

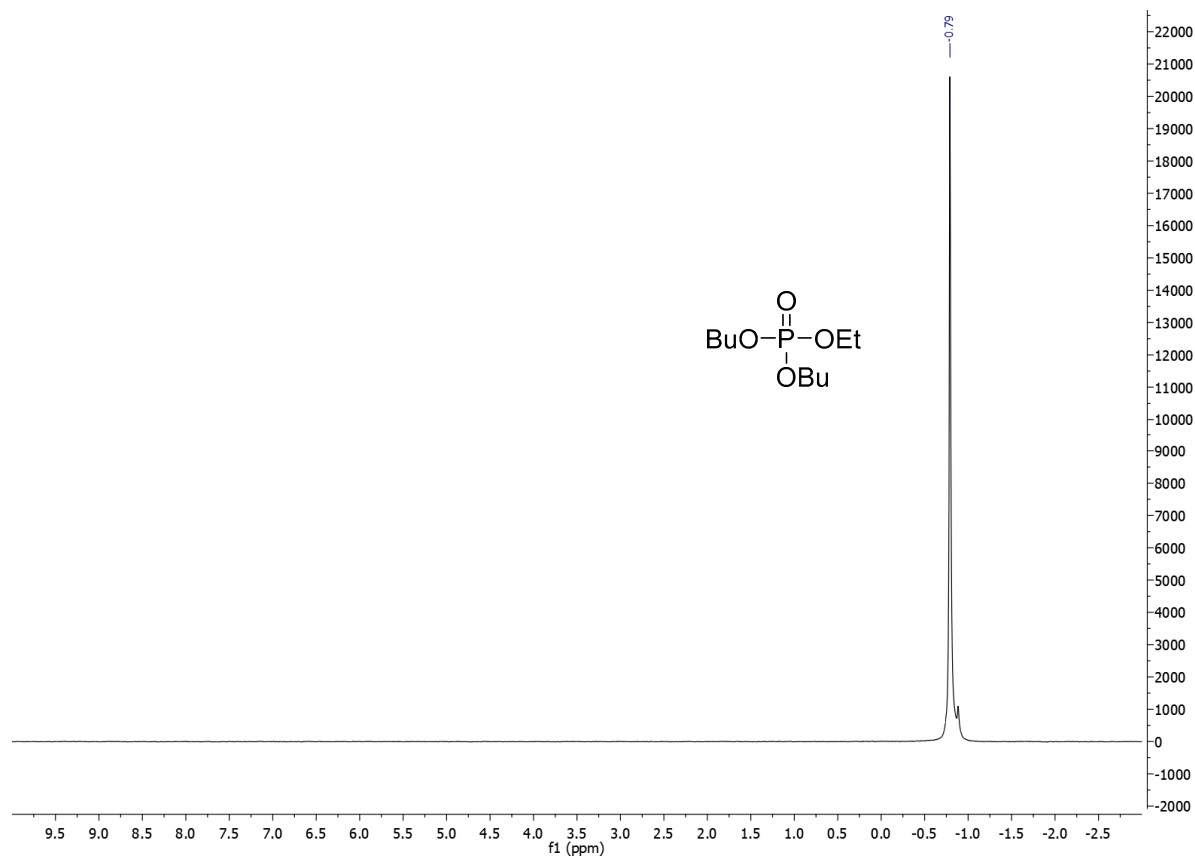
# Supporting Information

## A Theoretical Study on the Direct Esterification of Monoalkylphosphates and Dialkylphosphates; The Conversion of the Latter Species to Trialkylphosphates by Alkylating Esterification

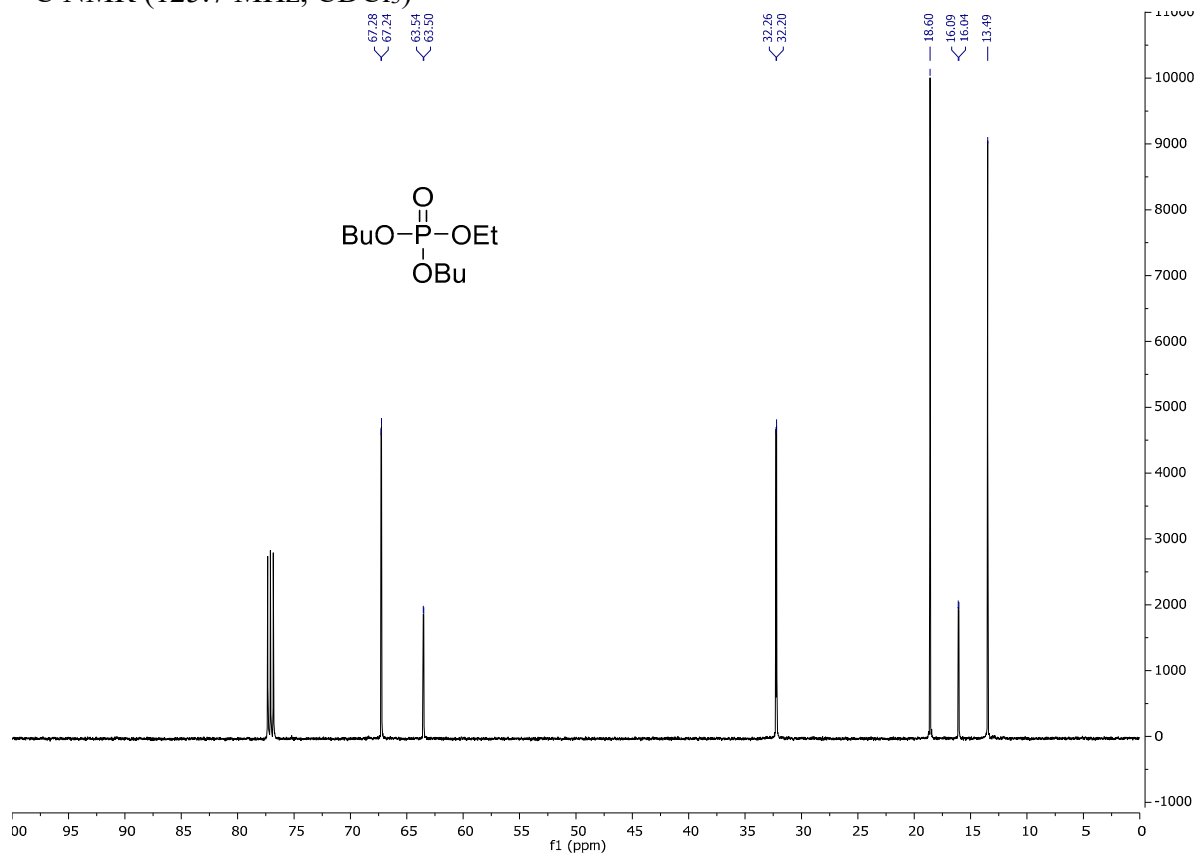
Péter Ábrányi-Balogh, Nikoletta Harsági, László Drahos and György Keglevich \*

### Content

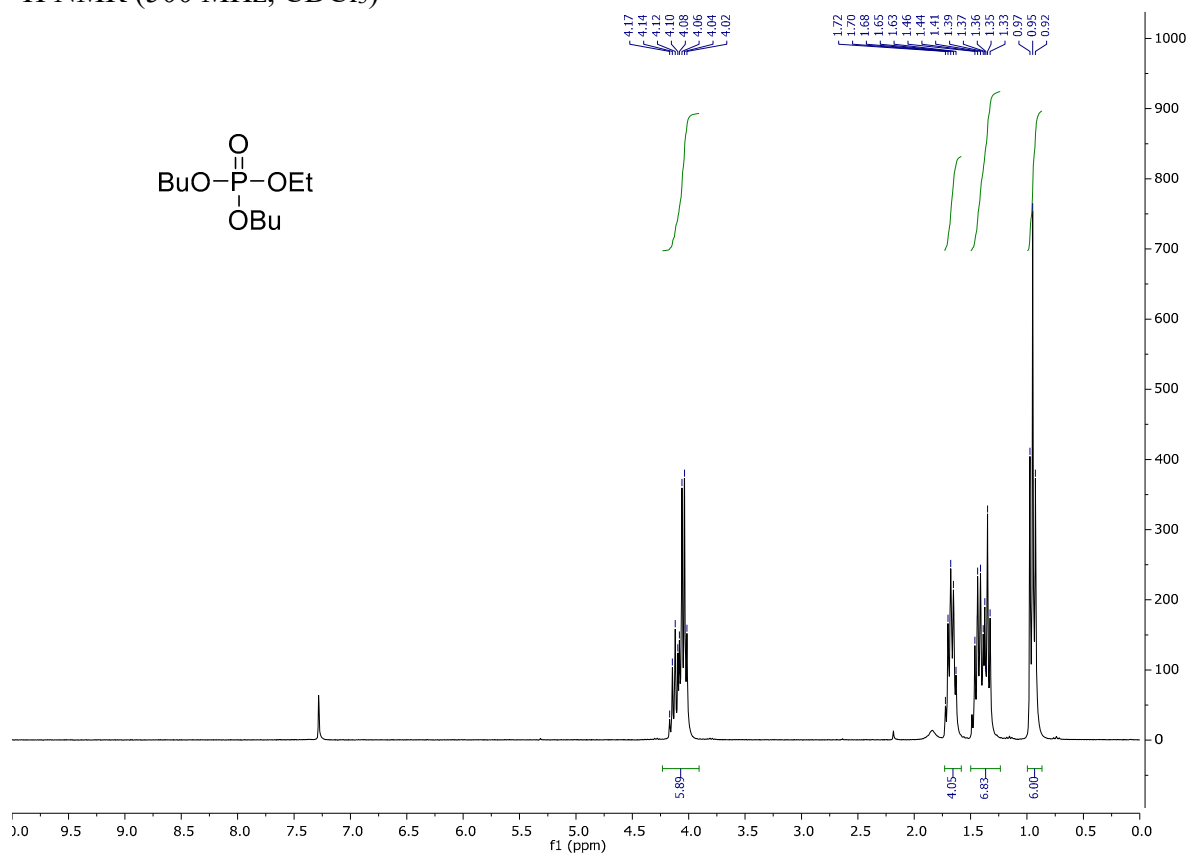
<b><sup>31</sup>P, <sup>13</sup>C and <sup>1</sup>H NMR spectra for the products (in CDCl<sub>3</sub>).....</b>	<b>2</b>
<i>Dibutyl-ethylphosphate (7a)</i> .....	2
<i>Dibutyl-propylphosphate (7b)</i> .....	4
<i>Dibutyl-isopropylphosphate (7c)</i> .....	6
<i>Dibutyl-pentylphosphate (7d)</i> .....	8
<i>Dipentyl-ethylphosphate (8a)</i> .....	10
<i>Dipentyl-propylphosphate (8b)</i> .....	12
<i>Dipentyl-isopropylphosphate (8c)</i> .....	14
<i>Dipentyl-butylphosphate (8d)</i> .....	16
<b>Computed raw data</b> .....	<b>18</b>
<b>Calculated data</b> .....	<b>18</b>
<b>XYZ geometries of computed species</b> .....	<b>19</b>

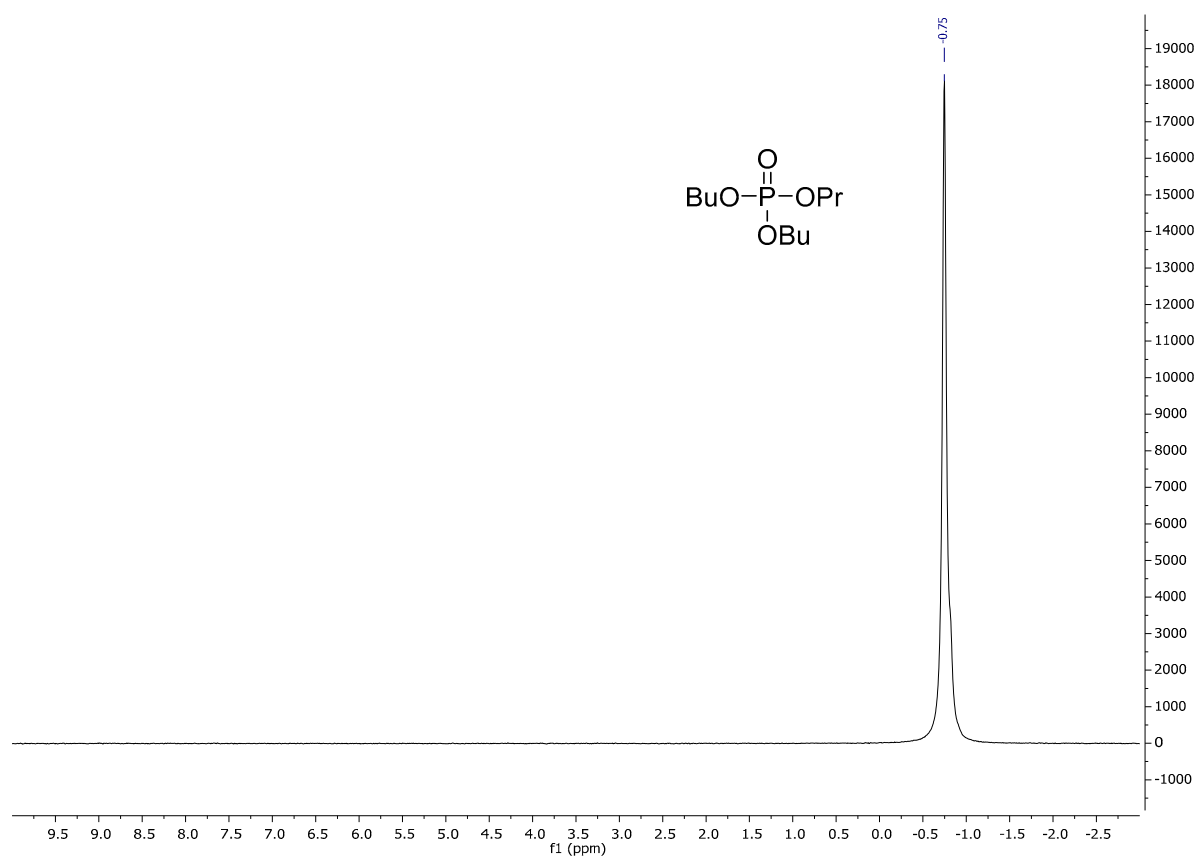
**$^{31}\text{P}$ ,  $^{13}\text{C}$  and  $^1\text{H}$  NMR spectra for the products (in  $\text{CDCl}_3$ )*****Dibutyl-ethylphosphate (7a)*** $^{31}\text{P}$  NMR (202.4 MHz,  $\text{CDCl}_3$ )

$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ )

