

Electronic Supporting Information

Ferrocenyl-Phosphonium Ionic Liquids - Synthesis, Characterisation and Electrochemistry

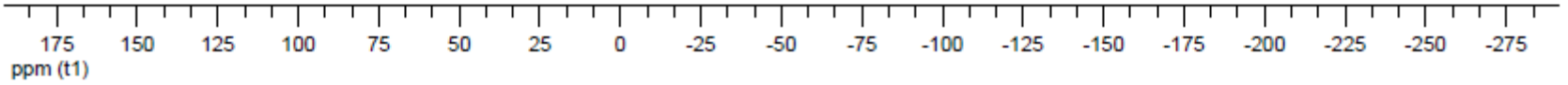
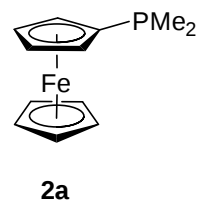
Paul Kübler^a and Jörg Sundermeyer^{*a}

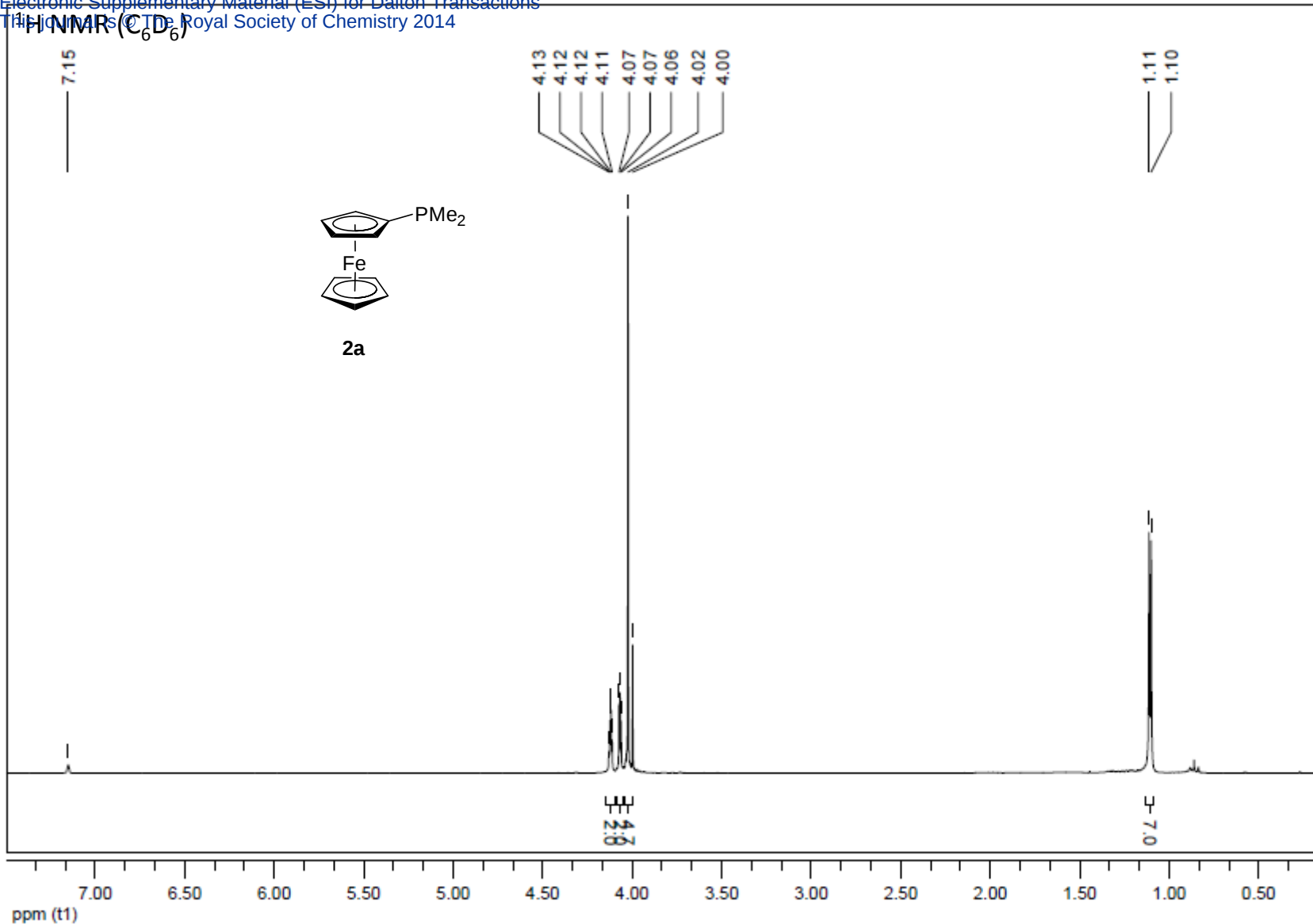
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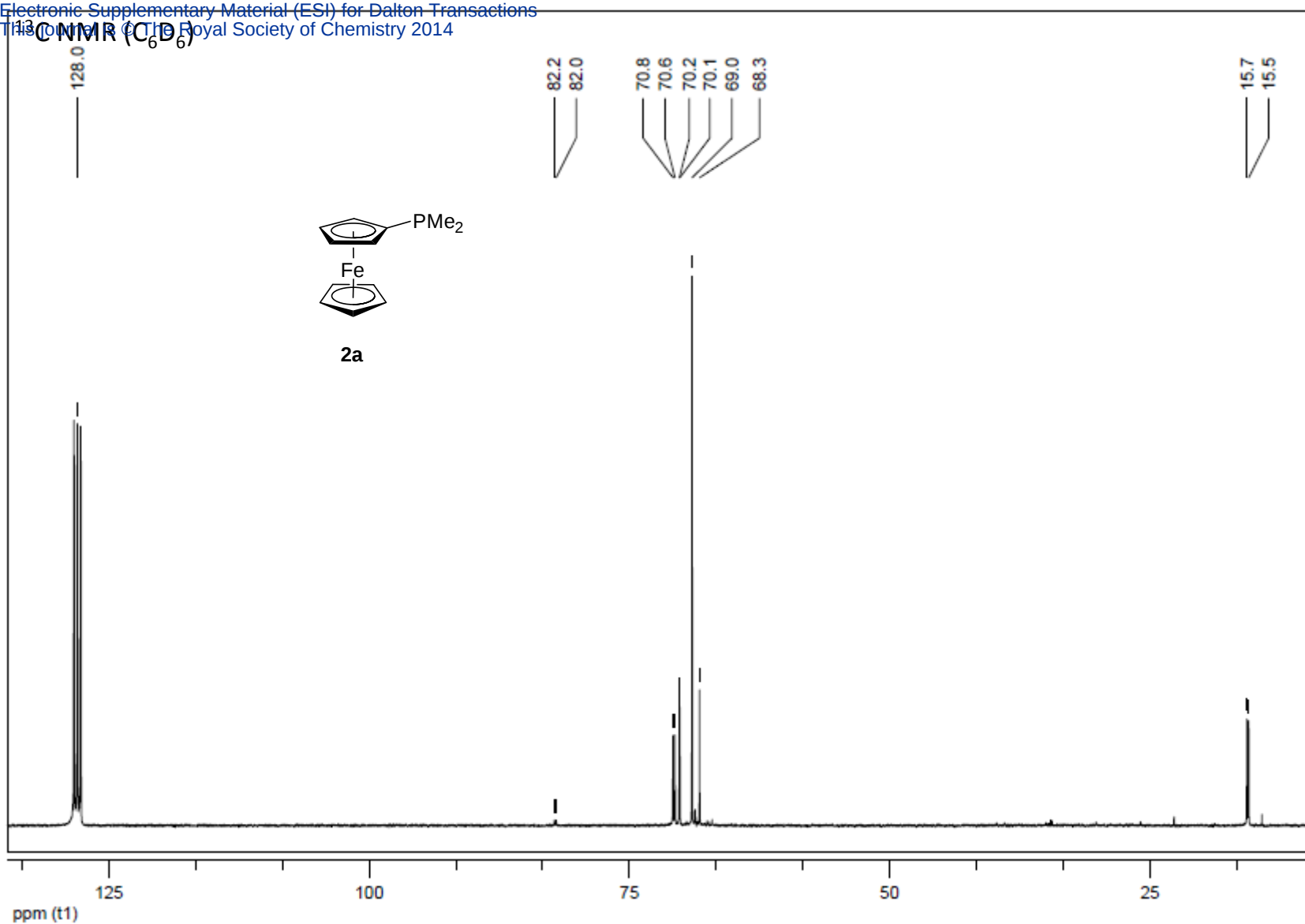
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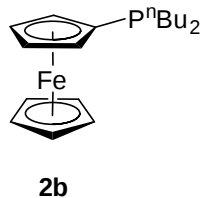
³¹P NMR (C₆D₆)







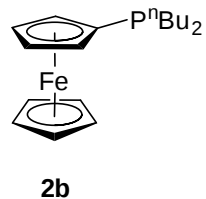
^{31}P NMR (C_6D_6)



