Appendices

Figure A1: IR Spectra of pure zeolite Y

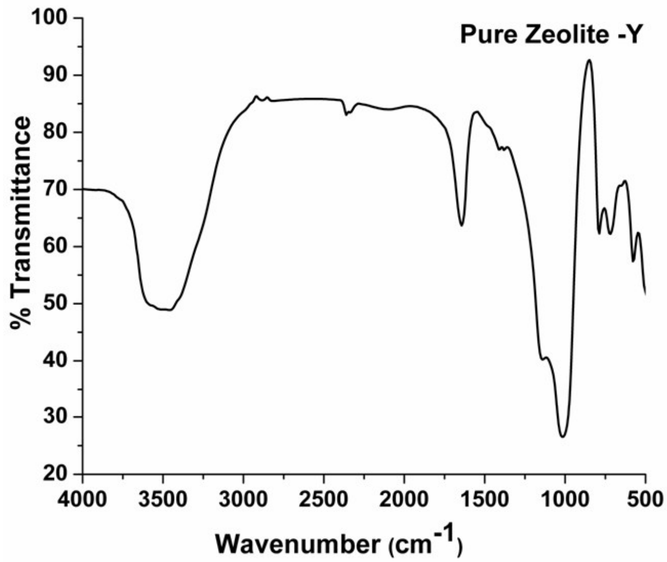


Figure A2: IR Spectra of metal exchanged zeolite -Y

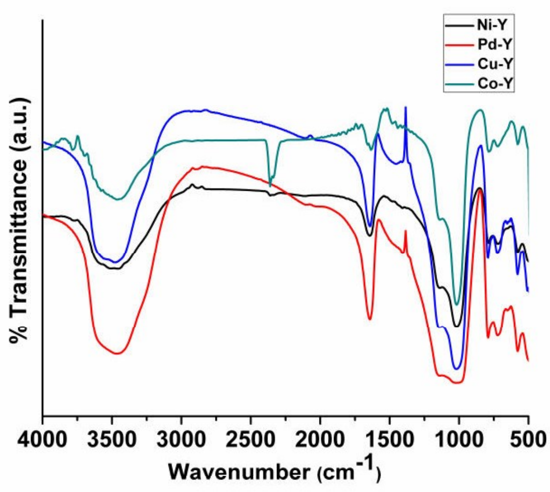


Figure A3: Solid state UV absorption spectra of pure zeolite Y and metal exchanged zeolite-Y

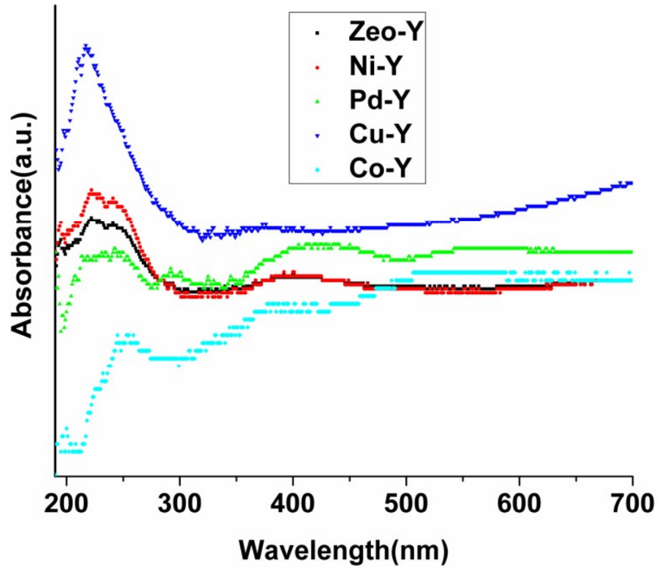


Figure A4: EDX data of pure zeolite Y

Element	Weight%	Atomic%
O K	51.34	63.89
Na K	8.39	7.27
Al K	10.09	7.45
Si K	30.18	21.40
Total	100	

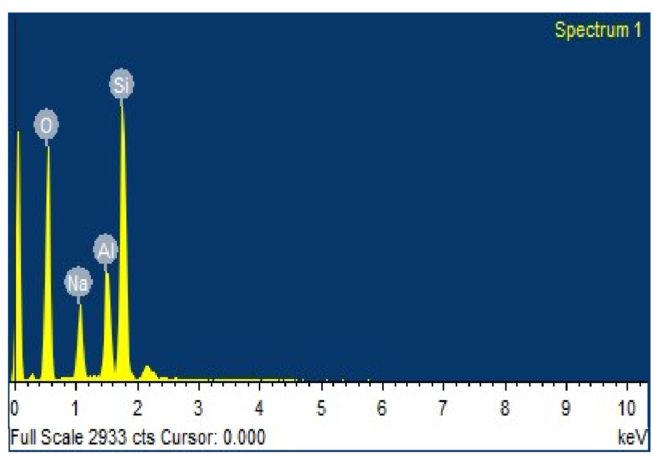


Figure A5: EDX data of NiL1-Y

Spectrum: s1_1

Element	Series	unn. C [wt.-%]	norm. C [wt.-%]	Atom. C [at.-%]	Error [%]
Silicon	K-series	13.54	16.18	10.09	0.6
Aluminium	K-series	6.03	7.21	4.68	0.3
Sodium	K-series	4.73	5.65	4.31	0.3
Carbon	K-series	5.86	7.00	10.21	0.7
Nickel	K-series	0.50	0.59	0.18	0.0
Nitrogen	K-series	6.03	7.20	9.01	0.9
Oxygen	K-series	47.00	56.17	61.52	5.2
	Total:	83.68	100.00	100.00	

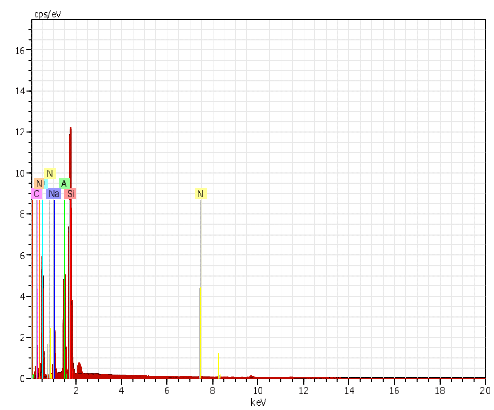


Figure A6: EDX data of NiL2-Y

Element	Weight %	Atomic%
C K	23.15	32.42
O K	46.14	48.51
Na K	4.87	3.57
Al K	7.67	4.78
Si K	17.66	10.58
Ni K	0.50	0.14
Totals	100.00	

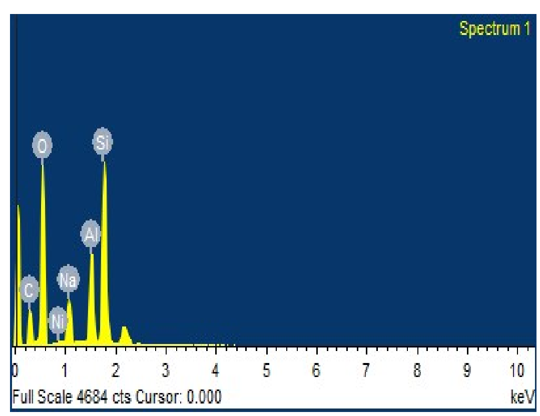


Figure A7: EDX data of NiL4-Y

Spectrum: s3_1

Element	Series	unn. C [wt.-%]	norm. C [wt.-%]	Atom. C [at.-%]	Error [%]
Silicon	K-series	4.07	4.07	2.29	0.2
Aluminium	K-series	5.39	5.39	3.15	0.3
Sodium	K-series	1.50	1.50	1.03	0.1
Carbon	K-series	14.92	14.92	19.62	5.0
Nickel	K-series	0.47	0.47	0.13	0.0
Nitrogen	K-series	7.65	7.65	8.62	2.9
Oxygen	K-series	65.99	65.99	65.15	20.4
	Total:	100.00	100.00	100.00	

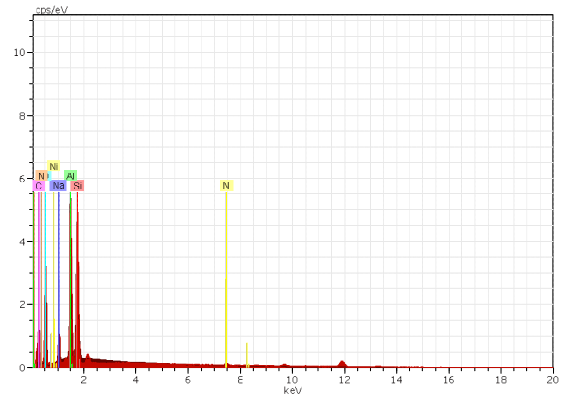


Figure A8: EDX data of NiL6-Y

Spectrum: s7_1

Element	Series	unn. C [wt.-%]	norm. C [wt.-%]	Atom. C [at.-%]	Error [%]
Silicon	K-series	12.47	13.67	8.21	0.6
Aluminium	K-series	5.65	6.19	3.87	0.3
Sodium	K-series	4.83	5.29	3.88	0.3
Carbon	K-series	11.48	12.58	17.66	1.3
Nickel	K-series	0.47	0.52	0.15	0.0
Nitrogen	K-series	7.07	7.75	9.33	1.0
Oxygen	K-series	49.27	53.99	56.90	5.4
	Total:	91.25	100.00	100.00	

