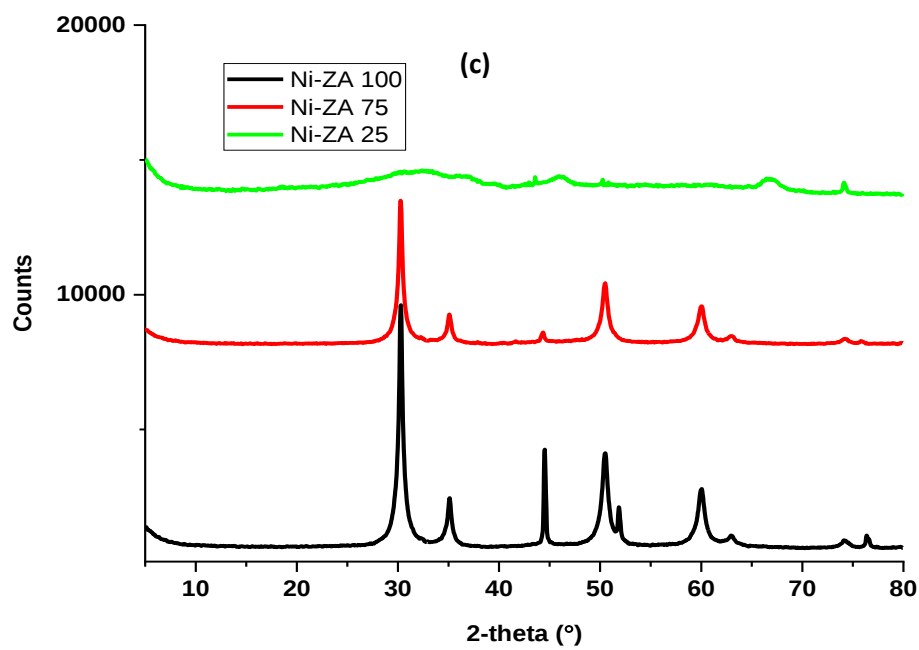
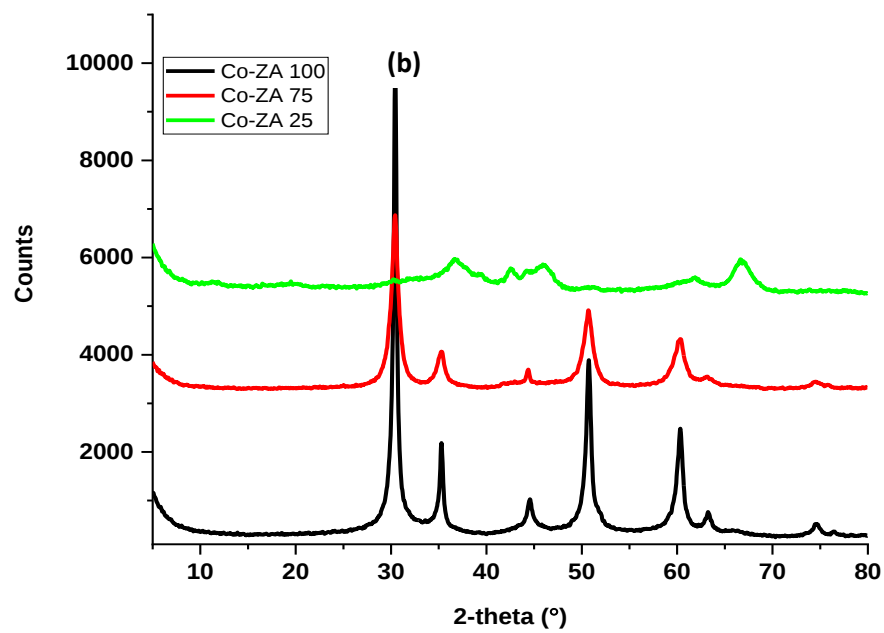




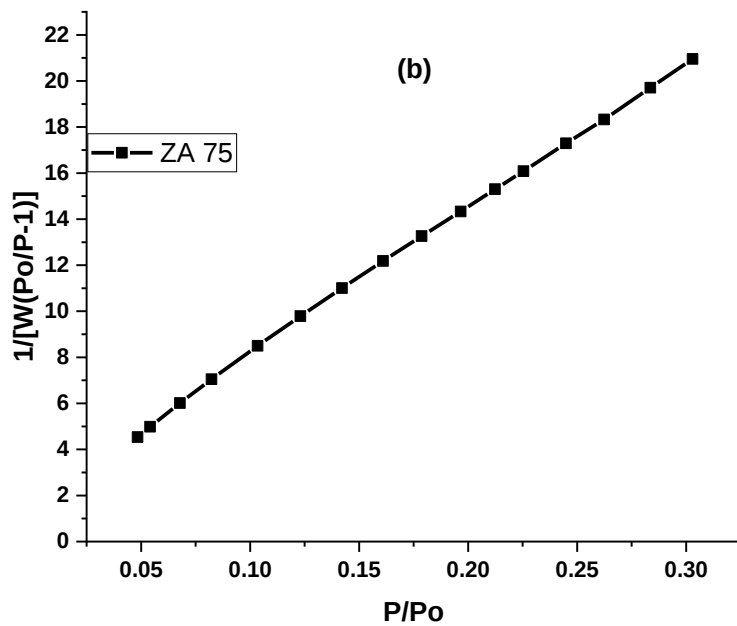
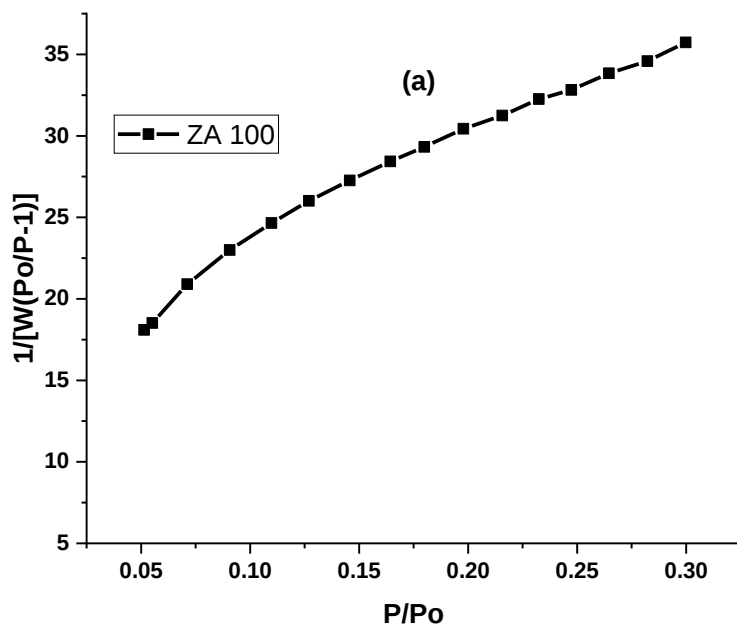