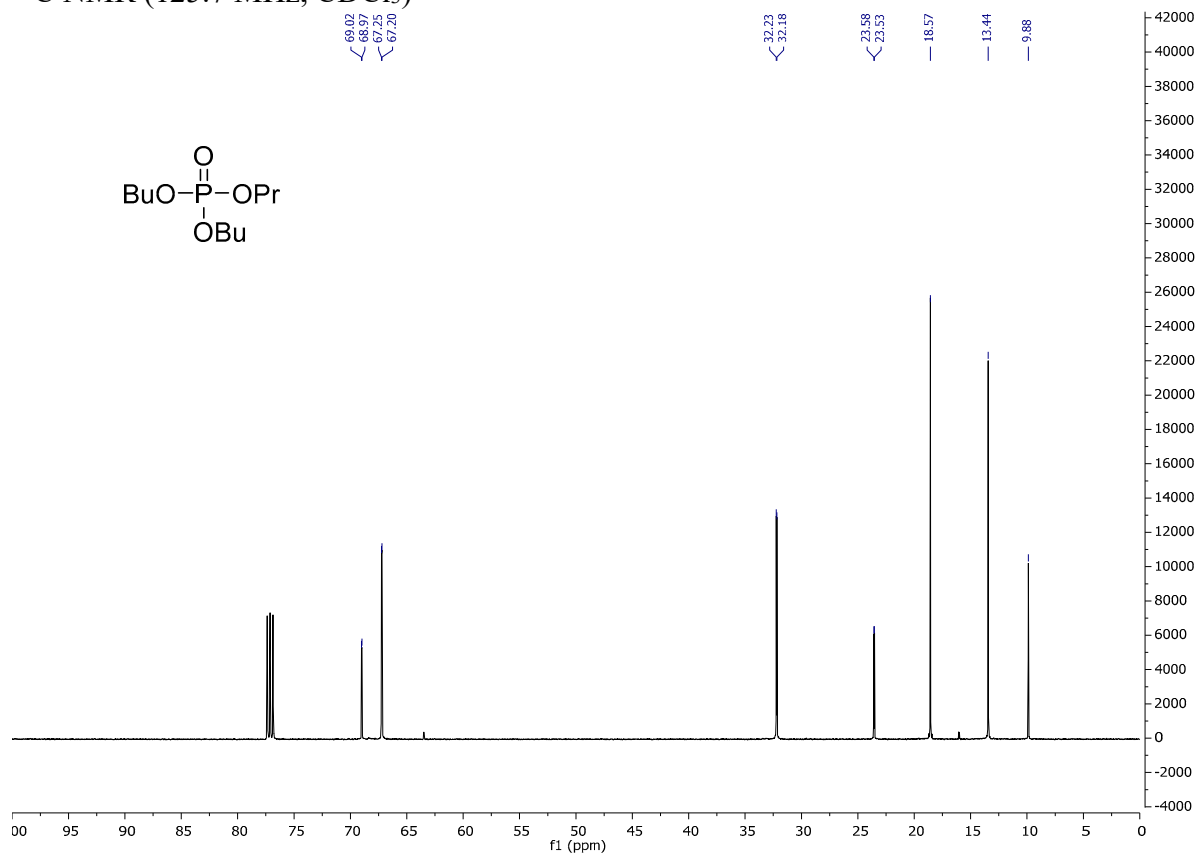


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

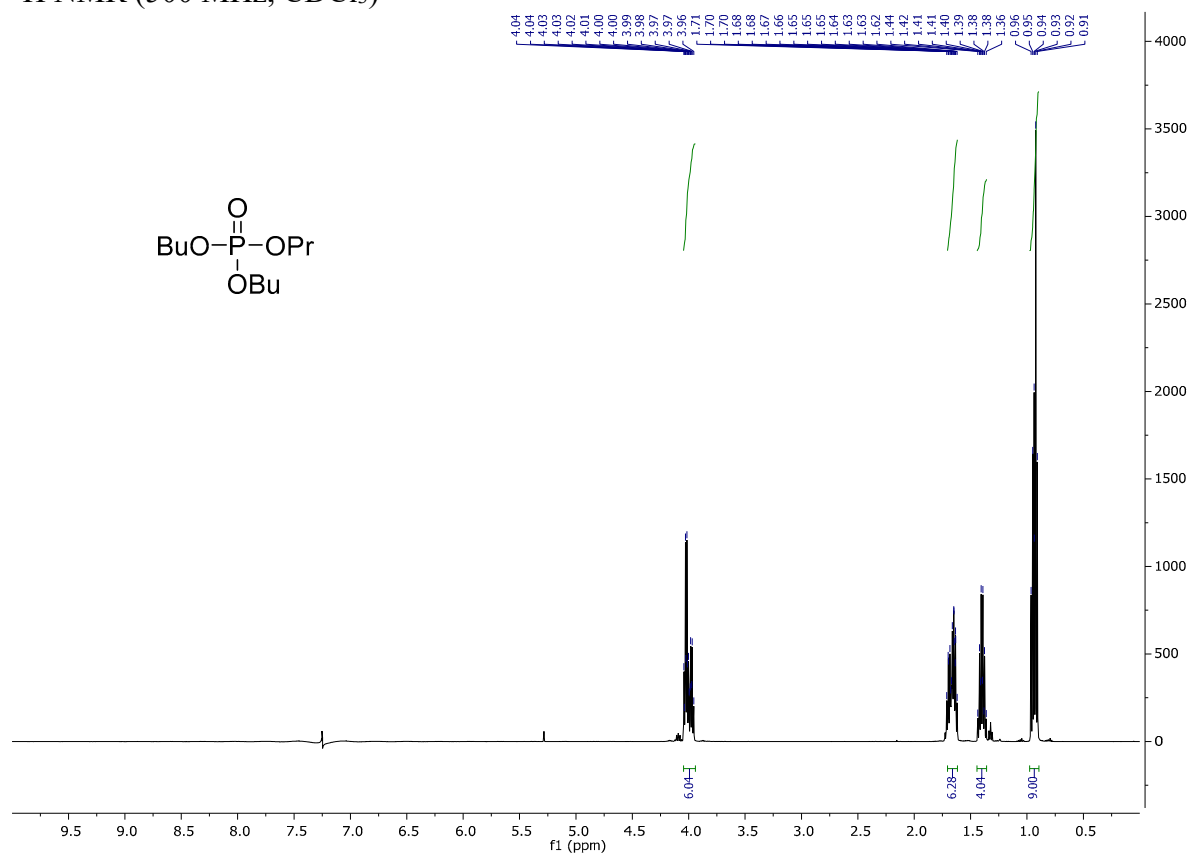


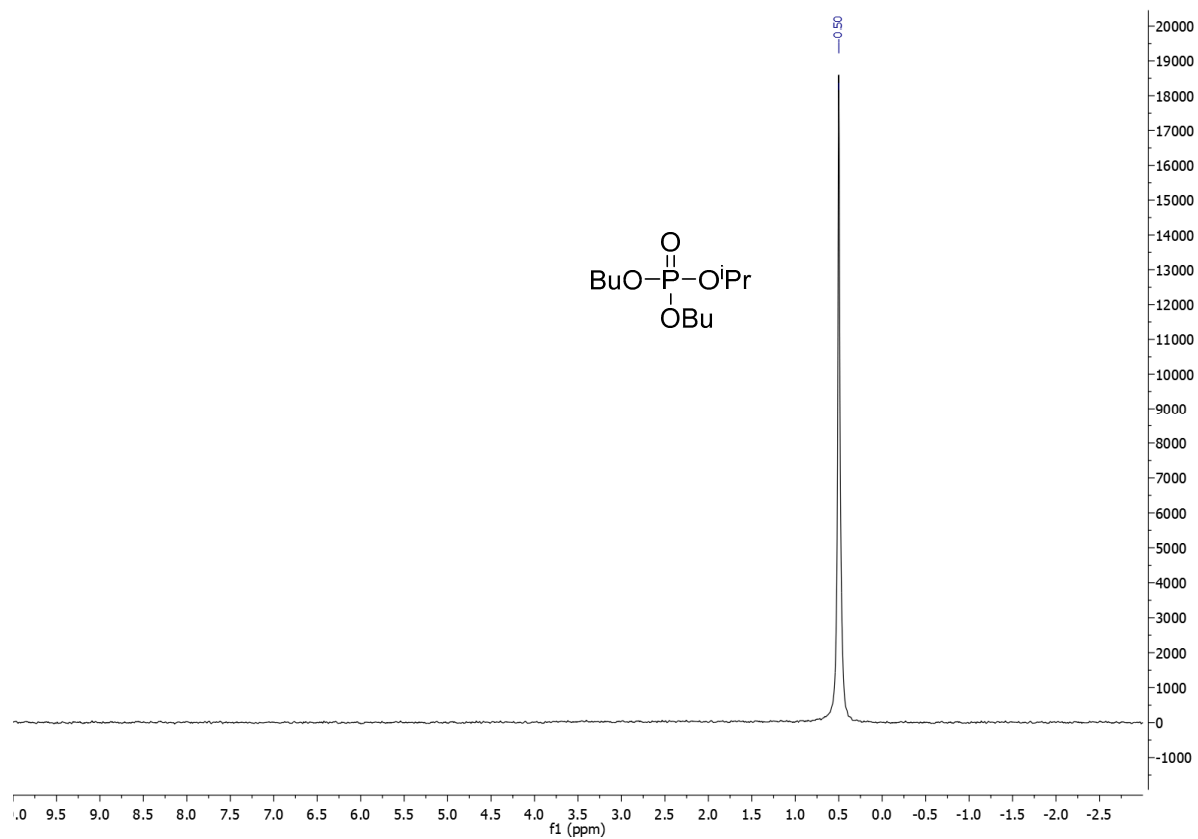
***Dibutyl-propylphosphate (7b)***<sup>31</sup>P NMR (202.4 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ )

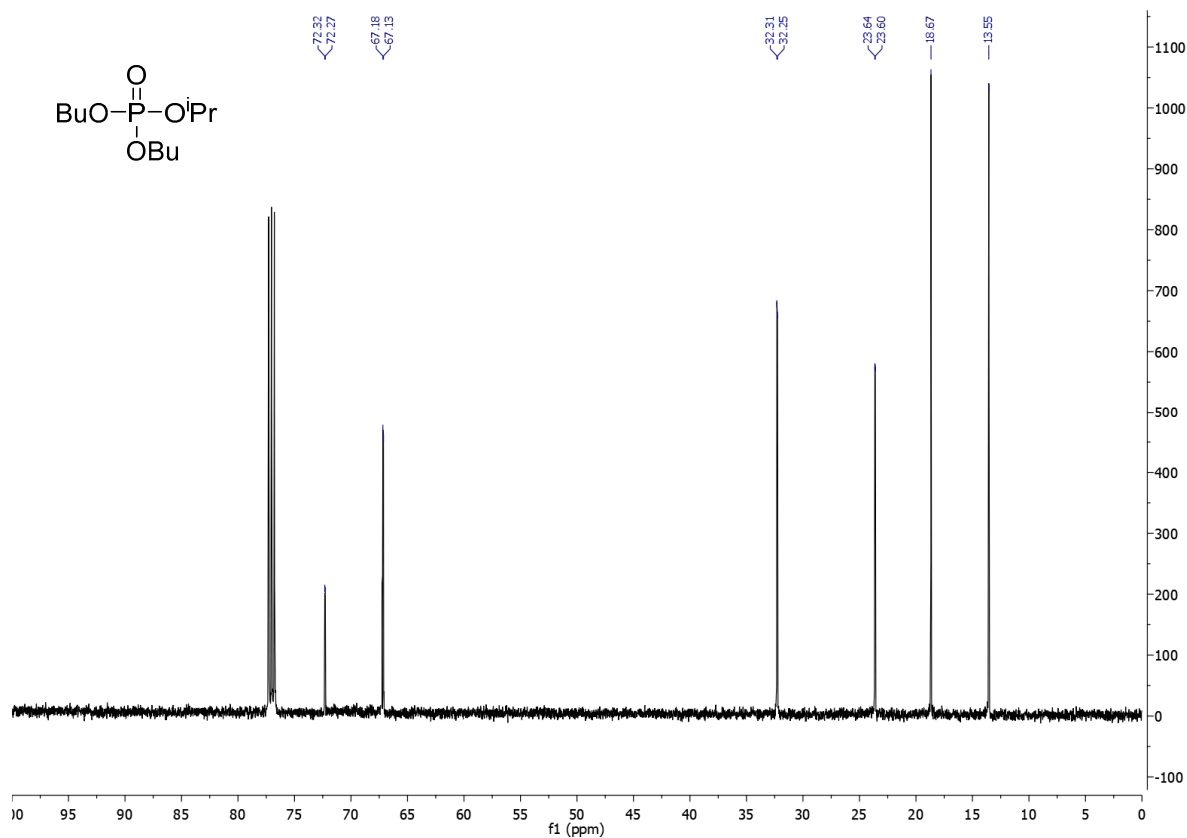


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

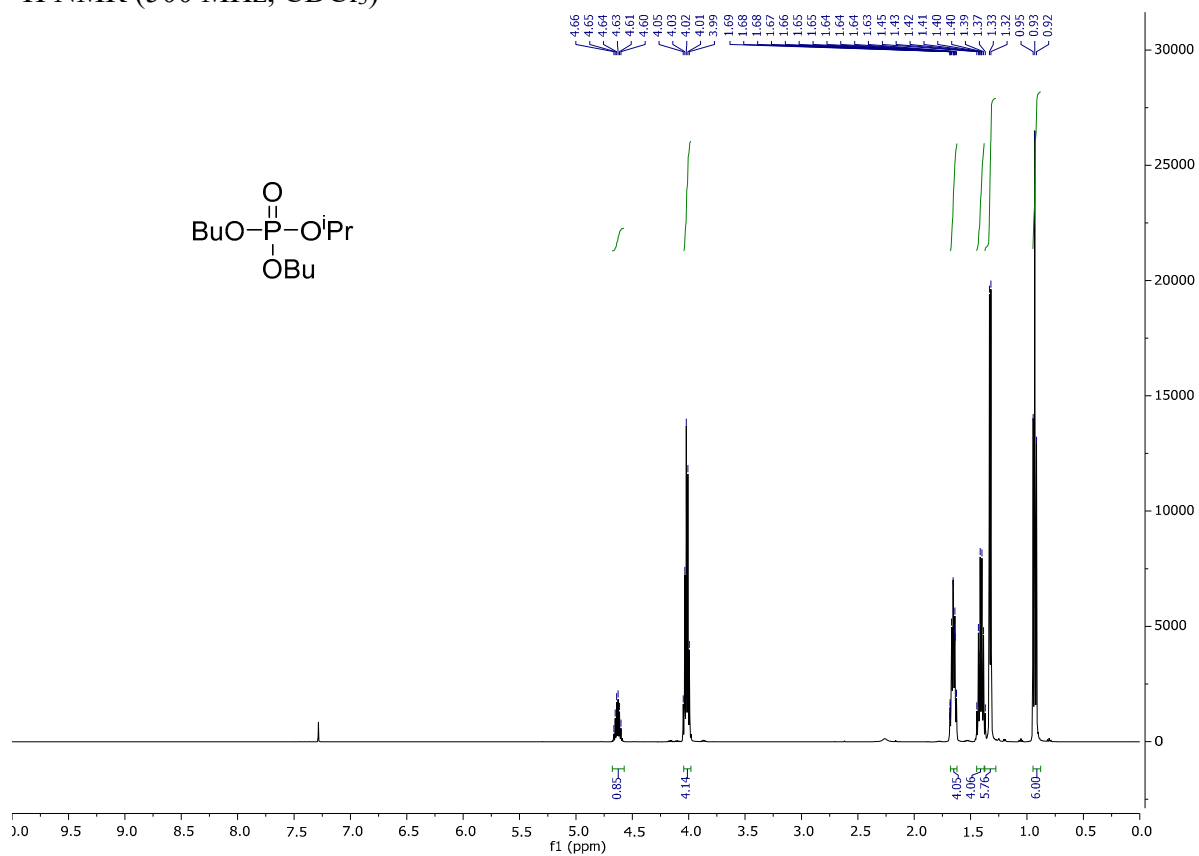


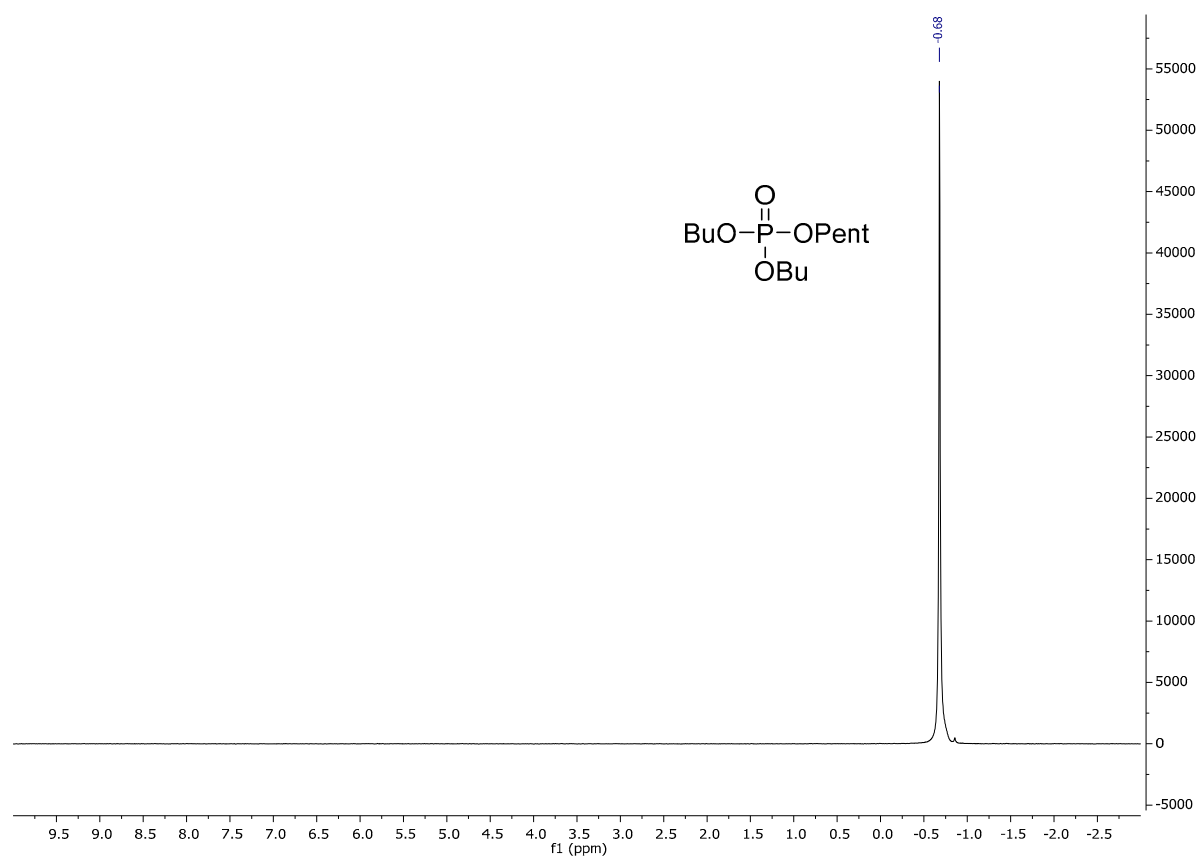
***Dibutyl-isopropylphosphate (7c)***<sup>31</sup>P NMR (202.4 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ )



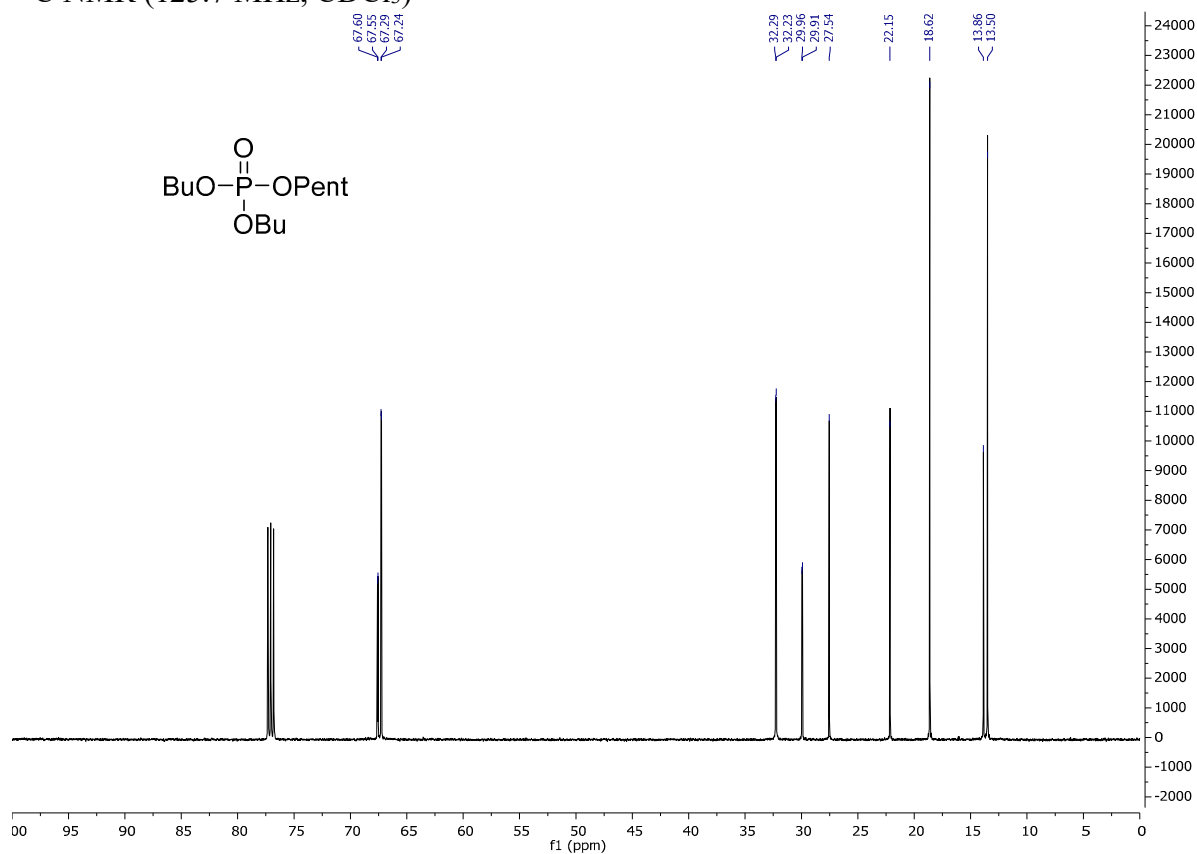
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