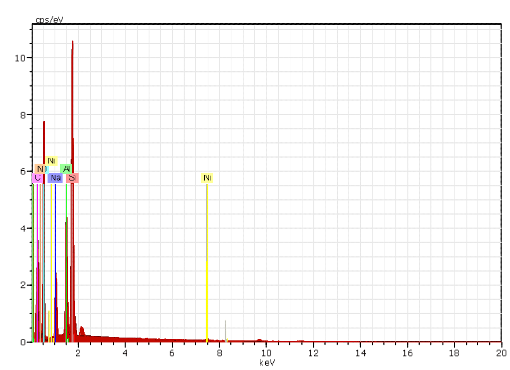
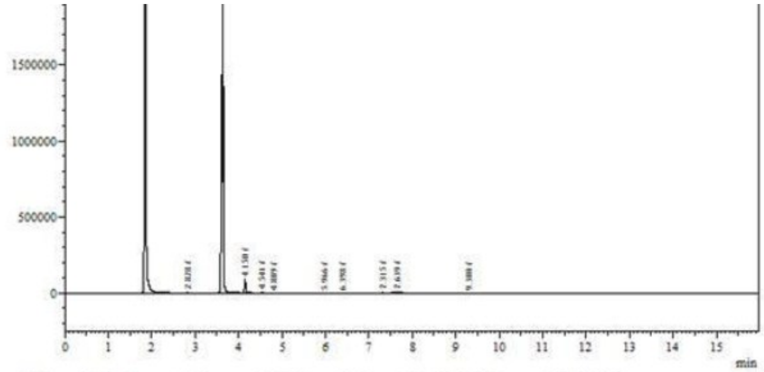
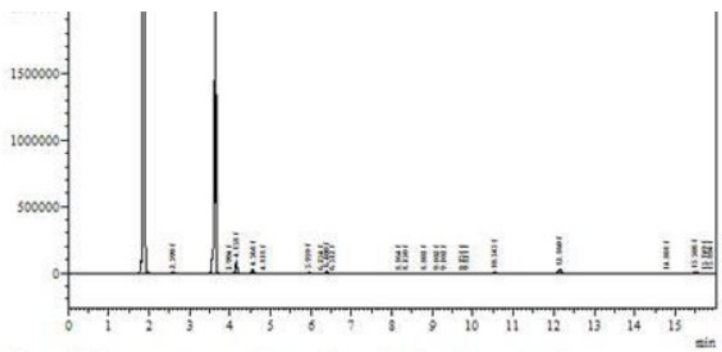


Figure A9: GC chromatogram of pure Zeolite-Y for styrene oxidation reaction



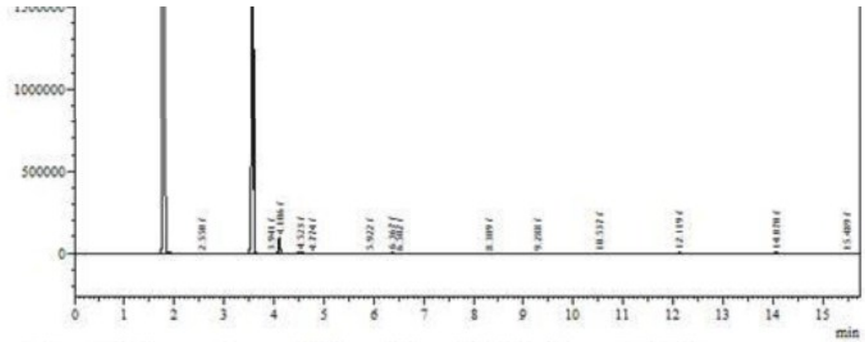
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.842	18582660	12461597	0.000		S		
2	2.828	3822	3941	0.000		TV		
3	3.637	4998638	2032312	0.000		S		
4	4.150	185981	87360	0.000		T		
5	4.541	4277	987	0.000		T		
6	4.809	1022	395	0.000		TV		
7	5.966	1364	392	0.000		V		
8	6.398	1629	464	0.000				
9	7.315	11045	966	0.000				
10	7.639	30640	2393	0.000		V		
11	9.300	2244	697	0.000				
Total		23823322	14591504					

Figure A10: GC chromatogram of NiL1 for styrene oxidation reaction



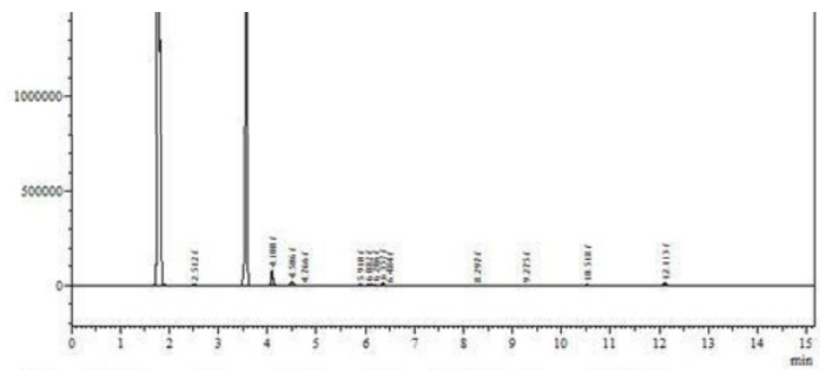
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.844	20349830	8044694	0.000		S		
2	2.590	22015	10316	0.000				
3	3.641	5543118	2153939	0.000				
4	3.994	1042	405	0.000				
5	4.158	249780	96370	0.000				
6	4.568	87965	24323	0.000		V		
7	4.818	2904	785	0.000		V		
8	5.959	23477	8559	0.000				
9	6.254	2674	952	0.000				
10	6.400	44032	15140	0.000		V		
11	6.532	1702	467	0.000		V		
12	8.164	1916	698	0.000				
13	8.350	5895	1412	0.000		V		
14	8.803	1687	428	0.000				
15	9.102	1364	373	0.000		V		
16	9.303	3834	973	0.000		V		
17	9.751	2566	810	0.000				
18	9.831	1875	385	0.000		V		
19	10.545	9717	3064	0.000				
20	12.160	117391	33259	0.000		S		
21	14.801	4418	738	0.000		V		

Figure A11: GC chromatogram of NiL2 for styrene oxidation reaction



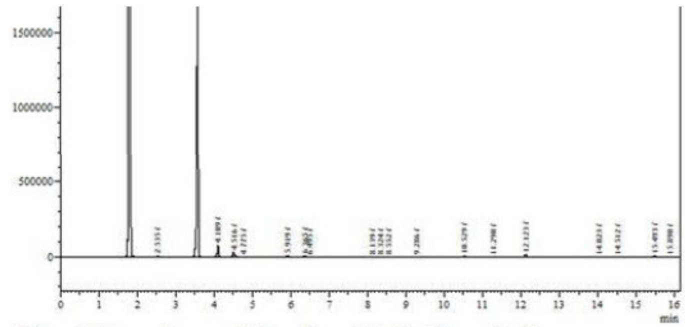
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.770	17392163	5931089	0.000				
2	2.550	2314	837	0.000				
3	3.580	5156416	2094413	0.000		V		
4	3.941	1057	343	0.000		V		
5	4.106	227815	91645	0.000		V		
6	4.523	43590	10315	0.000		V		
7	4.774	2214	674	0.000		V		
8	5.922	4430	1467	0.000		V		
9	6.367	8768	3179	0.000				
10	6.502	3857	1206	0.000		V		
11	8.309	2859	709	0.000		V		
12	9.288	2321	774	0.000				
13	10.537	3285	952	0.000		V		
14	12.119	7463	2577	0.000		V		
15	14.070	12492	1779	0.000				
16	15.489	4182	1207	0.000				
Total		22875226	8143166					

Figure A12: GC chromatogram of NiL4 for styrene oxidation reaction



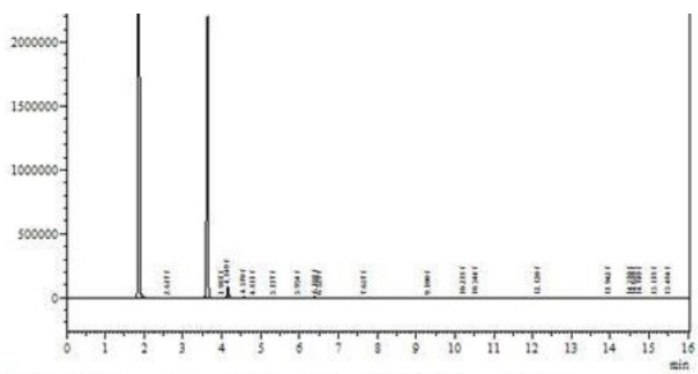
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.772	15041786	7039564	0.000		S		
2	2.512	10008	4140	0.000				
3	3.575	4138477	1716511	0.000				
4	4.100	188058	78284	0.000				
5	4.506	60486	18810	0.000		V		
6	4.766	1521	527	0.000		V		
7	5.910	18891	4808	0.000		V		
8	6.082	18471	2398	0.000		V		
9	6.206	7702	1496	0.000		V		
10	6.357	31411	11007	0.000		V		
11	6.484	2093	558	0.000		V		
12	8.297	2886	830	0.000		V		
13	9.275	2026	689	0.000		V		
14	10.518	5186	1638	0.000		V		
15	12.113	44569	14889	0.000				
Total		19573571	8896149					