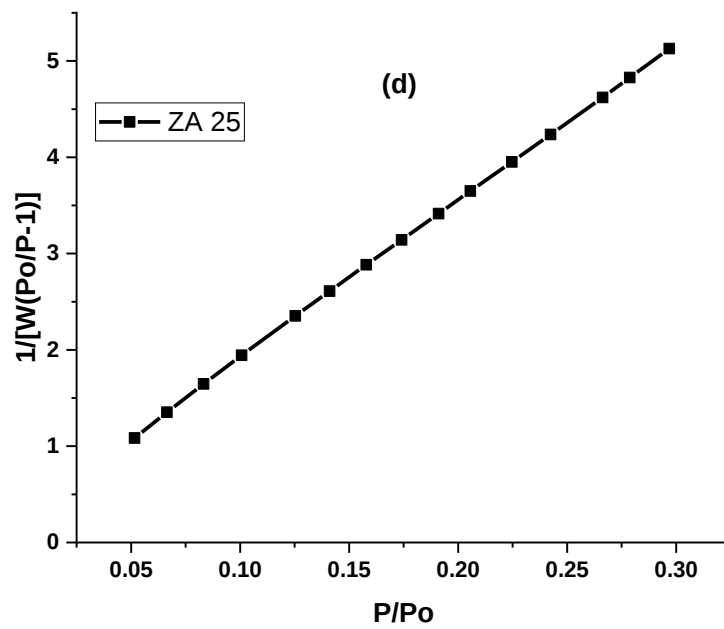
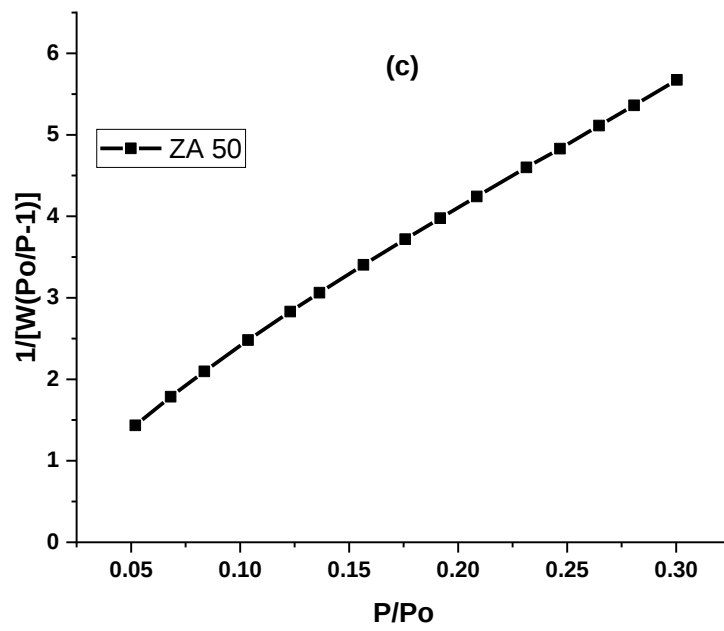
Appendix 9: XRD of reduced supported metal catalysts : (a) XRD of reduced Cu-ZA series catalysts (b) XRD of reduced Co-ZA series catalysts (c) XRD of reduced Ni-ZA series catalysts

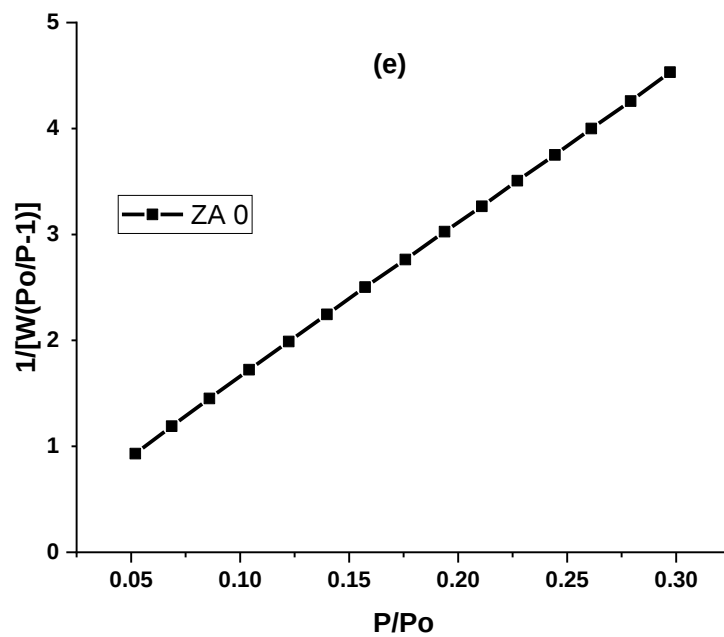




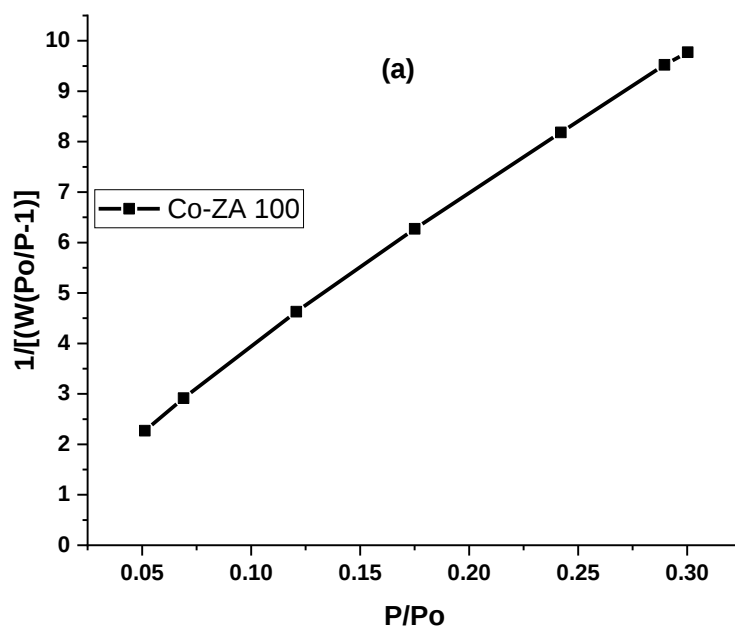
Appendix 10: BET plots of ZA series supports (a) ZA-100 (b) ZA-75 (c) ZA-50 (d) ZA-25 (e) ZA-0

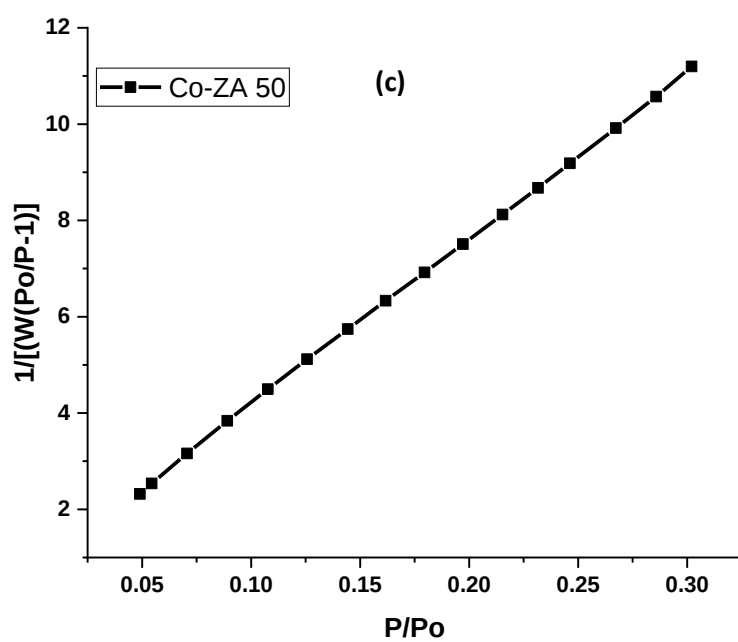
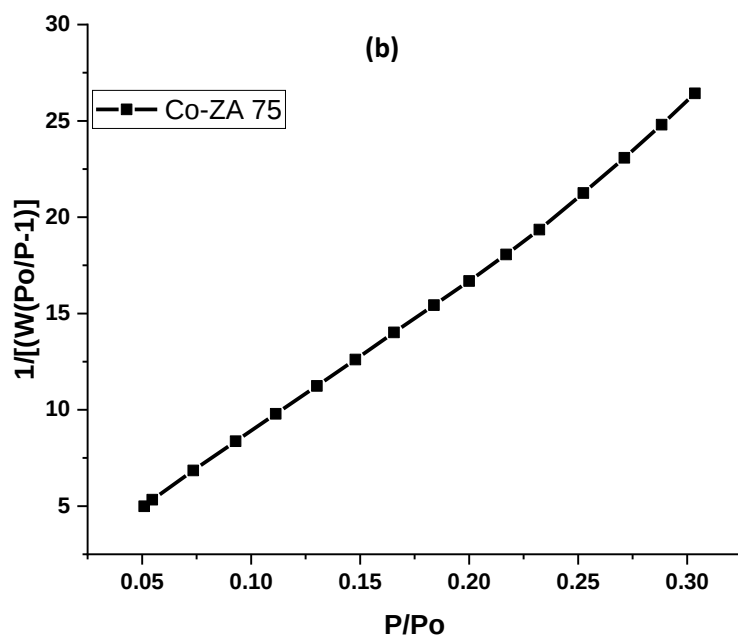