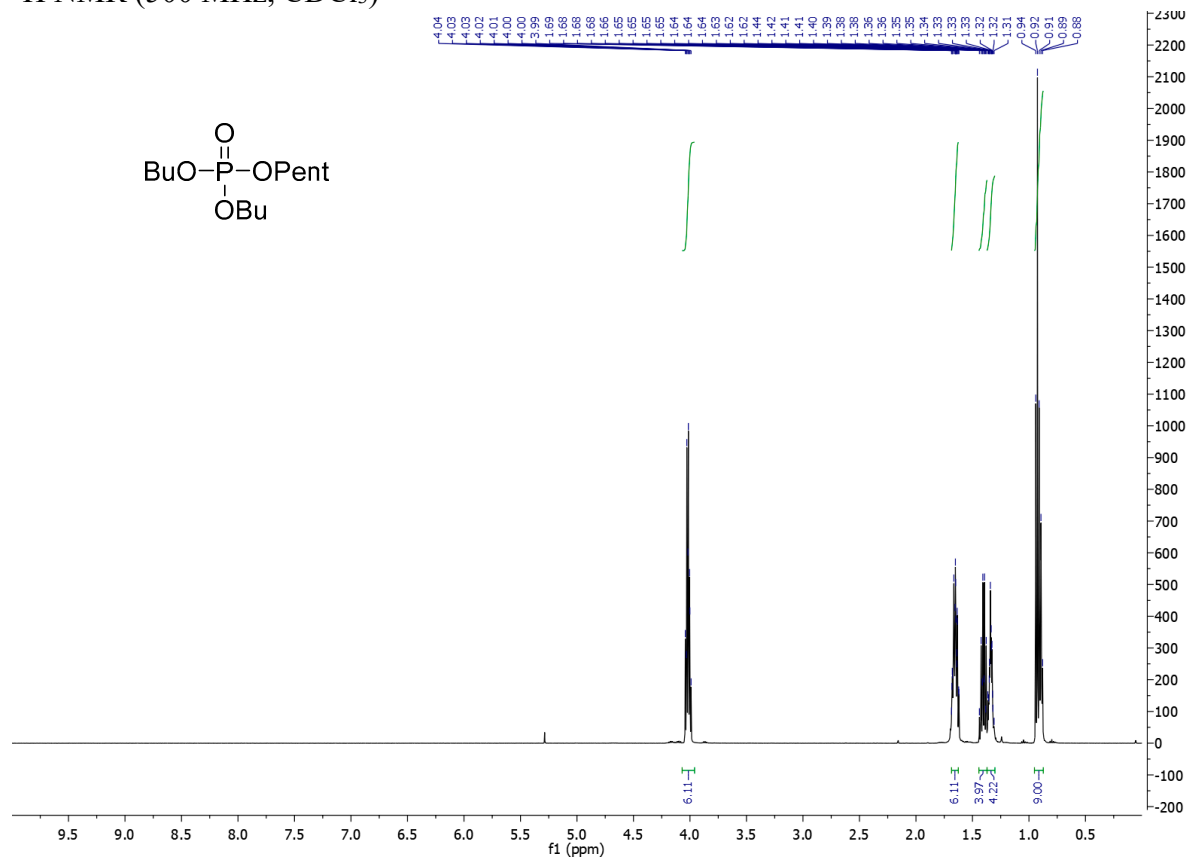
***Dibutyl-pentylphosphate (7d)***<sup>31</sup>P NMR (202.4 MHz, CDCl<sub>3</sub>)

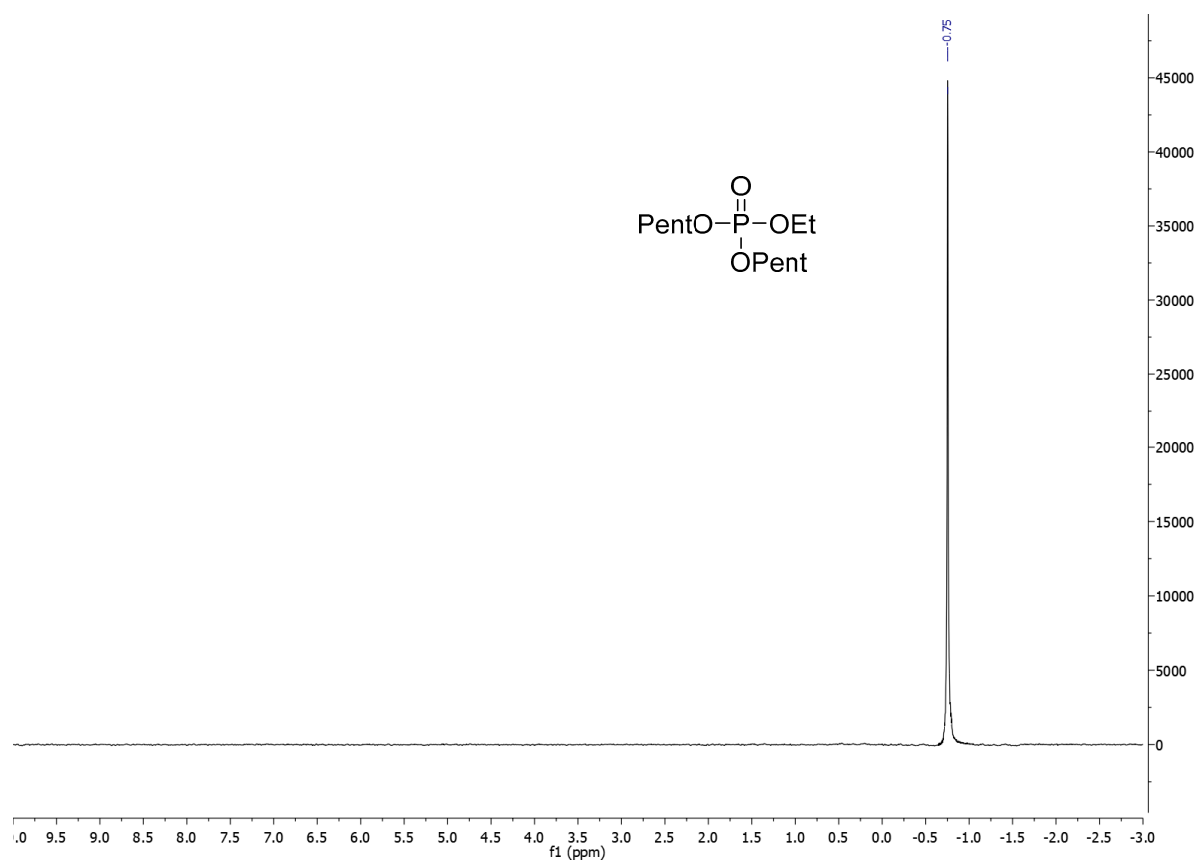


$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ )

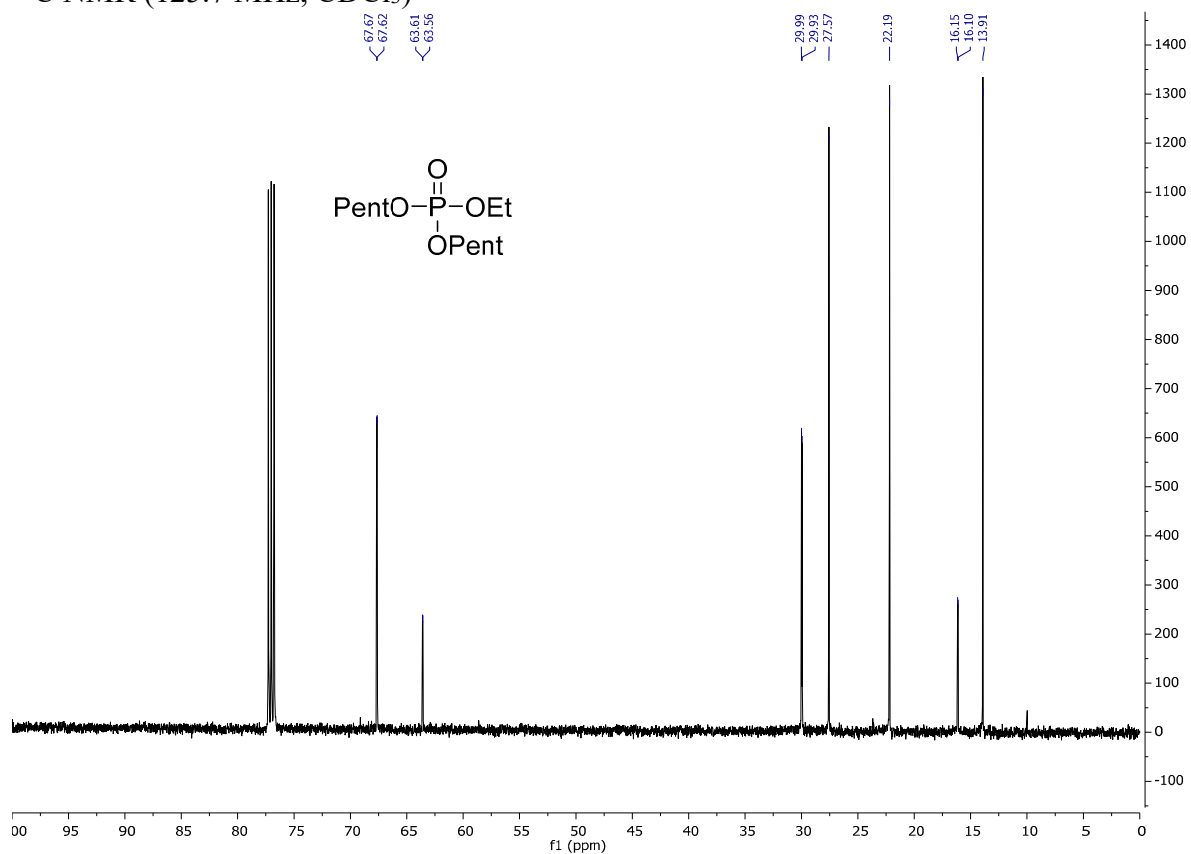


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

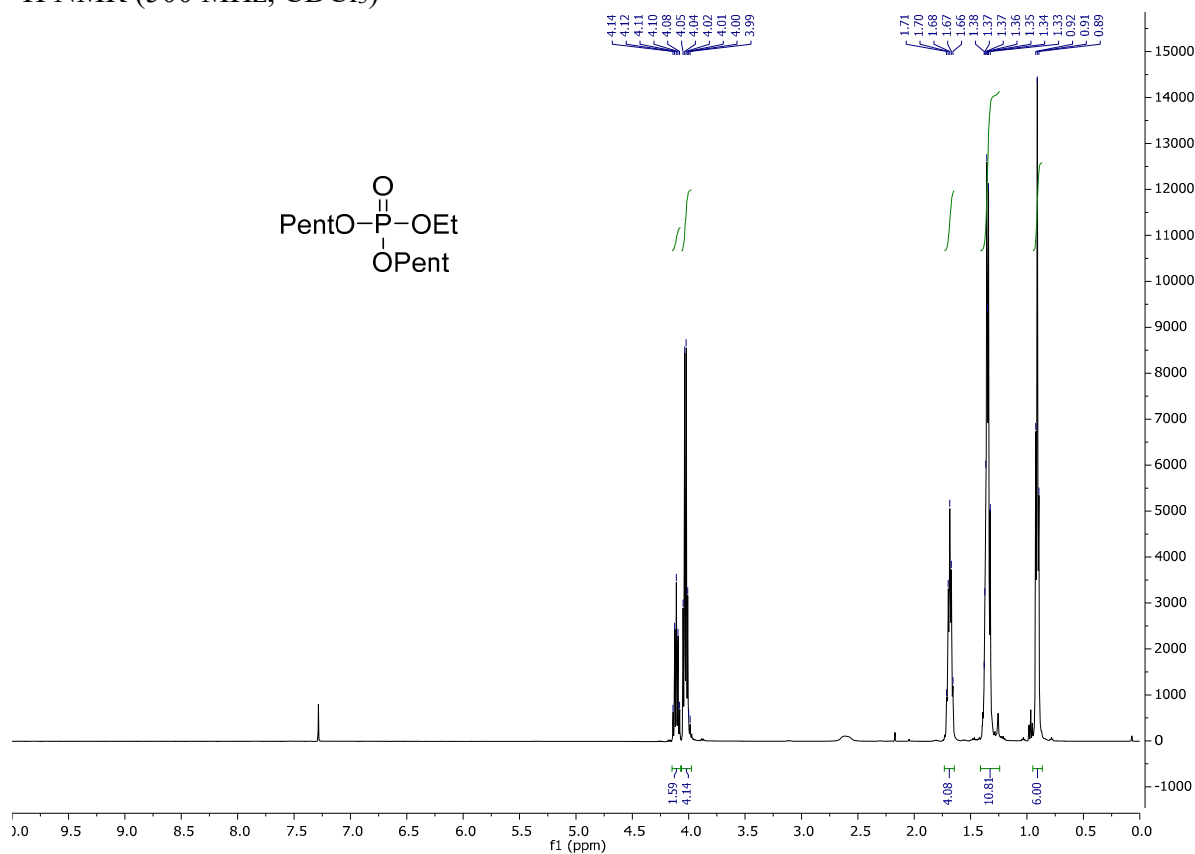


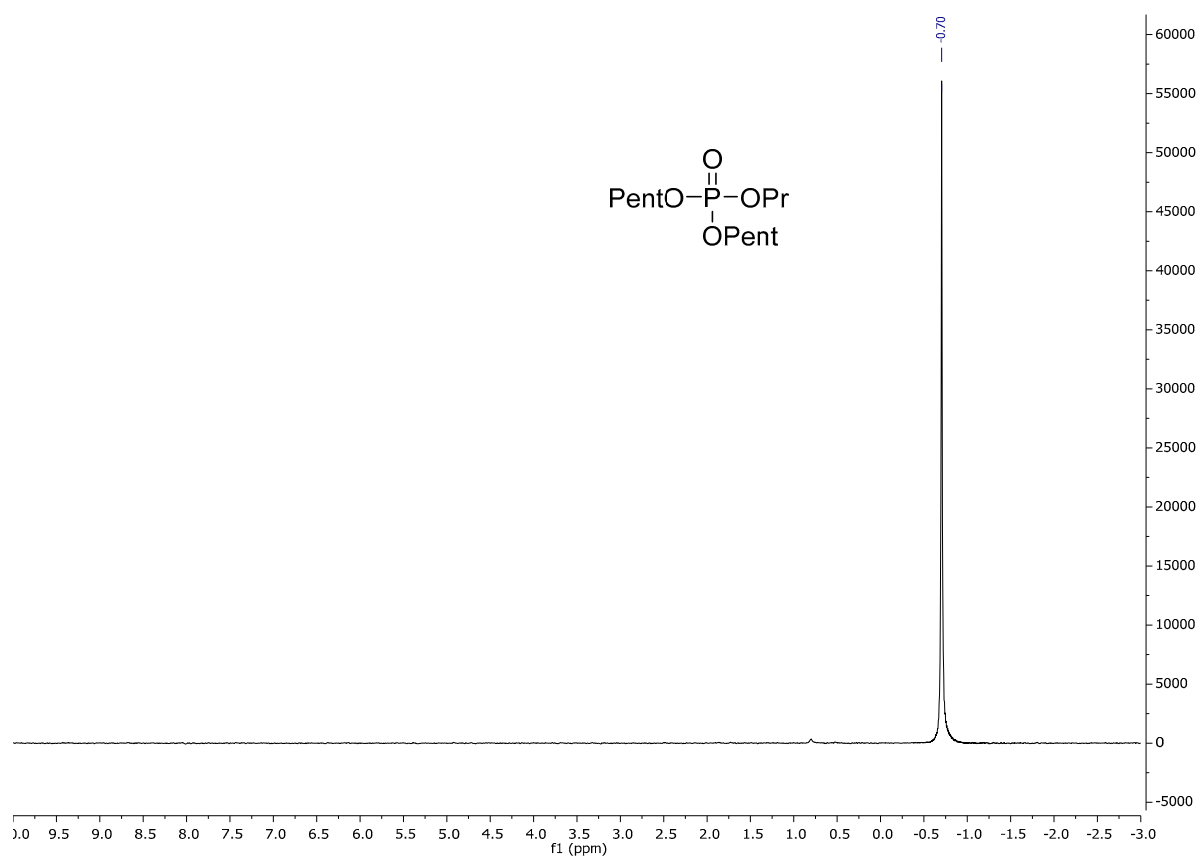
***Dipentyl-ethylphosphate (8a)***<sup>31</sup>P NMR (202.4 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ )

