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APPENDICES

Appendix A Calibration of sulfur compounds and sample of calculation.

A1 Calibration of sulfur compounds

From

$$n_i * RMR_i = A_i$$

$$n_{std} * RMR_{std} = A_{std}$$

$$\text{So, } RMR_i = \frac{A_i * n_{std} (RMR_{std})}{A_{std} * n_i}$$

$$Y_i = \frac{A_i / RMR_i}{\sum_{i=1}^n [A_i / RMR_i]}$$

Give $RMR_{std} = 1$

A_i = Peak area of component i

n_i = Concentration of component i (weight basis)

A_{std} = Peak area of standard component

n_{std} = Concentration of standard component (weight basis)

RMR_i = Respond factor of component i

RMR_{std} = Respond factor of standard component

Y_i = Concentration of component i from calibration

A2 Sample of calculation

A2.1 Calculation of adsorption amount of sulfur compound on zeolite

$$A = \frac{F * C_i}{100} - \left[\frac{C_f}{100} * \frac{F * (100 - C_i)}{(100 - C_f)} \right]$$

A = amount of sulfur compound adsorbed on zeolite (g)

C_i = sulfur concentration before adsorption (%)

C_f = sulfur concentration after adsorption (%)

F = amount of solution before adsorption (g)

Example: Adsorption of dibenzothiophene in decane on NaY zeolite at room temperature

A2.1.1 To convert concentration of sulfur compound before and after adsorption from ppm to percent

$$C_i = 2002 \text{ ppm} = 2002/10000 = 0.2002 \text{ percent}$$

$$C_f = 285 \text{ ppm} = 285/10000 = 0.0285 \text{ percent}$$

A2.1.2 To calculate the amount dibenzothiophene adsorbed on NaY zeolite

From, F = 34.24 g

So,

$$A = \frac{34.24 * 0.2002}{100} - \left[\frac{0.0285}{100} * \frac{34.24 * (100 - 0.2002)}{(100 - 0.0285)} \right] = 0.0588 \text{ g}$$

A2.1.3 To convert the amount of dibenzothiophene adsorbed on NaY zeolite to millimole

Molecular weight of dibenzothiophene = 184.26 mol/g

$$A = 0.0588 \text{ g} = (0.0588/184.26) * 1000 = 0.3191 \text{ millimole}$$

A2.1.4 To divide the amount adsorbed dibenzothiophene on zeolite with the amount of zeolite

From, NaY zeolite = 0.3941 g

So,

The amount of dibenzothiophene adsorbed on NaY zeolite

$$= 0.3191/0.3941$$

$$= 0.809 \text{ mmol/g}$$

Appendix B Experimental data.

Table B1 Calibration table of 3-methylthiophene in isooctane

No	Concentration of 3-methylthiophene (ppm)	%Area	A_i/A_{std}	n_{std}/n_i	RMR _i	Av.	SD.	All	
								Av.	SD.
1	1031.55000	0.06624	0.00066	968.41496	0.64190	0.64158	0.00040	0.62325	0.02436
		0.06622	0.00066	968.41496	0.64171				
		0.06616	0.00066	968.41496	0.64113				
2	1579.64000	0.09451	0.00095	632.05563	0.59792	0.59750	0.00079		
		0.09452	0.00095	632.05563	0.59798				
		0.09430	0.00094	632.05563	0.59659				
3	2164.68000	0.13621	0.00136	460.96205	0.62873	0.62822	0.00059		
		0.13596	0.00136	460.96205	0.62758				
		0.13613	0.00136	460.96205	0.62836				
4	1503.57000	0.09118	0.00091	664.08377	0.60606	0.60642	0.00041		
		0.09130	0.00091	664.08377	0.60686				
		0.09122	0.00091	664.08377	0.60633				
5	2708.50000	0.16238	0.00163	368.20805	0.59887	0.60099	0.00300		
		0.16353	0.00164	368.20805	0.60312				
6	203.34000	0.01358	0.00014	4916.87155	0.66780	0.66518	0.00516		
		0.01338	0.00013	4916.87155	0.65797				
		0.01362	0.00014	4916.87155	0.66977				
7	469.23000	0.02784	0.00028	2130.15103	0.59320	0.62288	0.00235		
		0.02764	0.00028	2130.15103	0.58894				
		0.02766	0.00028	2130.15103	0.58936				