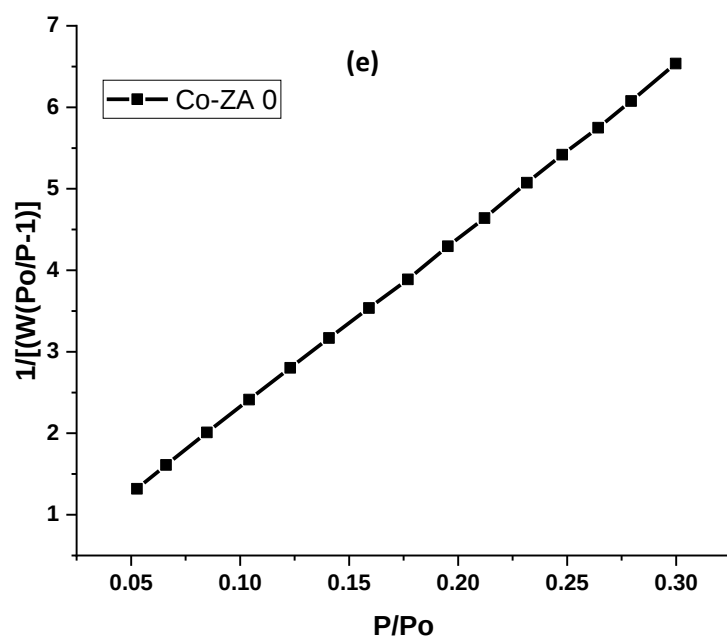
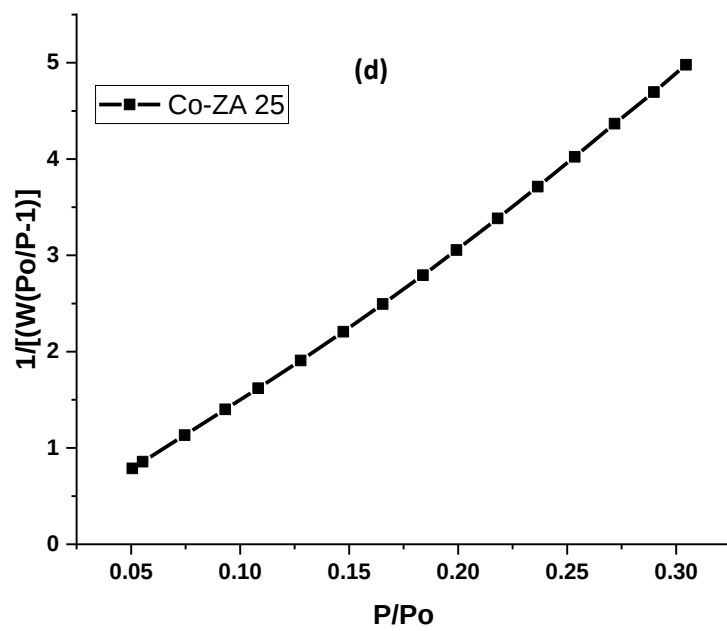




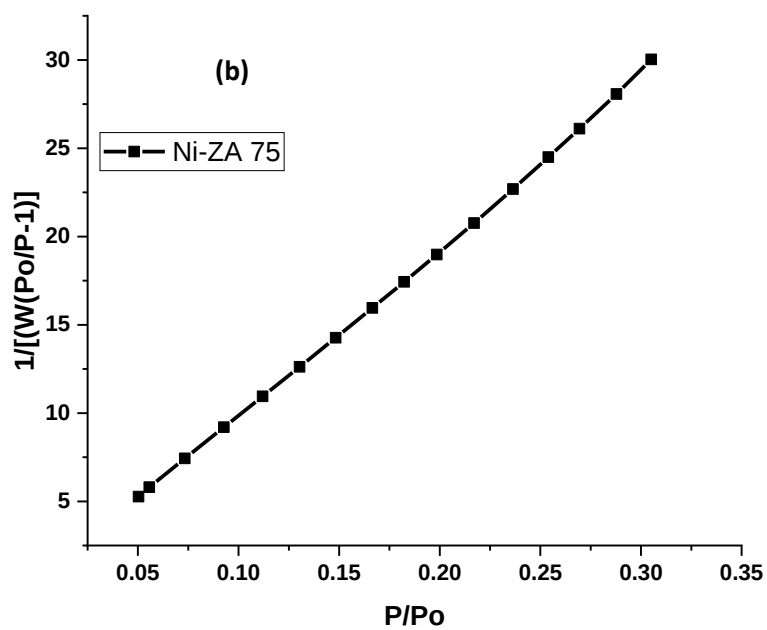
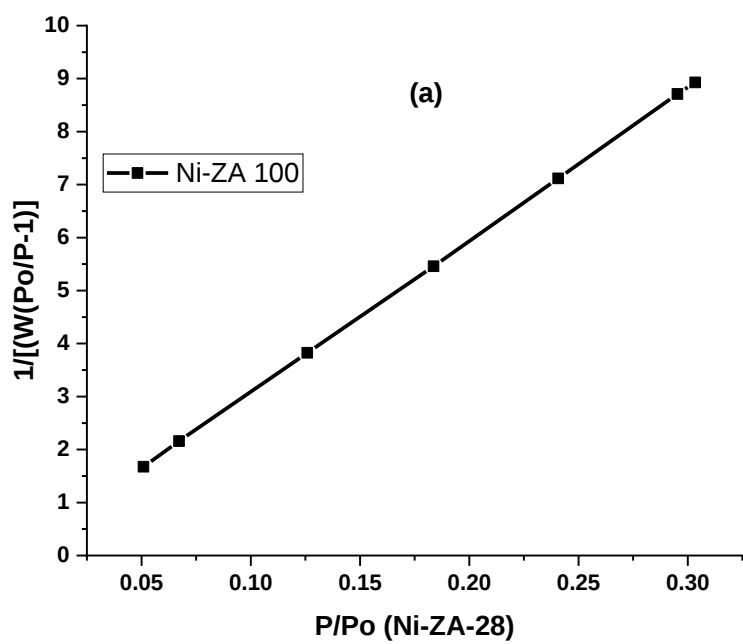
Appendix 11: BET plots of FP of Co-ZA series