Figure A13: GC chromatogram of NiL6 for styrene oxidation reaction



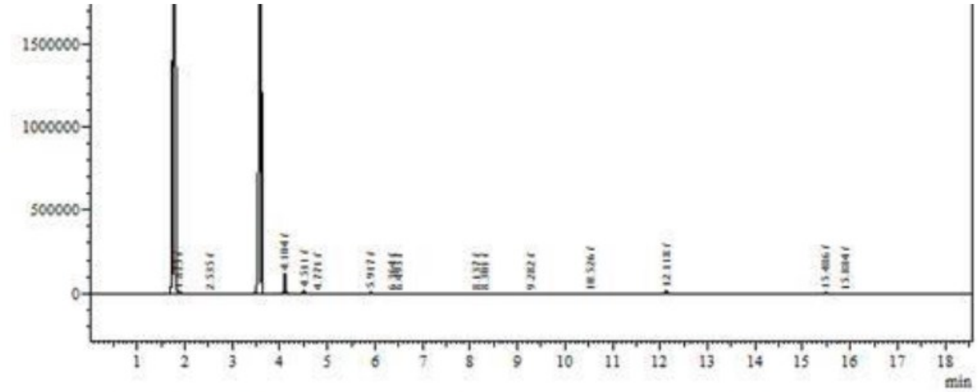
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.781	14889876	7100040	0.000		S		
2	2.535	4727	1835	0.000		S		
3	3.585	4287241	1830434	0.000				
4	4.109	186446	76975	0.000		V		
5	4.516	93132	28024	0.000		S		
6	4.775	1403	521	0.000		T		
7	5.919	13197	4304	0.000				
8	6.365	12670	4244	0.000		V		
9	6.495	4800	1425	0.000		V		
10	8.139	1612	605	0.000				
11	8.324	5487	1365	0.000		V		
12	8.552	1308	350	0.000		V		
13	9.286	2126	684	0.000		V		
14	10.529	6126	1958	0.000				
15	11.290	1451	249	0.000		V		
16	12.123	39644	13155	0.000				
17	14.023	1551	252	0.000				
18	14.512	1205	202	0.000				
19	15.493	15077	4611	0.000				
20	15.890	2320	657	0.000		V		
Total		19571399	9071890					

Figure A14: GC chromatogram of NiL1-Y for styrene oxidation reaction



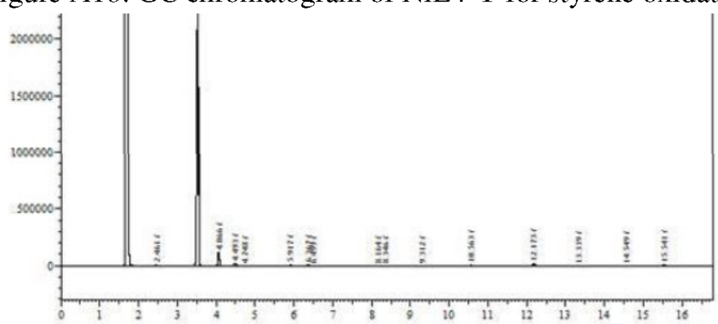
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.836	18386686	7067946	0.000		S		
2	2.617	1763	591	0.000				
3	3.632	5382270	2185316	0.000		V		
4	3.987	1235	340	0.000		V		
5	4.149	220086	81431	0.000		V		
6	4.570	16407	4084	0.000		V		
7	4.813	1801	620	0.000		V		
8	5.337	2520	520	0.000				
9	5.954	3896	1191	0.000		V		
10	6.393	6766	2374	0.000				
11	6.529	1988	567	0.000		V		
12	7.657	1825	450	0.000				
13	9.300	2212	755	0.000				
14	10.218	3422	791	0.000				
15	10.544	1966	573	0.000				
16	12.120	4253	1256	0.000				
17	13.942	3722	637	0.000				
18	14.510	3566	678	0.000				
19	14.610	1531	385	0.000		V		
20	14.749	2748	314	0.000		V		

Figure A15: GC chromatogram of NiL2-Y for styrene oxidation reaction



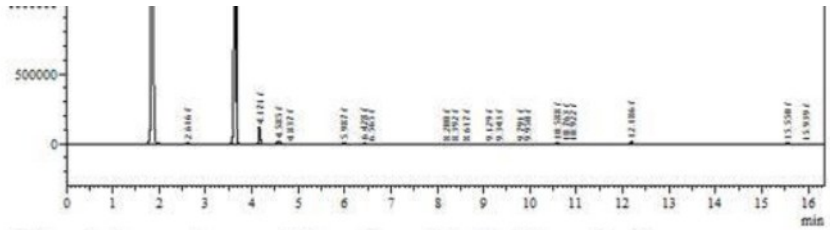
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.766	20229211	9102041	0.000		S		
2	1.875	5876	2873	0.000		T		
3	2.535	3952	1394	0.000				
4	3.586	5918142	2356582	0.000				
5	4.104	258972	114346	0.000				
6	4.511	49880	15376	0.000		V		
7	4.771	1932	764	0.000		V		
8	5.917	11549	4347	0.000		V		
9	6.364	3417	1000	0.000		V		
10	6.493	1446	442	0.000		V		
11	8.137	1555	613	0.000				
12	8.301	2102	716	0.000		V		
13	9.282	2736	940	0.000		V		
14	10.526	5283	1697	0.000				
15	12.118	36378	11993	0.000				
16	15.486	12478	3978	0.000				
17	15.884	1013	298	0.000				
Total		26545922	11619400					

Figure A16: GC chromatogram of NiL4-Y for styrene oxidation reaction



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.681	22697453	7138388	0.000		S		
2	2.461	11983	5089	0.000				
3	3.539	6910911	2535076	0.000				
4	4.066	312298	115572	0.000				
5	4.493	76792	22723	0.000		V		
6	4.748	2204	749	0.000		V		
7	5.917	17272	6238	0.000		V		
8	6.367	14766	4992	0.000		V		
9	6.499	2207	760	0.000		V		
10	8.164	1178	440	0.000				
11	8.346	4619	1166	0.000		V		
12	9.312	3203	1064	0.000		V		
13	10.563	7563	2491	0.000				
14	12.173	56486	18147	0.000				
15	13.339	3419	1063	0.000				
16	14.549	3856	378	0.000				
17	15.541	14079	4366	0.000		V		
Total		30140289	9858702					

Figure A17: GC chromatogram of NiL6-Y for styrene oxidation reaction



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.838	18677330	8223565	0.000				
2	2.616	10129	3083	0.000				
3	3.654	5997669	2378751	0.000				
4	4.171	280810	123395	0.000				
5	4.585	84792	21178	0.000				
6	4.837	2125	815	0.000		V		
7	5.987	16871	5994	0.000		V		
8	6.428	11918	4164	0.000		V		
9	6.565	3804	1136	0.000		V		
10	8.200	2423	894	0.000				
11	8.392	5901	1502	0.000		V		
12	8.617	1142	308	0.000		V		
13	9.129	1085	180	0.000				
14	9.343	3251	1051	0.000		V		
15	9.791	1037	361	0.000				
16	9.950	2228	451	0.000				
17	10.588	9334	2690	0.000				
18	10.763	2803	434	0.000		V		
19	10.922	7280	847	0.000		V		
20	12.186	54746	18470	0.000				
21	15.550	23206	7056	0.000				
22	15.939	3078	906	0.000		V		

Figure A18: EDX data of Pd-Y

Element	Weight%	Atomic%
C K	15.74	23.31
O K	47.06	52.33
Na K	6.40	4.95
Al K	7.94	5.23
Si K	22.21	14.06
Pd L	0.65	0.11
Totals	100.00	

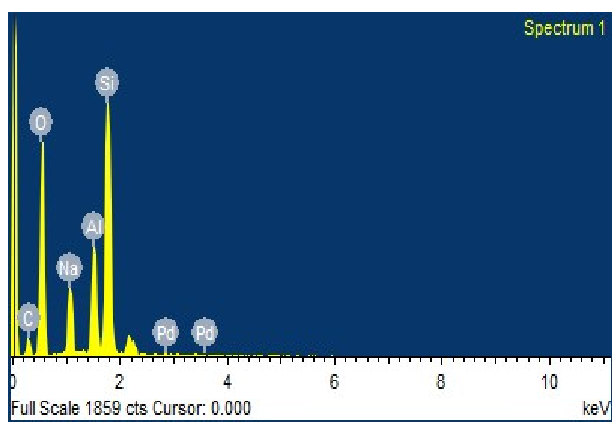


Figure A19: EDX data of PdL1-Y

Element	Weight%	Atomic%
C K	20.07	28.74
O K	46.75	50.25
Al K	7.04	4.48
Si K	20.09	12.30
Pd L	0.51	0.08
Totals	100.00	