-35.8

ppm (t1)

¹H NMR (CDCl₃)



4.18
4.15
4.10
4.08
4.00

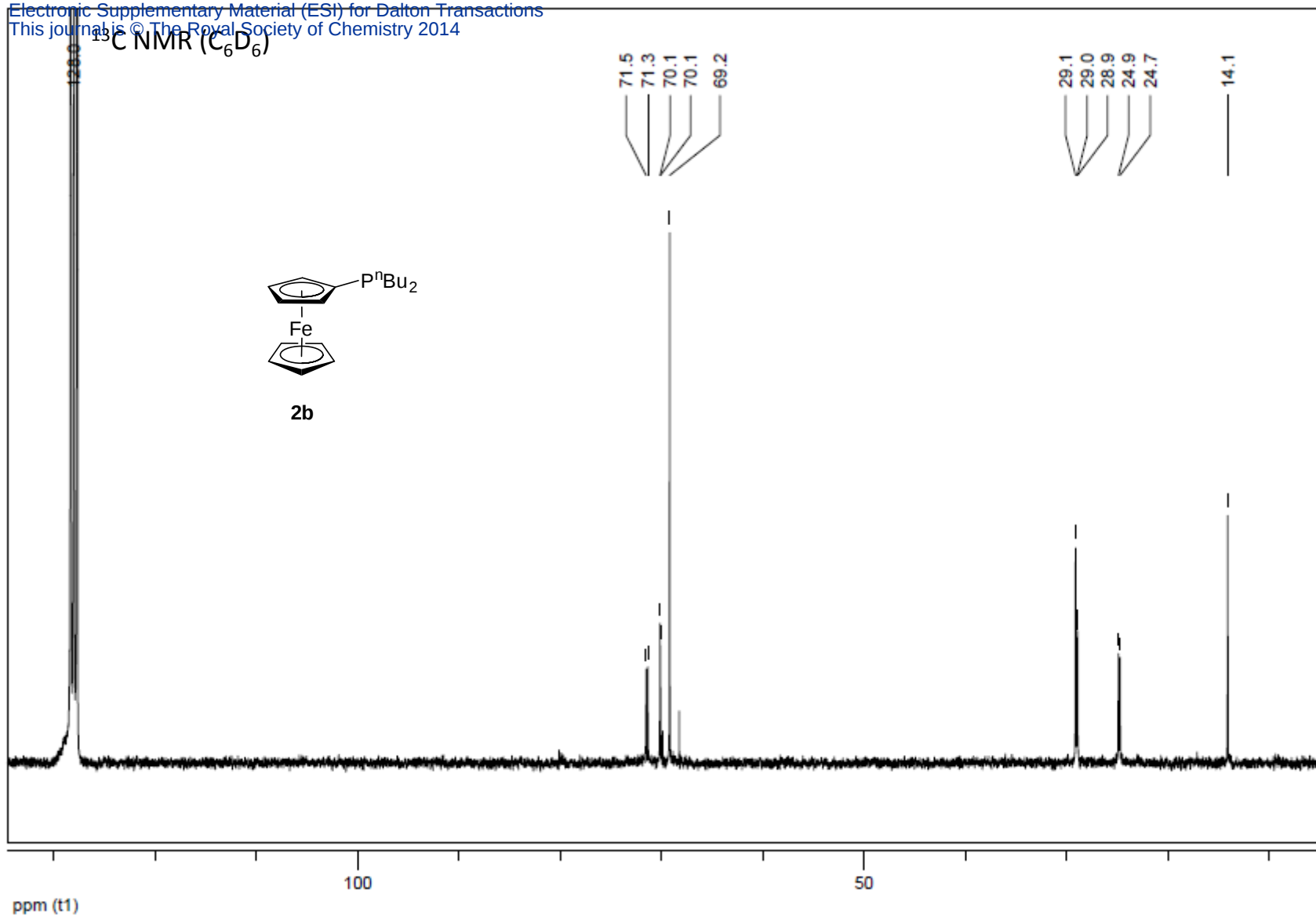
1.67
1.60
1.57
1.46
1.44
1.33
0.88

6.61
6.61
2.00

5.18
4.72
4.03

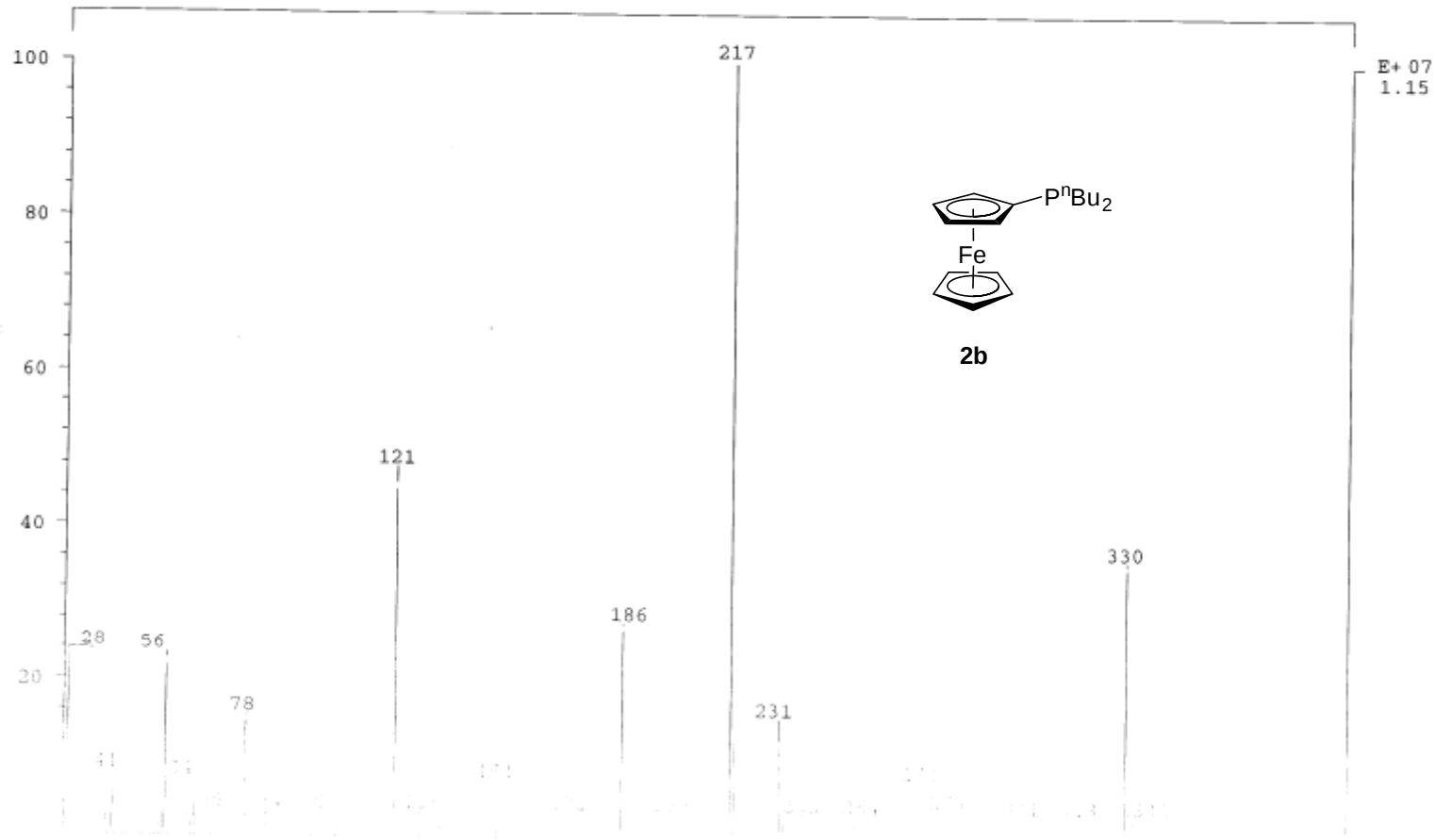
6.39

ppm (t1)



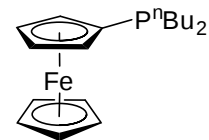
Samp: pk-C-96
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM
Oper: Ba Client: Kuebler
Base: 330.2 Inten: 4047054
Norm: 217.0 RIC: 64370351
Peak: 1000.00 mmu
Data: CMASS : converted