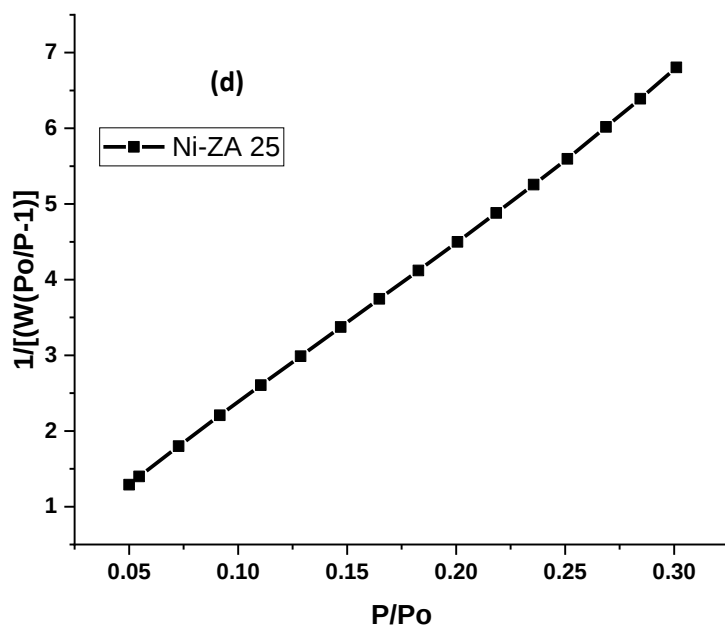
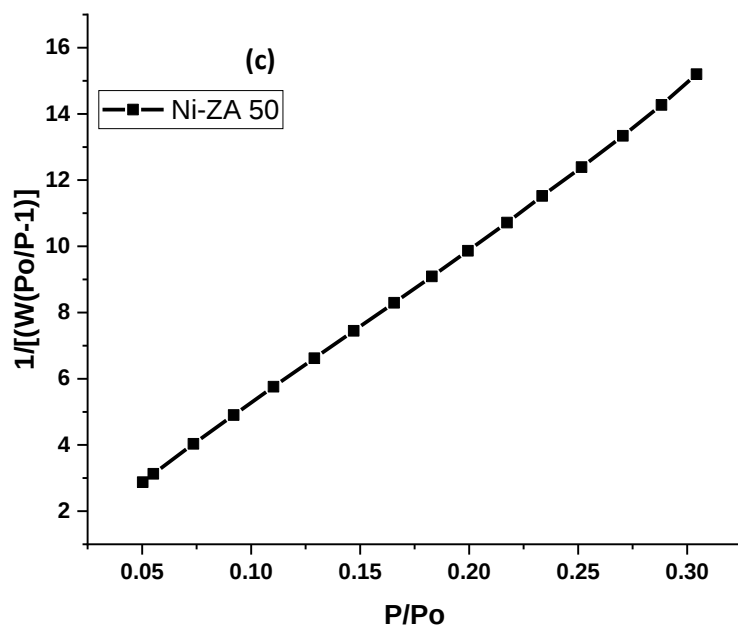


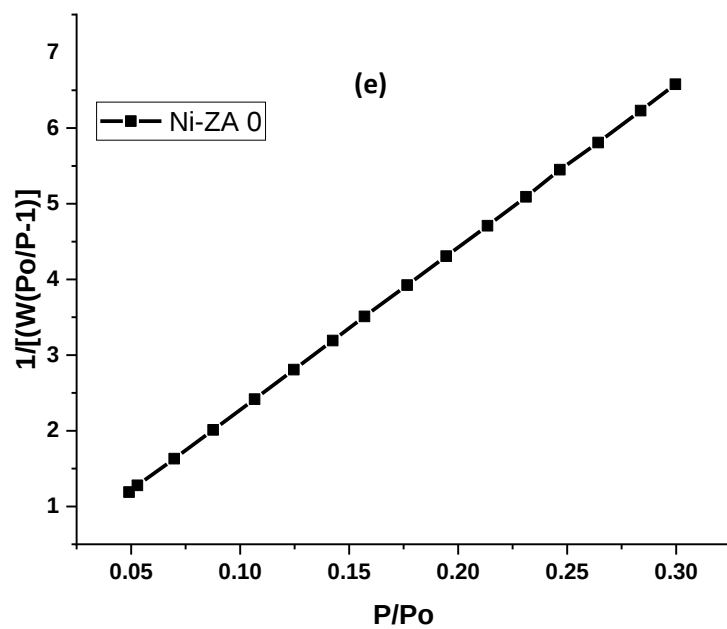




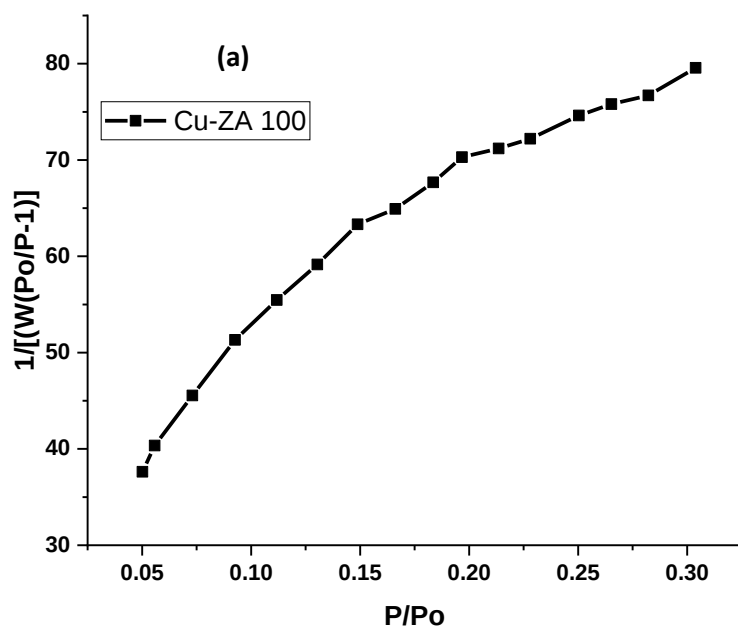
Appendix 12: BET plots of FP of Ni-ZA series

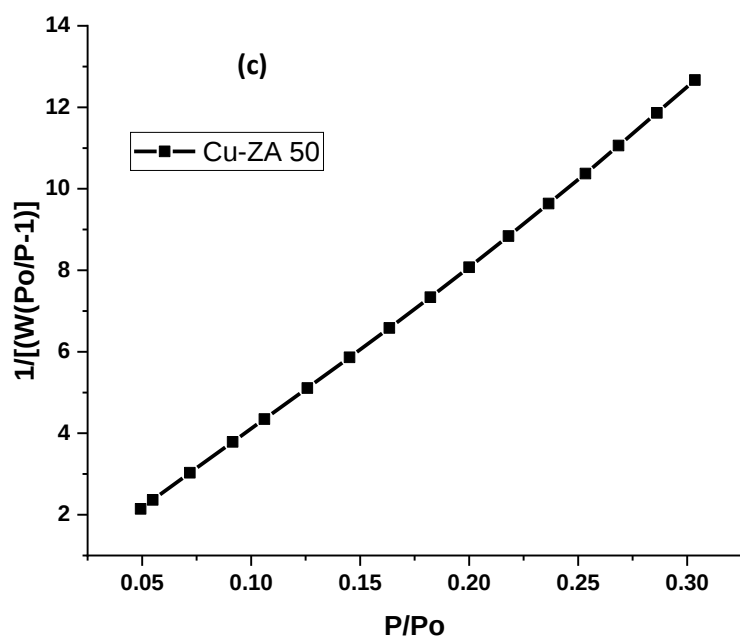
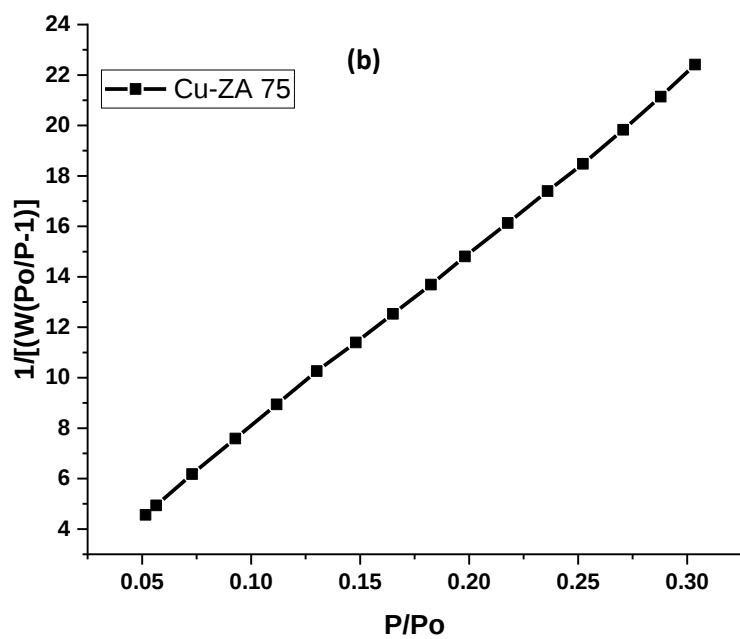