Table B2 Calibration table of benzothiophene in isooctane

No	Concentration of Benzothiophene (ppm)	%Area	A _i /A _{std}	n _{std} /n _i	RMR _i	Av.	SD.	All	
								Av.	SD.
1	1187.45	0.09490	0.00095	841.14072	0.79900	0.80291	0.00706	0.81278	0.00940
		0.09486	0.00095	841.14072	0.79866				
		0.09633	0.00096	841.14072	0.81105				
2	2147.94	0.17535	0.00176	464.56235	0.81604	0.82202	0.00662		
		0.17639	0.00177	464.56235	0.82089				
		0.17816	0.00178	464.56235	0.82914				
3	3178.23	0.26089	0.00262	313.64054	0.82040	0.81312	0.00630		
		0.25735	0.00258	313.64054	0.80924				
		0.25751	0.00258	313.64054	0.80974				
4	1029.58	0.08378	0.00084	970.26984	0.81357	0.80603	0.00730		
		0.08295	0.00083	970.26984	0.80551				
		0.08228	0.00082	970.26984	0.79900				
5	2109.70	0.17129	0.00172	473.00104	0.81159	0.81069	0.00225		
		0.17145	0.00172	473.00104	0.81235				
		0.17056	0.00171	473.00104	0.80813				
6	470.00	0.03898	0.00039	2126.65957	0.82930	0.82866	0.01055		
		0.03844	0.00038	2126.65957	0.81780				
		0.03943	0.00039	2126.65957	0.83887				
7	3021.27	0.24319	0.00244	329.98664	0.80445	0.80606	0.00929		
		0.24669	0.00247	329.98664	0.81606				
		0.24115	0.00242	329.98664	0.79769				
8	522.83	0.04127	0.00041	1911.66760	0.78927	0.80030	0.01019		
		0.04195	0.00042	1911.66760	0.80228				
		0.04232	0.00042	1911.66760	0.80936				

Table B3 Calibration table of dibenzothiophene in decane

No	Concentration of Dibenzothiophene (ppm)	%Area	A_i/A_{std}	n_{std}/n_i	RMR_i	Av.	SD.	All	
								Av.	SD.
1	1877.65	0.15776	0.00158	531.58062	0.83995	0.84007	0.00013	0.83854	0.00248
		0.15778	0.00158	531.58062	0.84005				
		0.15781	0.00158	531.58062	0.84021				
2	3372.25	0.28166	0.00282	295.53792	0.83476	0.83494	0.00105		
		0.28210	0.00283	295.53792	0.83607				
		0.28140	0.00282	295.53792	0.83399				
3	1091.84	0.09159	0.00092	914.88511	0.83871	0.83886	0.00014		
		0.09162	0.00092	914.88511	0.83899				
		0.09161	0.00092	914.88511	0.83889				
4	490.35	0.04122	0.00041	2038.35964	0.84056	0.84029	0.00047		
		0.04118	0.00041	2038.35964	0.83974				
		0.04122	0.00041	2038.35964	0.84056				

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Table B4 Adsorption isotherm of 3-methylthiophene in isooctane at 25 degree cetrigrade and fuel to adsorbent weight ratio 85

Zeolite	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
NaX	798	0.13	358	0.16	33.63	0.4028	0.374
NaX	991	0.10	453	0.13	33.68	0.3970	0.466
NaX	1493	0.07	791	0.15	33.14	0.4039	0.587
NaX	1928	0.18	1021	0.11	33.55	0.4092	0.759
NaX	2312	0.25	1368	0.04	34.03	0.4009	0.818
NaX	2926	0.04	1740	0.06	34.05	0.4054	1.017

Zeolite	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
NaY	520	0.73	229	0.44	34.22	0.3922	0.259
NaY	996	0.10	528	0.19	33.61	0.3937	0.407
NaY	1529	0.14	853	0.54	33.75	0.3932	0.593
NaY	2013	0.33	1196	0.08	34.21	0.3974	0.718
NaY	2517	0.32	1525	0.08	33.85	0.4082	0.840
NaY	3006	0.08	1921	0.08	33.23	0.4005	0.920

Table B5 Adsorption isotherm of benzothiophene in isooctane at 25 degree cetrigrade and fuel to adsorbent weight ratio 85

Zeolite	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
NaX	1135	0.98	125	1.21	33.1	0.3939	0.632
NaX	1506	0.56	229	1.13	34.67	0.3954	0.834
NaX	1953	0.65	409	1.27	34.09	0.3982	0.985
NaX	2469	0.50	739	0.86	33.70	0.4056	1.074
NaX	2915	0.33	1113	0.05	33.00	0.3968	1.118
NaX	3474	0.38	1702	0.55	33.51	0.3975	1.114

Zeolite	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
NaY	1055	0.46	185	0.82	33.8	0.3948	0.555
NaY	1499	0.53	303	0.50	33.74	0.3943	0.766
NaY	1990	1.33	573	0.53	34.46	0.3988	0.912
NaY	2506	0.52	946	0.84	33.27	0.3927	0.983
NaY	2891	0.64	1192	0.05	33.08	0.3936	1.065
NaY	3438	0.29	1711	0.33	33.16	0.3947	1.083

