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APPENDIX A

Proton NMR Chemical Shifts

Proton NMR chemical shifts

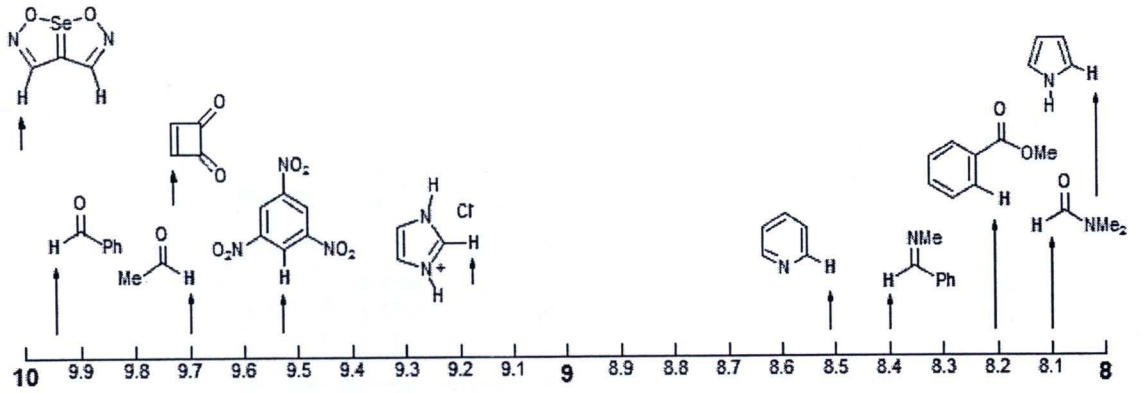


Figure A.1 Proton NMR chemical shifts range 8 – 10 ppm

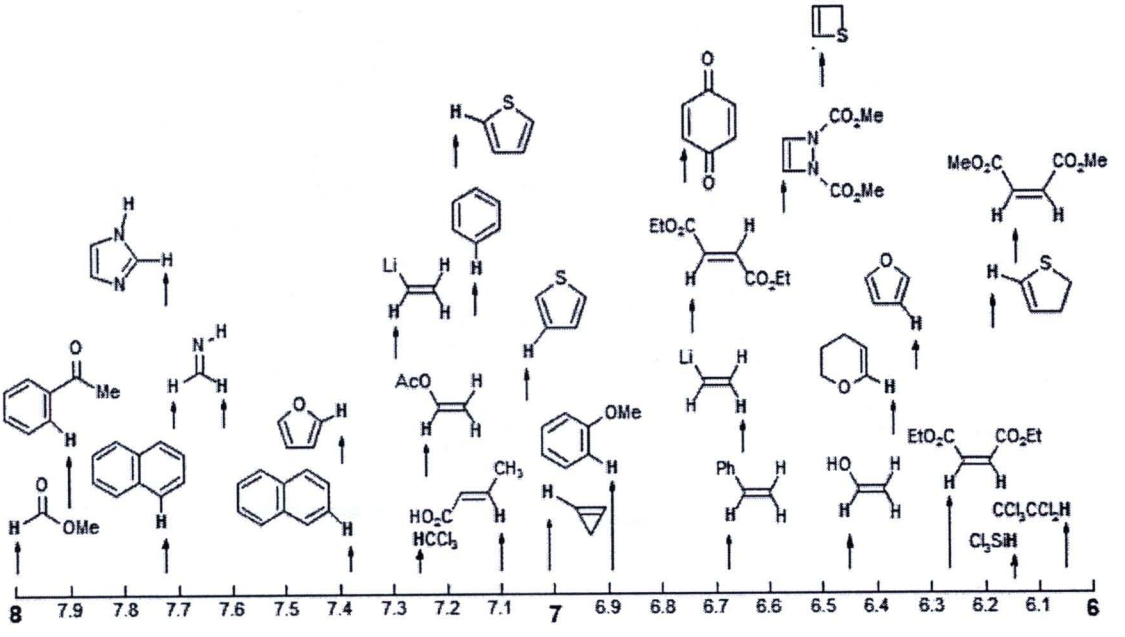


Figure A.2 Proton NMR chemical shifts range 6 – 8 ppm

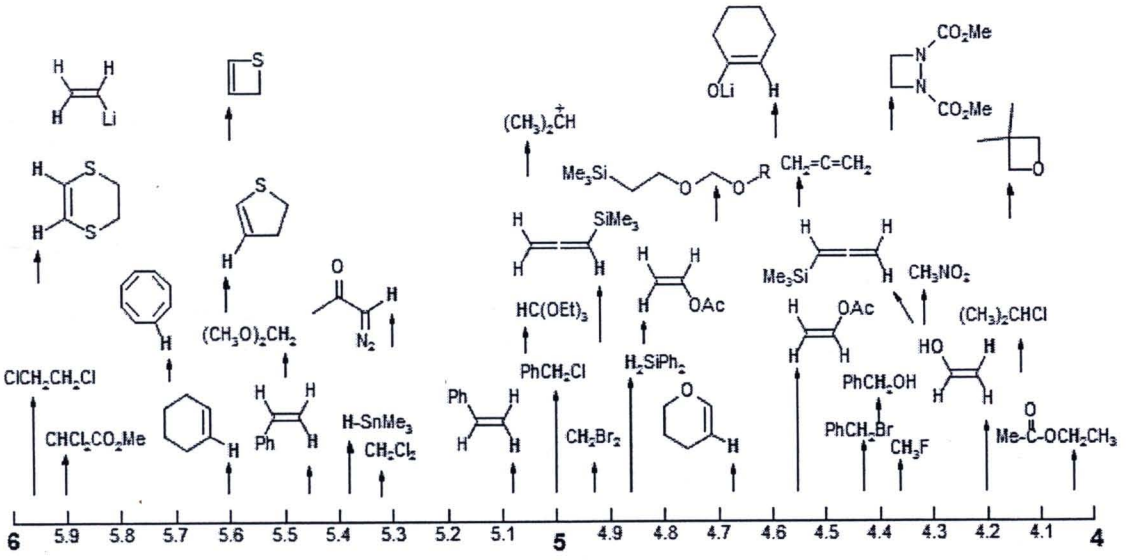


Figure A.3 Proton NMR chemical shifts range 4 – 6 ppm

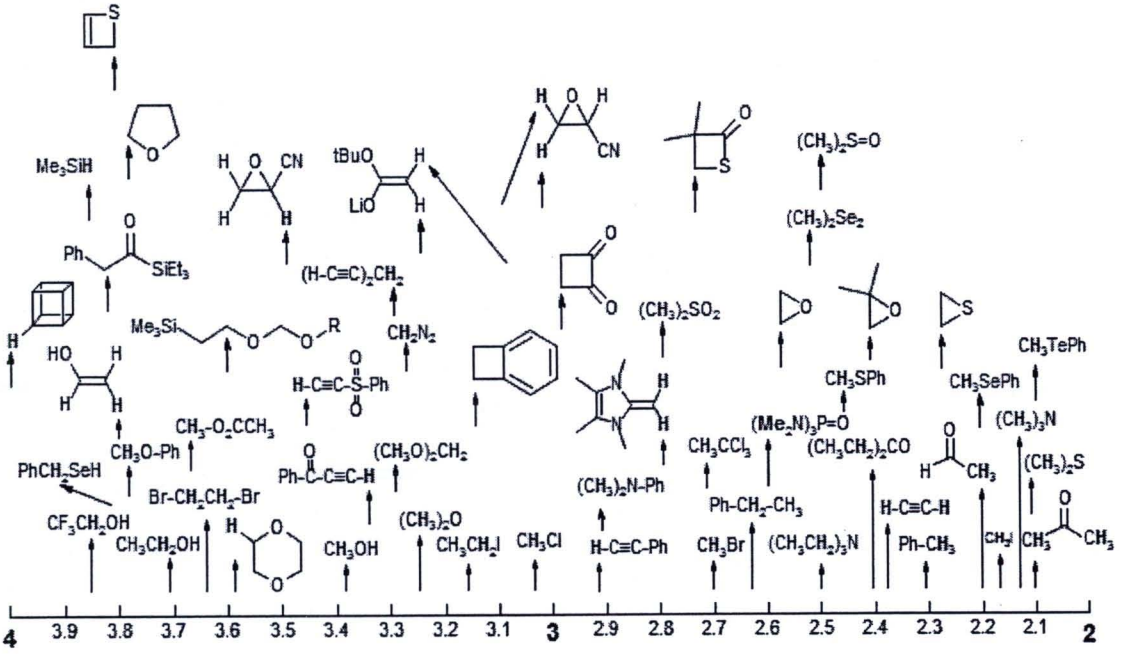


Figure A.4 Proton NMR chemical shifts range 2 – 4 ppm

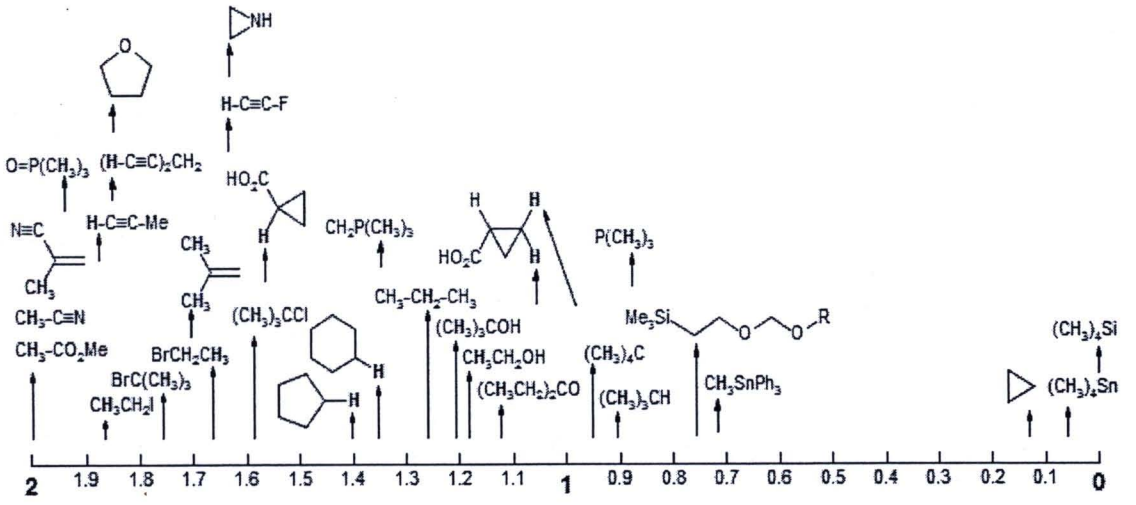


Figure A.5 Proton NMR chemical shifts range 0 – 2 ppm