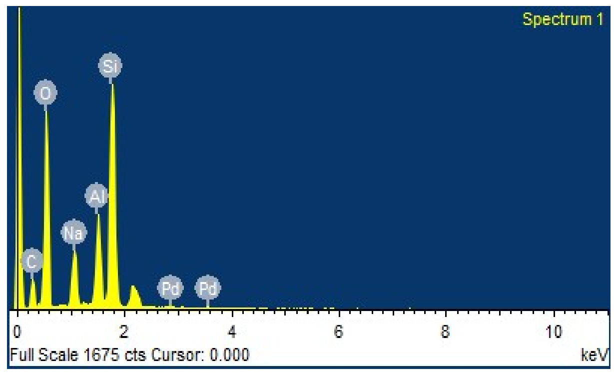


Figure A20: EDX data of PdL3-Y

Element	Weight%	Atomic%
C K	26.67	36.25
O K	46.64	47.59
Al K	5.53	3.34
Si K	16.01	9.31
Pd L	0.27	0.04
Totals	100.00	

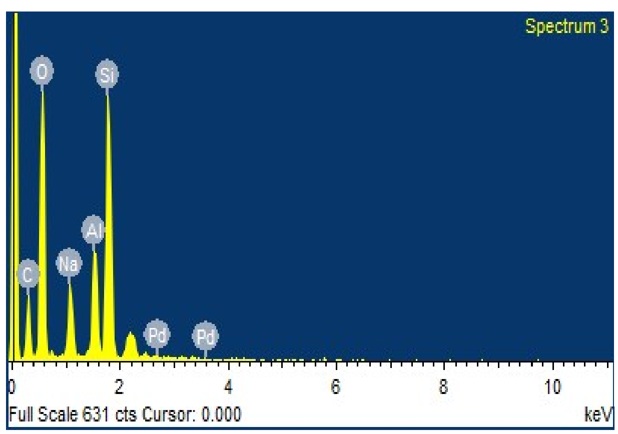


Figure A21: EDX data of PdL4-Y

Element	Weight%	Atomic%
C K	35.96	47.80
O K	35.39	35.32
Al K	10.82	6.40
Si K	13.95	7.93
Pd L	0.27	0.04
Totals	100.00	

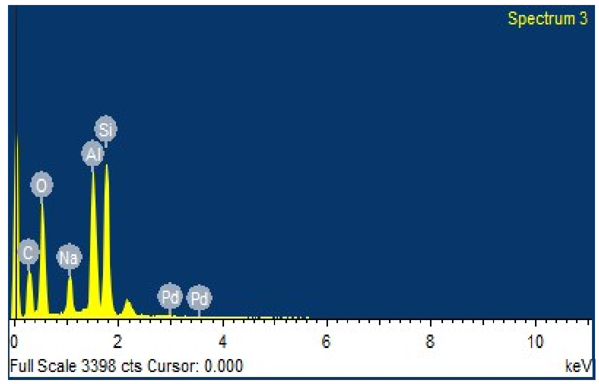


Figure A22: EDX data of PdL5-Y

Element	Weight%	Atomic%
C K	23.26	32.40
O K	47.04	49.18
Al K	6.38	3.96
Si K	17.75	10.57
Pd L	0.26	0.04
Totals	100.00	

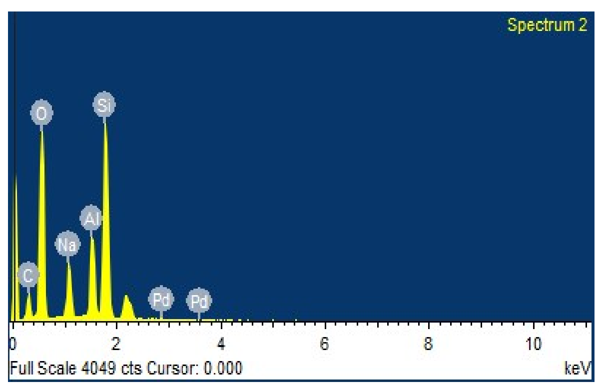


Figure A23: EDX data of PdL6-Y

Element	Weight%	Atomic%
C K	20.14	28.72
O K	47.03	50.35
Al K	6.97	4.43
Si K	19.47	11.87
Pd L	0.22	0.04
Totals	100.00	

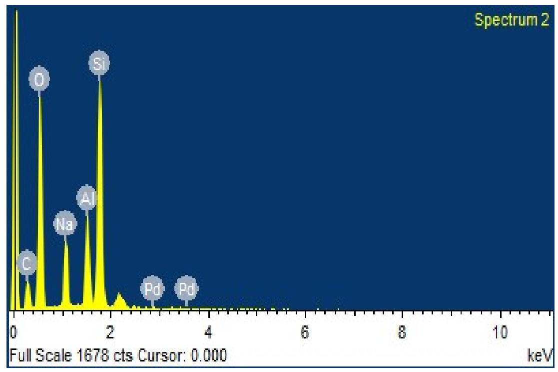
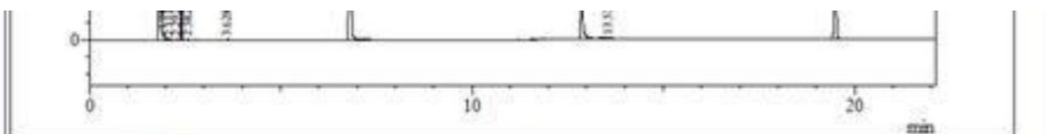
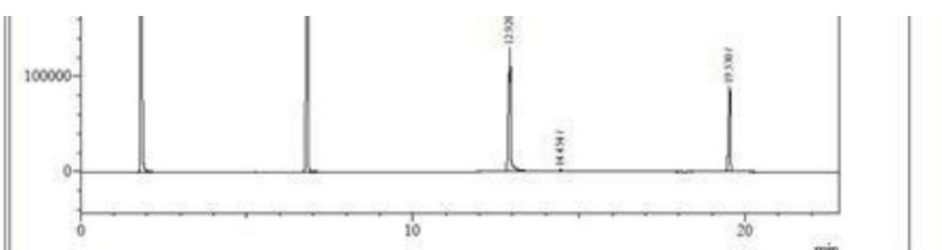


Figure A24: GC chromatogram of pure Zeolite-Y for sulfoxidation reaction



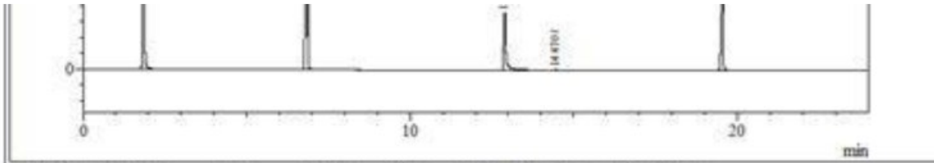
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.837	19635917	14357920	0.000		SV		
2	1.944	4127	3964	0.000		T		
3	2.111	2158	1285	0.000		T		
4	2.292	1451	851	0.000		T		
5	2.398	70977	48330	0.000		T		
6	2.582	1714	1193	0.000		TV		
7	3.628	1235	689	0.000				
8	6.844	1482651	431414	0.000				
9	12.867	246880	57490	0.000				
10	13.574	53956	2658	0.000		V		
11	19.505	296498	78436	0.000		SV		
Total		21797564	14984230					

Figure A25: GC chromatogram of PdL1 for sulfoxidation reaction



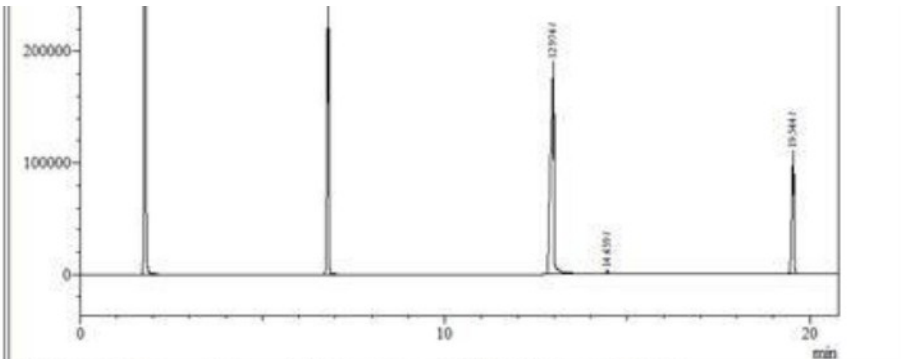
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.819	19493010	13565576	0.000		SV		
2	6.827	1098182	346613	0.000		S		
3	12.920	645601	129562	0.000		S		
4	14.454	9042	2258	0.000		S		
5	19.530	335596	88884	0.000		S		
Total		21581431	14132893					

Figure A26: GC chromatogram of PdL3 for sulfoxidation reaction



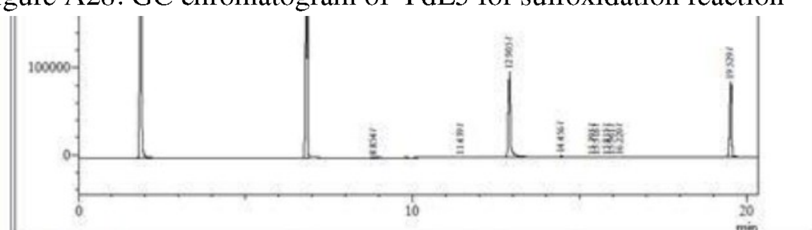
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.832	19747789	13999598	0.000		S		
2	6.848	1553763	433064	0.000		SV		
3	12.896	339016	72378	0.000		SV		
4	14.470	1909	516	0.000				
5	19.549	408704	104071	0.000				
Total		22051181	14609627					