Elapse: 06:27.2 49
Start: 50
Inlet:
Masses: 20 > 600
#peaks: 1885



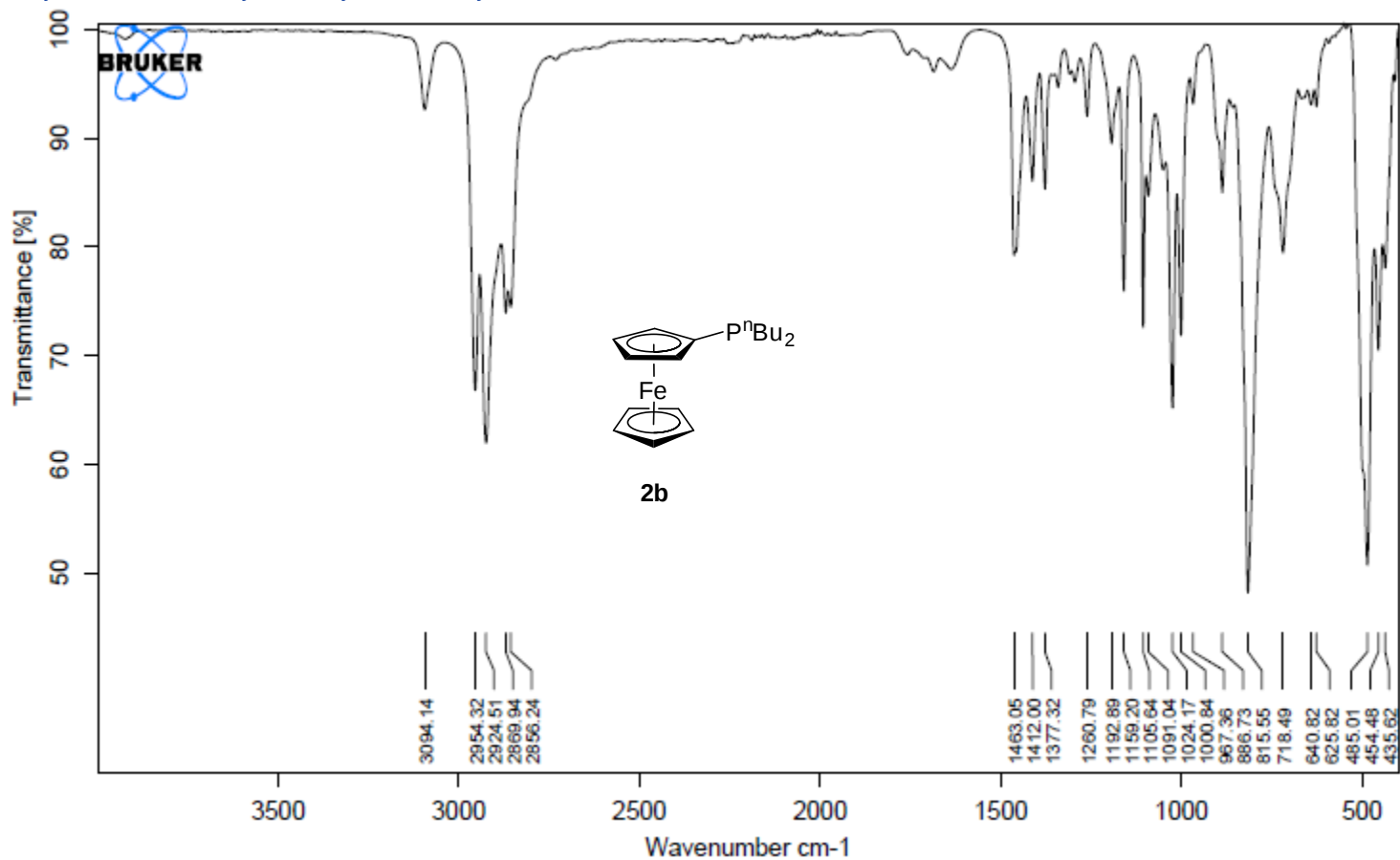
LIST: 13-pk-c-2761 31-Oct-13 Elapse: 02:07.9
Samp: pk-C-276.1 Start : 09:44:30
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM
Oper: Ba Client: Kuebler Inlet :
Limt: (318) C21.H35.P. . .
: (453) C22.H35.P.13C.54Fe.Fe
Peak: 1000.00 mmu R+D: -5.0 > 30.0

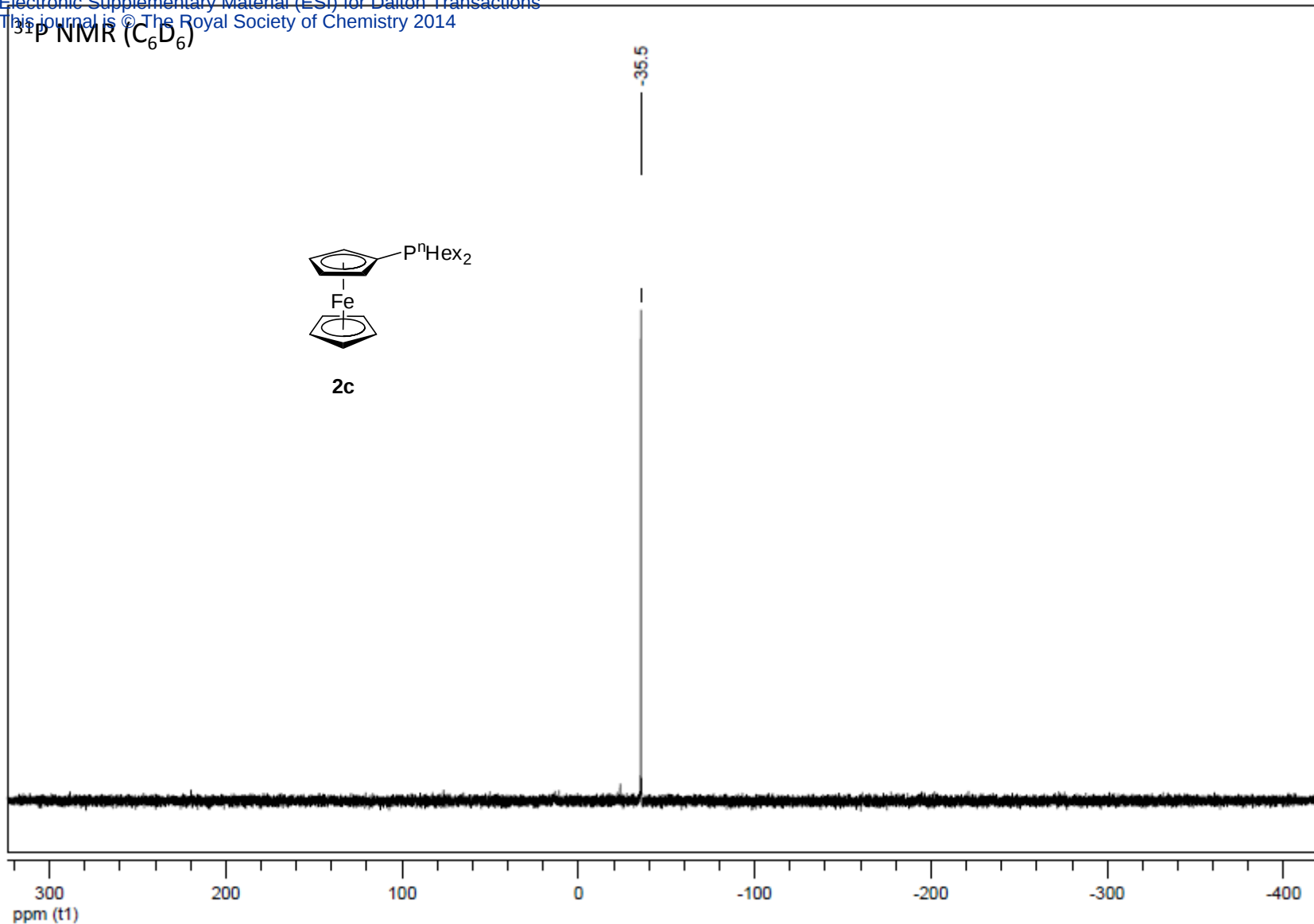
128103			(mmu)				
Mass	Intensity	%RA	%RIC	Delta	R+D	Composition	
384.1861	*	152718	0.60	0.04	1.1	6.0	C22.H35.P.54Fe
386.1818	*	2145998	8.38	0.61	0.8	6.0	C22.H35.P.Fe
387.1858	*	527509	2.06	0.15	0.2	6.0	C21.H35.P.13C.Fe