APPENDIX B

FT-IR absorption frequencies

Table B.1 Characteristic infrared absorption frequencies

Bond	Compound Type	Frequency range, cm^{-1}
C-H	Alkanes	2960-2850(s) stretch
		1470-1350(v) scissoring and bending
	CH_3 Umbrella Deformation	1380(m-w) - Doublet - isopropyl, *t*-butyl
C-H	Alkenes	3080-3020(m) stretch
		1000-675(s) bend
C-H	Aromatic Rings	3100-3000(m) stretch
	Phenyl Ring Substitution Bands	870-675(s) bend
	Phenyl Ring Substitution Overtones	2000-1600(w) - fingerprint region
C-H	Alkynes	3333-3267(s) stretch
		700-610(b) bend
C=C	Alkenes	1680-1640(m,w) stretch
C°C	Alkynes	2260-2100(w,sh) stretch
C=C	Aromatic Rings	1600, 1500(w) stretch
C-O	Alcohols, Ethers, Carboxylic acids, Esters	1260-1000(s) stretch
C=O	Aldehydes, Ketones, Carboxylic acids, Esters	1760-1670(s) stretch
O-H	Monomeric -- Alcohols, Phenols	3640-3160(s,br) stretch
	Hydrogen-bonded -- Alcohols, Phenols	3600-3200(b) stretch
	Carboxylic acids	3000-2500(b) stretch
N-H	Amines	3500-3300(m) stretch
		1650-1580 (m) bend
C-N	Amines	1340-1020(m) stretch
C=N	Nitriles	2260-2220(v) stretch
NO_2	Nitro Compounds	1660-1500(s) asymmetrical stretch
		1390-1260(s) symmetrical stretch