Figure A27: GC chromatogram of PdL4 for sulfoxidation reaction



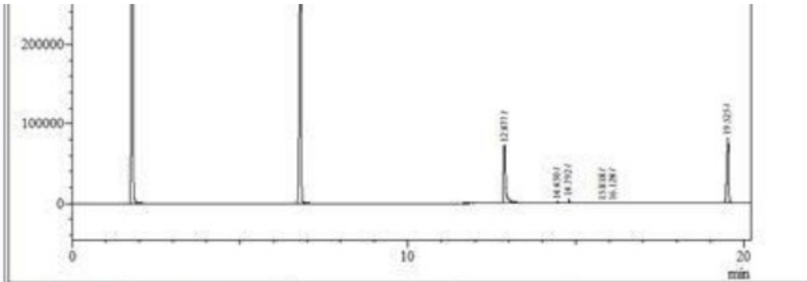
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.774	20249253	13837856	0.000		S		
2	6.805	877467	293773	0.000				
3	12.974	1227490	189257	0.000		S		
4	14.459	12894	3471	0.000				
5	19.544	434971	109936	0.000		S		
Total		22802075	14434293					

Figure A28: GC chromatogram of PdL5 for sulfoxidation reaction



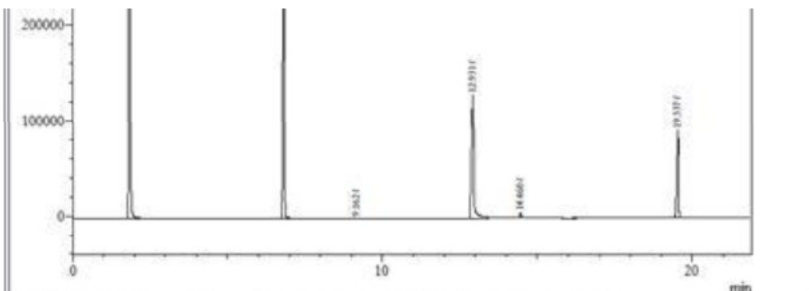
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.851	17979524	12893584	0.000		S		
2	6.837	1084652	334533	0.000				
3	8.854	2359	221	0.000				
4	11.439	1379	206	0.000				
5	12.905	473249	98524	0.000		S		
6	14.456	8341	2195	0.000		S		
7	15.395	1346	202	0.000				
8	15.516	4398	510	0.000		V		
9	15.815	1713	198	0.000		V		
10	15.961	1391	243	0.000		V		
11	16.220	1059	141	0.000		V		
12	19.529	324420	86128	0.000				
Total		19883831	13416685					

Figure A29: GC chromatogram of PdL6 for sulfoxidation reaction



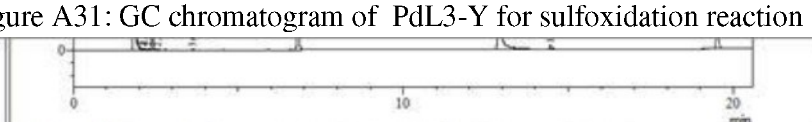
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.777	18309475	13039948	0.000		S		
2	6.810	1215546	370668	0.000				
3	12.877	347221	73038	0.000		S		
4	14.450	6552	1661	0.000				
5	14.792	4670	4641	0.000				
6	15.818	4530	434	0.000				
7	16.128	4033	299	0.000		V		
8	19.525	305206	81238	0.000				
Total		20197233	13571927					

Figure A30: GC chromatogram of PdL1-Y for sulfoxidation reaction



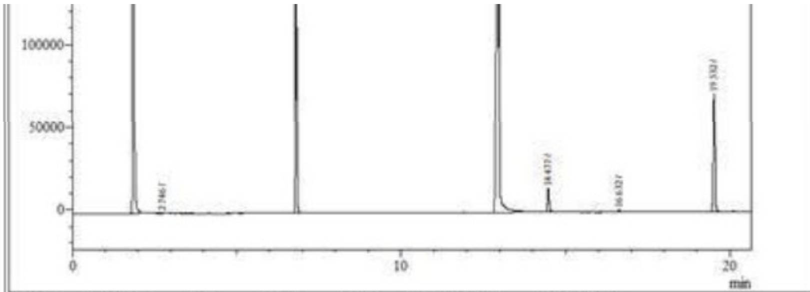
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.830	18278718	12146133	0.000		S		
2	6.829	950607	310596	0.000		S		
3	9.162	1031	178	0.000				
4	12.931	700999	128764	0.000		S		
5	14.460	20047	5226	0.000				
6	19.537	335637	91043	0.000		S		
Total		20287039	12681940					

Figure A31: GC chromatogram of PdL3-Y for sulfoxidation reaction



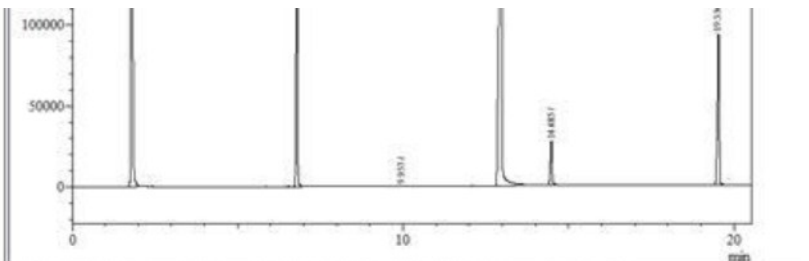
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.839	17894233	12429159	0.000		S		
2	2.114	1872	1214	0.000		T		
3	2.154	1281	680	0.000		TV		
4	2.296	1318	749	0.000		T		
5	2.403	68289	42504	0.000		T		
6	2.588	1350	852	0.000		TV		
7	3.635	1278	597	0.000				
8	6.827	678405	234963	0.000		S		
9	12.957	893741	156003	0.000		S		
10	14.469	11530	3088	0.000				
11	19.539	312566	83704	0.000				
Total		19865863	12953513					

Figure A32: GC chromatogram of PdL4-Y for sulfoxidation reaction



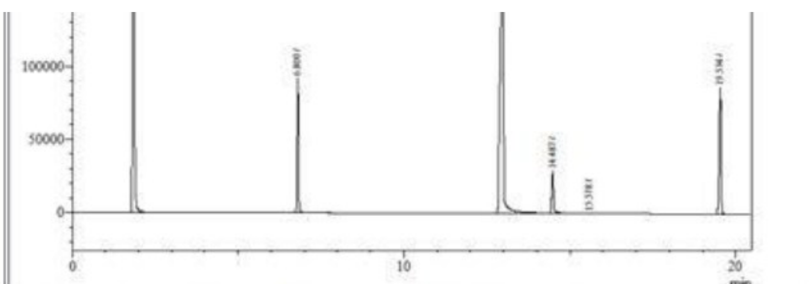
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.849	18682585	12853446	0.000		S		
2	2.746	1610	309	0.000				
3	6.817	425507	158911	0.000				
4	12.978	1128352	178415	0.000		S		
5	14.477	53886	14454	0.000		S		
6	16.632	1250	1267	0.000		V		
7	19.532	268312	71159	0.000		S		
Total		20561502	13277961					

Figure A33: GC chromatogram of PdL5-Y for sulfoxidation reaction



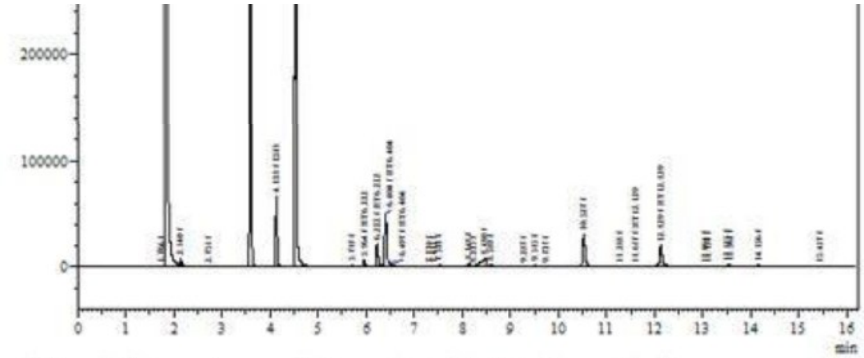
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.784	18902281	12877748	0.000		S		
2	6.793	464222	165740	0.000		S		
3	9.957	1036	115	0.000		V		
4	12.970	1132788	181401	0.000		S		
5	14.485	98440	26749	0.000		S		
6	19.536	353576	92265	0.000		S		
Total		20952343	13344018					

Figure A34: GC chromatogram of PdL6-Y for sulfoxidation reaction



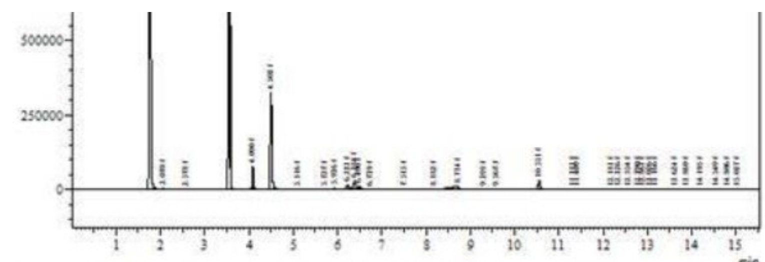
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.832	20412565	13839227	0.000		S		
2	6.800	252077	91544	0.000		S		
3	12.988	1351005	200733	0.000		S		
4	14.487	113850	28976	0.000		S		
5	15.578	1979	210	0.000				
6	19.534	326744	85820	0.000				
Total		22458220	14246510					