Table B6 Adsorption isotherm of dibenzothiophene in decane at 25 degree cetrigrade and fuel to adsorbent weight ratio 85

Zeolite	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
NaX	1113	0.05	90	0.00	34.84	0.3978	0.486
NaX	1493	0.03	156	0.00	34.40	0.3971	0.629
NaX	1985	0.05	270	0.37	34.31	0.3970	0.806
NaX	2479	0.02	470	0.00	34.48	0.3956	0.951
NaX	2971	0.03	831	0.06	34.80	0.3985	1.015
NaX	3582	0.02	1263	0.00	34.29	0.3980	1.060

Zeolite	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
NaY	1003	0.20	82	0.00	34.24	0.3961	0.432
NaY	1488	0.20	158	0.36	34.51	0.3968	0.628
NaY	2002	0.07	285	0.20	34.24	0.3941	0.809
NaY	2497	0.10	525	0.11	34.60	0.3972	0.933
NaY	3019	0.05	841	0.18	34.38	0.3951	1.020
NaY	3506	0.06	1259	0.12	34.40	0.3981	1.055

Table B7 Effect of temperature on 3-methylthiophene adsorption at fuel to adsorbent weight ratio 85

Zeolite	Temperature (degree centigrade)	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaX	25	3000	-	1822	-	-	-	0.99
NaX	50	2976	0.05	2189	0.30	33.93	0.3973	0.687
NaX	80	3016	0.15	2445	0.29	33.78	0.3978	0.496

Zeolite	Temperature (degree centigrade)	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaY	25	3000	-	1903	-	-	-	0.917
NaY	50	3040	0.07	2259	0.14	33.91	0.3987	0.684
NaY	80	2990	0.12	2419	0.13	33.81	0.3989	0.495

*: The adsorbed amount is calculated from adsorption isotherm at 25 degree centigrade

Table B8 Effect of temperature on benzothiophene adsorption at fuel to adsorbent weight ratio 85

Zeolite	Temperature (degree centigrade)	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaX	25	3000	-	1157	-	-	-	1.113
NaX	50	3039	0.20	1540	0.06	34.46	0.4020	0.958
NaX	80	3040	0.01	1655	0.372	34.49	0.4052	0.883

Zeolite	Temperature (degree centigrade)	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaY	25	3000	-	1302	-	-	-	1.05
NaY	50	2984	0.15	1481	0.06	34.49	0.4022	0.960
NaY	80	3038	0.23	1636	0.05	34.29	0.4039	0.888

*: The adsorbed amount is calculated from adsorption isotherm at 25 degree centigrade

Table B9 Effect of temperature on dibenzothiophene adsorption at fuel to adsorbent weight ratio 85

Zeolite	Temperature (degree centigrade)	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaX	25	3000	-	747	-	-	-	1.01
NaX	50	2981	0.08	974	0.83	34.75	0.4088	0.927
NaX	80	3026	0.39	1161	0.13	34.34	0.4035	0.862

Zeolite	Temperature (degree centigrade)	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaY	25	3000	-	916	-	-	-	1.02
NaY	50	3013	0.03	987	0.23	33.73	0.3980	0.932
NaY	80	2992	0.15	1127	0.22	33.78	0.3991	0.858

*: The adsorbed amount is calculated from adsorption isotherm at 25 degree centigrade

Table B10 Effect of fuel to adsorbent weight ratio on 3-methylthiophene adsorption at 25 degree centigrade

Zeolite	Fuel to adsorbent Weight ratio	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaX	85	3000	-	1822	-	-	-	0.99
NaX	40	2999	0.17	935	0.15	33.90	0.8431	0.845
NaX	20	2989	0.16	411	0.00	33.89	1.6952	0.526

Zeolite	Fuel to adsorbent Weight ratio	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaY	85	3000	-	1903	-	-	-	0.917
NaY	40	3009	0.17	1062	0.15	33.95	0.8510	0.793
NaY	20	3012	0.44	416	0.77	34.00	1.7003	0.529

*: The adsorbed amount is calculated from adsorption isotherm at fuel to adsorbent weight ratio 85

Table B11 Effect of fuel to adsorbent weight ratio on benzothiophene adsorption at 25 degree centigrade

Zeolite	Fuel to adsorbent Weight ratio	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaX	85	3000	-	1157	-	-	-	1.113
NaX	40	3036	0.46	337	1.63	34.38	0.8596	0.804
NaX	20	3021	0.44	53	5.72	34.19	1.7091	0.442

Zeolite	Fuel to adsorbent Weight ratio	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaY	85	3000	-	1302	-	-	-	1.05
NaY	40	2984	0.28	344	0.21	34.50	0.8632	0.786
NaY	20	3000	0.09	50	2.00	34.65	1.7341	0.439

*: The adsorbed amount is calculated from adsorption isotherm at fuel to adsorbent weight ratio 85