APPENDIX C

Experiments summary

Table C.1 Synthesized experiments

sample	furfural	time	HCL	time	Water added	Drying method	Product weight	yield
	Ml		ml		ml		g	
1	0.83	2 hrs	0.024	1 hr	50	Oven heat	-	-
2	0.83	2 hrs	0.024	1 hr	50	Vacuum dry	0.17	0.1062
3	0.83	2 hrs	0.024	2 hrs	50	Vacuum dry	0.37	0.2312
4	0.83	2 hrs	0.024	1 day	50	Vacuum dry	0.41	0.2562
5	0.83	2 hrs	0.024	4 days	50	Vacuum dry	0.49	0.3062
6	0.83	2 hrs	0.024	2 hrs	500	Vacuum dry	0.32	0.2
7	0.83	18 hours			500	Vacuum dry	0.33	0.2062
8	0.83	2 hrs	0.072	2 hrs	500	Vacuum dry	0.41	0.2562
9	0.83	2 hrs	0.12	2 hrs	500	Vacuum dry	0.57	0.3562
10	0.83	15 mins	0.024	2 hrs	500	Vacuum dry	0.45	0.2812

Note: Each sample uses 1.2 g of urea in water solution 4 ml before incorporate furfural

APPENDIX D

Calculations

Material preparation

The synthesized of furfural and urea, represented as F and U, respectively.

Basis 1.2 g of U

Molecular weight of F and U was 96.085 and 60.06 g/mol, respectively

$$\frac{(1.2 \text{ g of U})}{(96.085 \text{ g/mol})} = 0.02 \text{ moles U (basis)}$$

1 to 2 molar ratio of F to U was selected in this study

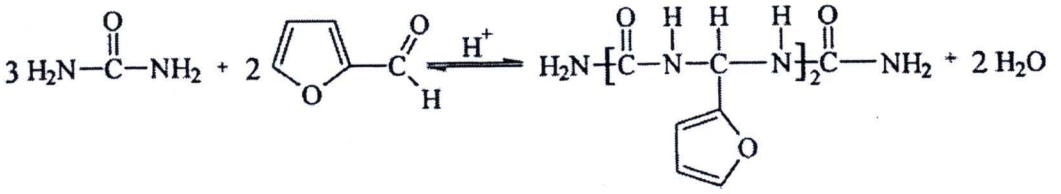
$$\begin{aligned} 2 \text{ moles of U} &= 1 \text{ mole of F} \\ 0.02 \text{ moles U} &= 0.01 \text{ mole of F} \\ \text{gram of F} &= (0.01 \text{ mole of F}) \times (96.085 \text{ g/mol}) \\ &= 0.961 \text{ g} \end{aligned}$$

The density of F was 1.1594 g/ml

$$\begin{aligned} \text{volume of F} &= \frac{(0.961 \text{ g of F})}{(1.1594 \text{ g/ml})} \\ &= 0.829 \text{ ml} \end{aligned}$$

Yield calculation

3 moles of urea reacted with 2 moles of furfural. According to the basis of 1.2 g of urea, urea was a limiting reagent because furfural was excess.



The yield of this reaction was calculated as following:

According to the material preparation calculations, 0.02 mole of U and 0.01 mole of F were used in the experiment. Since F was a limiting reagent, only 0.015 mol of U was reacted in this reaction.

$$\begin{aligned} \text{U (feed)} &= \text{U (react)} + \text{U (unreact)} \\ 1.2 \text{ g} &= (0.015 \text{ mol U} \times 60.06 \text{ g/mol}) + \text{U (unreact)} \\ \text{U (unreact)} &= 0.2991 \text{ g} \end{aligned}$$

Molecular weights of DFTU and water was 198 g/mol and 18 g/mol, respectively

Mass conservation

$$\text{mass (in)} = \text{mass (out)}$$

$$\text{U (in)} + \text{F (in)} = \text{DFTU (product)} + \text{water} + \text{U(unreact)}$$

$$1.2\ \text{g} + 0.961\ \text{g} = \text{DFTU} + (0.01\text{mol} \times 18\ \text{g/mol}) + 0.2991\ \text{g}$$

$$\text{DFTU} = 1.6819\ \text{g}$$

$$\text{The conversion of this reaction} = \frac{1.6819\ \text{g}}{2.161\ \text{g}}$$

$$= 0.78$$

Yield of product can be calculated by: (calculation for sample 1)

$$\frac{\text{Actual product weight}}{\text{Desired prodduct weicht}} = \frac{0.3\ \text{g}}{1.6819\ \text{g}}$$