Figure A35: GC chromatogram of CuL1 for styrene oxidation reaction



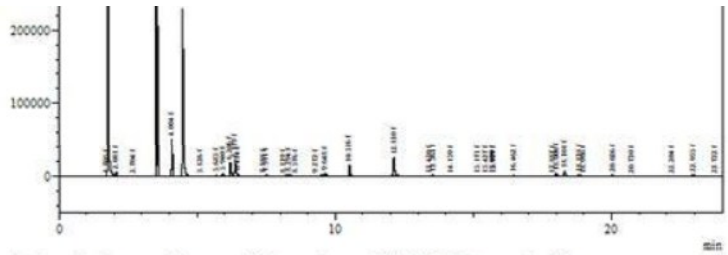
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.766	1361	793	0.000				
2	1.828	14129963	8404433	0.000		SV		
3	2.140	8030	5555	0.000		T		
4	2.751	1504	223	0.000		T		
5	3.593	615704	289650	0.000	ppm		1	styrene
6	4.138	151053	65774	0.000	ppm	S	2	ISD
7	4.538	819836	321539	0.000	ppm	S	3	BZA
8	5.717	3168	1040	0.000				
9	5.964	17753	6002	0.000	ppm	V	4	RT6.232
10	6.232	62032	21512	0.000	ppm		4	RT6.232
11	6.404	161382	50554	0.000	ppm	SV	5	RT6.404
12	6.497	1237	619	0.000	ppm	T	5	RT6.404
13	7.330	1371	236	0.000		V		
14	7.413	1113	264	0.000		V		
15	7.531	5019	1676	0.000		V		
16	8.148	10184	3578	0.000				
17	8.235	2067	730	0.000		V		
18	8.480	54757	6990	0.000		V		
19	8.589	8469	1443	0.000		V		
20	9.287	1609	432	0.000				

Figure A36: GC chromatogram of CuL3 for styrene oxidation reaction



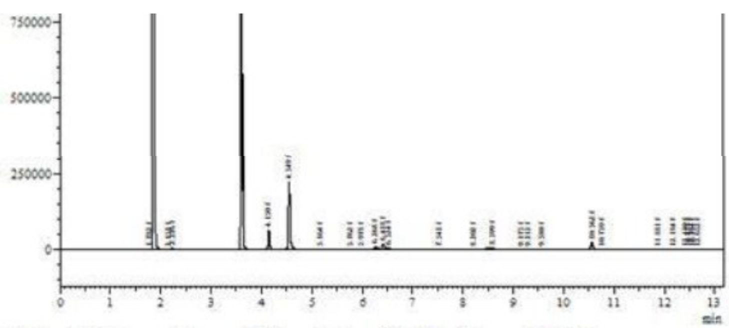
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.757	17316607	12255492	0.000		S		
2	2.070	4151	2967	0.000		T		
3	2.578	1041	221	0.000				
4	3.553	2053877	1020274	0.000		S		
5	4.090	166444	78177	0.000		T		
6	4.503	852307	319888	0.000		S		
7	5.116	5460	1038	0.000		T		
8	5.727	2322	487	0.000		TV		
9	5.936	15081	4147	0.000		TV		
10	6.233	63618	13483	0.000		T		
11	6.384	92209	29376	0.000		TV		
12	6.490	42211	8616	0.000		TV		
13	6.739	2050	335	0.000		TV		
14	7.515	9473	1398	0.000				
15	8.182	5607	1541	0.000				
16	8.714	155942	10684	0.000		SV		
17	9.291	2103	493	0.000		TV		
18	9.567	2731	884	0.000				
19	10.551	103482	29760	0.000		S		
20	11.313	1137	275	0.000		TV		
21	11.409	4864	606	0.000		TV		
22	12.181	2519	683	0.000		V		

Figure A37: GC chromatogram of CuL4 for styrene oxidation reaction



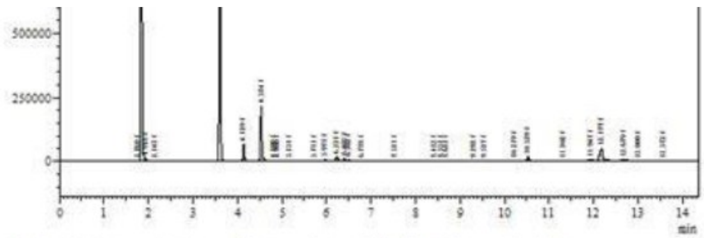
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.705	1174	776	0.000				
2	1.767	11920724	8680267	0.000		SV		
3	2.081	6620	5258	0.000		T		
4	2.704	1156	202	0.000				
5	3.547	713114	389850	0.000		S		
6	4.094	104312	50497	0.000		V		
7	4.493	579681	227169	0.000		S		
8	5.126	1222	235	0.000		T		
9	5.685	4126	1158	0.000				
10	5.940	11139	2890	0.000		V		
11	6.206	60103	18822	0.000				
12	6.379	70459	22353	0.000		V		
13	6.474	15203	3579	0.000		V		
14	7.388	1720	321	0.000				
15	7.511	3822	1158	0.000		V		
16	8.139	1581	534	0.000				
17	8.294	24128	2190	0.000		V		
18	8.576	2665	571	0.000		V		
19	9.272	1077	296	0.000		V		
20	9.648	34128	3085	0.000				
21	10.516	50495	14877	0.000		S		

Figure A38: GC chromatogram of CuL6 for styrene oxidation reaction



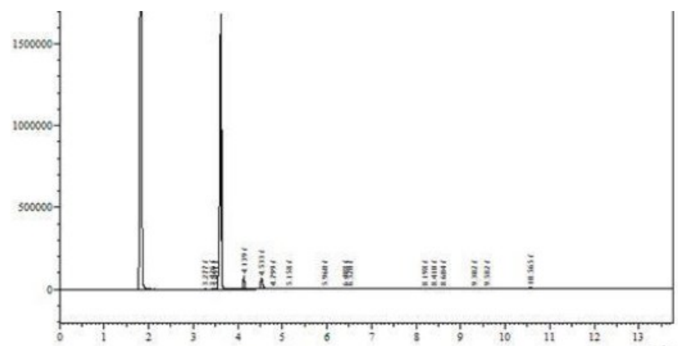
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.782	1530	865	0.000				
2	1.843	13495899	9011038	0.000		SV		
3	2.153	2454	1623	0.000		T		
4	2.236	9436	5694	0.000		T		
5	3.617	1883505	965600	0.000		S		
6	4.150	134280	60941	0.000		T		
7	4.549	576828	222067	0.000		S		
8	5.164	3356	711	0.000		T		
9	5.762	2945	628	0.000				
10	5.978	9565	2613	0.000		V		
11	6.268	46813	9546	0.000				
12	6.418	58241	17613	0.000		V		
13	6.524	34576	6564	0.000		V		
14	7.543	2950	700	0.000				
15	8.202	3655	1042	0.000				
16	8.599	85632	7054	0.000		SV		
17	9.175	1352	180	0.000		T		
18	9.312	1548	405	0.000		TV		
19	9.580	3203	726	0.000		V		
20	10.562	72836	21434	0.000				
21	10.759	5555	643	0.000		V		
22	11.881	1086	315	0.000				

Figure A39: GC chromatogram of CuL1-Y for styrene oxidation reaction



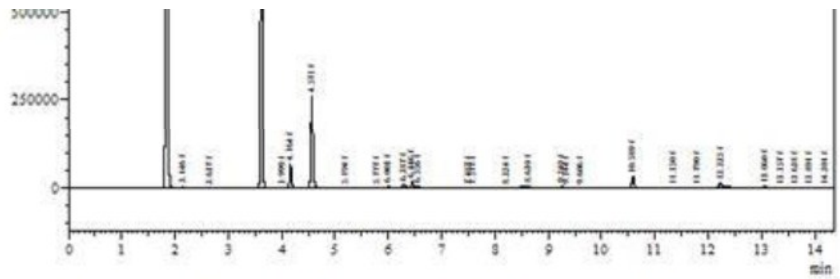
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.769	1592	847	0.000				
2	1.831	15445750	11238239	0.000		SV		
3	1.938	4331	4024	0.000		T		
4	2.143	2510	1839	0.000		T		
5	3.608	2105582	1086192	0.000		T		
6	4.139	141075	67961	0.000		TV		
7	4.534	517242	213873	0.000		T		
8	4.800	2844	747	0.000		TV		
9	4.900	1102	296	0.000		TV		
10	5.151	4652	686	0.000		TV		
11	5.711	2948	826	0.000				
12	5.971	12877	3259	0.000		V		
13	6.231	47329	15169	0.000		V		
14	6.405	28754	9216	0.000		V		
15	6.502	20152	3990	0.000		V		
16	6.778	1230	350	0.000		V		
17	7.531	1801	542	0.000		V		
18	8.412	11240	1257	0.000				
19	8.551	5048	821	0.000		V		
20	8.681	3889	510	0.000		V		
21	9.292	1538	407	0.000				
22	9.537	2796	710	0.000				
23	10.219	4166	1088	0.000		V		
24	10.529	62912	17199	0.000		S		