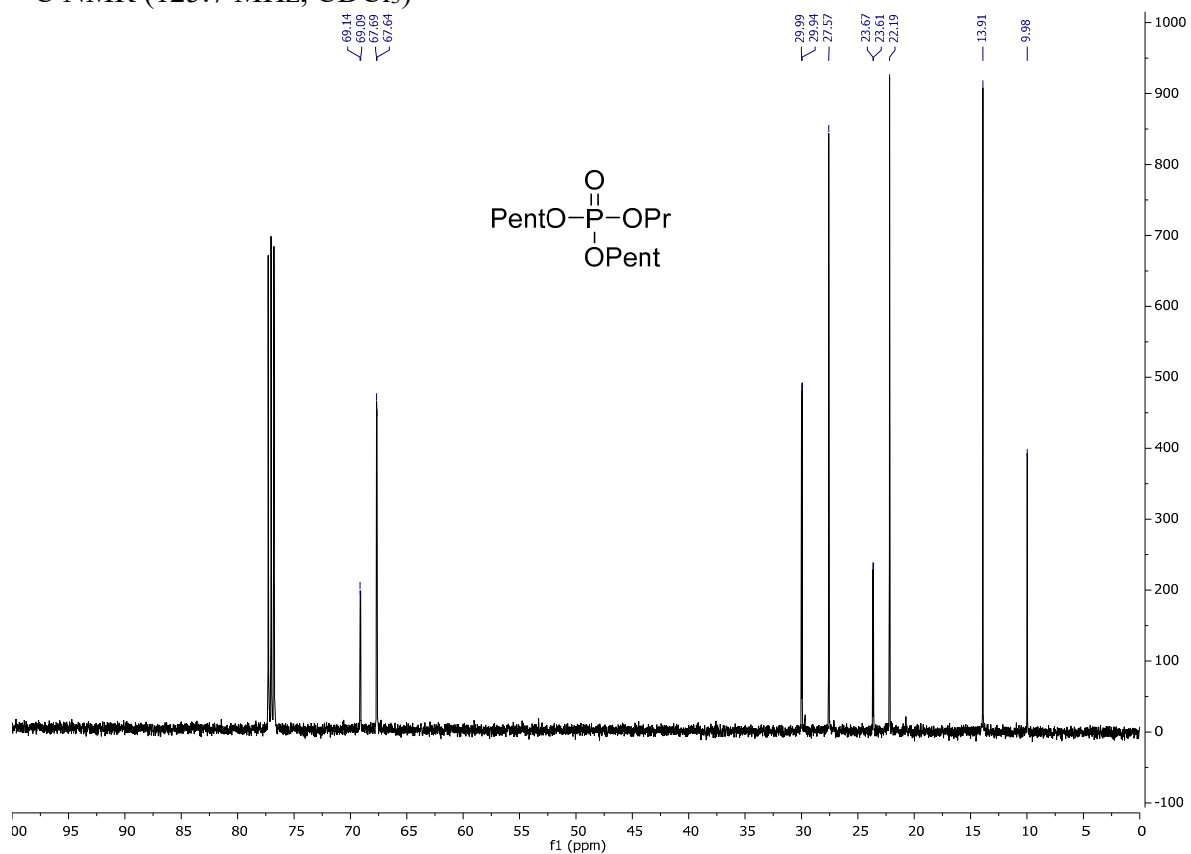


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

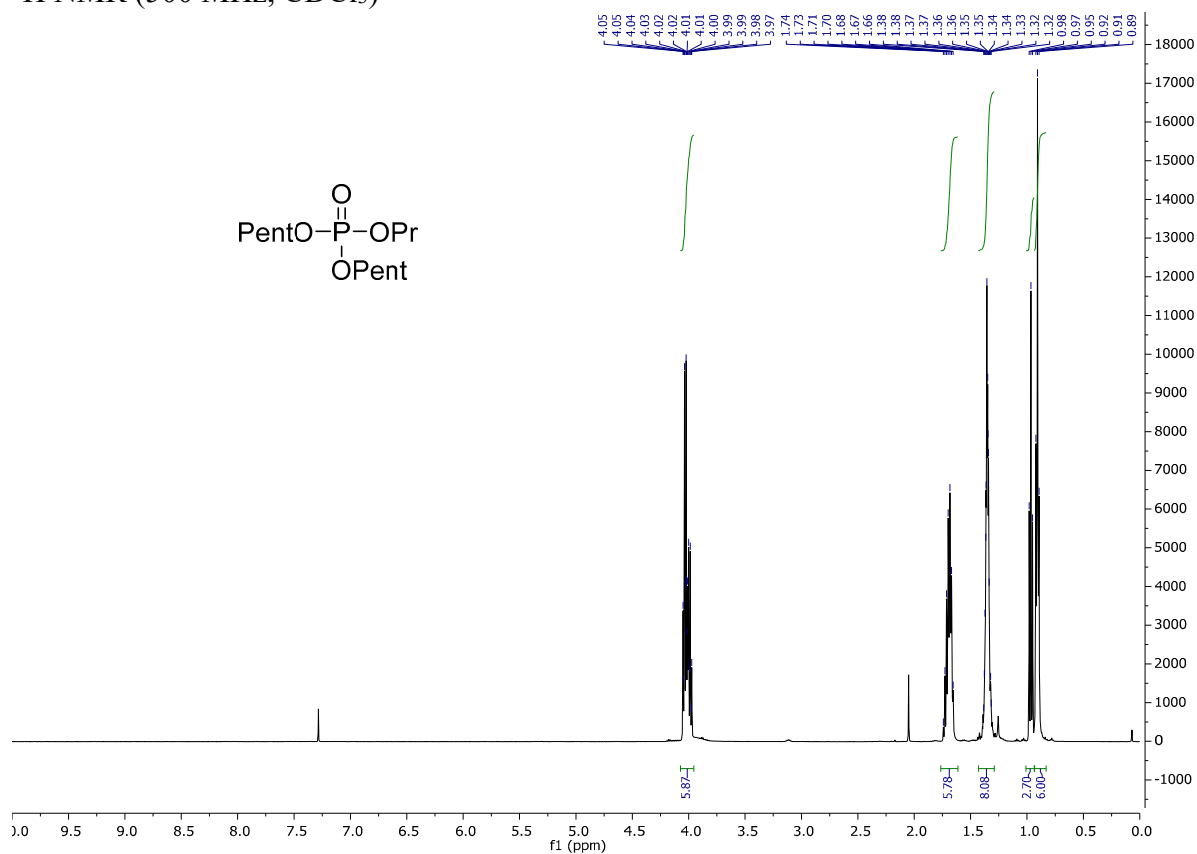


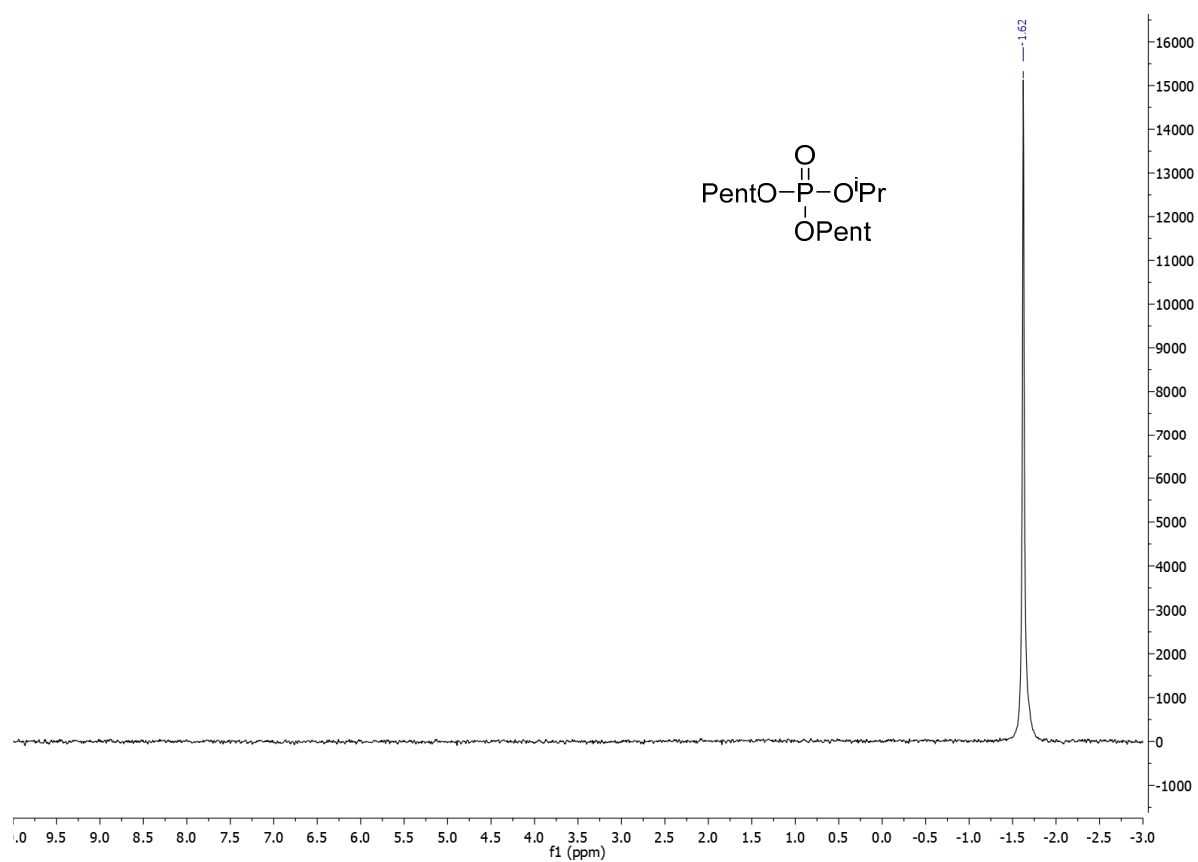
***Dipentyl-propylphosphate (8b)***<sup>31</sup>P NMR (202.4 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ )

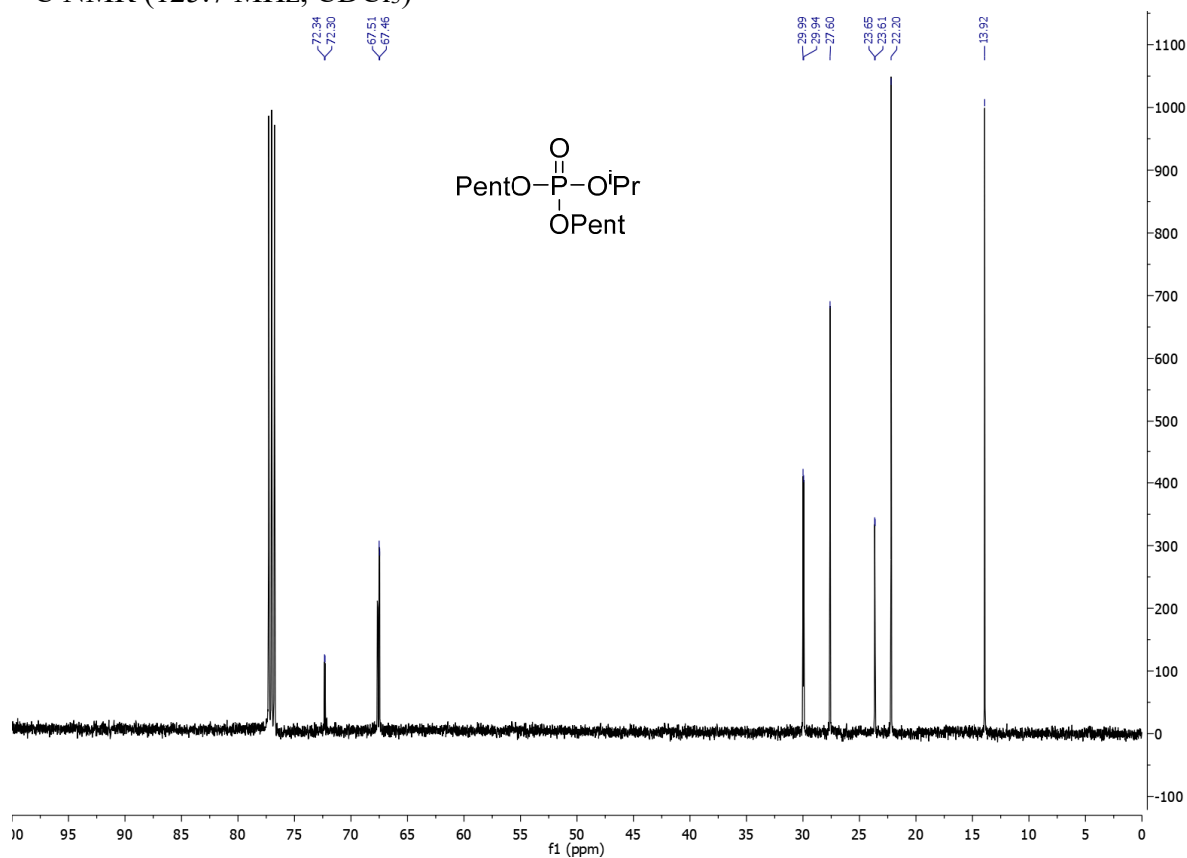


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

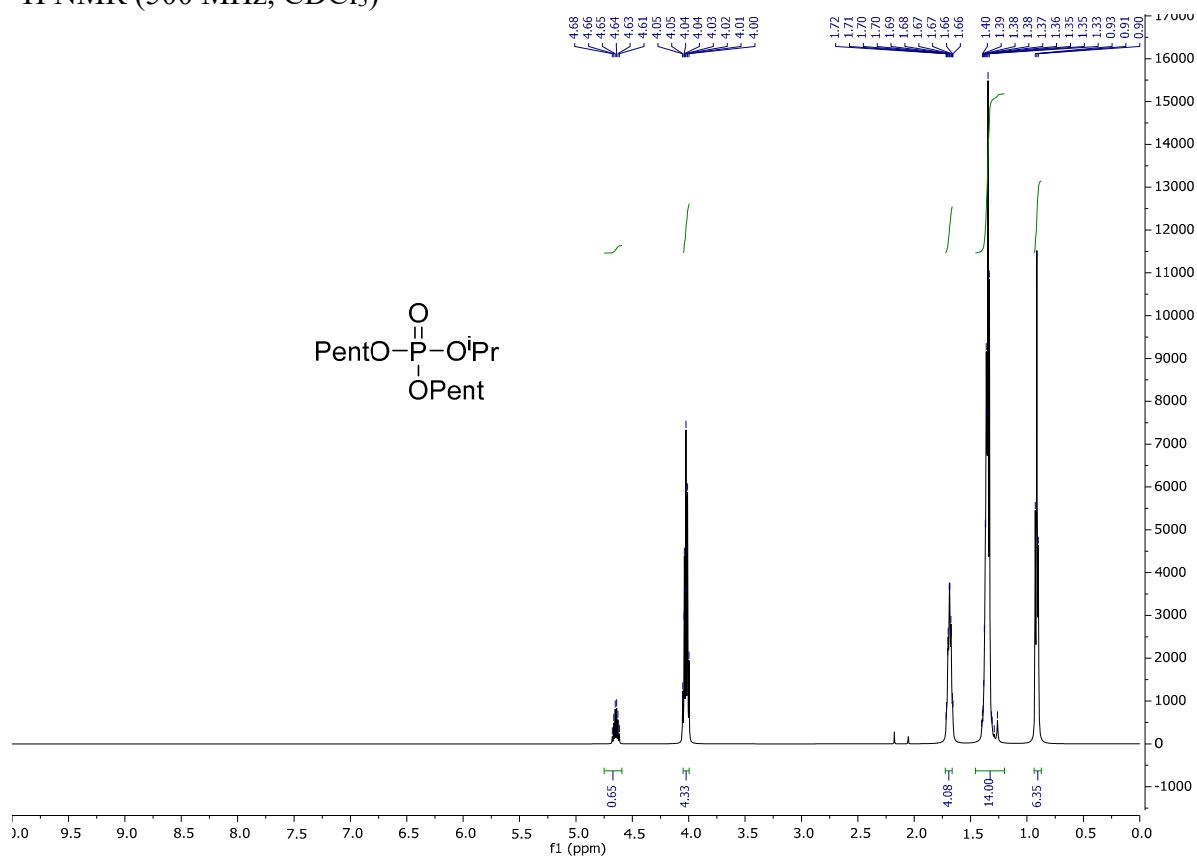


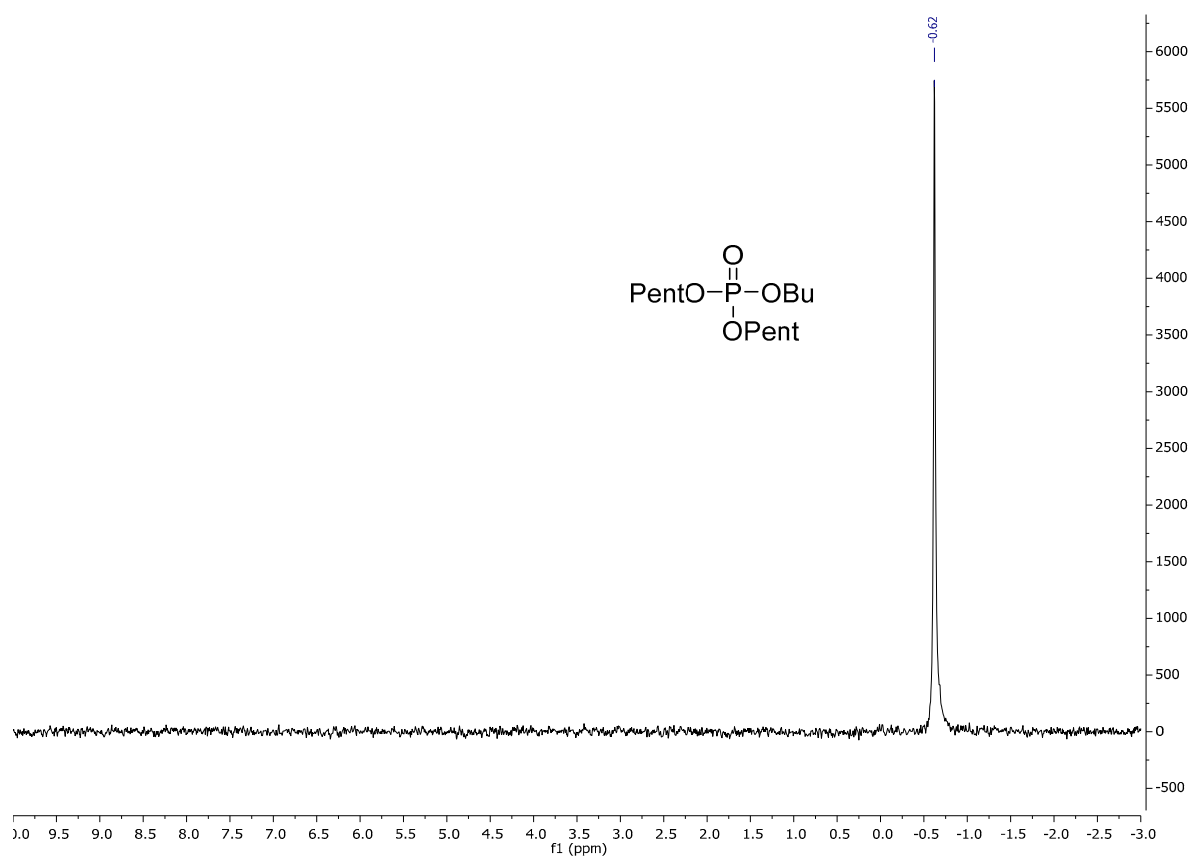
***Dipentyl-isopropylphosphate (8c)***<sup>31</sup>P NMR (202.4 MHz, CDCl<sub>3</sub>)

$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ )

