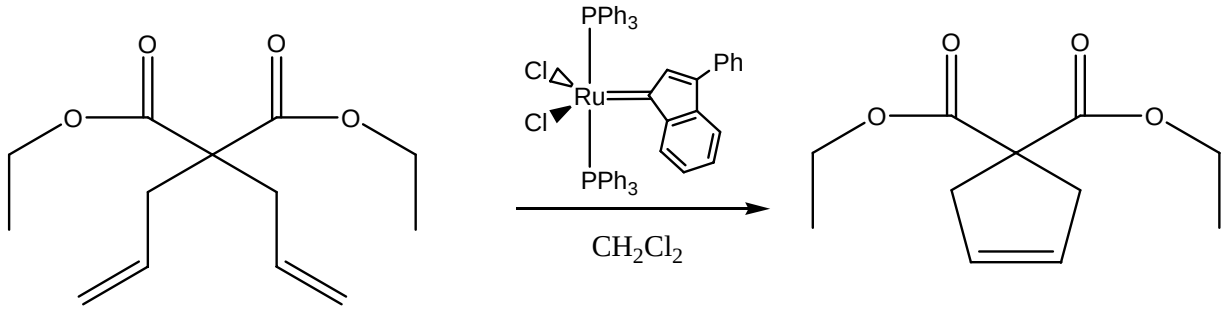
Chem 213 T6
Problem V

Ring closing metathesis reactions can be successful with a variety of catalysts and substrates. In the current research project a series of ruthenium catalysts are being investigated to compare their efficiency on diethyl diallyl malonate.

The reaction was first successfully done using the trans-$P(C_6H_{11})_3$ version of the catalyst. The reaction is now being repeated using the trans-PPh_3 version of the catalyst, and the resulting product is characterized by NMR.