Figure A40: GC chromatogram of CuL3-Y for styrene oxidation reaction



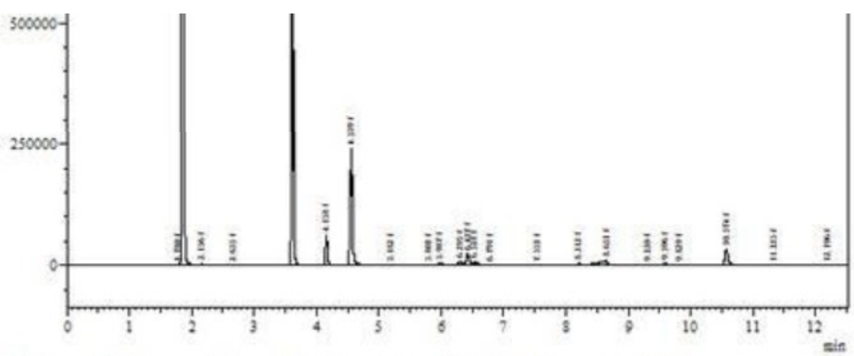
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.819	16372798	11004288	0.000		S		
2	3.277	1364	414	0.000		V		
3	3.426	1476	324	0.000		V		
4	3.491	1135	394	0.000		V		
5	3.617	3878888	1637052	0.000		SV		
6	4.139	180882	79590	0.000		T		
7	4.533	223653	68076	0.000		T		
8	4.799	2381	547	0.000		TV		
9	5.158	1701	331	0.000		TV		
10	5.960	6726	1113	0.000				
11	6.408	16808	3362	0.000				
12	6.520	15362	2547	0.000		V		
13	8.198	4337	1406	0.000				
14	8.410	6106	1125	0.000		V		
15	8.604	2756	371	0.000		V		
16	9.302	1675	521	0.000		V		
17	9.582	2398	672	0.000		V		
18	10.565	41843	10139	0.000				
Total		20762289	12812272					

Figure A41: GC chromatogram of CuL4-Y for styrene oxidation reaction



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.832	16192032	10453821	0.000		S		
2	2.146	4225	2816	0.000		T		
3	2.637	2116	451	0.000				
4	3.627	1965649	952613	0.000				
5	3.999	1314	292	0.000		V		
6	4.164	153936	66918	0.000		SV		
7	4.571	715461	260046	0.000		SV		
8	5.194	3194	685	0.000		T		
9	5.777	2697	643	0.000		V		
10	6.003	13472	3543	0.000		V		
11	6.287	39745	10408	0.000		V		
12	6.446	62217	19840	0.000		V		
13	6.556	26604	5953	0.000		SV		
14	7.487	2622	456	0.000				
15	7.577	3352	760	0.000		V		
16	8.224	5258	1622	0.000		V		
17	8.630	84214	7402	0.000		SV		
18	9.249	12713	5065	0.000		V		
19	9.344	3012	567	0.000		V		
20	9.606	5121	1449	0.000		V		
21	10.589	99008	31216	0.000		S		
22	11.350	1866	429	0.000		V		

Figure A42: GC chromatogram of CuL6-Y for styrene oxidation reaction



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.780	2751	1788	0.000				
2	1.845	13111006	8981850	0.000		SV		
3	2.156	3232	2131	0.000		T		
4	2.655	1447	266	0.000				
5	3.619	1370957	705111	0.000				
6	4.158	134975	60510	0.000		S		
7	4.559	630471	238639	0.000		S		
8	5.182	4072	892	0.000		T		
9	5.803	4191	607	0.000		V		
10	5.987	17616	4769	0.000		V		
11	6.295	34377	6537	0.000				
12	6.427	75388	22788	0.000		V		
13	6.538	30089	4975	0.000		V		

Figure A43: EDX data of Co-Y

Element	Weight%	Atomic%
O K	50.97	63.93
Na K	7.65	6.68
Al K	10.14	7.54
Si K	29.97	21.41
Co K	1.28	0.44
Totals	100.00	

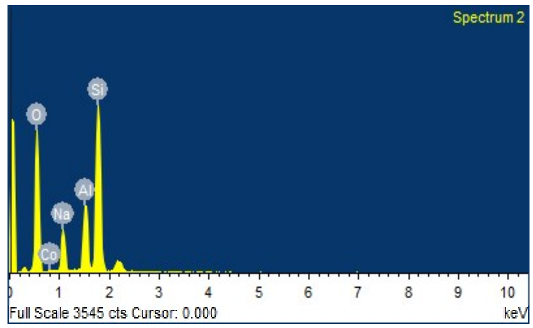


Figure A44: EDX data of CoL1-Y

```
Spectrum: c1

Element     Series   unn. C norm. C Atom. C Error
                     [wt.%]  [wt.%]  [at.%]   [%]
-------------------------------------------------
Cobalt     K-series    0.35    0.35    0.10   0.0
Aluminium  K-series    4.10    4.10    2.48   0.2
Silicon    K-series    9.12    9.12    5.29   0.4
Oxygen     K-series   70.59   70.59   71.85  21.8
Carbon     K-series    9.74    9.74   13.20   3.5
Nitrogen   K-series    6.10    6.10    7.09   2.4
-------------------------------------------------
            Total:  100.00  100.00  100.00
```

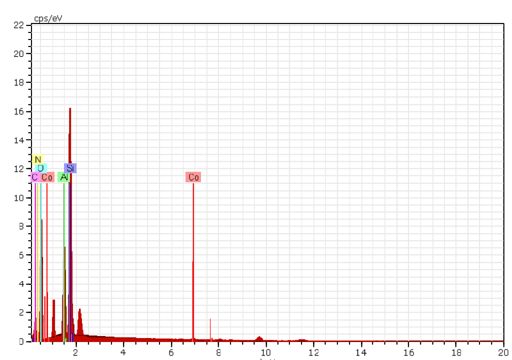


Figure A45: EDX data of CoL2-Y

Spectrum: c2_1

Element	Series	unn. C [wt.-%]	norm. C [wt.-%]	Atom. C [at.-%]	Error [%]
Carbon	K-series	23.13	23.13	29.15	7.3
Nitrogen	K-series	10.43	10.43	11.27	3.5
Aluminium	K-series	2.28	2.28	1.28	0.1
Silicon	K-series	5.34	5.34	2.88	0.3
Cobalt	K-series	0.31	0.31	0.08	0.0
Oxygen	K-series	58.51	58.51	55.35	17.9
	Total:	100.00	100.00	100.00	

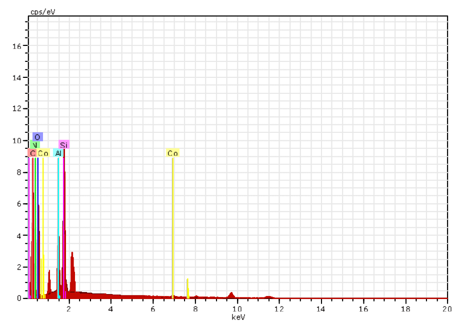


Figure A46: EDX data of CoL3-Y

Element	Weight%	Atomic%
C K	31.16	42.23
O K	40.82	41.55
Na K	0.51	0.36
Al K	2.80	1.69
Si K	24.19	4.20
Co K	0.52	0.14
Totals	100.00	

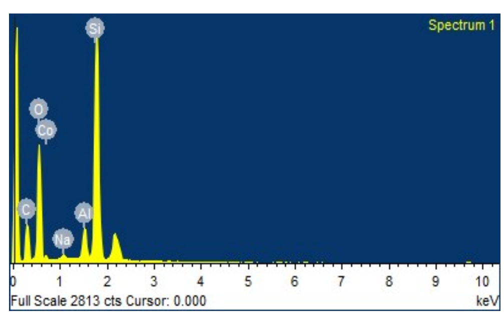


Figure A47: EDX data of CoL4-Y

Spectrum: c4_1

Element	Series	unn. C [wt.-%]	norm. C [wt.-%]	Atom. C [at.-%]	Error [%]
Carbon	K-series	10.97	10.97	14.70	3.9
Nitrogen	K-series	9.07	9.07	10.42	3.3
Aluminium	K-series	6.05	6.05	3.61	0.3
Silicon	K-series	6.40	6.40	3.67	0.3
Cobalt	K-series	0.37	0.37	0.10	0.0
Oxygen	K-series	67.12	67.13	67.50	20.7
	Total:	100.00	100.00	100.00	

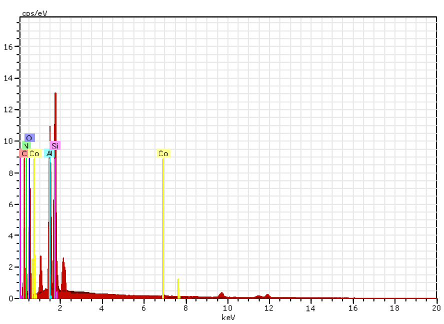


Figure A48: EDX data of CoL5-Y

Element	Weight%	Atomic%
C K	50.46	61.63
O K	31.86	29.21
Al K	2.94	1.60
Si K	14.25	4.10
Co K	0.49	0.12
Totals	100.00	