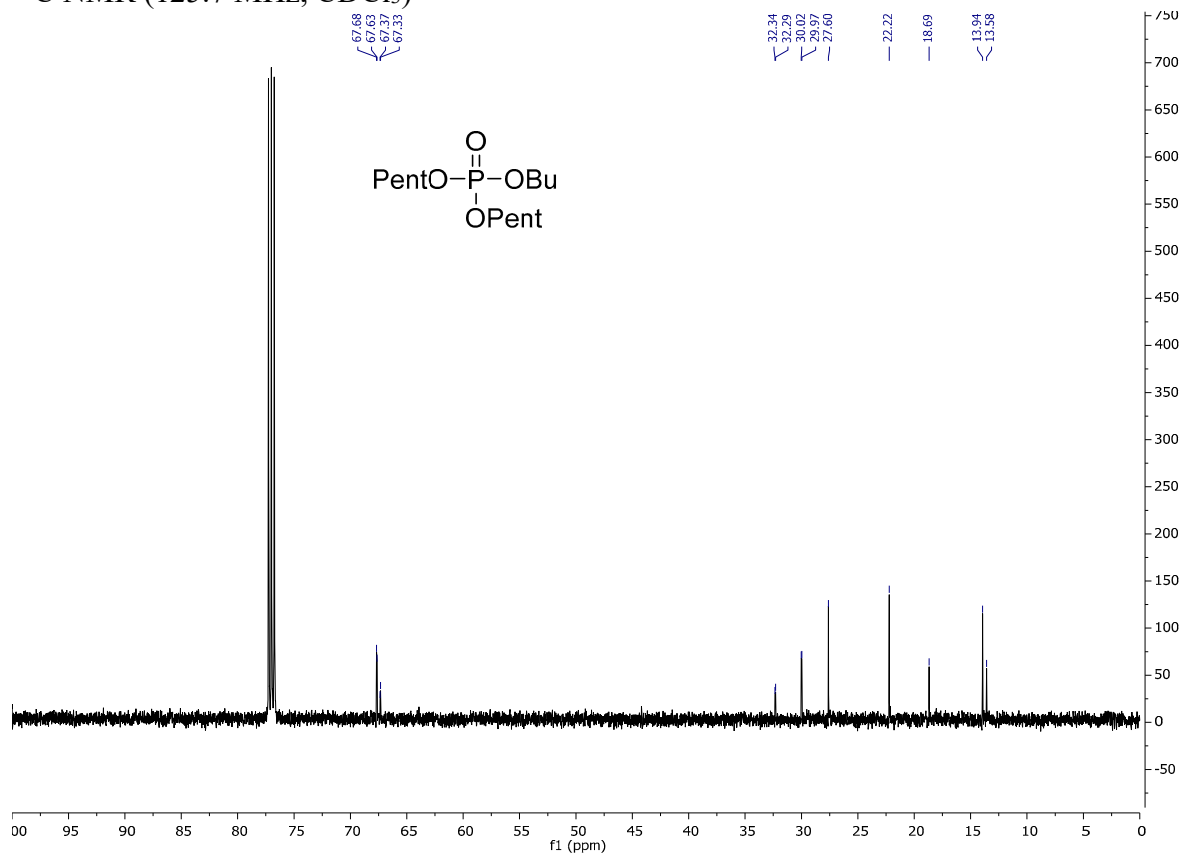
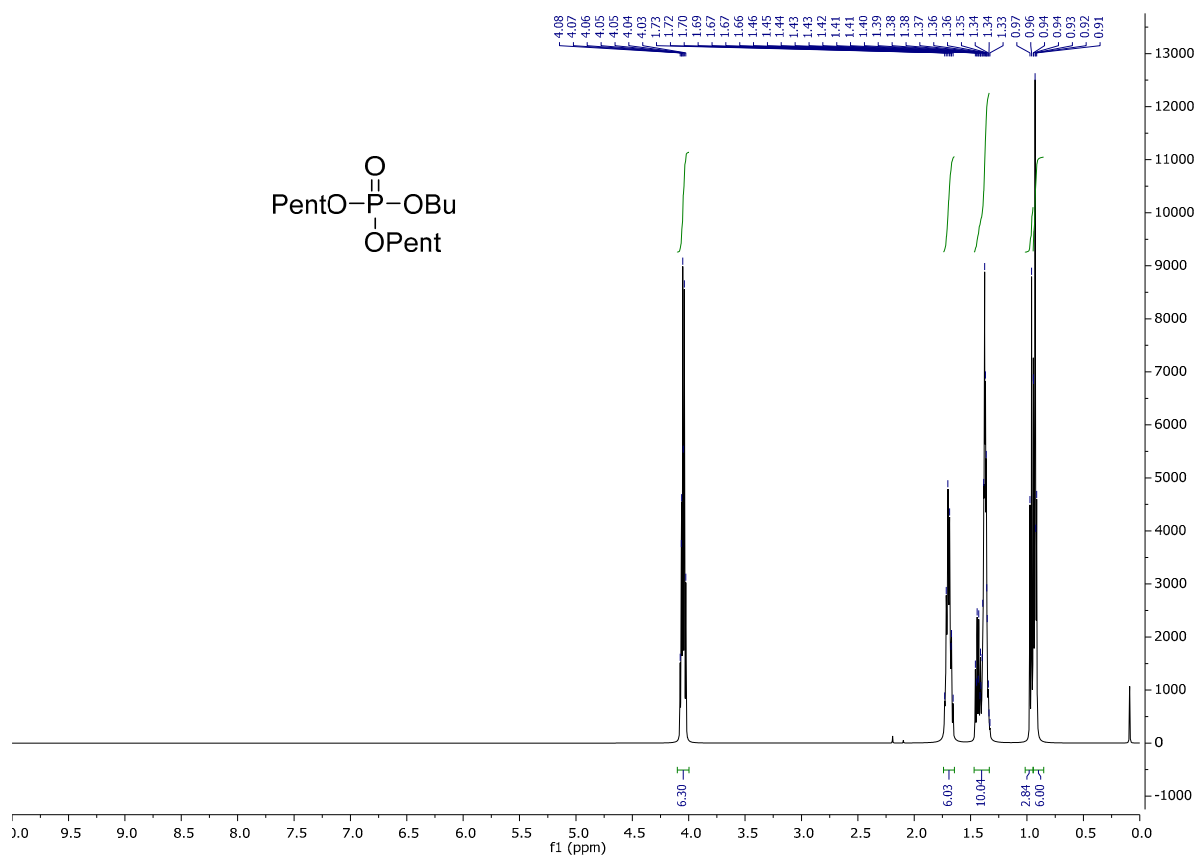


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



***Dipentyl-butylphosphate (8d)***<sup>31</sup>P NMR (202.4 MHz, CDCl<sub>3</sub>)



$^{13}\text{C}$  NMR (125.7 MHz,  $\text{CDCl}_3$ ) $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

## Computed raw data

**Table S1.** Computed energies (E), zero point energies, internal energies (U), enthalpies (H) and Gibbs free energies (G) given in Hartree as well as entropies (S) given in Cal mol<sup>-1</sup> K<sup>-1</sup> at M06-2X/6-311+G(d,p) basis set considering an SMD solvent method using the parameter set of the appropriate alcohols for small molecules.

R <sup>1</sup>	R <sup>2</sup>	Nr.	E	ZPE	U	H	G	S	S <sub>vib</sub>	Imaginary frequency
Et	OH	4	-1832.03936	-1831.63504	-1831.56924	-1831.56774	-1831.76164	257.2	175.1	
		TS1	-1832.00095	-1831.59698	-1831.53313	-1831.53163	-1831.71938	249.1	166.9	-404.8
		5	-1832.00210	-1831.59619	-1831.53164	-1831.53014	-1831.72058	252.6	170.6	
		TS2	-1831.97390	-1831.56989	-1831.50566	-1831.50416	-1831.69239	249.7	167.7	-274.26
		6	-1832.03718	-1831.63607	-1831.56876	-1831.56726	-1831.77024	269.3	186.8	
	Et	4	-1989.21851	-1988.70167	-1988.62204	-1988.62054	-1988.85118	306.0	222.5	
		TS1	-1989.16998	-1988.65756	-1988.58459	-1988.58310	-1988.79323	278.8	195.3	-435.19
		5	-1989.18797	-1988.66776	-1988.59145	-1988.58995	-1988.80168	280.9	197.7	
		TS2	-1989.14976	-1988.63259	-1988.55580	-1988.55431	-1988.77044	286.7	203.5	-1457
		6	-1989.21540	-1988.69712	-1988.61659	-1988.61509	-1988.84543	305.6	222.3	
Bu	OH	4	-2067.86444	-2067.28842	-2067.20432	-2067.20282	-2067.44100	316.0	231.4	
		TS1	-2067.82478	-2067.24984	-2067.16884	-2067.16735	-2067.39283	299.1	214.6	-583.24
		5	-2067.82883	-2067.25088	-2067.16737	-2067.16587	-2067.40208	313.4	228.8	
		TS2	-2067.79419	-2067.22143	-2067.14246	-2067.14096	-2067.36295	294.5	209.9	-268.25
		6	-2067.86565	-2067.29051	-2067.20601	-2067.20451	-2067.44532	319.5	234.8	
	Bu	4	-2382.26215	-2381.46013	-2381.34976	-2381.34826	-2381.65304	404.3	317.7	
		TS1	-2382.21612	-2381.41506	-2381.30855	-2381.30706	-2381.59759	385.4	298.8	-107.86
		5	-2382.22466	-2381.41944	-2381.31188	-2381.31038	-2381.60504	390.9	304.3	
		TS2	-2382.1973	-2381.39386	-2381.28544	-2381.28394	-2381.57748	389.4	302.9	-245.46
		6	-2382.25350	-2381.44981	-2381.33899	-2381.33749	-2381.63956	400.7	314.3	

## Calculated data

**Table S2.** Calculated  $\Delta G$  and  $\Delta S$  values in kJ mol<sup>-1</sup> and J mol<sup>-1</sup> K<sup>-1</sup>, respectively.

R <sup>1</sup>	R <sup>2</sup>	Nr.	2*(1/2) + 2 MeOH	4	TS1	5	TS2	6	2/3 + 1/2 + H <sub>2</sub> O + 2 MeOH
Et	OH	$\Delta G$	0.0	165.6	276.5	265.4	339.3	143.0	-4.9
		$\Delta S$	0.0	348.3	313.8	329.2	317.0	397.1	34.3
	Et	$\Delta G$	0.0	158.1	310.1	280.0	369.9	181.1	7.4
		$\Delta S$	0.0	395.0	281.3	291.2	315.7	394.3	17.2
Bu	OH	$\Delta G$	0.0	159.1	285.4	253.3	355.9	147.8	-7.8
		$\Delta S$	0.0	375.2	305.0	364.2	147.8	389.5	42.5
	Bu	$\Delta G$	0.0	156.3	301.8	274.3	346.6	191.7	-15.4
		$\Delta S$	0.0	439.7	360.9	383.7	377.7	425.7	71.4

## XYZ geometries of computed species

R = Et, OH, monoalkylation

4

P	2.00738600	-0.29008500	0.49584900
P	-1.56068400	1.25114800	-0.88786000
O	1.13200200	3.09905000	0.35254200
H	0.22853100	3.07490100	-0.03495000
O	-3.38466100	-1.49505800	-0.72833800
H	-2.46895500	-1.85718000	-0.77908500
O	-0.91831500	-2.50019800	-0.52148600
H	-0.31148400	-2.04938300	0.09510100
O	1.22333600	-1.49965400	0.85006200
O	-1.22260000	2.70351700	-0.91293300
O	3.57978400	-0.52576400	0.51987400
O	1.81878900	0.96620400	1.38603500
H	1.49640200	1.86545800	0.93691200
O	1.67063800	0.13109800	-1.02810400
H	2.32664000	0.70714800	-1.45180600
O	-3.09308500	0.98888800	-1.06417400
H	-3.31129000	-0.01211200	-0.94385500
O	-0.87601800	0.35922200	-2.00565200
O	-1.07520200	0.52749000	0.44721500
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C	-0.14242000	-2.95586600	-1.62506300
C	4.11669100	-1.75899400	-0.03500100
C	-1.39063100	1.12358300	1.73540100
C	2.05281300	3.51824600	-0.66239900
H	3.80236700	-2.58360100	0.60704300
H	3.69741000	-1.90430000	-1.03453000
H	2.00569400	4.60178000	-0.78206300
H	3.05399900	3.23276000	-0.33819100
H	1.82235400	3.03463800	-1.61493300
H	0.55286200	-3.74056500	-1.31276300
H	-0.82973000	-3.36558700	-2.36612500
H	0.42347500	-2.13779600	-2.08042400
H	-4.63311400	-2.80082300	0.26427700
H	-3.18091200	-2.31981700	1.15670100
C	-4.75318000	-0.83876500	1.15402400
H	-5.24202700	-1.20799800	2.05853500
H	-4.09264400	-0.01326800	1.43062900
H	-5.52370300	-0.45782300	0.47836700
H	-0.68171600	1.93409500	1.91507500
H	-2.40067100	1.54073900	1.69576000
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H	6.05002600	-2.53946500	-0.48794200
H	5.91060100	-0.78633300	-0.71660200
H	6.01928600	-1.46636600	0.92299000
C	-1.28247000	0.04135100	2.77921600
H	-1.97552100	-0.77451300	2.55891700
H	-0.26657400	-0.35527900	2.81761200
H	-1.53301400	0.45718600	3.75794600
H	0.07104800	0.18601600	-1.82160400

TS1

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P	-1.99806900	0.27289800	-0.68343200
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H	-1.10936600	2.29349900	-1.02412100
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H	-1.12957800	-2.12064200	-0.18508600

O	-0.13885200	-2.83632900	-0.21396900
H	0.64009900	-2.28092500	0.14436000
O	1.80886100	-1.48494200	0.59490100
O	-1.92192700	1.77963500	-1.29346400
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O	1.41091600	1.07932500	0.83866400
H	0.74142300	2.30152900	-0.05761500
O	2.33771100	0.02165200	-1.31984000
H	2.70025100	0.86082400	-1.63774600
O	-3.34595300	0.00485100	-1.50873600
H	-3.64602200	-0.91181500	-1.45231200
O	-0.59465900	-0.25584000	-1.26288200
O	-2.06211000	0.63015700	0.86749700
C	-2.84076600	-1.92636400	1.06912700
C	0.17231100	-3.25149900	-1.55120400
C	4.73703400	-0.83378100	0.56169900
C	-2.27861700	1.95331300	1.42100500
C	1.10166900	3.17077600	-1.79568700
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H	4.73551400	-1.08160700	-0.50394400
H	0.76454200	4.08400800	-2.28719400
H	2.15647500	3.28373300	-1.52972800
H	0.99069500	2.33614700	-2.49736600
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H	6.85235100	-1.01703500	0.82710600
H	6.31764500	0.62164200	0.41015600
H	6.05509000	-0.01131200	2.04976900
C	-2.43056300	1.77186200	2.91099900
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P	2.11378400	0.09693700	0.25645600
P	-2.16759900	0.23398300	-0.55152000
O	0.04725300	3.09601300	-0.61287500
H	-1.45257500	2.35585200	-0.76665300
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H	-0.81006500	-2.13315500	-0.77066000
O	0.10901200	-2.59200200	-0.86710700
H	0.79582700	-1.98269600	-0.23843500
O	1.53448400	-1.28089200	0.54815300
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O	3.61500400	0.14014900	0.81755100
O	1.41620600	1.30995600	0.78918800
H	0.56378200	2.45979000	-0.06794700
O	2.25297700	0.13861300	-1.35188500
H	2.54491900	0.99258900	-1.70206900

O	-3.71275300	0.08566200	-0.99902900	H	-2.37210400	4.08807800	-1.43301400
H	-3.99157400	-0.83808200	-1.03939400	H	-1.36744500	3.93335900	0.03174100
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O	-1.76128800	0.38279600	0.99141000	H	0.50114900	-1.71643800	4.12390800
C	-2.42394900	-2.18665800	0.89965800	H	-0.12710100	-0.34009400	3.17582700
C	0.54214400	-2.67555800	-2.23779500	H	3.77202800	-2.59541200	1.59940100
C	4.50937400	-0.96949600	0.57307900	H	2.88591700	-2.69049900	0.06821600
C	-1.89465100	1.56993400	1.80429000	C	4.81336500	-1.72315500	-0.07108100
C	0.76351000	3.32668800	-1.82089800	H	5.35422200	-2.65204400	-0.26987900
H	4.15946600	-1.82830900	1.15015000	H	4.60790400	-1.24101900	-1.02986500
H	4.47978800	-1.22183600	-0.49089600	H	5.45582100	-1.07055300	0.52387600
H	0.25384800	4.12111600	-2.36691300	H	0.92713700	0.10005400	-2.68974900
H	1.78785900	3.64696300	-1.60895000	H	2.68040100	-0.14009600	-2.86191800
H	0.79139700	2.43063000	-2.45046000	C	-5.24467700	-2.24639700	-0.96103900
H	1.47649000	-3.23414700	-2.25021600	H	-5.83156400	-3.03039000	-0.47730400
H	-0.21938300	-3.21395800	-2.79974600	H	-5.79151200	-1.30446800	-0.88402900
H	0.68744600	-1.67868700	-2.65098400	H	-5.12707800	-2.50226000	-2.01597500
H	-2.27999500	-3.24721800	0.67982600	C	1.50462500	-1.94884400	-3.07011000
H	-1.71397500	-1.89695600	1.67697500	H	2.33209400	-2.62640800	-2.84751600
C	-3.84971000	-1.94413700	1.35433400	H	0.58021100	-2.37213300	-2.66981400
H	-4.03185600	-2.53080400	2.25822800	H	1.40595000	-1.86593500	-4.15515000
H	-4.03096800	-0.89372400	1.59334100	C	0.43738000	1.91758900	1.31140200
H	-4.56835500	-2.26791400	0.59607300	H	-0.21666700	1.69233400	2.15354200
H	-1.19910900	2.33210000	1.45032000	H	-0.18601600	2.12743000	0.44519200
H	-2.91460700	1.94860300	1.71486000	C	1.36504400	3.06072700	1.65992300
C	5.89454400	-0.54552600	0.99686700	H	2.02180900	2.77887700	2.48643000
H	6.59560200	-1.36678500	0.83301300	H	1.97582800	3.37664700	0.81303300
H	6.22702300	0.31739300	0.41608700	H	0.76109600	3.91345600	1.98044100
H	5.90767600	-0.28497800	2.05740100	C	-2.88935600	1.35463300	1.09827500
C	-1.57400900	1.15677800	3.22060000	H	-2.54462400	1.86028900	1.99997000
H	-2.27673900	0.39780900	3.57238800	H	-2.61570600	1.95927400	0.22929800
H	-0.55952800	0.75599600	3.27952900	C	-4.37998400	1.09578300	1.14265900
H	-1.64284600	2.02624700	3.87834200	H	-4.71986800	0.60188800	0.22985700
H	-0.78044100	0.75743300	-2.15293600	H	-4.63683800	0.47842700	2.00589900
<b>TS2</b>				H	-4.90455900	2.05018400	1.23327500
P	-1.78018100	-0.56294200	-0.34507200	H	2.96105800	1.89489700	-0.70218300
P	2.28677300	0.27652700	0.07295100	<b>6</b>			
O	-0.58338400	3.05172300	-1.69643000	P	2.03520600	-0.39241200	-0.16891300
H	1.07884100	2.37002400	-1.15806000	P	-2.23232900	0.26303600	-0.21684300
O	2.79417700	-0.90691500	1.11242600	O	4.10505900	1.19694800	2.21161400
H	1.31867400	-1.56009200	1.87474100	H	0.29431400	0.47057400	0.84888900
O	0.46889400	-2.00458900	2.07087700	O	-1.82081800	-0.97035400	-1.11431700
H	-0.35563100	-1.84216600	0.90930800	H	-0.83731100	2.91312400	-2.10696400
O	-0.96512000	-1.82453700	0.05767300	O	0.75657900	2.50872200	-1.98474900
O	1.83782200	1.76243500	-1.18492800	H	0.90649500	1.54300600	-1.94334600
O	-3.13331800	-1.12286800	-0.97512200	O	1.46159500	-0.07887300	-1.51037400
O	-1.16773500	0.38483400	-1.31494900	O	-1.08929400	0.93846500	0.48241100
H	-1.00485300	2.18135300	-1.56876000	O	2.04778900	-1.95858100	0.13503200
O	-2.14695700	0.10747400	1.05762000	O	1.25308400	0.19656700	1.05835700
O	3.58546400	1.14270100	-0.01125400	H	3.78985500	0.71684400	2.98735600
O	1.12763300	0.66858700	1.09172800	O	3.51782800	0.11606900	-0.02158300
O	1.87462900	-0.75802000	-1.05814200	H	3.77538000	0.47683300	0.89173500
C	3.54057600	-2.06194100	0.67640900	O	-3.03485300	1.19889800	-1.16235300
C	-0.09349600	-1.42862000	3.25490100	H	-2.52010000	2.02527500	-1.55633700
C	-3.89932100	-2.14463600	-0.28665100	O	-1.80958700	3.12164000	-2.13014500
C	1.75273000	-0.57796100	-2.48851600	O	-3.27647000	-0.37120200	0.79756100
C	-1.34560600	4.06582400	-1.05554300	C	-1.14826300	-2.12985200	-0.54332300
H	-3.34623700	-3.08377700	-0.35141000	C	1.33272800	3.07322600	-0.80726500
H	-4.00031300	-1.86242300	0.76535100	C	2.51618400	-2.88736000	-0.87406500
H	-0.87153400	5.02257300	-1.27733900	C	-3.76213400	0.41801400	1.91786000