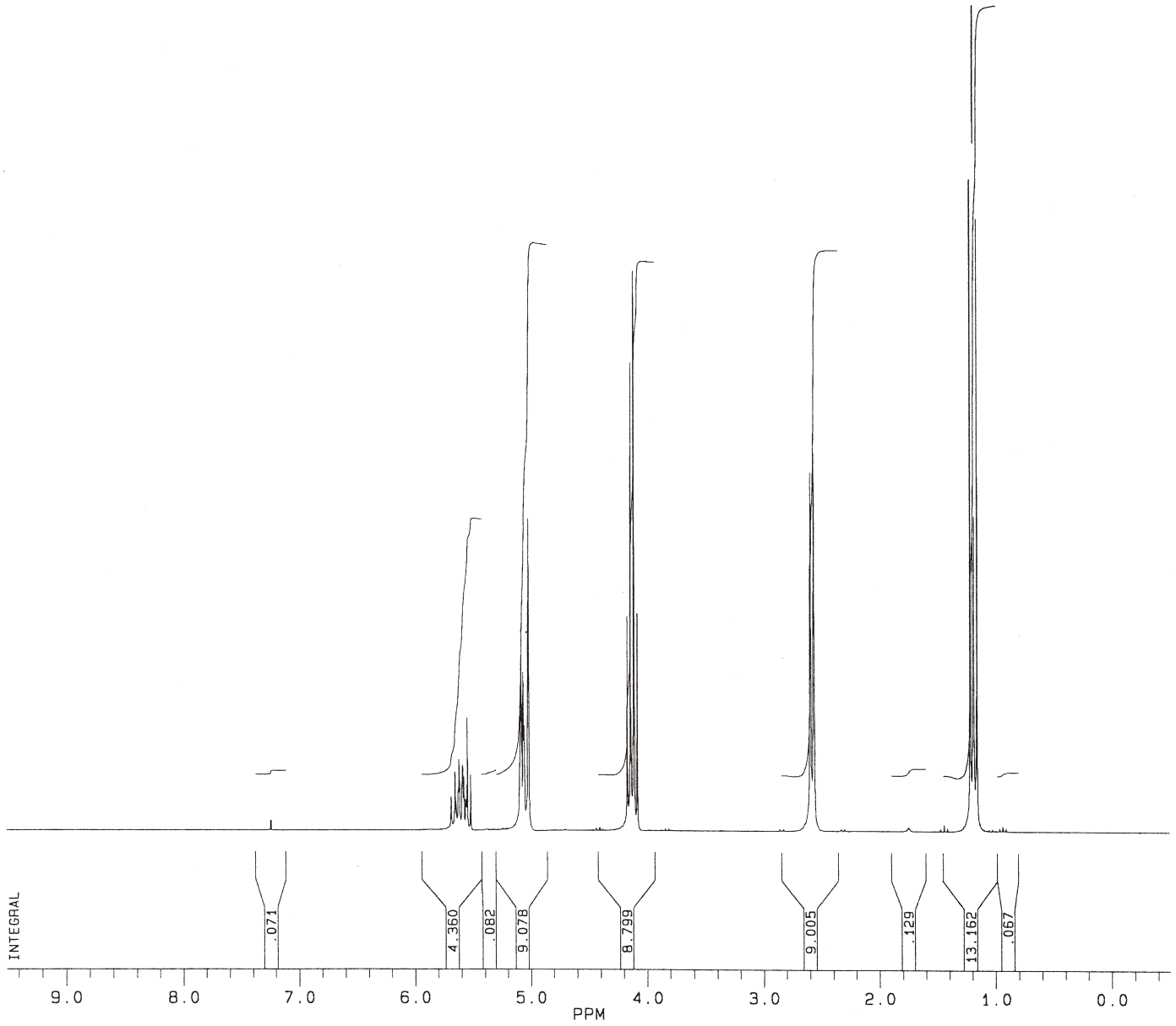
diethyl diallyl malonate

Based on the spectra of the resultant reaction, can you help figure out what has happened? Did the reaction go to completion, or is there a mixture present? If there is a mixture, please quantify the major components. Write a report that explains your findings and identifies any unanswered questions and inconsistencies remaining in the spectra.