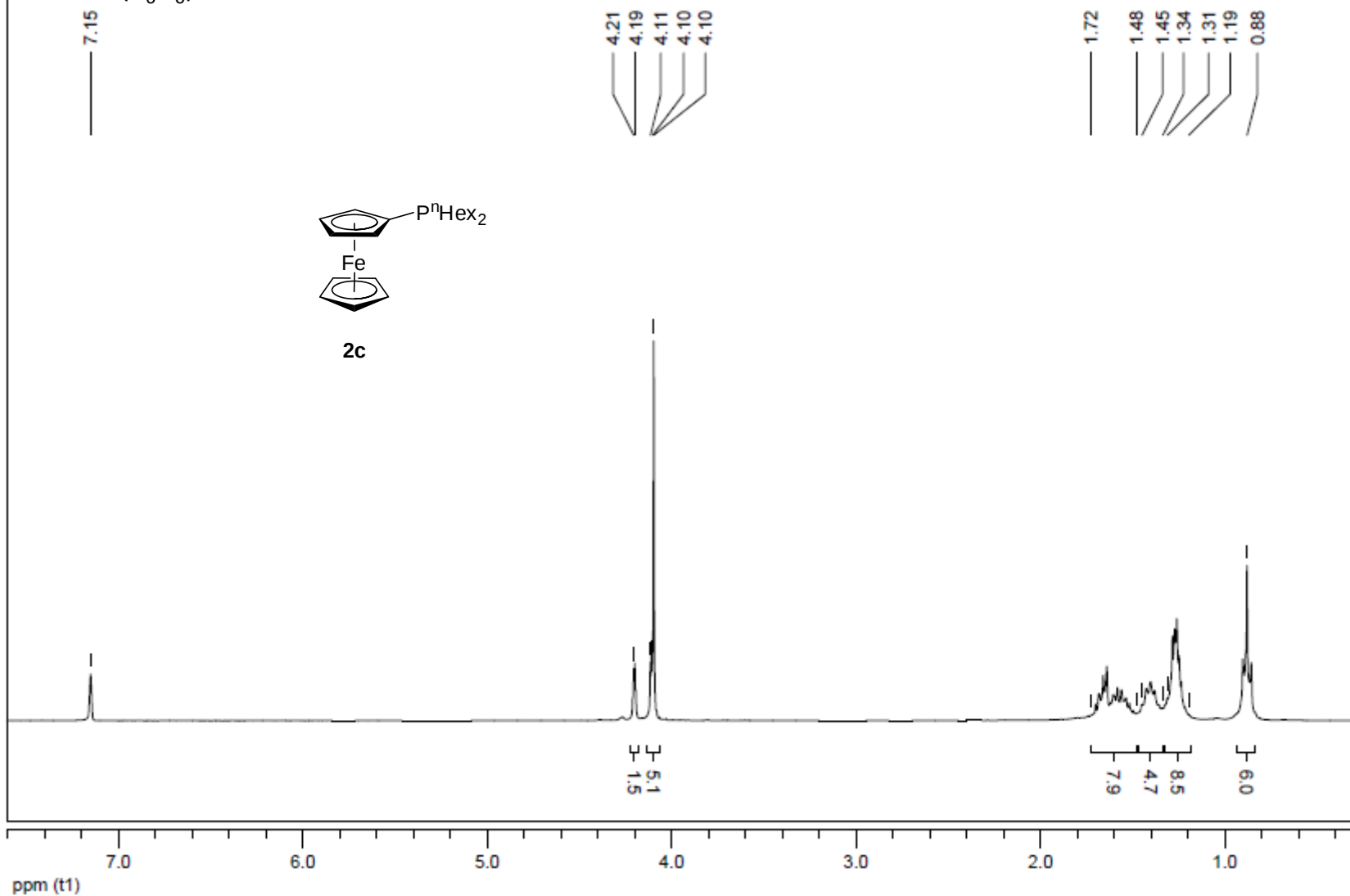
2b

IR (neat)

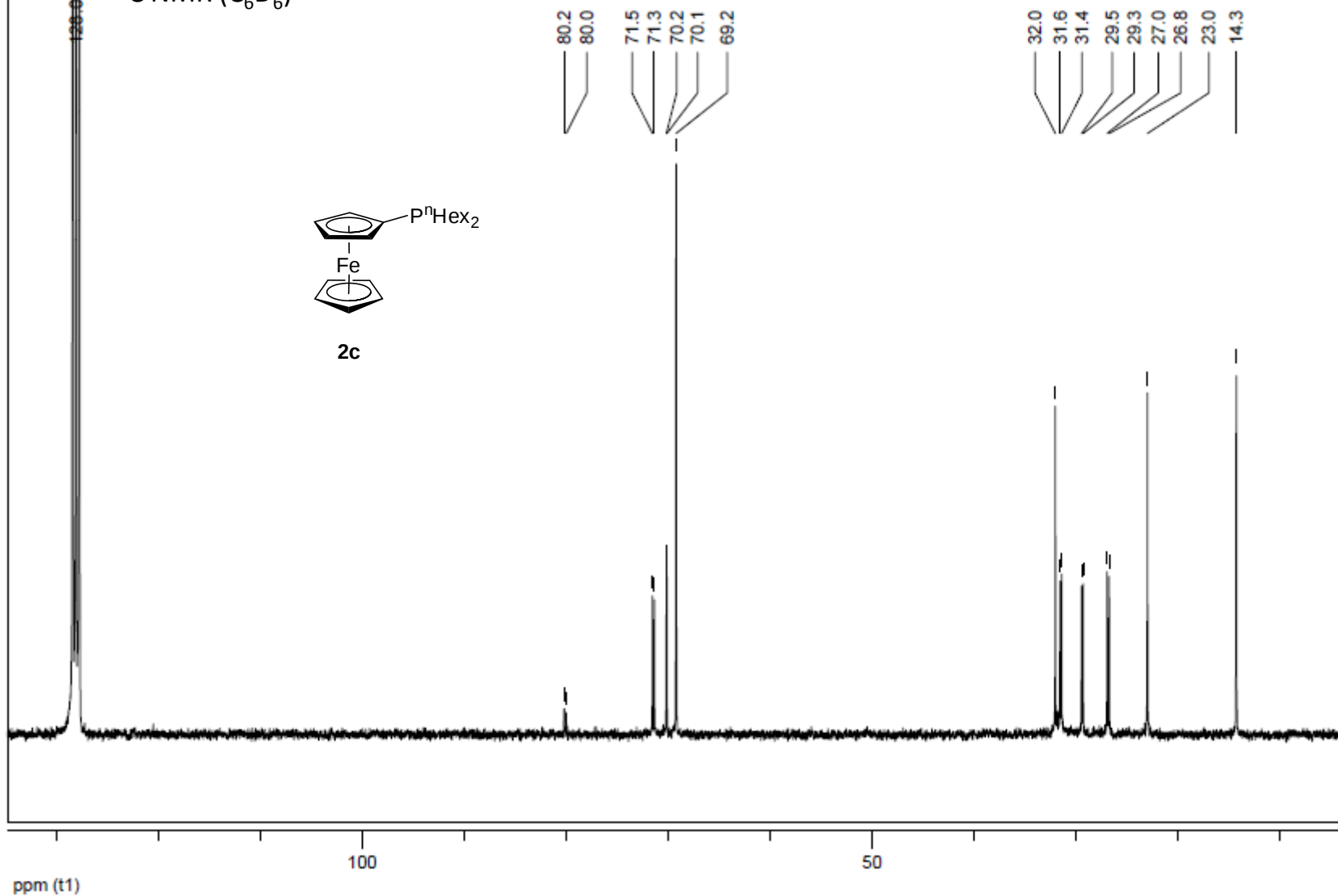
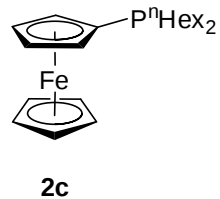




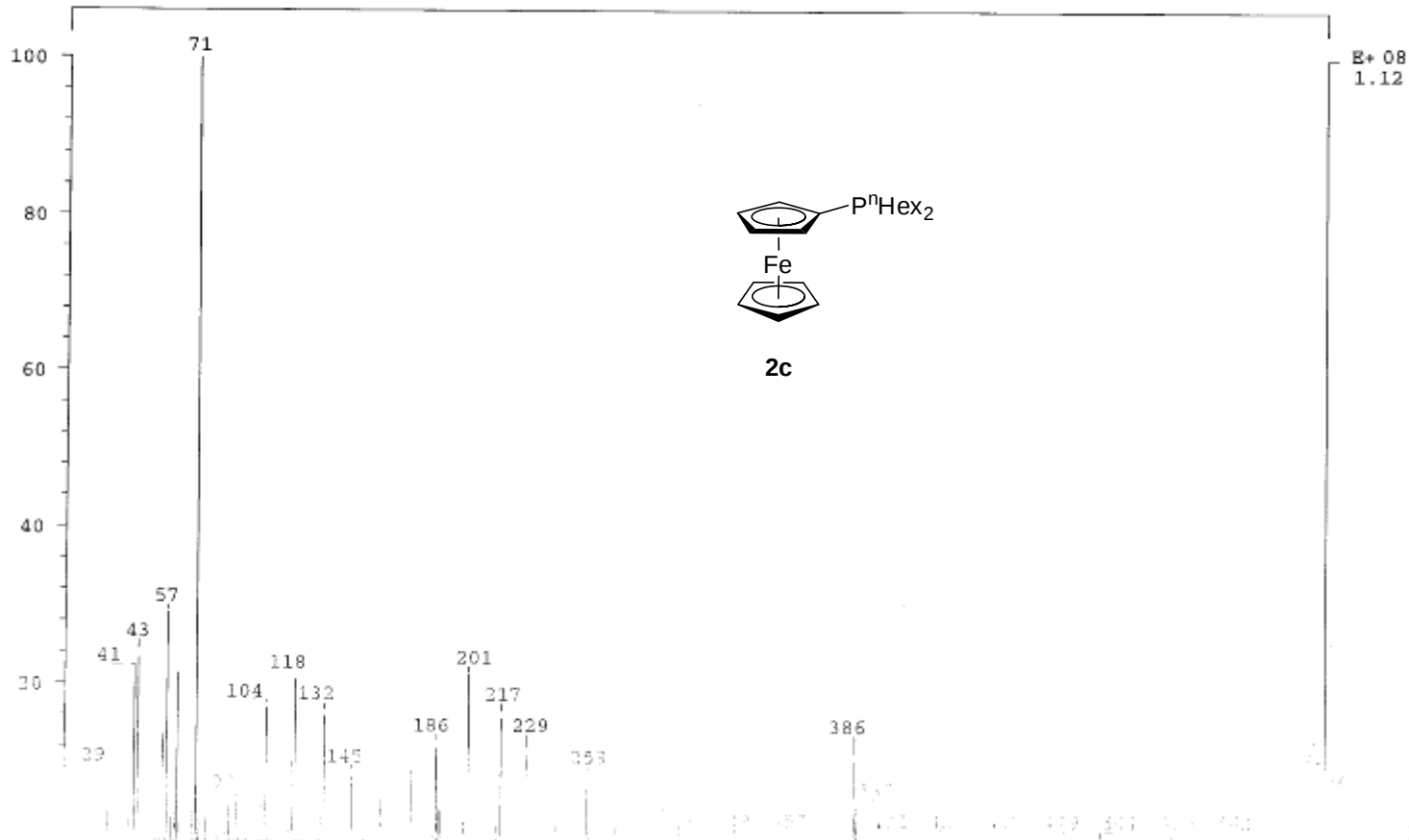
¹H NMR (C₆D₆)