C	3.54977400	2.51884200	2.21443700	H	5.97720000	-0.35520400	0.12050200
H	1.99510900	-2.67527900	-1.81086700	H	5.64659600	-1.71603800	1.19761600
H	3.58826700	-2.72912900	-1.01865100	C	-1.81009100	-0.53263600	1.72755400
H	3.94275600	3.02728500	1.33489800	H	-2.27639500	-1.07533500	0.89653100
H	2.45936100	2.48342400	2.16414200	H	-0.79949400	-0.93365100	1.84890600
H	3.86295600	3.05589800	3.11129000	H	0.63745300	1.68406200	-1.74892500
H	2.34926400	2.69733200	-0.66260800	C	-4.24780700	-1.83285800	-0.99814700
H	1.37437700	4.15465800	-0.94272100	H	-3.22834400	-2.21342000	-0.86523300
H	0.72743300	2.84441400	0.07487800	H	-4.63902800	-2.27421700	-1.92129000
H	-0.34256400	-2.36399600	-1.23900000	H	-2.71451800	1.38372900	1.28708600
H	-0.70998200	-1.85654200	0.42054900	H	-5.18192100	0.07299100	-1.41426800
C	-2.12671400	-3.27296500	-0.41390200	H	3.65507800	-2.32437300	-0.17918400
H	-1.60344200	-4.15661800	-0.04077400	C	-5.10465100	-2.24857600	0.19546000
H	-2.92946600	-3.02441700	0.28264600	H	-6.12269900	-1.86539000	0.06522400
H	-2.56070900	-3.51297400	-1.38676700	H	-4.70626400	-1.77469900	1.10064600
H	-2.92124900	0.61235900	2.58660800	C	-5.14183700	-3.76162800	0.38271800
H	-4.14418800	1.36762200	1.53451000	H	-5.73518100	-4.04122500	1.25691200
C	2.21914700	-4.28110700	-0.38057200	H	-5.58039700	-4.25201900	-0.49122700
H	2.56601700	-5.00971200	-1.11656100	H	-4.13317900	-4.16322100	0.51805700
H	2.73014100	-4.47269400	0.56522500	C	-2.61967900	-0.74966100	3.00309100
H	1.14442900	-4.41508400	-0.23686600	H	-2.15781600	-0.19572300	3.82769300
C	-4.84564300	-0.37922300	2.59832200	H	-3.62570300	-0.33525100	2.87065400
H	-5.67384800	-0.56689100	1.91243200	C	-2.71401800	-2.22879600	3.36532800
H	-4.45352500	-1.33409200	2.95460300	H	-3.30038600	-2.38089000	4.27469700
H	-5.22289100	0.18242000	3.45565600	H	-3.18776700	-2.79808100	2.55938100
H	-1.92780800	3.94316400	-1.63821300	H	-1.71926600	-2.65218600	3.53134100
<b>R = Bu, OH, monoalkylation</b>				C	6.37248600	-2.29139000	-0.75505100
<b>4</b>				H	5.95112000	-3.30133100	-0.71272000
P	1.90372300	-0.06675000	0.41950500	H	6.27188900	-1.95053900	-1.79104600
P	-1.18728600	2.35054200	-0.80527000	C	7.84766500	-2.33328600	-0.36889100
O	1.01064900	3.00768400	1.82142300	H	7.97213700	-2.69469400	0.65581600
O	-3.29127000	0.10652600	-2.16202700	H	8.41331500	-2.99513800	-1.02891300
H	-2.44668500	-0.40033500	-2.07888900	H	8.29505900	-1.33699600	-0.42950000
O	-0.95237300	-1.22535300	-1.95135400	H	1.23720400	1.61679700	1.76724200
H	-0.41488500	-1.15148000	-1.14147300	H	0.26772800	3.28638400	1.23908700
O	1.08565100	-1.18619400	-0.10815800	<b>TS1</b>			
O	-0.84089900	3.58490000	-0.04230900	P	1.86778000	1.01893500	0.55670200
O	3.41814800	-0.46316500	0.69931600	P	-1.73586300	0.62223800	-1.71084700
O	1.45678300	0.58432300	1.75526000	O	-0.16475000	3.75753700	-0.10836500
O	1.97554600	1.10342200	-0.69493000	O	-1.82028200	-1.22703900	-1.85583300
H	2.70278000	1.73529700	-0.58155600	H	-0.79588700	-1.67249500	-1.36590600
O	-2.62152200	2.40958300	-1.42155800	O	0.20525300	-2.03473700	-0.84609400
H	-2.92598400	1.50083000	-1.81843300	H	0.50340900	-1.28443800	-0.21906100
O	-0.24204200	2.00855900	-2.03232200	O	0.92206600	-0.15094900	0.65799000
O	-1.05664400	1.02869200	0.07642500	O	-1.67565200	2.24841000	-1.65920900
C	-4.20267400	-0.32377700	-1.13737100	O	3.36596200	0.56109200	0.91683000
C	-0.05915300	-1.19642200	-3.06022500	O	1.58406900	2.26921600	1.33584000
C	4.11128000	-1.33319200	-0.23438300	O	1.94262300	1.37928300	-1.03718200
C	-1.71937900	0.93323300	1.36379600	H	2.52142500	2.13183300	-1.22851600
C	2.17355700	3.76636800	1.47101200	O	-2.91341400	0.70477100	-2.79683000
H	3.98551700	-0.93732300	-1.24707100	H	-3.13489500	-0.13943800	-3.21046700
H	2.12142600	4.75690500	1.92593500	O	-0.24825600	0.36281100	-2.24107900
H	3.04446600	3.23613800	1.85775200	O	-2.09087700	0.34112200	-0.17539000
H	2.25570400	3.86822200	0.38577300	C	-3.00228300	-1.93287700	-1.41376400
H	0.43326600	-2.16489200	-3.18849100	C	1.25410800	-2.28729900	-1.79596100
H	-0.64334300	-0.97405900	-3.95446900	C	3.85278200	-0.70014100	0.40895700
H	0.70348300	-0.42243000	-2.93560800	C	-2.17172800	1.32504700	0.88079400
H	-3.91174700	0.13469700	-0.18414500	C	0.57853000	4.60513900	-0.97940900
H	-1.13441000	1.49556800	2.09649800	H	3.69339200	-0.73443200	-0.67407400
C	5.56950300	-1.37073900	0.16135000	H	-0.13318500	5.18946100	-1.56330500

H	1.21241200	5.28749700	-0.40764000	C	3.98341400	0.75254600	-0.51725300
H	1.20230000	4.02428600	-1.66644500	C	0.32109100	0.91918100	-2.75110900
H	2.01838600	-2.90113300	-1.31939900	C	-3.99066500	0.79225200	-0.55398100
H	0.81955100	-2.82929000	-2.63531200	C	1.02020800	-0.13875100	2.44542000
H	1.68196000	-1.34729800	-2.14710300	C	-0.61350900	-4.36538600	-1.56724900
H	-3.79607800	-1.20371600	-1.23217400	H	-3.67555800	0.78076300	-1.60211900
H	-1.19298600	1.79343500	1.00397900	H	-0.50137800	-3.57572200	-2.31715000
C	5.32546100	-0.81128500	0.73696900	H	-0.03724600	-5.23472900	-1.88538300
H	5.85924500	0.02102800	0.26588100	H	-1.66613100	-4.64931200	-1.49085100
H	5.45689300	-0.71544600	1.81988300	H	-0.71788800	1.20309800	-2.91687600
C	-2.55365700	0.58274400	2.14299300	H	0.97145500	1.57142500	-3.33724600
H	-3.52669300	0.09953300	1.99923700	H	0.46869100	-0.12027300	-3.05100700
H	-1.81503100	-0.20645100	2.32012900	H	3.94800800	1.08282000	0.52629400
H	0.39681700	1.06337700	-2.02748200	H	0.14125800	-0.74645400	2.22401900
C	-2.75205200	-2.74915500	-0.15773500	C	-5.49691100	0.85433200	-0.44028400
H	-2.30254900	-2.10326500	0.60328800	H	-5.92861300	-0.02926800	-0.92185600
H	-2.03640000	-3.54936100	-0.37439200	H	-5.77510500	0.82189500	0.61835100
H	-2.91088200	2.08345100	0.61480900	C	0.62581000	1.27602400	2.81241600
H	-3.31428700	-2.57769100	-2.24001600	H	1.52420900	1.84720200	3.07069300
H	3.28257700	-1.50762100	0.87755800	H	0.17321400	1.75191100	1.93690300
C	-4.05141000	-3.35050200	0.37338500	H	0.92951100	-2.69597100	-0.49920900
H	-4.51405700	-3.96828700	-0.40433000	C	3.88863800	1.94568400	-1.44965100
H	-4.75758700	-2.54216900	0.59305100	H	2.95817600	2.49013300	-1.25246600
C	-3.82586800	-4.18676800	1.62913700	H	3.84430900	1.58467600	-2.48378800
H	-4.76495100	-4.59673800	2.00865000	H	1.58408300	-0.60348600	3.25940400
H	-3.15153600	-5.02393300	1.42702400	H	4.92504000	0.21987900	-0.67829400
H	-3.37840300	-3.58184500	2.42341300	H	-3.51714100	1.63772500	-0.04870400
C	-2.60359500	1.52285300	3.34531800	C	5.07910000	2.88662100	-1.28059300
H	-1.62905900	2.00961400	3.46097900	H	6.00552300	2.33828800	-1.48256000
H	-3.33344100	2.31804100	3.15909500	H	5.13203400	3.21973300	-0.23820000
C	-2.96404800	0.78554000	4.63136900	C	4.98982300	4.09981500	-2.20139000
H	-2.99577200	1.46636300	5.48521100	H	5.84750600	4.76429800	-2.07157900
H	-3.94439700	0.30783300	4.54601200	H	4.96000500	3.79142900	-3.25053500
H	-2.22945400	0.00554400	4.85101700	H	4.08395400	4.67775200	-1.99673900
C	5.90650500	-2.14005900	0.25772700	C	-0.35884900	1.29204200	3.97902900
H	5.36802800	-2.96502700	0.73655600	H	-1.25001300	0.71729700	3.70324200
H	5.74222400	-2.24112800	-0.82072100	H	0.08799400	0.78480200	4.84129100
C	7.39688800	-2.25712200	0.56129900	C	-0.76230400	2.71043500	4.36974600
H	7.58328500	-2.18592500	1.63663900	H	-1.46235700	2.70913900	5.20867400
H	7.79957600	-3.21176200	0.21425100	H	0.11232100	3.29828800	4.66306300
H	7.95913800	-1.45771300	0.07033800	H	-1.24356100	3.22264900	3.53157500
H	0.45980600	3.29652700	0.49264700	C	-6.05076100	2.12289400	-1.08537700
H	-1.07340200	2.70236900	-1.01302700	H	-5.59775400	2.99887600	-0.60896700
<b>5</b>				H	-5.75715000	2.15131600	-2.14027600
P	-2.03513000	-0.91430300	-0.09855500	C	-7.56980400	2.20526500	-0.97291800
P	2.38918700	-1.28704200	0.36968000	H	-7.88366100	2.19865700	0.07485000
O	-0.10763300	-3.94592000	-0.30154400	H	-7.95355100	3.11929800	-1.43221500
O	2.89622500	-0.13954900	-0.78802500	H	-8.04504900	1.35456300	-1.46964600
H	1.48252200	0.68719800	-1.15772200	H	-0.78856100	-3.40881200	0.15184400
O	0.60011700	1.08699600	-1.35745500	H	2.21399300	-2.44984700	2.32296100
H	-0.36609100	0.60956900	-0.50694600	H	4.05340600	-2.51308400	1.09590500
O	-1.13578300	0.31650600	0.17587900	<b>TS2</b>			
O	1.85353500	-2.49780400	1.42930100	P	-1.83506600	-0.72206300	-0.16752800
O	-3.53967900	-0.42775600	0.08513200	P	2.14262800	-1.20149400	-0.10862800
O	-1.82542500	-2.12572300	0.74243900	O	-0.13133100	-3.51890900	-1.49499400
O	-1.82092900	-1.17907000	-1.66481200	O	2.82109800	0.12329500	-0.76713700
H	-2.27458700	-1.96470300	-2.00394200	H	1.48122400	1.20890700	-1.31426100
O	3.94144200	-1.73545900	0.53494700	O	0.60307900	1.56719600	-1.52564800
O	1.44918600	-1.88814900	-0.77171100	H	-0.29041100	0.89169700	-0.59436400
O	1.85040000	-0.05664300	1.26928900	O	-0.86076600	0.45197800	0.15240400

O	1.31416900	-3.12590100	0.56526200	P	2.10647300	-0.83929300	0.01046600
O	-3.31422100	-0.16523900	0.05704700	P	-2.12868600	-0.94741000	0.87672000
O	-1.65871700	-1.95610300	0.63270900	O	-0.36498000	-3.87949000	-0.25354900
O	-1.66188100	-0.90698200	-1.75042200	O	-2.46698600	0.58796200	1.12434700
H	-2.20375400	-1.61335300	-2.13214800	H	-0.87981900	1.62861600	0.96878200
O	3.45515900	-2.10135000	-0.13424400	O	0.04795200	1.91605700	0.97344800
O	1.06080800	-1.31597700	-1.22512900	H	0.87490000	1.02418000	0.05508500
O	1.75056200	-0.51647900	1.25519700	O	1.41611100	0.44474200	-0.58553100
C	4.00799100	0.73750100	-0.21973100	O	-2.70544100	-4.17231900	1.09519600
C	0.34366700	1.36798100	-2.91971400	O	3.67155900	-0.60803500	-0.10344800
C	-3.72678400	1.09195300	-0.52887000	O	1.72791000	-2.10178800	-0.67791400
C	0.84252800	-0.92586300	2.30688400	O	1.85281300	-0.81541200	1.58039600
C	-1.47023900	-3.86907300	-1.83152200	H	0.89533700	-0.95305000	1.76703900
H	-3.55397100	1.05264600	-1.60905700	O	-3.21209900	-1.74378700	1.67753100
H	-1.67169200	-3.47880700	-2.82956000	O	-0.70913200	-1.19289800	1.23721600
H	-1.57890000	-4.95648800	-1.85270000	O	-2.48041400	-1.29129800	-0.63271300
H	-2.18128000	-3.44555400	-1.11926400	C	-3.74896100	1.17181000	0.75615100
H	-0.66568900	1.72725900	-3.11767400	C	0.48899800	1.98203700	2.33478000
H	1.05506000	1.94615900	-3.51291200	C	4.29238100	0.55456300	0.50028400
H	0.41490700	0.31055700	-3.17996600	C	-1.55464000	-1.01458800	-1.71839900
H	3.92871300	0.77129000	0.87048800	C	-0.21330200	-4.46016600	-1.54309000
H	-0.05404800	-1.34815200	1.85264200	H	4.26384200	0.43157600	1.58622500
C	-5.19357700	1.29257100	-0.22022600	H	0.77457400	-4.91590300	-1.65488300
H	-5.75972700	0.44372800	-0.61800700	H	-0.97255400	-5.23661400	-1.64838000
H	-5.33024500	1.29870500	0.86621500	H	-0.35562500	-3.71660700	-2.33263300
C	0.52134700	0.30579900	3.12507300	H	1.57169500	2.10590300	2.32126000
H	1.43875400	0.68820700	3.58540900	H	0.03225000	2.84000700	2.83269200
H	0.13536600	1.08272600	2.45808700	H	0.23393900	1.06552500	2.87151200
H	0.49981800	-2.16296700	-1.32896000	H	-4.11510900	0.67881600	-0.14834900
C	4.12134600	2.13136800	-0.79978500	H	-0.56509200	-1.37973100	-1.43315000
H	3.26787500	2.73129800	-0.46489500	C	5.71428900	0.64455000	-0.00504400
H	4.06667100	2.06321500	-1.89232900	H	6.24002600	-0.28314100	0.24374100
H	1.34447100	-1.67880900	2.91814700	H	5.69983800	0.73384500	-1.09617600
H	4.86980200	0.12492500	-0.49689400	C	-1.52275100	0.45871700	-2.06846300
H	-3.11712600	1.89182500	-0.09926300	H	-2.54493200	0.81284800	-2.24447200
C	5.42629300	2.80795000	-0.38726300	H	-1.11699700	1.02875900	-1.22579300
H	6.27136600	2.21351500	-0.75011200	H	0.27919600	-3.15239200	-0.17693100
H	5.49829600	2.82269500	0.70576300	C	-3.52956800	2.64975600	0.52615100
C	5.52815900	4.23065000	-0.92810000	H	-2.78355500	2.77844600	-0.26665300
H	6.47812500	4.69456300	-0.65235600	H	-3.11987300	3.09525500	1.43964100
H	5.45527700	4.23816300	-2.01953800	H	-1.92833600	-1.61045400	-2.55168100
H	4.72195300	4.85664300	-0.53535300	H	-4.44396500	0.98389600	1.57717500
C	-0.51381000	-0.01479200	4.20082700	H	3.71879600	1.44426000	0.22355600
H	-1.43767100	-0.35278800	3.71916900	C	-4.82722300	3.35431300	0.13803400
H	-0.15675400	-0.84842500	4.81569300	H	-5.57155400	3.20625200	0.92752400
C	-0.80467300	1.18928200	5.09133200	H	-5.23289800	2.89240000	-0.76851600
H	-1.60613600	0.97462500	5.80225300	C	-4.61522200	4.84654500	-0.09647500
H	0.08290200	1.47595500	5.66263800	H	-5.54780100	5.34080000	-0.37829100
H	-1.10995600	2.05204600	4.49218400	H	-4.23651000	5.33298900	0.80687000
C	-5.71902900	2.59562300	-0.81827000	H	-3.88950900	5.01567800	-0.89718800
H	-5.16558400	3.43958400	-0.39291500	C	-0.65931000	0.70878800	-3.30321600
H	-5.52570200	2.60442500	-1.89644100	H	0.31712300	0.23257700	-3.16390500
C	-7.21158700	2.78056000	-0.56308400	H	-1.12369000	0.23067200	-4.17198800
H	-7.42463400	2.79895000	0.50952900	C	-0.47064300	2.19920700	-3.56580100
H	-7.57540500	3.71636900	-0.99382100	H	0.12742200	2.37486300	-4.46306400
H	-7.78647500	1.96123900	-1.00404900	H	-1.43566400	2.69657100	-3.70213900
H	0.09976000	-3.72042500	-0.56248600	H	0.03740400	2.67803600	-2.72320400
H	1.33980800	-3.24331700	1.51853300	C	6.44587100	1.83697900	0.60737900
H	3.19811400	-2.99275600	0.16925300	H	5.90281200	2.75748900	0.36770300
				H	6.44032900	1.74305800	1.69861500