Attached spectra of "diethyl diallyl malonate rxn" in $CDCl_3$:

^{1}H nmr	MA260S.112
^{13}C nmr	MA261S.112
DEPT-135	MA262S.112
COSY	MA264112.smx
HETCOR	MA267112.smx

KELLI DIETHYL DIALLYLMALONATE CDCL3



MA260S.112
AU PROG:
XOO.AU
DATE 26-5-8

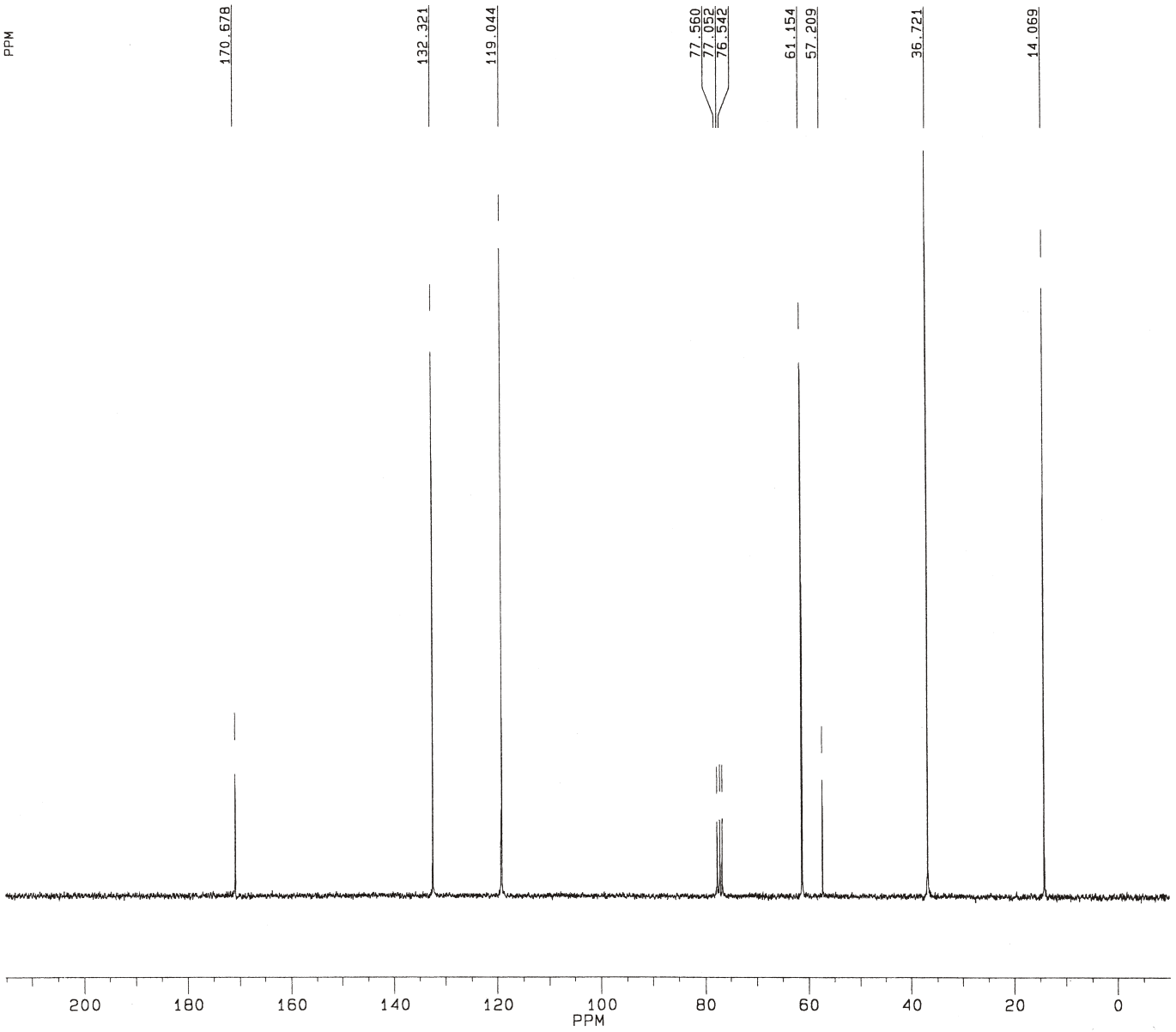
SF 250.133
SY 250.0
O1 4360.000
SI 16384
TD 16384
SW 5000.000
HZ/PT .610