^{13}C NMR (C_6D_6)

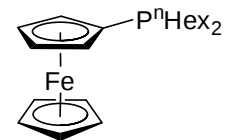


SPEC: 13-pk-c-2761 31-Oct-13 Elapse: 02:53.4 22
Samp: pk-C-276.1 Start : 09:44:30 22
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM
Oper: Ba Client: Kuebler Inlet :
Base: 71.0 Inten : 112112640 Masses: 20 > 600
Norm: 71.0 RIC : 770735299 #peaks: 1440
Peak: 1000.00 mmu

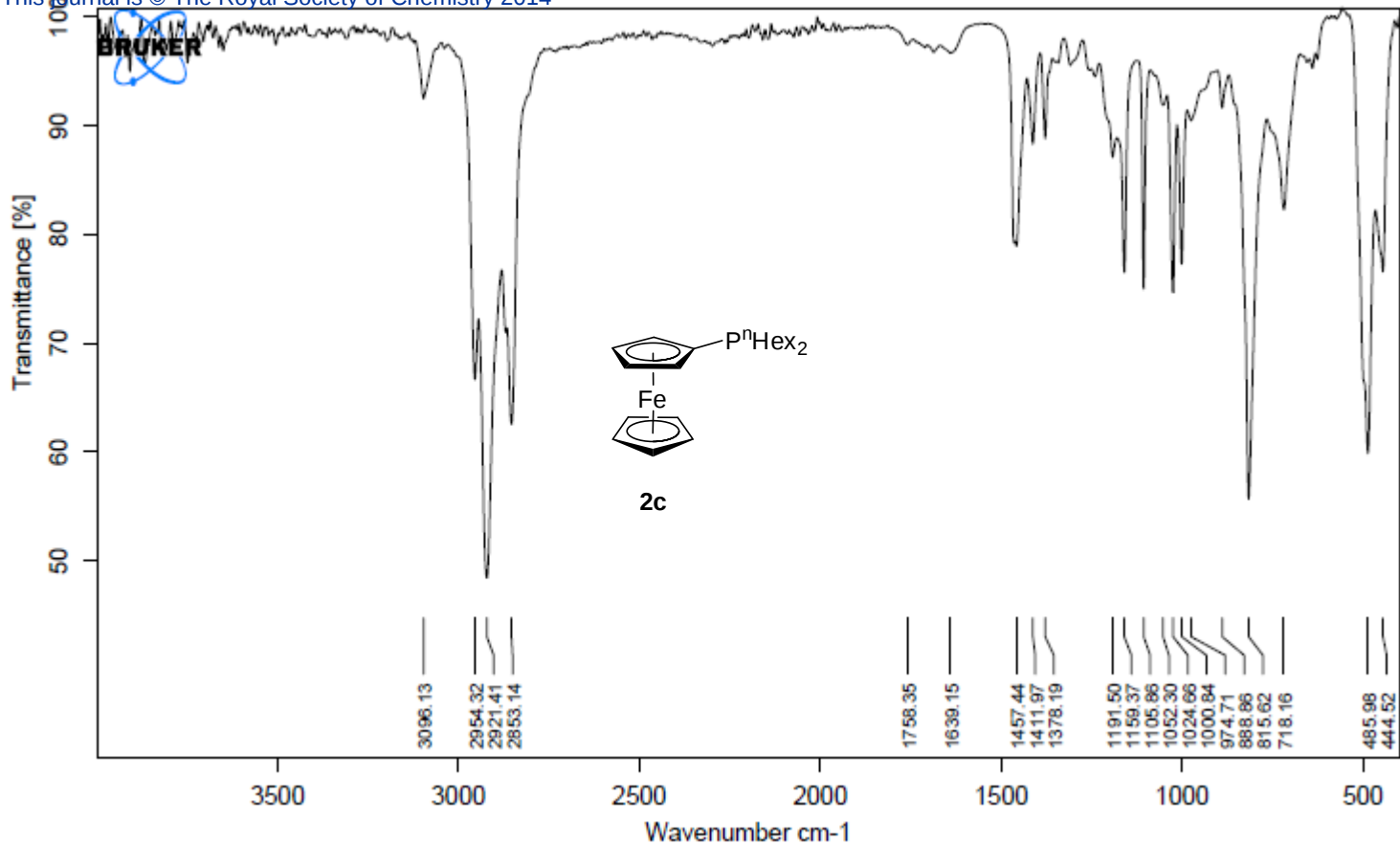


LIST: 13-pk-c-2761 31-Oct-13 Elapse: 02:07.9
Samp: pk-C-276.1 Start : 09:44:30
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM
Oper: Ba Client: Kuebler Inlet :
Limt: (318) C21.H35.P. . .
: (453) C22.H35.P.13C.54Fe.Fe
Peak: 1000.00 mmu R+D: -5.0 > 30.0

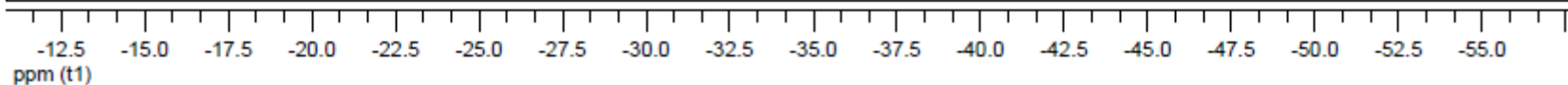
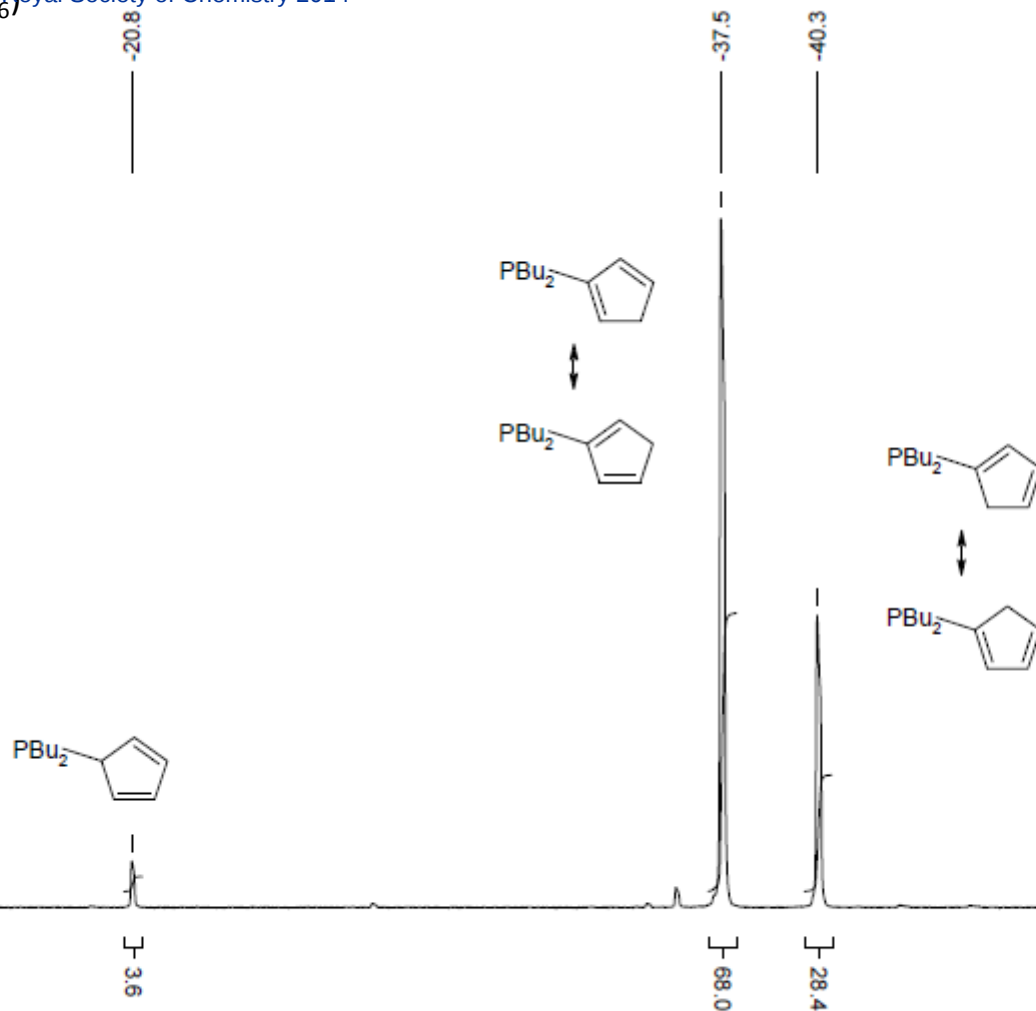
128103		(mmu)				
Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
384.1861 *	152718	0.60	0.04	1.1	6.0	C22.H35.P.54Fe
386.1818 *	2145998	8.38	0.61	0.8	6.0	C22.H35.P.Fe
387.1858 *	527509	2.06	0.15	0.2	6.0	C21.H35.P.13C.Fe