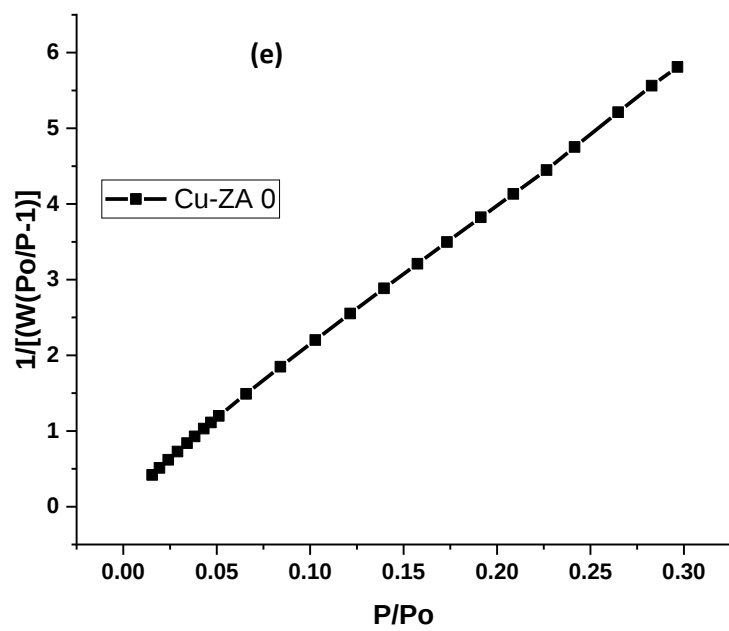
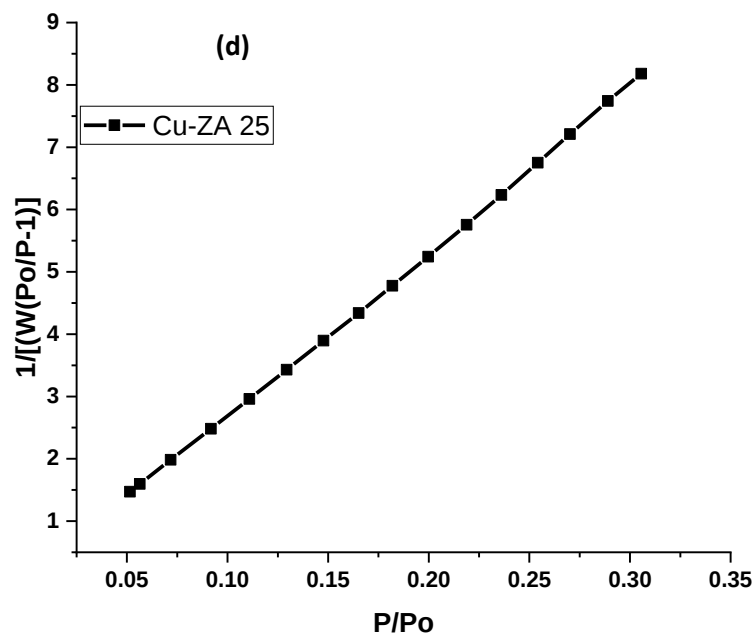




Appendix 13: BET plots of FP of Cu-ZA series

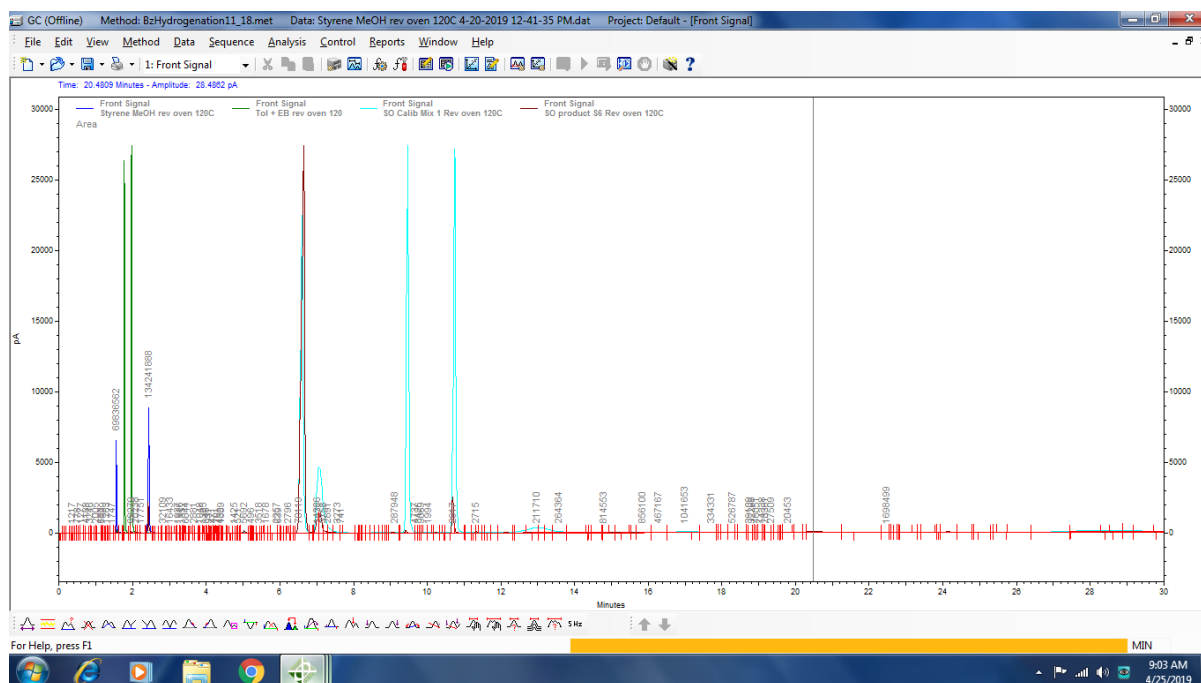






Appendix 14: GC Chromatogram of analysis of products of transformation of Styrene oxide

HP-INNOWAX capillary column 0.25 mm, ID 30 m length



Peak Table of products of styrene oxide reaction Gas Chromatographic analysis.