PW 0.0
RD 0.0
AQ 1.638
RG 1
NS 16
TE 297

FW 6300
O2 0.0
DP 63L PO

LB .250
GB 0.0
CX 21.00
CY 15.00
F1 9.502P
F2 -.498P
HZ/CM 119.106
PPM/CM .476
SR 2858.54

KELLI DIETHYL DIALLYLMALONATE CDCL3



MA261S.112
AU PROG:
X02.AU
DATE 26-5-8

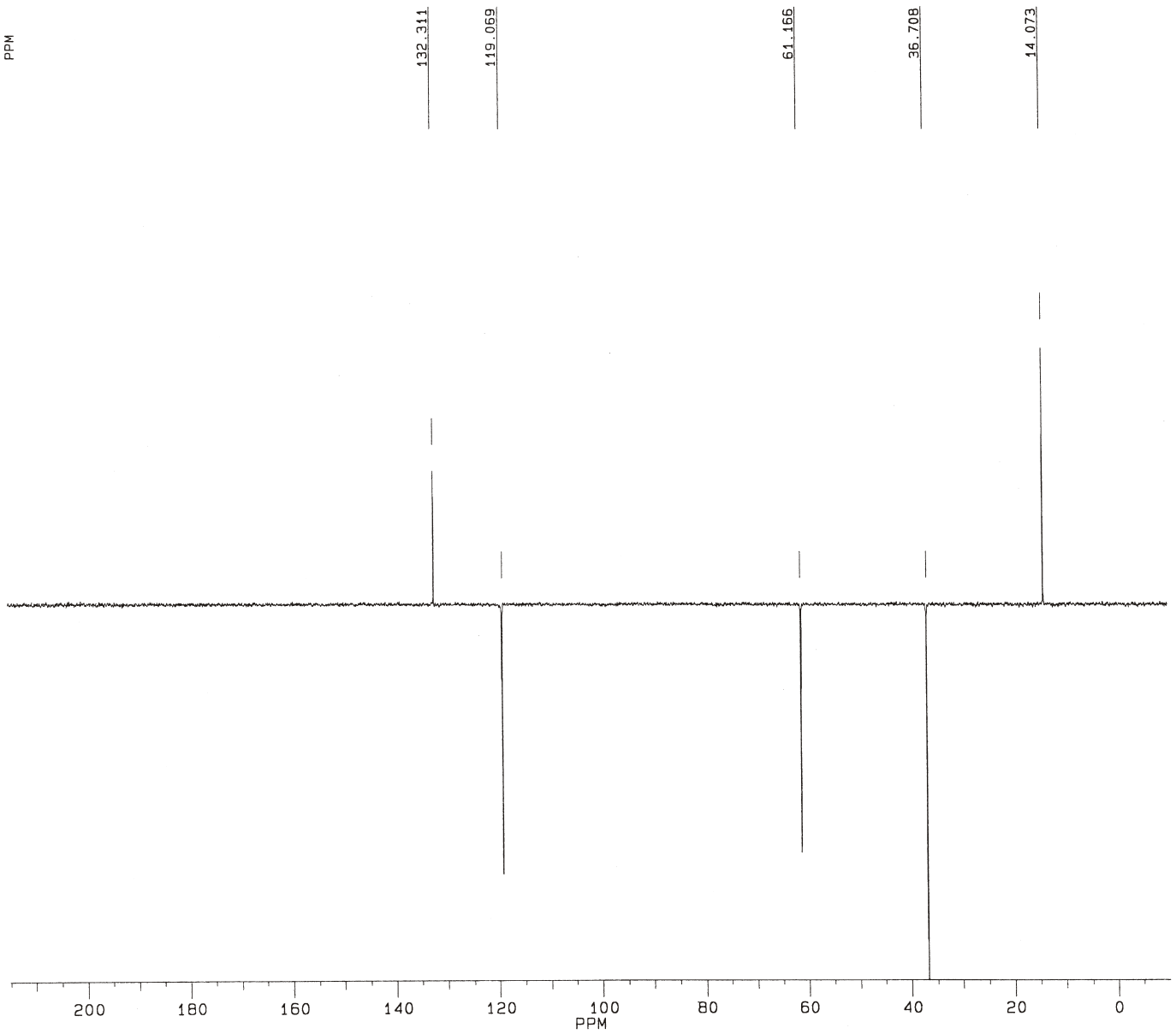
SF 62.896
SY 62.0
O1 2400.000
SI 32768
TD 32768
SW 15625.000
HZ/PT .954