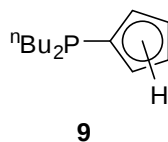
2c



³¹P NMR (CDCl₃)

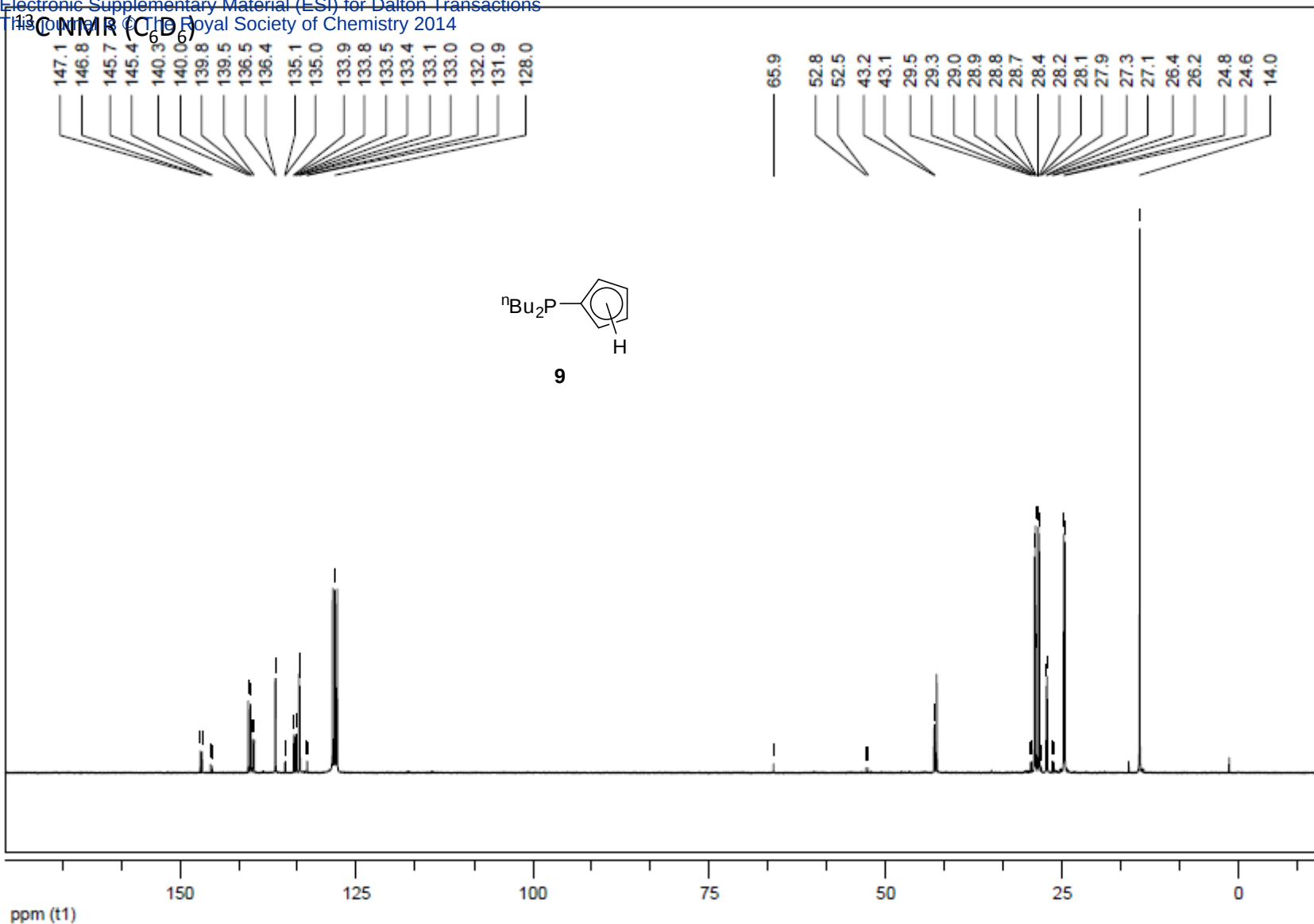
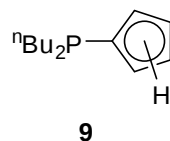


¹H NMR (CDCl₃)

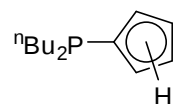


ppm (t1)

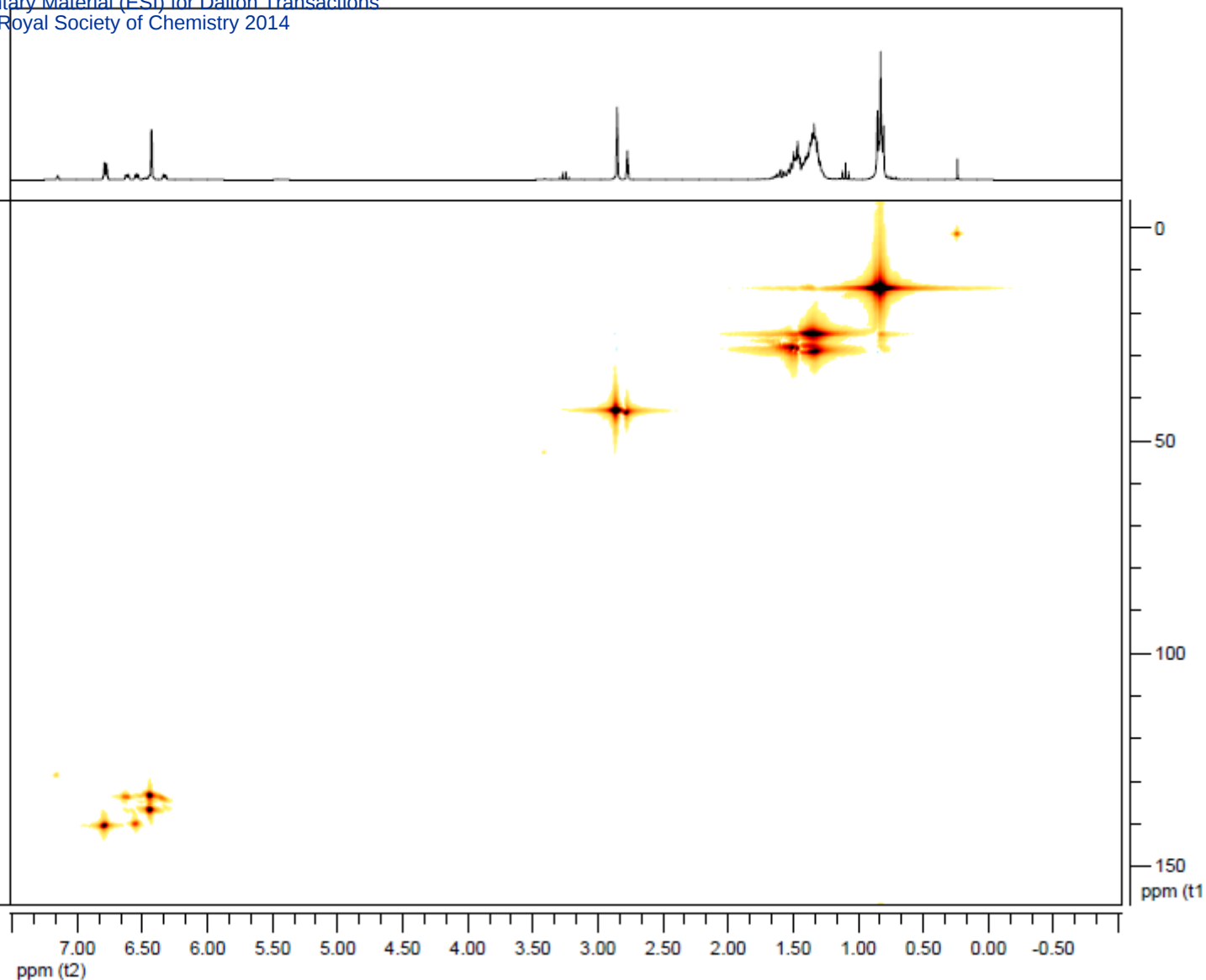
¹³C NMR (CDCl₃)