Table B12 Effect of fuel to adsorbent weight ratio on dibenzothiophene adsorption at 25 degree centigrade

Zeolite	Fuel to adsorbent Weight ratio	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaX	85	3000	-	747	-	-	-	1.01
NaX	40	3012	0.10	106	0.00	34.36	0.8610	0.629
NaX	20	3021	0.17	30	4.71	33.44	1.6715	0.324

Zeolite	Fuel to adsorbent Weight ratio	Initial Concentration(ppmw)	%RSD	Final Concentration(ppmw)	%RSD	Solution Amount(g)	Adsorbent Amount(g)	Adsorbed Amount(mmol/g)
*NaY	85	3000	-	916	-	-	-	1.02
NaY	40	3019	0.62	117	1.97	33.63	0.8413	0.629
NaY	20	3040	0.10	29	2.48	33.40	1.7217	0.326

*: The adsorbed amount is calculated from adsorption isotherm at fuel to adsorbent weight ratio 85

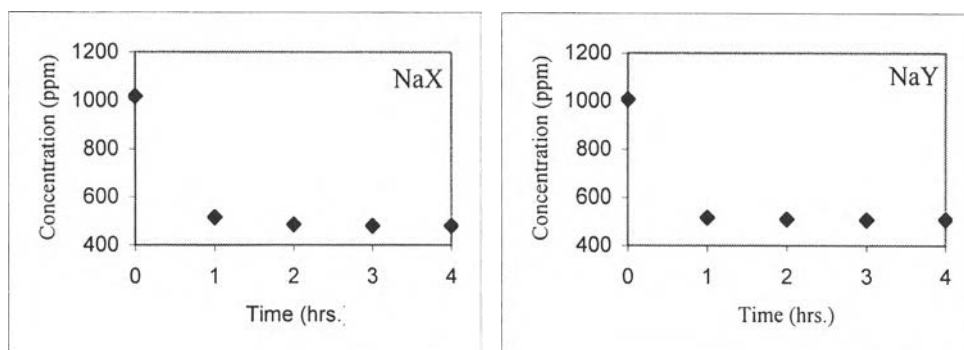


Figure B1 Adsorption of 3-methylthiophene in isooctane on zeolites.

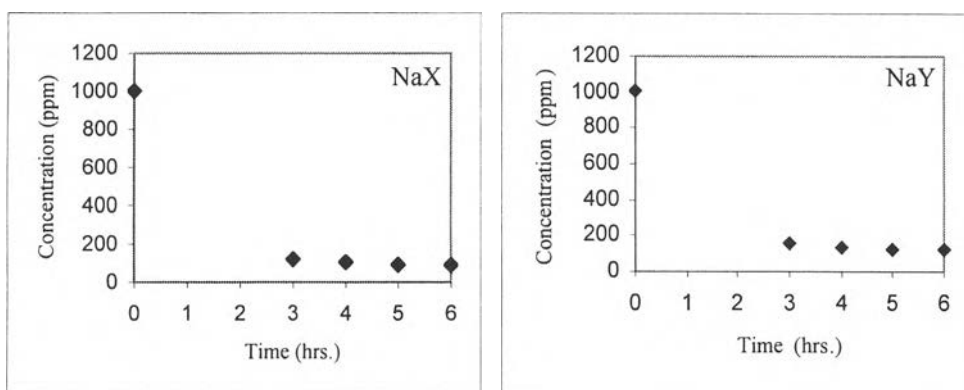


Figure B2 Adsorption of benzothiophene in isooctane on zeolites.

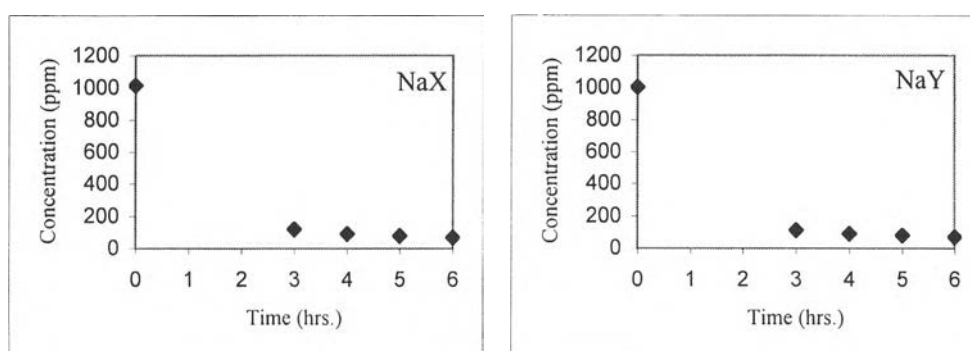


Figure B3 Adsorption of dibenzothiophene in decane on zeolites.

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