PW 0.0
RD 0.0
AQ 1.049
RG 200
NS 400
TE 297

FW 19600
O2 3980.000
DP 18H DO

LB 1.600
GB 0.0
CX 21.00
CY 14.00
F1 215.007P
F2 -9.992P
HZ/CM 673.884
PPM/CM 10.714
SR -4044.93

KELLI DIETHYL DIALLYLMALONATE CDCL3

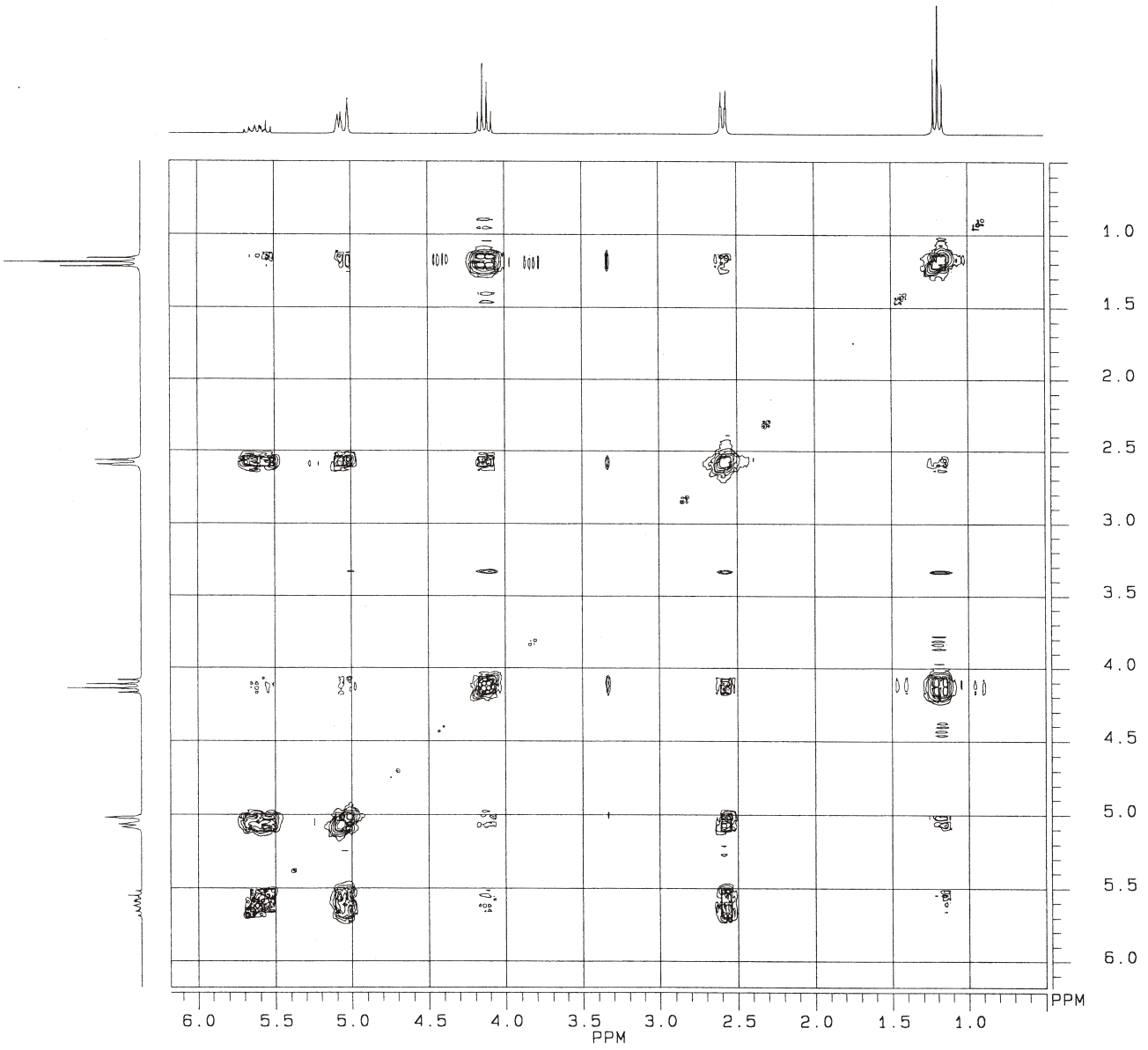


BRUKER

MA262S.112
AU PROG:
X09.AU
DATE 26-5-8

SF	62.896
SY	62.0
O1	2400.000
SI	32768
TD	32768
SW	15625.000
HZ/PT	.954
PW	0.0
RD	0.0
AQ	1.049
RG	200
NS	400
TE	297
FW	19600
O2	3980.000
DP	18H DO
LB	1.600
GB	0.0
CX	21.00
CY	7.00
F1	215.007P
F2	-9.992P
HZ/CM	673.884
PPM/CM	10.714
SR	-4044.93