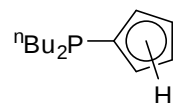
HMQC NMR



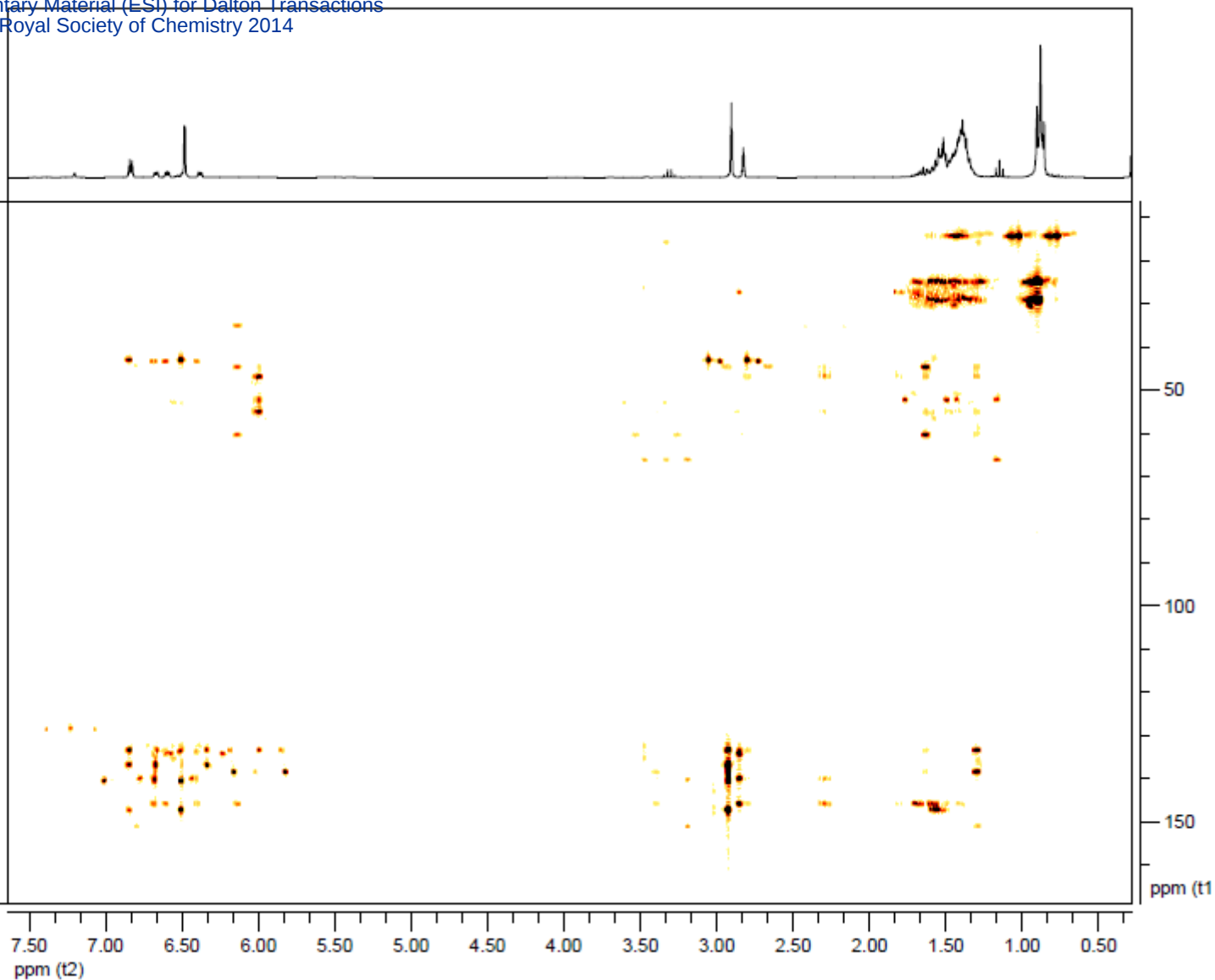
9



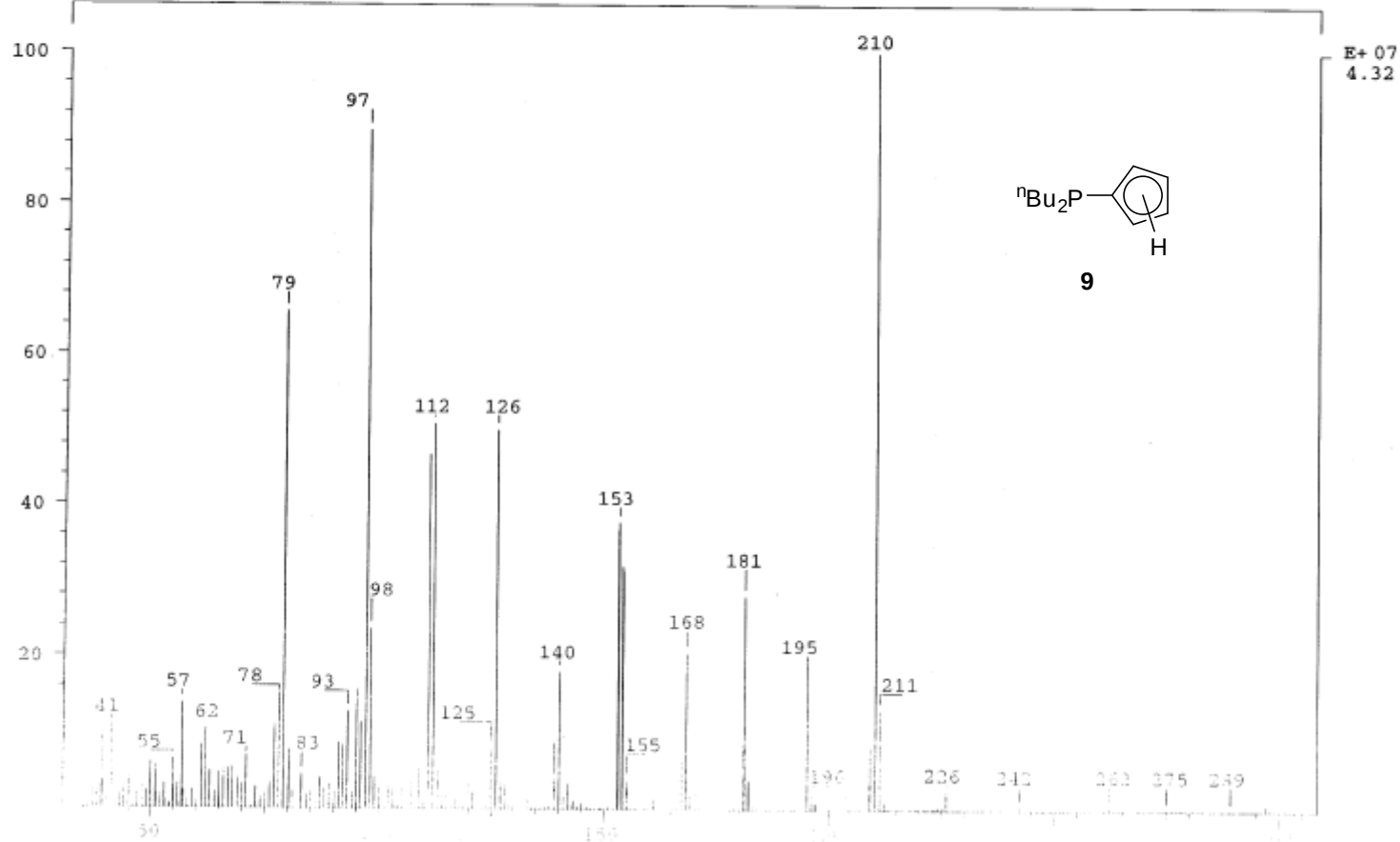
HMBC NMR



9

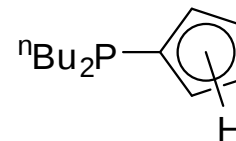


SPEC: 12-hr-pk189-cl 05-Oct-12 REG : 10:59.8 #9
Samp: pk-L-89 Start : 13:00:49 95
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM
Oper: K1 Client: Kuebler Inlet :
Base: 210.2 Inten : 43165344 Masses: 20 > 600
Norm: 210.2 RIC : 514865096 #peaks: 623
Peak: 1000.00 mmu
Data: +/85>88 - /1>11 (CMass : converted |CMass : converted |CMass :