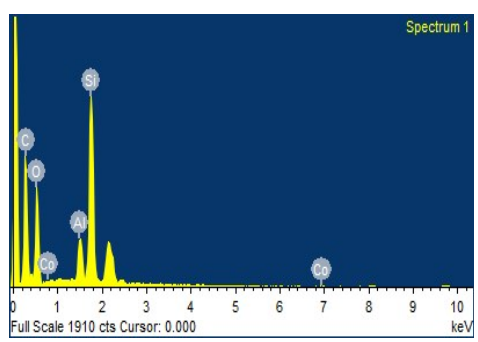
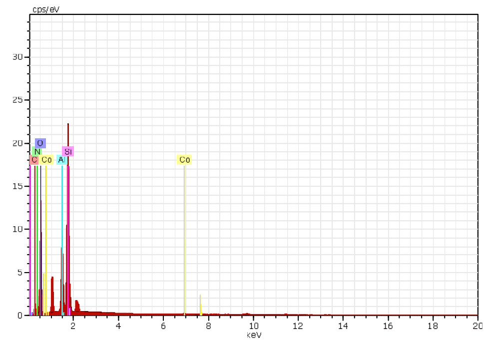


Figure A49: EDX data of CoL6-Y

Spectrum: c6_1

Element	Series	unn. C [wt.-%]	norm. C [wt.-%]	Atom. C [at.-%]	Error [%]
Carbon	K-series	4.62	4.62	6.53	2.3
Nitrogen	K-series	7.11	7.11	8.62	3.0
Aluminium	K-series	5.88	5.88	3.70	0.3
Silicon	K-series	12.84	12.84	7.77	0.6
Cobalt	K-series	0.61	0.61	0.17	0.0
Oxygen	K-series	68.94	68.95	73.20	21.6
	Total:	100.00	100.00	100.00	



LIST OF PUBLICATIONS

1. **Choudhary, A.**; Das, B.; Ray, S., "Encapsulation of a Ni salen complex in zeolite Y: an experimental and DFT study". ***Dalton Trans***. 2015, *44* (8), 3753-3763.

2. **Choudhary, A.**; Das, B.; Ray, S., "Enhanced catalytic activity and magnetization of encapsulated nickel Schiff-base complexes in zeolite-Y: a correlation with the adopted non-planar geometry". ***Dalton Trans***. 2016, 45, 18967-18976

3. **Choudhary, A**.; Das, B.; Ray, S., "Encapsulated Schiff Base Nickel Complex in Zeolite Y: Correlation Between Catalytic Activities and Extent of Distortion Supported by Experimental and DFT Studies". ***Inorg. Chim. Acta.*** 2017, 462, 256-265.

4. **Choudhary, A**.; Kumari, S.; Ray, S., "Tuning of Catalytic Property Controlled by the Molecular Dimension of Palladium–Schiff Base Complexes Encapsulated in Zeolite Y" ***ACS Omega,*** 2017, *2* (10), 6636–6645

5. **Choudhary, A**.; Kumari, S.; Ray, S., "The Functionality of the Hybrid Systems Driven by Molecular Dimension of the Guest Copper Schiff-Base Complexes Entrapped in Zeolite-Y" **(Submitted)**

6. **Choudhary, A**.; Kumari, S.; Ray, S.,"Cobalt Schiff-base Complexes Encapsulated in Zeolite Y and their Catalytic Activity for the dye degradation. "(**manuscript under preparation)**

LIST OF PAPER PRESENTED IN SYMPOSIUM AND CONFERANCES

(1) **Choudhary, A**.; Ray, S "Encapsulation of metal Complex in Zeolite" Organized by Department of Chemistry at Birla Institute of Technology and Science, Pilani Campus, Pilani. (26th March, **2011**)

(2) **Choudhary, A**.; Das, B.; Ray, S "Design and Synthesis of Nanostructral Heterogeneous catalyst And Characterization" Organized by IIT Bombay.(5-8th may 2012, **Won best oral presentation award)**

(3) **Choudhary, A**.; Das, B.; Ray, S "Study of Host – Guest systems prepared by "Ship in Bottle complexes" synthesis and its Characterization" Organized by Department of Chemistry at Birla Institute of Technology and Science, Pilani Campus, Pilani. (March. 2013)

(4) **Choudhary, A**.; Das, B.; Ray, S "Spectroscopic and Magnetic Studies of 'Ship-in-a-Bottle' Ni(II) Schiff base Complexes in Zeolite Y" at Department of Chemistry, Mohanlal Sukhadia University, Udaipur. (2nd – 5th March, 2013).

(5) **Choudhary, A**.; Das, B.; Ray, S "Experimental and Theoretical studies of 'Ship-in-a-Bottle' Ni(II) Schiff base Complexes in Zeolite Y" at BITS Pilani department of Physics, (March, 2014)

(6) **Choudhary, A**.; Das, B.; Ray, S "Experimental and Theoretical Evidence for Encapsulation Ni Salen complex in Zeolite Y" A National Conference on NANO- And FUNCTIONAL MATERIALS, Organized by Department of Chemistry at Birla Institute of Technology and Science, Pilani Campus, Pilani. (7 – 8th November, 2014).

(7) **Choudhary, A**.; Das, B.; Ray, S "Effect of Host Supercage on the Encapsulated Complexes in Zeolite Y: Experimental and DFT Study" at national conference "FACSI-15", at on university of Rajasthan, Jaipur. (13-14th March)

(8) **Choudhary, A**.; Das, B.; Ray, S "Effect of Encapsulation on the Optical, Magnetic and catalytic properties of the square planar nickel Schiff-base in zeolite Y." at International conference on Nascent Developments in Chemical Sciences, Organized by Department

of Chemistry at Birla Institute of Technology and Science, Pilani Campus, Pilani. (16th – 18th October, **2015**).

(9) **Choudhary, A**.; Das, B.; Ray, S "Encapsulated Schiff Base Nickel Complexes in Zeolite Y: Correlation between Catalytic Activities and Extent of Distortion Supported by Experimental and DFT Studies" at National Conference on New Frontiers in Chemistry - From Fundamentals to Applications, (NFCFA-2015), Department of Chemistry, BITS Pilani K.K. Birla Goa Campus. (18-19 December. 2015.)

(10) **Choudhary, A**.; Kumari, S.; Ray, S "The Synthesis and Characterization of Heterogeneous Catalyst and its Application for the Rhodamine B Degradation" at International conference on Recent Trends in Chemical Sciences (ICRCS-2017), Govt engineering college, Bikaner. (12-13 January, 2017)

- **Workshops**

(1) Workshop on Advanced Characterization Techniques MR-12 (held in IIT Bombay in May, 2012).

(2) Workshop on Analytical Instruments for Chemical & Environmental Engineers – WAICEE-2013 held in BITS Pilani.

BRIEF BIOGRAPHY OF THE SUPERVISOR

Prof. Saumi Ray, Associate Professor, Department of Chemistry, Birla Institute Technology and Science, Pilani (BITS Pilani), Pilani Campus, has around 12 years of teaching and research experience. Her current research interests are in the field of Material Chemistry and Computational Fluid Dynamics. She completed her B.Sc. from Bethune College, University of Calcutta (1991) and M.Sc. from Department of Chemistry, University of Calcutta (1993). She received her Ph.D. degree from Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India (2003) under the supervision of Prof. S. Vasudevan. During her doctoral studies she worked on zeolites with a detailed understanding of 'Host-guest' Chemistry and Molecular Recognitions, ultimately leading to design and synthesize advanced materials for different practical purposes like catalysis, separation, molecular sensing. **Prof. Saumi Ray** has joined BITS Pilani in 2005 and has supervised a Ph.D student (Dr. Priya C Sande) under the field of Computational Fluid Dynamics. She is currently supervising two Ph.D students, as a result of her research accomplishment she has published research papers in peer reviewed journals, presented papers and delivered lectures in national and international conferences. She has successfully completed one research project as PI.

BRIEF BIOGRAPHY OF THE CANDIDATE

Ms Archana Choudhary completed her B.Sc. from IMGVSN College, Pilani, University of Rajasthan, Jaipur, India (2001-2004) and M.Sc. from Department of Chemistry, Banasthali Vidyapeeth , Banasthali, India (2004-2006).

Further she completed her M. Phil in Chemistry from Dept of Chemistry, Dungar College Bikaner, University of Bikaner, India (2007-2008) under the supervision of **Prof. Ravi Shankar Verma**. She has published one national journal during the M. Phil course.

She has qualified NET (LS) in chemical sciences in June, 2010. In January 2011, she joined the Department of Chemistry, BITS Pilani for her doctoral research under the supervision of **Prof. Saumi Ray**. During her doctoral studies, she joined as DST-JRF fellow in DST-FAST TRACK project. Currently she has published four research articles in well renowned international journals and her two more publications are in pipeline. She has presented papers in ten conferences/symposiums and attended two workshops. Her research interest lies in designing of zeolite encapsulated heterogeneous systems to obtain better tunable reactivity with advantages of the robustness of host so that they can play a vital role in the field of catalysis field.