$$= 0.12$$

APPENDIX E

UV-vis raw data

UV-vis spectroscopy

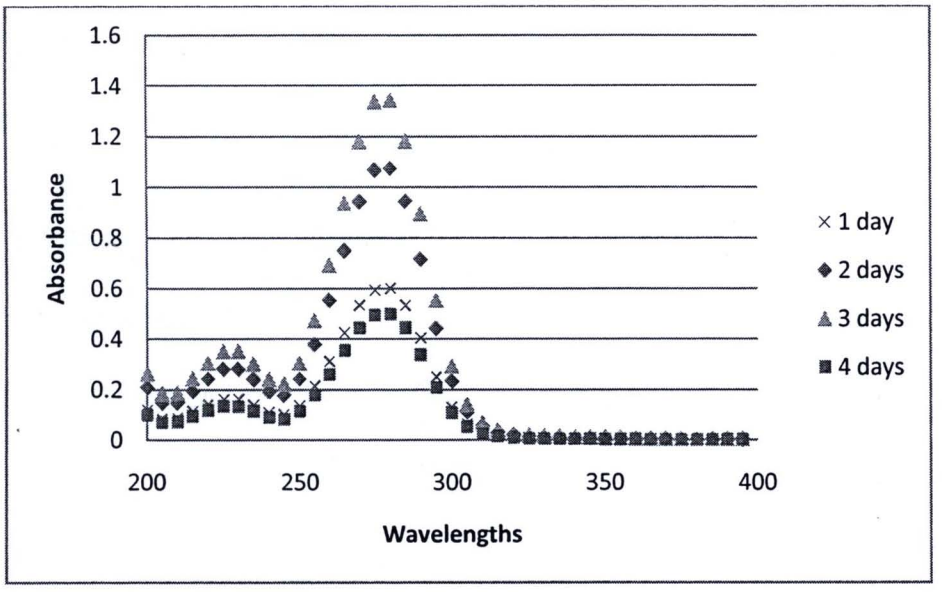


Figure E.1 UV absorption of the release of furfural in furfural-urea complex in 4 days

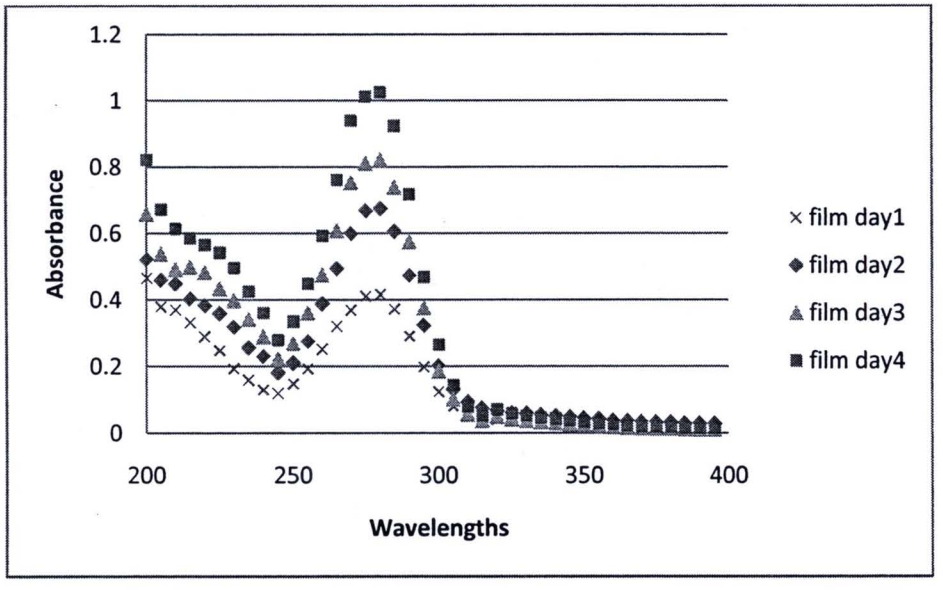


Figure E.2 UV absorption of the release of furfural in furfural-urea complex imbedded with PBSA polymer in 4 days

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King Mongkut's University of Technology Thonburi
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Surname/Family Name.....Niyomthamkij.....
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○ Doctoral Degree
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