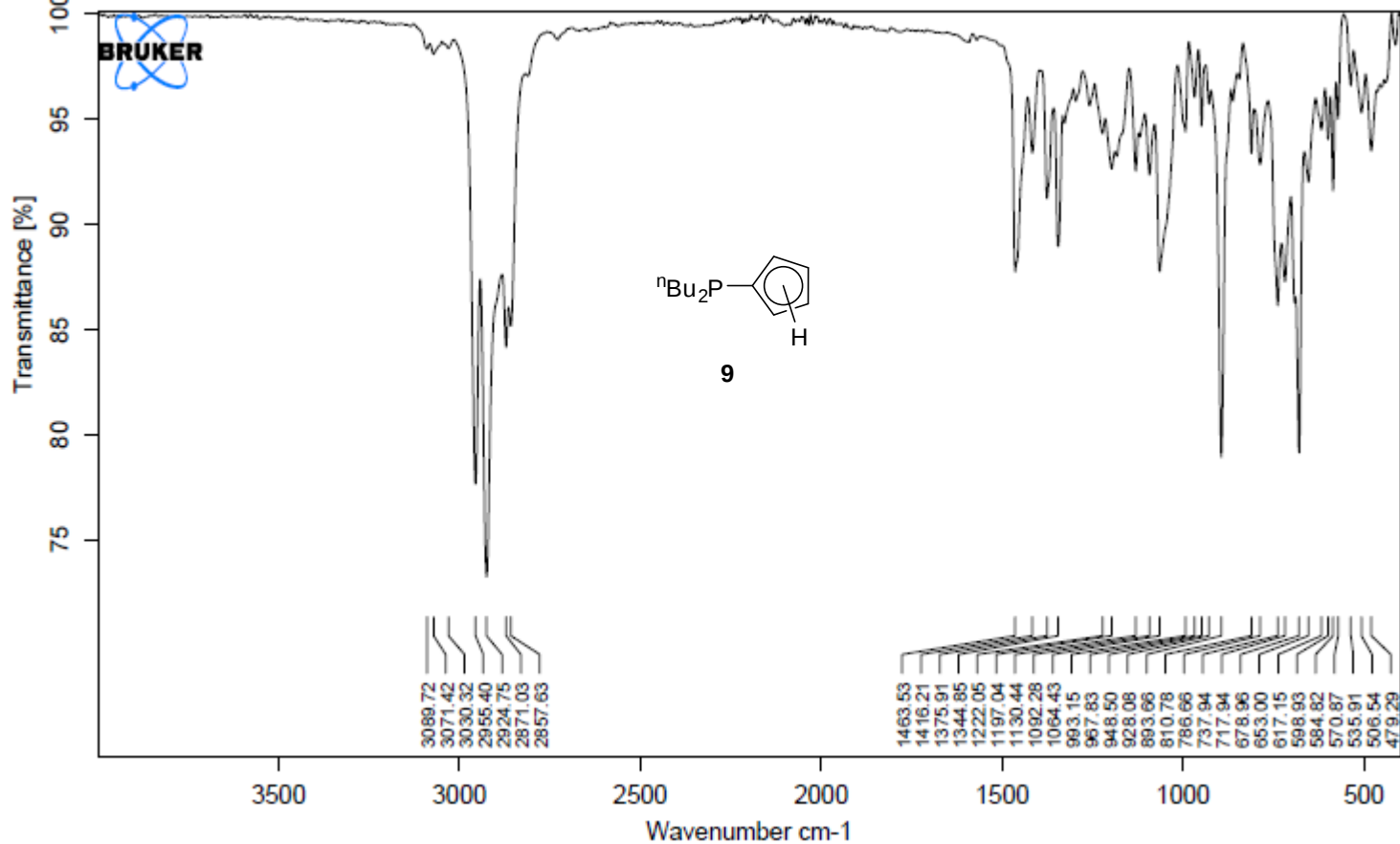
12-hr-pk189-c1
PK-L-89
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM
Opex: K1 Client: Kuebler
Limit: (198) C12.H23.P.
Limit: (223) C13.H23.P.13C
Peak: 1000.00 mmu R+D: -5.0 > 30.0
Data: CMASS : converted

05-Oct-12 Elapse: 05:41.9 43
Start : 13:00:49 95
Inlet :

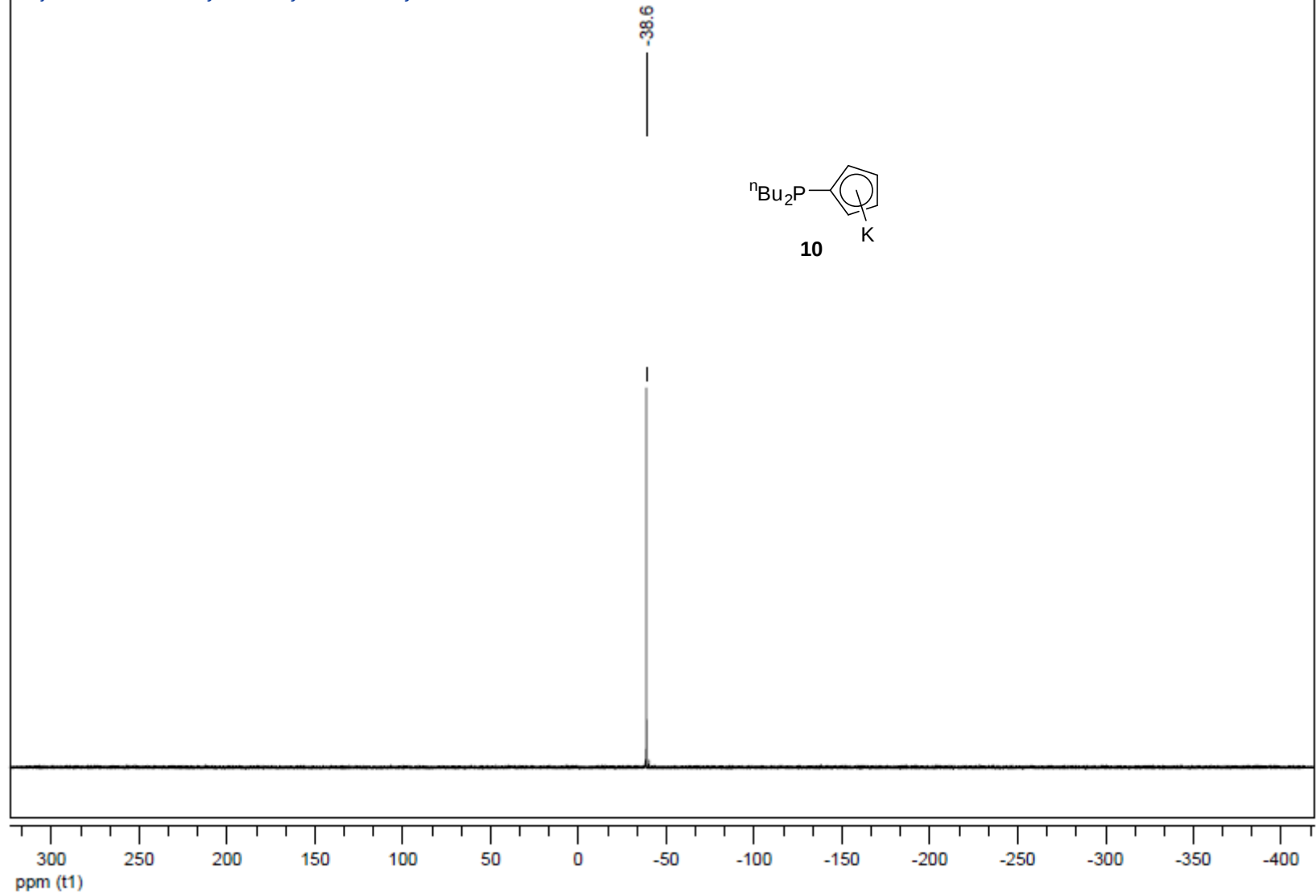


9

		88967		(mmu)			
Mass	Intensity	%RA	%RIC	Delta	R+D	Composition	
210.1539	* 8896512	100.00	3.51	-0.2	3.0	C13.H23.P	
211.1576	* 1349663	15.17	0.53	-0.5	3.0	C12.H23.P.13C	



³¹P NMR (THF-d₈)



¹H NMR (THF-d₈)