C	7.88363600	1.94468500	0.10932000	H	-6.05206300	0.37378900	0.23523200
H	7.91236800	2.06864800	-0.97693100	H	-6.18786100	-0.46668600	-1.32640000
H	8.39576900	2.79892000	0.55851500	H	-6.85166100	-1.20698200	0.14196000
H	8.45135600	1.04375900	0.35881300	C	3.72771600	-1.88913600	0.51004900
H	-1.84748100	-4.10922600	0.61509300	H	3.52685700	-2.61880000	1.29404300
H	-3.32813400	-4.57150800	0.47610400	H	3.35858700	-2.28539700	-0.43933500
H	-3.11634900	-2.74853600	1.51107100	C	5.19791100	-1.54254100	0.44081700
<b>R = Et, Et, dialkylaton</b>				H	5.39335800	-0.80947200	-0.34517600
<b>4</b>				H	5.54420000	-1.14370100	1.39668300
P	2.32817700	0.23704600	-0.24415400	H	5.76860000	-2.44687300	0.21579400
P	-2.14487600	-0.85199100	-0.33737600	<b>TS1</b>			
O	0.43655000	-2.86938600	-1.22484600	P	-2.67615600	0.27605200	0.27111400
H	-0.94414100	-2.39328700	-1.35799700	P	2.20279800	-0.35347900	-0.30069400
O	-3.03068900	1.63725500	1.91840800	O	-0.54609300	-1.84673800	-1.99272800
H	-3.94078200	1.82795400	2.17277400	O	2.27928700	1.60284800	-0.35900900
O	-0.04506900	0.41273800	2.30841500	H	1.06275200	1.99520900	-0.53925900
H	0.81935100	0.88149200	1.30895400	O	-0.01274900	2.29518100	-0.70623900
O	1.49428700	1.25465000	0.58319600	O	-3.04780600	-0.62995300	1.53342000
O	-1.89833300	-1.98537600	-1.39419800	O	2.07221700	-1.99407300	-0.35943900
O	3.51656300	1.08285400	-0.87485800	O	-2.55350600	-0.51452400	-1.00153200
O	1.64888200	-0.50665600	-1.34414500	O	-1.45528100	1.06860700	0.72486300
H	0.98443300	-2.05991800	-1.34236200	H	0.56893600	-0.93044000	-1.71205300
O	2.94287100	-0.72205000	0.87263500	O	-3.94670700	1.25497000	0.19789800
O	-3.66835000	-0.46106300	-0.53287400	O	3.76786600	-0.22099300	-0.56684600
O	-1.75615000	-1.20628600	1.05944800	O	1.20413700	-0.14125700	-1.49400600
H	-0.75715700	-0.12712100	1.89111000	H	-0.65171500	1.68683500	-0.01282700
O	-1.37279700	0.45273600	-0.79294500	O	1.73922400	-0.15066000	1.21486600
C	-2.52474700	2.76735200	1.20686000	C	2.79848100	2.36406600	0.73170800
C	0.62115900	-0.38773300	3.29189000	C	-0.25301600	3.68396300	-0.46537800
C	4.33962300	1.93986800	-0.03996500	C	0.89874600	-1.09118000	1.93864000
C	-1.39308700	0.90942800	-2.17133600	C	-0.41731500	-3.24929900	-1.75642900
C	0.67696300	-3.39335700	0.08587100	H	-1.33944000	-3.75973000	-2.04417000
H	3.73653700	2.79911100	0.25967000	H	0.39986400	-3.62049100	-2.37433100
H	4.63507800	1.38106100	0.85218400	H	-0.19654200	-3.45717700	-0.70695800
H	-0.20208700	-3.96683100	0.38235400	H	0.38711100	4.27212100	-1.12407600
H	1.54743000	-4.05204100	0.07311000	H	-1.29753300	3.90245400	-0.69488100
H	0.83445400	-2.58294900	0.80305100	H	-0.05012700	3.94492300	0.57649800
H	1.50319700	0.16191800	3.61995800	H	2.77036200	3.41227000	0.41372900
H	-0.04136800	-0.55328000	4.14326400	H	2.13410500	2.26608900	1.59780300
H	0.92750600	-1.34808500	2.87020700	C	4.22052100	2.00928800	1.12873000
H	-2.45012800	3.62782000	1.88147600	H	4.59510900	2.77859600	1.80949400
H	-1.51456700	2.49269800	0.89506300	H	4.27531900	1.04703200	1.64109800
C	-3.38562400	3.10890000	0.00632800	H	4.87251800	1.97687200	0.25341700
H	-2.98117000	3.97786500	-0.51935000	H	0.03559200	-1.34095500	1.31853100
H	-3.43084900	2.26566000	-0.68741800	H	1.47515300	-1.99649700	2.13723000
H	-4.40450300	3.35131500	0.32451100	C	0.49006500	-0.42055100	3.22674000
H	-0.94513900	0.13300500	-2.79578500	H	1.37092000	-0.08651200	3.78014900
H	-2.43434400	1.05525300	-2.47088300	H	-0.15708700	0.43390300	3.02782600
C	5.53994600	2.35599800	-0.85254800	H	-0.05665700	-1.13445600	3.84742200
H	6.17285300	3.01235200	-0.25109300	C	4.69676800	-1.33581100	-0.60270900
H	6.12655100	1.48443800	-1.15049100	H	4.41321900	-2.00594400	-1.41468600
H	5.22955500	2.89844400	-1.74790800	H	4.64509300	-1.87281300	0.34720800
C	-0.61021600	2.19673000	-2.24002600	C	6.07154700	-0.75177200	-0.81705100
H	-1.02420000	2.93777000	-1.55336400	H	6.10727200	-0.18073000	-1.74691600
H	0.43868100	2.02690400	-1.99096300	H	6.35043800	-0.09963200	0.01268700
H	-0.66426300	2.59461300	-3.25603100	H	6.80040800	-1.56300700	-0.88064900
C	-4.72228100	-1.29888400	0.01086100	C	-4.29494000	1.92017000	-1.03975200
H	-4.54400100	-1.42379200	1.08134800	H	-4.66986000	2.90051900	-0.74500900
H	-4.67516600	-2.27460400	-0.47915400	H	-3.39481400	2.06299500	-1.64373100
C	-6.03293200	-0.60242500	-0.25412900	C	-5.34495600	1.13124700	-1.78826100



H	-4.95690700	0.15839900	-2.09599500	C	-0.55907200	1.78414500	-1.66653000
H	-6.22774600	0.98192000	-1.16231700	H	0.31452000	1.49038500	-2.24764400
H	-5.64395200	1.68273800	-2.68314800	H	-0.22274100	2.39118900	-0.82553800
H	-1.27287500	-1.47547700	-1.43482600	C	-1.56062100	2.51600000	-2.53258000
C	-4.15467800	-1.56112500	1.44220000	H	-1.89334500	1.87621700	-3.35383300
H	-4.63785300	-1.53494700	2.41896700	H	-2.43061200	2.83416800	-1.95509600
H	-4.87009400	-1.20210900	0.69683500	H	-1.08676400	3.40349700	-2.95949100
C	-3.65180500	-2.94656900	1.10600600	C	2.87215100	1.59415100	-0.77589200
H	-2.92389400	-3.28088900	1.84873700	H	2.36131800	2.25769400	-1.47517100
H	-4.48962800	-3.64816600	1.10426400	H	2.70277100	1.96728200	0.23793400
H	-3.18513900	-2.96369100	0.11855800	C	4.34965000	1.50910600	-1.09102400
H	2.49685800	-2.48965400	0.35242300	H	4.87174500	0.88018500	-0.36680300
<b>5</b>				H	4.50546500	1.10458500	-2.09365800
P	1.92429900	-0.59857100	0.37090000	H	4.78595800	2.51040200	-1.05110600
P	-2.29238900	0.36093100	-0.12496200	<b>TS2</b>			
O	0.08600800	2.60069000	1.67002600	P	-1.78018100	-0.56294200	-0.34507200
H	-1.38982400	2.14494600	0.92740600	P	2.28677300	0.27652700	0.07295100
O	-2.43264700	-1.25959200	-0.87059700	O	-0.58338400	3.05172300	-1.69643000
H	-1.24943300	-1.70067000	-1.49910000	H	1.07884100	2.37002400	-1.15806000
O	-0.37336600	-2.14424400	-1.88223700	O	2.79417700	-0.90691500	1.11242600
H	0.38782800	-2.01780700	-1.11002200	H	1.31867400	-1.56009200	1.87474100
O	1.31075300	-1.87875900	-0.17606900	O	0.46889400	-2.00458900	2.07087700
O	-2.23829600	1.88190400	0.49997700	H	-0.35563100	-1.84216600	0.90930800
O	3.36186300	-0.96381000	0.99382700	O	-0.96512000	-1.82453700	0.05767300
O	1.19166000	0.18423700	1.41715700	O	1.83782200	1.76243500	-1.18492800
H	0.64945200	1.80655100	1.54681400	O	-3.13331800	-1.12286800	-0.97512200
O	2.24280500	0.30097200	-0.92633700	O	-1.16773500	0.38483400	-1.31494900
O	-3.80365000	0.67656600	-0.60498300	H	-1.00485300	2.18135300	-1.56876000
H	-4.16221500	-0.03489300	-1.15045400	O	-2.14695700	0.10747400	1.05762000
O	-1.08739400	0.52841900	-1.18559500	O	3.58546400	1.14270100	-0.01125400
O	-1.98455100	-0.41582300	1.24416300	O	1.12763300	0.66858700	1.09172800
C	-2.97269800	-2.41100300	-0.19265700	O	1.87462900	-0.75802000	-1.05814200
C	0.04515500	-1.51495700	-3.10878700	C	3.54057600	-2.06194100	0.67640900
C	4.25125300	-1.84285400	0.27008300	C	-0.09349600	-1.42862000	3.25490100
C	-2.04890800	0.13254000	2.57949800	C	-3.89932100	-2.14463600	-0.28665100
C	0.79740000	3.79051700	1.35470800	C	1.75273000	-0.57796100	-2.48851600
H	3.82143700	-2.84714000	0.27193600	C	-1.34560600	4.06582400	-1.05554300
H	4.33082300	-1.49724500	-0.76534800	H	-3.34623700	-3.08377700	-0.35141000
H	0.13841000	4.63355400	1.56566400	H	-4.00031300	-1.86242300	0.76535100
H	1.69508400	3.88404100	1.97243600	H	-0.87153400	5.02257300	-1.27733900
H	1.08519000	3.82517100	0.29924300	H	-2.37210400	4.08807800	-1.43301400
H	0.56554800	-2.26036300	-3.70813400	H	-1.36744500	3.93335900	0.03174100
H	-0.84142800	-1.16484100	-3.63587100	H	-1.10389500	-1.82134500	3.36469600
H	0.70824100	-0.67861200	-2.88586900	H	0.50114900	-1.71643800	4.12390800
H	-2.96529100	-3.20325300	-0.94545900	H	-0.12710100	-0.34009400	3.17582700
H	-2.29603900	-2.69783300	0.61499400	H	3.77202800	-2.59541200	1.59940100
C	-4.38202500	-2.21275400	0.32932500	H	2.88591700	-2.69049900	0.06821600
H	-4.72315000	-3.15051100	0.77491600	C	4.81336500	-1.72315500	-0.07108100
H	-4.42943900	-1.43764500	1.09714300	H	5.35422200	-2.65204400	-0.26987900
H	-5.07282200	-1.95715300	-0.47900600	H	4.60790400	-1.24101900	-1.02986500
H	-1.25945400	0.87320900	2.70604600	H	5.45582100	-1.07055300	0.52387600
H	-3.01814600	0.61584900	2.71753100	H	0.92713700	0.10005400	-2.68974900
C	5.59257400	-1.81584900	0.96165000	H	2.68040100	-0.14009600	-2.86191800
H	6.28821500	-2.47558800	0.43825700	C	-5.24467700	-2.24639700	-0.96103900
H	6.00646600	-0.80516000	0.96369300	H	-5.83156400	-3.03039000	-0.47730400
H	5.49973200	-2.16067000	1.99375500	H	-5.79151200	-1.30446800	-0.88402900
C	-1.86568400	-1.02731800	3.52850700	H	-5.12707800	-2.50226000	-2.01597500
H	-2.66046100	-1.76592800	3.39989200	C	1.50462500	-1.94884400	-3.07011000
H	-0.90088400	-1.51137500	3.36062300	H	2.33209400	-2.62640800	-2.84751600
H	-1.89534500	-0.66246000	4.55781100	H	0.58021100	-2.37213300	-2.66981400

H	1.40595000	-1.86593500	-4.15515000	H	1.77909400	-0.60592200	-4.09707000
C	0.43738000	1.91758900	1.31140200	H	0.18900000	-0.07916100	-3.49584600
H	-0.21666700	1.69233400	2.15354200	H	1.22904300	1.05667300	-4.37637400
H	-0.18601600	2.12743000	0.44519200	C	1.03920300	1.07984900	1.99586300
C	1.36504400	3.06072700	1.65992300	H	-0.00228300	1.30726300	2.22112500
H	2.02180900	2.77887700	2.48643000	H	1.56036000	2.00615000	1.74391300
H	1.97582800	3.37664700	0.81303300	C	1.70803200	0.34920600	3.13912600
H	0.76109600	3.91345600	1.98044100	H	1.20711100	-0.59890800	3.34658900
C	-2.88935600	1.35463300	1.09827500	H	2.76258800	0.15512100	2.92831900
H	-2.54462400	1.86028900	1.99997000	H	1.65414300	0.97126900	4.03585900
H	-2.61570600	1.95927400	0.22929800	C	-2.84441200	1.22688300	1.42044700
C	-4.37998400	1.09578300	1.14265900	H	-2.32381100	1.52385700	2.33112500
H	-4.71986800	0.60188800	0.22985700	H	-2.77440000	2.04397600	0.69760700
H	-4.63683800	0.47842700	2.00589900	C	-4.27996500	0.85016700	1.70654900
H	-4.90455900	2.05018400	1.23327500	H	-4.81423900	0.59802000	0.78801500
H	2.96105800	1.89489700	-0.70218300	H	-4.32176100	-0.00012500	2.39112300
<b>6</b>				H	-4.78600300	1.69715300	2.17631700
P	-1.85554500	-0.10369700	-0.64383300	H	3.25070000	2.47778000	-0.07408200
P	2.26524200	-0.24361500	0.04787700	<b>R = Et, OH, monoalkylation</b>			
O	0.18481200	3.21751800	-0.40233000	<b>4</b>			
H	1.99166700	3.31166500	-0.33464700	P	-2.01660300	-0.06968300	-0.34486300
O	2.40041800	-1.73586700	0.57915500	P	1.88435000	0.43326400	0.07063300
H	0.74009800	-2.30201800	1.41562000	O	0.35192600	3.46101500	0.15085600
O	-0.18771700	-2.57336100	1.32507600	H	0.44823400	1.48309600	-1.73243900
H	-0.72719400	-1.88739400	0.13871000	O	2.31928500	-0.58156400	1.29317100
O	-1.10701400	-1.46933300	-0.72675000	H	0.79665200	-0.87144500	2.30349500
O	2.95981600	3.38536600	-0.25458300	O	-0.10319600	-1.18691600	2.50661500
O	-3.27527200	-0.34572500	-1.32864200	H	-0.82614000	-1.19428300	1.24494200
O	-1.22327800	1.06765100	-1.30729300	O	-1.36201100	-1.29567800	0.35998000
H	-0.34469300	2.44020100	-0.66543500	O	1.31645000	1.82538200	-1.47023300
O	-2.11068000	0.07828800	0.91760800	O	-3.41641500	-0.60959500	-0.88032200
O	3.45452800	0.62479300	0.24439400	O	-1.29055500	0.56990700	-1.46971700
O	0.96359200	0.25933700	0.79685700	H	0.79881500	3.02036300	-0.65512900
O	1.82545100	-0.45049200	-1.45480900	O	-2.33852400	0.91338900	0.87909900
C	3.09758800	-2.78160400	-0.16258600	H	-2.62284600	1.80092600	0.61453900
C	-0.89978800	-2.35016500	2.54777600	O	3.27851100	1.18039400	-0.14621000
C	-4.04905700	-1.53011400	-1.00737900	H	3.93566800	0.92897600	0.52136500
C	1.85925600	0.67974700	-2.37575400	O	0.78533100	1.11487600	0.95721800
C	-0.52776000	3.98263700	0.55982200	O	1.51067000	-0.71694300	-0.94001700
H	-3.55910400	-2.38856100	-1.47077500	C	2.92529800	-1.87718100	1.07505600
H	-4.05389200	-1.66685100	0.07806400	C	-0.69597800	-0.34233800	3.49920400
H	0.10231700	4.82857500	0.83969600	C	-4.29311300	-1.37358900	-0.01370600
H	-1.46373200	4.36881200	0.14413000	C	1.71083100	-0.76878900	-2.37616500
H	-0.74929800	3.39993100	1.45905300	C	-0.93801400	3.93323900	-0.22287200
H	-1.91742900	-2.70814800	2.39303700	H	-3.84275400	-2.35593900	0.14110400
H	-0.43567800	-2.91688700	3.35688900	H	-4.37152900	-0.86106400	0.94881900
H	-0.92574400	-1.28793900	2.79803700	H	-1.52679900	4.08689100	0.68321200
H	3.04969000	-3.64528500	0.49843000	H	-0.85576000	4.88591900	-0.75315700
H	2.51731700	-2.98824400	-1.06331900	H	-1.44818400	3.21207000	-0.86995300
C	4.52615700	-2.40707900	-0.48184400	H	-1.74722700	-0.61958000	3.57418200
H	5.01677500	-3.27065300	-0.93668600	H	-0.20974700	-0.50415200	4.46287300
H	4.57811200	-1.57754200	-1.19115500	H	-0.61376700	0.70797800	3.21360600
H	5.06912100	-2.13584500	0.42587400	H	3.06188900	-2.27900800	2.07937200
H	1.31085700	1.50923800	-1.92418700	H	2.21218600	-2.50747100	0.54040800
H	2.90366300	0.96708900	-2.51418500	C	4.25062100	-1.80358600	0.34586000
C	-5.44386200	-1.32844200	-1.54450100	H	4.67303500	-2.80938900	0.28443700
H	-6.04516300	-2.21497000	-1.33087100	H	4.13862100	-1.42462900	-0.67335900
H	-5.91892300	-0.46403400	-1.07588700	H	4.95924400	-1.16962500	0.88587100
H	-5.42012700	-1.17687300	-2.62557700	H	0.84857500	-0.30766200	-2.85547500
C	1.22279300	0.22839200	-3.66444800	H	2.60999000	-0.20483300	-2.62641200