Peak #	Component	GC retention time (min)
1	Toluene	1.77
2	EB	1.96
3	Styrene	2.41
4	Styrene Oxide (SO)	6.47
5	Phenylacetaldehyde (PAA)	7.01
6	1-Phenylethanol (1-PEA)	9.37
7	2-Phenyl ethanol (2-PEA)	10.67
8	Heavy ends	14.55 - 29.76

Appendix 15: Table of conversion of transformation of styrene oxide on supported metal catalysts

Conversion of styrene oxide (%)						
TOS (h)	1	2	3	4	5	6
Ni-ZA 100	28.85	28.59	23.34	21.09	18.72	17.48
Ni-ZA 75	58.79	43.62	43.20	30.39	24.66	25.58
Ni-ZA 50	92.14	97.57	97.95	97.98	97.95	97.35
Ni-ZA 25	98.00	97.94	97.99	97.99	97.98	97.77
Ni-ZA 0	96.90	97.09	97.25	96.96	96.81	95.69
TOS (h)	1	2	3	4	5	6
Co-ZA 100	20.00	22.12	23.15	24.11	33.86	27.59
Co-ZA 75	36.12	17.91	16.21	19.70	14.25	12.00
Co-ZA 50	94.70	96.01	97.51	95.96	93.56	91.64
Co-ZA 25	96.78	97.89	97.94	97.88	98.00	97.91
Co-ZA 0	95.51	96.48	97.10	97.27	97.20	96.89
TOS (h)	1	2	3	4	5	6
Cu-ZA 100	23.23	21.44	8.55	8.71	7.97	3.29
Cu-ZA 75	17.37	11.93	5.71	6.24	6.61	5.01
Cu-ZA 50	85.00	83.70	84.20	83.40	83.50	83.00
Cu-ZA 25	93.00	93.30	92.50	92.00	93.60	92.20
Cu-ZA 0	98.00	96.70	97.40	97.93	97.89	97.96

Appendix 16 : Table of product selectivity – transformation of styrene oxide

Selectivity to Products (mol fraction)								
Catalyst	PAA	2-PEA	1-PEA	Styrene	EB	Toluene	Heavies	Total
Ni-ZA 100	0.284	0.267	0.013	0.375	0.033	0.007	0.022	1.001
Ni-ZA 75	0.331	0.216	0.014	0.304	0.07	0.009	0.057	1.001
Ni-ZA 50	0.059	0.309	0.003	0.045	0.43	0.108	0.046	1.000
Ni-ZA 25	0.109	0.356	0.001	0.158	0.312	0.021	0.044	1.001
Ni-ZA 0	0.106	0.34	0.002	0.043	0.351	0.019	0.085	0.946

Catalyst	PAA	2-PEA	1-PEA	Styrene	EB	Toluene	Heavies	Total
Co-ZA 100	0.161	0.174	0.01	0.575	0.011	0.001	0.069	1.001
Co-ZA 75	0.281	0.212	0.019	0.392	0.02	0.002	0.075	1.001
Co-ZA 50	0.069	0.289	0.005	0.502	0.085	0.006	0.043	0.999
Co-ZA 25	0.019	0.317	0.002	0.436	0.098	0.004	0.124	1.000
Co-ZA 0	0.136	0.256	0.009	0.208	0.227	0.005	0.159	1.000

Catalyst	PAA	2-PEA	1-PEA	Styrene	EB	Toluene	Heavies	Total
Cu-ZA 100	0.319	0.048	0.031	0.344	0.034	0.002	0.223	1.001
Cu-ZA 75	0.605	0.053	0.036	0.211	0.006	0.001	0.089	1.001
Cu-ZA 50	0.511	0.056	0.016	0.296	0.028	0.002	0.09	0.999
Cu-ZA 25	0.269	0.13	0.004	0.393	0.023	0.001	0.18	1.000
Cu-ZA 0	0.160	0.335	0.01	0.369	0.031	0.003	0.139	1.047

Appendix 17: Effect of process parameters on transformation of styrene oxide (a) Effect of temperature (b) Effect of Pressure (c) Effect of WHSV

(a) Effect of temperature on conversion of Styrene oxide (SO) (mole percent) and selectivity to products (mole fraction)

Temp (°C)	SO conversion (mol%)	S-PEA	S-PAA	Styrene	Seb	Shv	Total
95	14.3	0.18	0.3	0.25	0.05	0.21	0.99
115	45.8	0.25	0.28	0.17	0.07	0.18	0.95
130	97.4	0.33	0.25	0.15	0.09	0.16	0.98
165	97.5	0.41	0.22	0.11	0.11	0.14	0.99
200	97.9	0.43	0.18	0.1	0.12	0.12	0.95

Reaction conditions: Pressure 10 kg/cm² g, WHSV 6h⁻¹, H₂/SO 5.2 molar

(b) Effect of Pressure on conversion of Styrene oxide (SO) (mole percent) and selectivity to products (mole fraction)

Pressure (kg/cm ²)	XSO	S-PEA	S-PAA	Styrene	Seb	Shv	Total
0	38.5	0.05	0.65	0.2	0.005	0.1	1.005
4	45.8	0.2	0.47	0.15	0.02	0.15	0.99
8	62.6	0.3	0.4	0.12	0.025	0.17	1.015
10	85	0.3	0.45	0.07	0.023	0.15	0.993
16	95.4	0.37	0.39	0.06	0.035	0.15	1.005

Reaction conditions: Temperature 150°C, WHSV 6h⁻¹, H₂/SO 5.2 molar

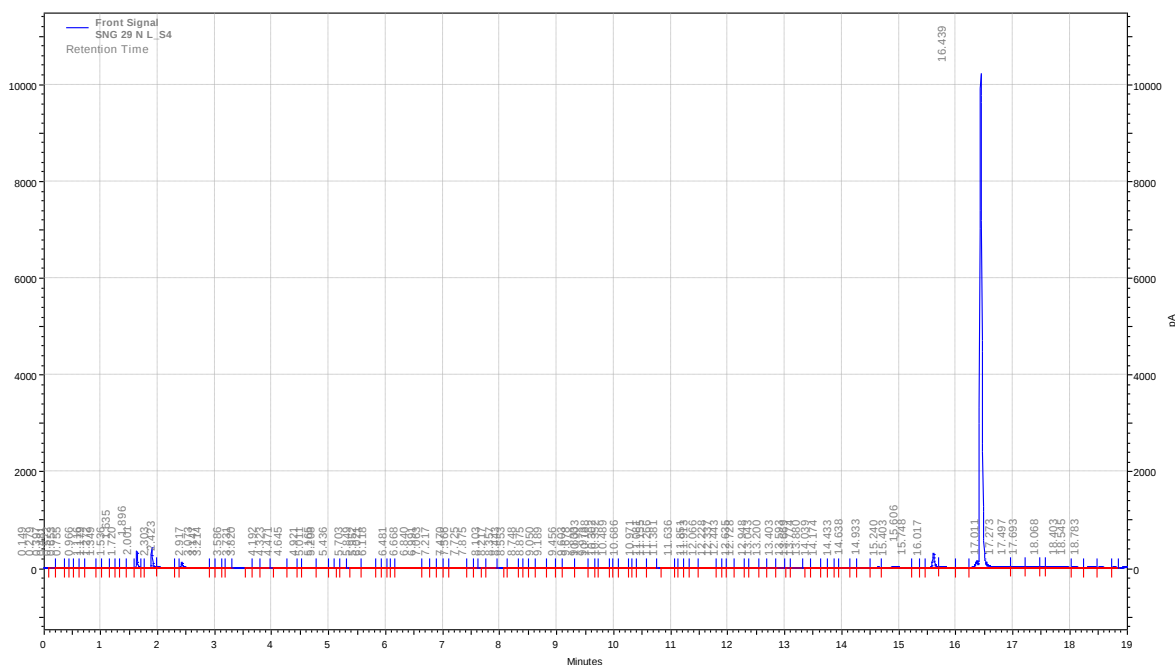
(c) Effect of WHSV on conversion of Styrene oxide (SO) (mole percent) and selectivity to products (mole fraction)