KELLI DIETHYL DIALLYLMALONATE CDCL3

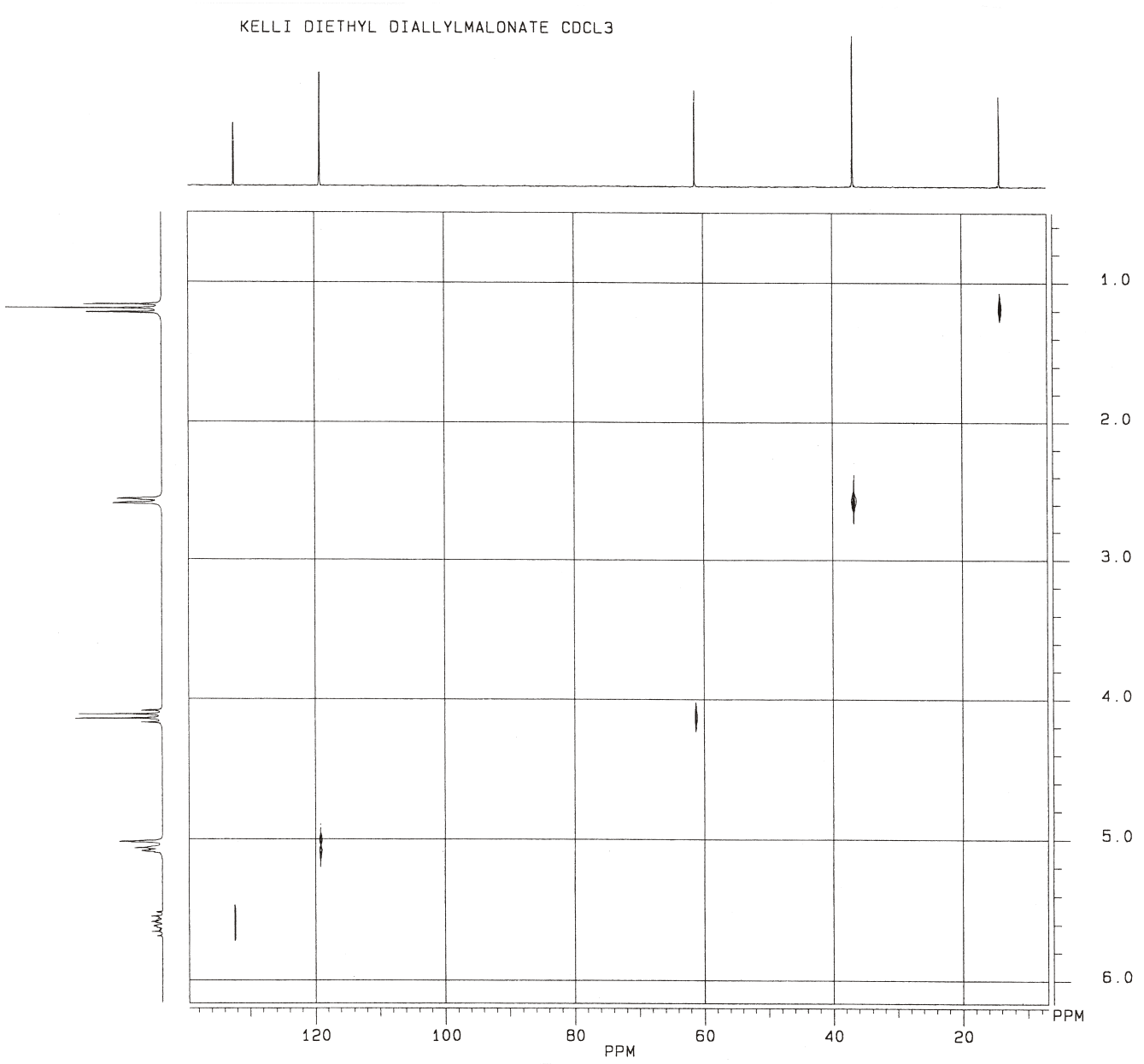


BRUKER

MA264112.SMX
F1 PROJ:
PROJH1.001
F2 PROJ:
PROJH1.001
AU PROG:
Z27.AU
DATE 26-5-8

SI2	1024
SI1	512
SW2	1420.455
SW1	710.227
ND0	1

WDW2	S
WDW1	S
SSB2	0
SSB1	0
MC2	M
PLIM ROW:	
F1	6.176P
F2	.497P
AND COLUMN:	
F1	6.176P
F2	.497P
D1	1.8440000
P1	18.00
RGA	
RD	0.0
PW	0.0
DE	502.00
NS	8
DS	2
D0	.0000030
P3	9.00
NE	128
IN	.0007040



MA267112.SMX
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PROJH1.001
F2 PROJ:
PROJX.001
AU PROG:
Z28.AU
DATE 26-5-8

SI2	4096
SI1	512
SW2	8333.333
SW1	708.416
ND0	2

WDW2	G
WDW1	S
LB2	2.000
GB2	0.0
SSB1	10
MC2	M
PLIM ROW:	
F1	139.422
F2	6.928
AND COLUMN:	
F1	6.161
F2	.497

D1	.885000
S3	0H
P1	20.00
D0	.000003
P6	11.80
D2	.003450
P5	5.90
D4	.001720
S2	18H
RGA	
RD	0.0
PW	0.0
DE	87.70
NS	16
DS	2
P9	100.00
NE	128
IN	.000352