C	-5.63513600	-1.47719100	-0.69447500	H	3.63919400	2.45652300	1.69988900
H	-6.31012300	-2.07254300	-0.07565700	H	4.53265800	1.34257300	0.64901600
H	-6.07410000	-0.48769600	-0.83699800	C	3.30799800	2.77465500	-0.42507200
H	-5.53481500	-1.96510100	-1.66625900	H	2.33780300	3.26433500	-0.28089600
C	1.83794700	-2.22865500	-2.73744400	H	3.23016700	2.14547800	-1.31620200
H	2.69908800	-2.68098400	-2.24036300	H	-2.24503900	2.07175800	-1.37269900
H	0.93582200	-2.77520900	-2.45390600	C	4.39543500	3.83115900	-0.62941500
H	1.97260700	-2.31949000	-3.81785900	H	5.36171000	3.33529900	-0.77352300
H	0.49066300	2.06458200	0.69592900	H	4.18053600	4.36733300	-1.55808000
<b>TS1</b>				C	4.49479800	4.83459800	0.51918300
P	2.51676600	-0.48214200	0.28248200	H	4.83908900	4.36534600	1.44407300
P	-2.05074200	-0.11928800	-0.83809400	H	5.19772900	5.63549900	0.27751700
O	0.82545300	0.37579000	-2.97015200	H	3.52062000	5.29298300	0.71771500
O	-2.23189200	-1.84110500	0.03053300	C	6.37867600	-3.12041400	-0.96723700
H	-0.92732700	-2.56869900	-0.08708900	H	5.70061100	-3.69194100	-1.61024200
O	0.00925400	-2.99873100	-0.05701200	H	6.66878500	-3.78541600	-0.14644500
O	2.50973200	0.94384900	0.97885500	C	7.61679400	-2.71370000	-1.76057700
O	-1.81509200	1.27692900	-1.71029500	H	7.34565500	-2.07663100	-2.60726700
O	2.66913900	-0.46974600	-1.20671200	H	8.31650700	-2.15533800	-1.13207600
O	1.21485000	-1.10807800	0.83362800	H	8.14186600	-3.58769300	-2.15340800
H	-0.39782100	-0.31392400	-2.28203800	C	-4.50029700	-1.65982400	3.08287700
O	3.77075800	-1.18196200	0.98572500	H	-4.50768800	-2.74244900	3.25178000
O	-3.61994900	-0.28021400	-1.11188900	H	-3.76476400	-1.24082400	3.77915500
O	-1.00635200	-0.90410800	-1.72938400	C	-5.88039700	-1.08548000	3.39010500
H	0.72895800	-1.98329300	0.35765900	H	-5.88778900	0.00123800	3.26374900
O	-1.63445000	0.45833800	0.59547200	H	-6.63457500	-1.50418700	2.71695400
C	-2.67332400	-1.94302100	1.37819400	H	-6.18727000	-1.30555000	4.41576600
C	0.03308700	-4.04803800	0.91500600	C	-6.90155900	1.21667600	-2.15152200
C	-0.79965600	1.62661000	0.79223100	H	-6.86227200	2.12771500	-1.54454300
C	0.87663000	1.79625200	-3.08370900	H	-6.61586100	1.50341900	-3.16926200
H	1.82057600	2.10616600	-3.54031600	C	-8.32313000	0.66274900	-2.15406500
H	0.05308300	2.10804000	-3.72532100	H	-8.38830600	-0.23635800	-2.77358700
H	0.76801300	2.27618700	-2.10728200	H	-8.63881300	0.39472200	-1.14173100
H	-0.75218900	-4.77346800	0.69565100	H	-9.03481700	1.39331600	-2.54597000
H	1.00336300	-4.54176900	0.85314800	C	0.46690900	2.88812300	2.54508500
H	-0.10584200	-3.64921300	1.92368500	H	-0.18262700	3.76928200	2.51020400
H	-2.68657700	-3.01636200	1.60607600	H	1.22459400	3.02399800	1.76620400
H	-1.94448100	-1.47427400	2.05250400	C	1.15133000	2.80005500	3.90531600
C	-4.05927200	-1.37414200	1.64920400	H	0.41697300	2.66265500	4.70474100
H	-4.06188000	-0.29263600	1.47720200	H	1.83986400	1.95032600	3.93573000
H	-4.77377400	-1.81426900	0.94475200	H	1.72177500	3.70584200	4.12589900
H	0.06164300	1.56672300	0.12002100	<b>5</b>			
H	-1.37804100	2.52447300	0.55630500	P	2.51181200	-0.47514500	0.25092400
C	-0.35500900	1.63679300	2.23721700	P	-2.06678700	-0.21378600	-0.74239300
H	-1.23617300	1.59692800	2.88710700	O	0.80869300	0.41401600	-3.03868000
H	0.24160400	0.74046500	2.42942700	O	-2.22381100	-1.73463500	0.02604900
C	-4.48909300	0.76011700	-1.61404200	H	-0.80307100	-2.68326600	-0.24610000
H	-4.17721400	1.03923800	-2.62221400	O	0.08885900	-3.09556200	-0.16039800
H	-4.42054100	1.63376500	-0.95835400	O	2.46706300	0.94232500	0.95396600
C	-5.89621600	0.20247300	-1.61069500	O	-1.81017300	1.20445600	-1.63890200
H	-5.91753500	-0.70663600	-2.22097500	O	2.64221400	-0.47116600	-1.23730800
H	-6.16677100	-0.08188300	-0.58823200	O	1.21658200	-1.12964600	0.81636900
C	4.41313700	-2.33405600	0.38615500	H	-0.47108800	-0.32390500	-2.26415100
H	4.68367900	-2.98169900	1.22142600	O	3.77301900	-1.15455000	0.95347200
H	3.69861500	-2.86810500	-0.24781600	O	-3.64988900	-0.28941100	-1.07039000
C	5.63833400	-1.91237600	-0.39809600	O	-0.99217400	-0.94070500	-1.68451300
H	5.33429300	-1.24328000	-1.20979200	H	0.80530400	-1.96559200	0.33015900
H	6.30222800	-1.34653400	0.26491600	O	-1.64754700	0.45333200	0.66846400
H	1.55029100	0.08034900	-2.37658500	C	-2.68550300	-1.92770900	1.36544800
C	3.59008200	1.88649300	0.77180600	C	0.04660700	-4.11440200	0.84475800

C	-0.83935500	1.63495300	0.84102800	H	-6.81686000	2.19985100	-1.54895400
C	0.86277900	1.83603200	-3.09648900	H	-6.52046900	1.62337700	-3.18236500
H	1.80350600	2.16822800	-3.54543600	C	-8.28724800	0.79371500	-2.26484600
H	0.03512000	2.17423900	-3.71996200	H	-8.35071900	-0.07882200	-2.92148000
H	0.75892200	2.27856100	-2.10169500	H	-8.64807700	0.49477200	-1.27649400
H	-0.73601300	-4.83887500	0.61335100	H	-8.96605400	1.55646000	-2.65374400
H	1.01345400	-4.61740800	0.84156700	C	0.47967000	2.90710400	2.55160200
H	-0.13123500	-3.68030900	1.83236100	H	-0.17685000	3.78376700	2.54508400
H	-2.68455400	-3.01315200	1.50555400	H	1.20474100	3.05168800	1.74374500
H	-1.95867700	-1.49787200	2.06293100	C	1.21891900	2.82030300	3.88293500
C	-4.07706600	-1.39146300	1.66513900	H	0.51851600	2.67455600	4.71086500
H	-4.09706200	-0.30305900	1.54726200	H	1.91438800	1.97551400	3.88250800
H	-4.79096100	-1.80915200	0.94756100	H	1.79104000	3.72967700	4.08410000
H	0.00223900	1.60232500	0.14310800	<b>TS2</b>			
H	-1.44273200	2.52314200	0.62937500	P	-2.56502200	0.15376400	-0.78531600
C	-0.34323300	1.65070300	2.27056700	P	2.34764100	-0.16600900	-0.96718500
H	-1.19885600	1.60029100	2.95314700	O	0.36911600	-2.65817100	-2.57678900
H	0.26897100	0.75947700	2.43808800	O	2.49813100	1.43967400	-1.26186300
C	-4.47209200	0.77309000	-1.58352900	H	0.93926600	2.02619400	-2.06401600
H	-4.12244400	1.06585400	-2.57547300	O	-0.00601500	2.19645000	-2.23363000
H	-4.40961600	1.63601200	-0.91153200	O	-2.54495500	-0.98922000	0.31753700
C	-5.89443000	0.25510500	-1.64143300	O	2.07713400	-2.33331000	-0.79724700
H	-5.91998600	-0.63705900	-2.27646100	O	-3.57035600	-0.03049800	-1.86403800
H	-6.20743700	-0.04929300	-0.63686600	O	-1.05361500	0.14282800	-1.18938900
C	4.42518200	-2.30888600	0.36599800	H	1.04196200	-1.25258300	-2.43986400
H	4.70209000	-2.94287700	1.20941800	O	-2.78338700	1.51275700	0.03116800
H	3.71413900	-2.85648900	-0.26011100	O	3.90343200	-0.46241300	-0.93339200
C	5.64503100	-1.88456500	-0.42445400	O	1.56196900	-0.39143400	-2.30354800
H	5.33343400	-1.23384800	-1.24820500	H	-0.67463900	0.97117900	-1.65741800
H	6.30062700	-1.29877600	0.22930700	O	1.62694600	-0.00479400	0.42592900
H	1.52317900	0.10090800	-2.44738400	C	2.82628000	2.40908400	-0.24216100
C	3.54307600	1.90050000	0.78656000	C	-0.41030400	3.36728800	-1.51419200
H	3.55441600	2.46408900	1.71939400	C	0.78514000	-0.89602700	1.19891800
H	4.49476100	1.36762500	0.69120800	C	-0.97700800	-2.86436100	-2.15404700
C	3.28738100	2.79184900	-0.41346100	H	-1.11081100	-2.55906000	-1.11328900
H	2.31104100	3.27539800	-0.29294200	H	-1.63637200	-2.26767500	-2.78669000
H	3.23686200	2.16698800	-1.30977200	H	-1.24669300	-3.92002400	-2.25505400
H	-2.25166100	1.99471400	-1.30865100	H	0.20082500	4.22234400	-1.80889400
C	4.37413600	3.85531300	-0.58194200	H	-1.44982200	3.56400400	-1.77590300
H	5.34587300	3.36544500	-0.70873100	H	-0.33077400	3.20951300	-0.43488600
H	4.17771000	4.39938800	-1.51005600	H	2.86406600	3.35820600	-0.78093200
C	4.44185000	4.84718600	0.57888900	H	2.00170900	2.44966000	0.47521300
H	4.76620800	4.36952500	1.50675800	C	4.14457200	2.15824800	0.46547000
H	5.14713000	5.65318400	0.36231300	H	4.08871600	1.23517700	1.05260800
H	3.46133400	5.29958700	0.75921900	H	4.93411200	2.02170500	-0.28052000
C	6.40146600	-3.09318100	-0.97083200	H	0.16327500	-1.47406200	0.51826000
H	5.73236500	-3.68418100	-1.60553000	H	1.43243600	-1.56646400	1.76907700
H	6.69728700	-3.74001000	-0.13764800	C	-0.06041000	-0.03221800	2.10723300
C	7.63690200	-2.68498900	-1.76750700	H	0.58584300	0.61543600	2.70938100
H	7.36060300	-2.06783300	-2.62718200	H	-0.68885900	0.61503500	1.48703600
H	8.32642000	-2.10535200	-1.14703500	C	4.59492900	-1.44576800	-0.12703900
H	8.17522500	-3.55926500	-2.14131000	H	4.54407900	-2.40609400	-0.63855600
C	-4.49609000	-1.75646900	3.08771300	H	4.09399100	-1.52661600	0.84235100
H	-4.47199100	-2.84558800	3.20509500	C	6.02736700	-0.98369200	0.03672900
H	-3.76630300	-1.34925600	3.79657600	H	6.46778800	-0.83013700	-0.95431700
C	-5.88887100	-1.23556000	3.43037400	H	6.04678500	-0.02229700	0.55876500
H	-5.92758800	-0.14498600	3.35282800	C	-3.81156200	2.47211700	-0.31385900
H	-6.63693600	-1.64539400	2.74523600	H	-3.44296600	3.42494800	0.06955200
H	-6.17981400	-1.50951400	4.44755800	H	-3.89329300	2.53833600	-1.40142700
C	-6.85376600	1.31017400	-2.18708600	C	-5.13939700	2.10755200	0.31696500

H	-5.47926100	1.14622800	-0.08466100	H	-0.56978400	-0.75352400	-2.54368100
H	-4.99683800	1.98362300	1.39639700	O	1.68712400	-0.31010700	0.94841200
H	0.98660500	-2.84246200	-1.80625400	C	1.48103100	2.15605800	-0.68097000
C	-3.77076800	-1.62608200	0.74934900	C	-0.42649200	0.94457900	-4.31001500
H	-3.66709900	-1.74465200	1.82855000	C	0.46463000	-0.97330400	1.38218600
H	-4.62354800	-0.96842300	0.55241800	C	-1.38197900	-3.76156500	-0.24715700
C	-3.93103800	-2.95847200	0.04190800	H	-1.53484600	-3.04741000	0.56761500
H	-3.07802600	-3.59656800	0.29992000	H	-2.11143500	-3.56478700	-1.03674000
H	-3.89446600	-2.78248000	-1.03815000	H	-1.53490700	-4.77187200	0.13523800
H	2.30173300	-2.69888700	0.06234800	H	0.22257100	1.40797300	-5.05523300
C	-5.23945600	-3.65958800	0.41084100	H	-1.23657800	0.41822200	-4.81398900
H	-6.08372800	-3.02663400	0.11625100	H	-0.84463000	1.71396200	-3.65530700
H	-5.31605000	-4.57616700	-0.18069700	H	1.04803900	2.75335100	-1.48405700
C	-5.34796800	-4.00629600	1.89509800	H	0.72336200	1.99589800	0.08908700
H	-5.40239800	-3.11115300	2.52003900	C	2.72128800	2.81352300	-0.11492000
H	-6.24466200	-4.59847700	2.09312700	H	3.13697600	2.19559100	0.68789600
H	-4.48168900	-4.59076900	2.22072300	H	3.48170200	2.89378300	-0.89889300
C	-6.19420300	3.17943900	0.04956200	H	-0.14332100	-1.22108700	0.50964400
H	-6.31447700	3.30714400	-1.03172800	H	0.76539400	-1.89623300	1.88345800
H	-5.84151500	4.13923800	0.44244100	C	-0.28343900	-0.04676400	2.31304100
C	-7.53933800	2.82917500	0.67775000	H	0.41029600	0.35117700	3.06109100
H	-7.92446600	1.88787800	0.27507900	H	-0.66521100	0.80087500	1.73390500
H	-7.44520200	2.71540300	1.76168500	C	4.62319200	-1.20690500	0.23123500
H	-8.28325200	3.60599300	0.48547400	H	4.67132700	-2.04562400	-0.46900300
C	4.49440800	3.32204400	1.39024200	H	4.15938300	-1.53919900	1.16527300
H	4.55420800	4.24592700	0.80495100	C	5.99177800	-0.61575700	0.48011400
H	3.68981000	3.46343700	2.12033400	H	6.38697500	-0.22742100	-0.46437800
C	5.81434100	3.08877500	2.11955500	H	5.89324800	0.22865900	1.17033500
H	5.76603700	2.18695100	2.73712900	C	-2.02731900	2.51576600	-0.96230600
H	6.63462200	2.96251800	1.40679600	H	-1.21033100	3.22940000	-1.07678900
H	6.06356200	3.92898700	2.77217500	H	-2.72299300	2.64246500	-1.79627700
C	6.84607600	-2.01185300	0.81512600	C	-2.72249000	2.70080200	0.37228300
H	6.37416400	-2.19074000	1.78756100	H	-3.52431100	1.96086400	0.48149400
H	6.83415300	-2.96650000	0.27855000	H	-2.00081400	2.52262300	1.17676100
C	8.28712000	-1.55532800	1.02126600	H	1.42444600	-3.95819200	0.29872000
H	8.78337400	-1.38772500	0.06107300	C	-4.11460800	-0.81608000	0.43405400
H	8.32216300	-0.61819500	1.58450000	H	-4.12897200	-0.63477300	1.50904700
H	8.86519600	-2.30058800	1.57280700	H	-4.72113500	-0.05186600	-0.05976400
C	-0.93695200	-0.89441400	3.01687800	C	-4.60036300	-2.20885100	0.08464500
H	-0.31857900	-1.34340900	3.80096500	H	-4.00642300	-2.94383400	0.63952400
H	-1.35954200	-1.72134600	2.43663400	H	-4.42560700	-2.38039600	-0.98275500
C	-2.06879300	-0.08452600	3.64052300	H	2.85584800	-3.47503700	0.15292100
H	-1.67508300	0.75670700	4.21908100	C	-6.08529500	-2.39496100	0.40250600
H	-2.72131600	0.32272500	2.86146400	H	-6.67418900	-1.69149100	-0.19619200
H	-2.67975900	-0.69618300	4.30945300	H	-6.38158100	-3.39844700	0.08465400
<b>6</b>				C	-6.41613300	-2.21439200	1.88335100
P	-2.28684000	-0.08654000	-1.36662500	H	-6.26566000	-1.18247700	2.21060400
P	2.23792700	-0.42275600	-0.53289800	H	-7.45867000	-2.47246100	2.08438800
O	-0.05306700	-3.69755300	-0.74981100	H	-5.78528400	-2.85825800	2.50438600
O	1.75817200	0.87325600	-1.31429600	C	-3.31065700	4.10379900	0.50458500
H	0.96652300	0.42166000	-3.00486900	H	-4.03449100	4.27076400	-0.30018400
O	0.30574600	-0.02862500	-3.55539400	H	-2.51491700	4.84493500	0.37251100
O	-2.72558400	-0.64963600	0.05198700	C	-3.98639500	4.30873400	1.85709000
O	2.29673000	-4.00448200	0.73230900	H	-4.79605200	3.58721300	2.00041500
O	-3.42204800	0.16873300	-2.28929000	H	-3.27047600	4.17452800	2.67323200
O	-1.19508100	-1.12097300	-1.82108600	H	-4.41067000	5.31178900	1.94368600
H	0.12735800	-2.80198200	-1.07453200	C	2.37973100	4.19855900	0.43289200
O	-1.40374800	1.21238300	-1.07045800	H	1.96225300	4.81388400	-0.37134100
O	3.79244100	-0.17259900	-0.36200600	H	1.59768900	4.10140500	1.19436900
O	1.86360600	-1.65972700	-1.25838500	C	3.59772200	4.89295000	1.03398400

H	4.01507200	4.30465900	1.85606500
H	4.38225000	5.02351300	0.28319100
H	3.33894900	5.87999500	1.42444200
C	6.95025600	-1.65476500	1.05770600
H	6.52987800	-2.06329900	1.98289700
H	7.04196300	-2.49087800	0.35645000
C	8.32874400	-1.06383100	1.33676300
H	8.77353500	-0.66404800	0.42094100
H	8.26310900	-0.24725500	2.06139400
H	9.00994100	-1.81671000	1.74015400
C	-1.43627000	-0.77485900	3.00554400
H	-1.02841000	-1.48611500	3.73132100
H	-1.99098900	-1.36188600	2.26680900
C	-2.38364000	0.19697600	3.70160100
H	-1.85207500	0.79167500	4.45092400
H	-2.82625200	0.89084900	2.97958800
H	-3.19744100	-0.32935400	4.20728400