WHSV (h ⁻¹)	XSO	S-PEA	S-PAA	Styrene	Seb	Shv	Total
6	95.3	0.27	0.27	0.27	0.04	0.17	1.02
12	65	0.17	0.25	0.27	0.2	0.08	0.97
18	55	0.22	0.4	0.17	0.05	0.13	0.97
24	40	0.17	0.5	0.15	0.027	0.15	0.997
36	29	0.13	0.6	0.08	0.025	0.12	0.955

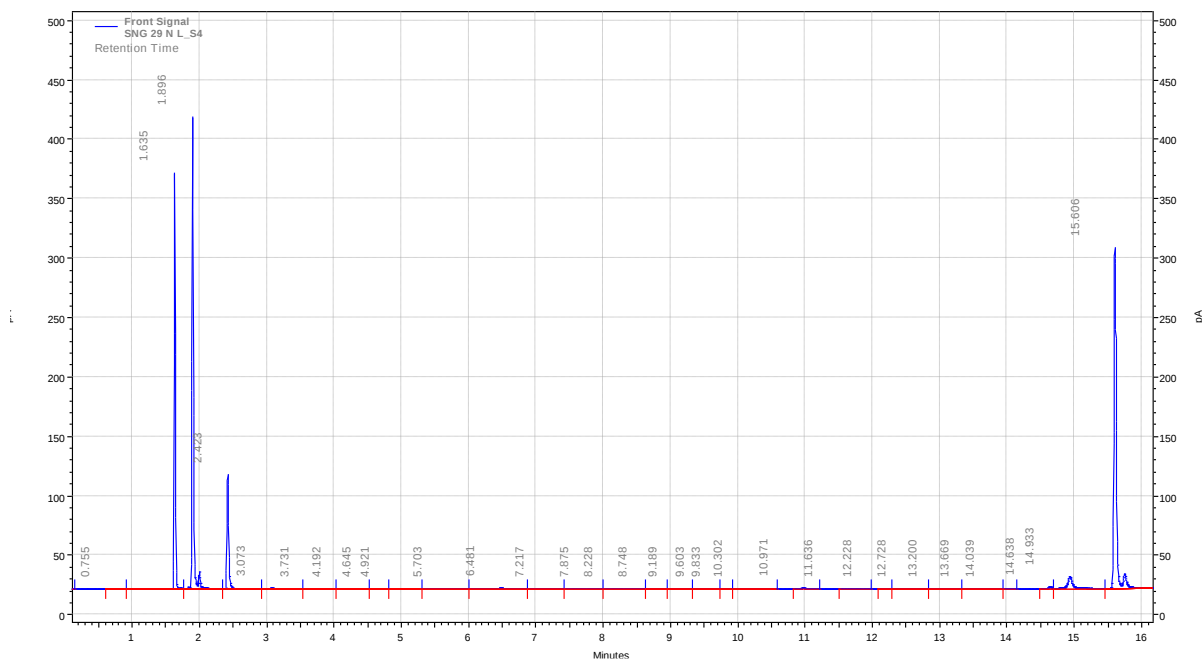
Reaction conditions: Temperature 150°C, Pressure 10 kg/cm² g, H₂/SO 5.2 molar

Appendix 18: GC Chromatogram of analysis of products of hydrodeoxygenation of m-cresol

DB-1 capillary column 0.25 mm ID, 30m length



Zoom in image of chromatogram



Peak Table: m-cresol Hydrodeoxygenation Gas Chromatographic analysis

Ret time (min)	Component
1.247	Methane
1.428	BENZENE
1.631	CYCLOHEXANE
1.718	TOLUENE
1.831	Me-CYCLOHEXANE
3.03	Di-Me-cyclohexane
5.961	CYCLOHEXANONE
6.261	ME-CYCLOHEXANONE
8.044	CYCLOHEXANOL
8.5	Me-CYCLOHEXANOL
10.589	Di-Me-CYCLOHEXANONE
11.4	Di-Me-CYCLOHEXANOL
15.53	PHENOL

16.445	m-cresol
16.7	Xylenol
17.347-18.4	Heavies

Appendix 19: Table of conversion and product selectivity m-cresol HDO on (a) Co catalysts (b) Ni catalysts (c) Cu catalyst

(a) Conversion and product selectivity of HDO of m-cresol over Co supported on bicomponent zirconia-alumina catalysts

Catalyst >>>	Co-ZA 100	Co-ZA 75	Co-ZA 50	Co-ZA 25	Co-ZA 0
Conversion (%)	1.90	4.10	4.30	4.74	5.44
Product selectivity (wt%)					
Lights	1.25	0.16	0.57	0.96	0.04
Benzene	0.00	0.00	0.00	34.68	0.00
Cyclohexane	26.24	59.83	53.89	0.12	21.61
Toluene	13.74	3.25	7.47	18.06	28.33
Methyl-cyclohexane	4.15	1.25	1.68	4.08	2.68
Cyclohexanone	0.10	0.01	0.04	0.04	0.04
Methylcyclohexanone	3.66	1.21	2.69	2.46	7.67
Cyclohexanol	0.05	0.02	0.08	0.02	0.00
Methylcyclohexanol	4.72	1.07	3.84	4.18	6.84
Phenol	13.37	16.76	9.70	18.17	19.51
Xylenol	32.36	15.64	19.56	16.70	12.88
Heavies	0.01	0.64	0.11	0.30	0.21
Total	99.67	99.84	99.63	99.77	99.82

(b) Conversion and product selectivity of HDO of m-cresol over Ni supported on bicomponent zirconia-alumina catalysts

Catalyst >>>	Ni-ZA 100	Ni-ZA 75	Ni-ZA 50	Ni-ZA 25	Ni-ZA 0
Conversion (%)	2.08	3.91	9.32	9.76	14.00
Product selectivity (wt%)					
Lights	0.10	0.10	1.05	3.37	13.52
Benzene	13.26	10.38	12.01	18.31	6.97
Cyclohexane	17.05	44.06	17.69	2.63	3.68
Toluene	0.13	8.08	9.24	16.00	7.25
Methyl-cyclohexane	0.50	1.58	2.07	3.30	4.23
Cyclohexanone	0.01	0.00	0.01	0.06	0.00
Methylcyclohexanone	2.39	1.42	0.99	0.79	0.90
Cyclohexanol	0.00	0.01	0.01	0.00	0.02
Methylcyclohexanol	3.65	2.43	1.18	0.41	1.41
Phenol	18.85	11.70	44.38	44.46	51.20
Xylenol	43.34	19.24	10.81	9.96	10.13
Heavies	0.90	0.66	0.43	0.59	0.48
Total	100.17	99.66	99.87	99.89	99.79

(c) Conversion and product selectivity of HDO of m-cresol over Cu supported on bicomponent zirconia-alumina catalysts

Catalyst >>>	Cu-ZA 100	Cu-ZA 75	Cu-ZA 50	Cu-ZA 25	Cu-ZA 0
Conversion (%)	1.05	1.98	2.13	2.25	2.45
Product selectivity (wt%)					
Lights	0.48	0.05	0.06	0.01	0.18
Benzene	0.00	13.58	70.64	2.47	0.00
Cyclohexane	0.92	17.52	0.13	70.24	62.67
Toluene	2.30	26.16	0.80	0.19	0.96
Methyl-cyclohexane	1.72	3.70	0.68	0.73	0.67
Cyclohexanone	0.28	0.01	0.09	0.05	0.02
Methylcyclohexanone	4.79	1.44	13.05	2.28	8.54
Cyclohexanol	0.10	0.02	0.00	0.05	0.02
Methylcyclohexanol	6.72	1.11	4.37	2.23	3.31
Phenol	30.57	17.34	3.83	12.39	6.61
Xylenol	51.48	18.39	6.25	9.17	15.72
Heavies	0.40	0.49	0.05	0.08	1.25
Total	99.74	99.82	99.95	99.90	99.95

Appendix 20: Summary of Material Safety Data of chemicals used in this work

(a) Styrene oxide, Phenylacetaldehyde, 2-Phenylethanol

Chemical >>>	Styrene oxide	Phenylacetaldehyde	2-Phenylethanol
CAS #	96-09-3	122-78-1	60-12-8
Boiling Point (C)	194 C	195C	219-221 C
Flash Point (C)	74 C	86 C	102 C
AIT	498 C	NA	NA
LEL / HEL	1.10% / 22.0%	NA	NA
Classification			
Flammable Liquid	Cat 4	Cat 4	
Acute toxicity oral			Cat 4
Acute Dermal toxicity	Cat 4		
Acute Inhalation toxicity (Vapor)	Cat 3		
Skin corrosion/irritation	Cat 2	Cat 1B	
Eye damage/irritation	Cat 2	Cat 1	Cat 2
Skin sensitization	Cat 1	Cat 1	
Germ cell mutagenicity	Cat 1B		
Carcinogenicity	Cat 1B		
Reproductive			
Risk Phrases	45-21-36	22-43	22/36
Safety Phrases	53-45 Note E	20/21; 24/25; 36/37/39	
Hazard statements	H312/319/350	H320/314/317/412	H302/319

(a) 1-Phenylethanol, Styrene, Ethylbenzene, Toluene

Chemical >>>	1-Phenylethanol	Styrene	Ethylbenzene	Toluene
CAS #	98-85-1	100-42-5	100-41-4	108-88-3
Boiling Point (C)	204 C	145C	136.1 C	110.6 C
Flash Point (C)	86 C	31 C	23 C	4 C
AIT	NA	490 C	430 C	480 C
LEL / HEL	NA	1.2% / 8.9%	1.0 / 7.8%	1.2% / 8%
Classification				
Flammable Liquid	Cat 4	Cat 3	Cat 2	Cat 2
Acute toxicity oral	Cat 4			
Acute Dermal toxicity	Cat 5			
Acute Inhalation toxicity (Vapor)		Cat 4	Cat 4	Cat 1
Skin corrosion/irritation	Cat 2	Cat 2		Cat 2
Eye damage/irritation	Cat 1	Cat 2		
Skin sensitization				
Germ cell mutagenicity				
Carcinogenicity				
Reproductive				Cat 2
Risk Phrases				
Safety Phrases				
Hazard statements	H227/302/313/315/318	H226/332/315/319/361d/372/304	H225/332/373/304/412	H225/304/315/336/361d/373

(b) m-cresol, Phenol, Xylenol 2,6

Chemical	m-cresol	Phenol	Xylenol 2,6
CAS #	108-39-4	108-95-2	576-26-1
Boiling Point (C)	202 C	181 C	203 C
Flash Point (C)	86 C	79 C	86 C
AIT	559 C	715 C	NA
LEL / HEL	NA	1.3/9/5%	
Classification			
Flammable Liquid	Cat 4		
Acute toxicity oral	Cat 3	Cat 3	Cat 3
Acute Dermal toxicity	Cat 3		Cat 3
Acute Inhalation toxicity (Vapor)		Cat 3	
Skin corrosion/irritation	Cat 1B	Cat 3	Cat 1B
Eye damage/irritation	Cat 1	Cat 1	Cat 1
Skin sensitization			
Germ cell mutagenicity		Cat 2	
Carcinogenicity			
Specific Organ specificity	Cat 3	Cat 2	
Risk Phrases			
Safety Phrases			
Hazard statements	H301/311/ 314	H301/331/311/314/ 318/341/373/411	H301/311/314/318/4 11

(c) Benzene, Toluene, Cyclohexane

Chemical	Benzene	Toluene	Cyclohexane
CAS #	71-43-2	108-88-3	110-82-7
Boiling Point (C)	80 C	110.6 C	80 C
Flash Point (C)	-10.99 C	4 C	-20 C
AIT	562 C	480 C	260 C
LEL / HEL	1.3% / 8%	1.2% / 8%	1.3% / 8.4%
Classification			
Flammable Liquid	Cat 2	Cat 2	Cat 2
Acute toxicity oral			
Acute Dermal toxicity			
Acute Inhalation toxicity (Vapor)		Cat 1	
Skin corrosion/irritation	Cat 2	Cat 2	Cat 2
Eye damage/irritation	Cat 2		
Skin sensitization			
Germ cell mutagenicity	Cat 1B		
Carcinogenicity	Cat 1		
Specific Organ specificity	Cat 1	Cat 2	STOT SE 3
Risk Phrases			
Safety Phrases			
Hazard statements	H225/315/319/340/350/372 /304/412	H225/304/315/336/36 1d/373	H225/315/336 /304

(d) Methyl cyclohexane, Cyclohexanol, Cyclohexanone

Chemical	Methyl cyclohexane	Cyclohexanol	Cyclohexanone
CAS #	10120-28-2	108-93-0	108-94-1
Boiling Point (C)	100.9 C	160 C	154.3 C
Flash Point (C)	-4 C	68 C	44 C
AIT		NA	420 C
LEL / HEL	1.1%/6.7%	NA	1.3% / 9.4%
Classification			
Flammable Liquid	Cat 2		Cat 3
Acute toxicity oral		Cat 4	Cat 4
Acute Dermal toxicity			Cat 4
Acute Inhalation toxicity (Vapor)		Cat 4	Cat 4
Skin corrosion/irritation	Cat 2	Cat 2	Cat 2
Eye damage/irritation			Cat 1
Skin sensitization			
Germ cell mutagenicity			
Carcinogenicity			
Specific Organ specificity	STOT SE 3	Cat 3	
Risk Phrases			
Safety Phrases			
Hazard statements	H225/315/336/304/400/411	H302/322/315/335/	H226/302/312/322/315/318

(e) Methyl cyclohexanol, Methyl cyclohexanone, Methane

Chemical	Methyl cyclohexanol	Methyl cyclohexanone	Methane
CAS #	583-59-5	583-60-8	74-82-8
Boiling Point (C)	163-166 C	165.1 C	-161 C
Flash Point (C)	58 C	48 C	-188 C
AIT	296 C	NA	537C
LEL / HEL	NA	NA	4.4/15%
Classification			
Flammable Liquid	Cat 3	Cat 3	Cat 1
Acute toxicity oral	Cat 4		
Acute Dermal toxicity			
Acute Inhalation toxicity (Vapor)	Cat 4	Cat 4	
Skin corrosion/irritation			
Eye damage/irritation	Cat 2		
Skin sensitization			
Germ cell mutagenicity			
Carcinogenicity			
Specific Organ specificity			
Risk Phrases			
Safety Phrases			
Hazard statements		H226/332	H220/280