

Supporting Information

**The First Manganese Catalyzed Isomerization of Allylic/Homo-allylic
Alcohols to Ketones**

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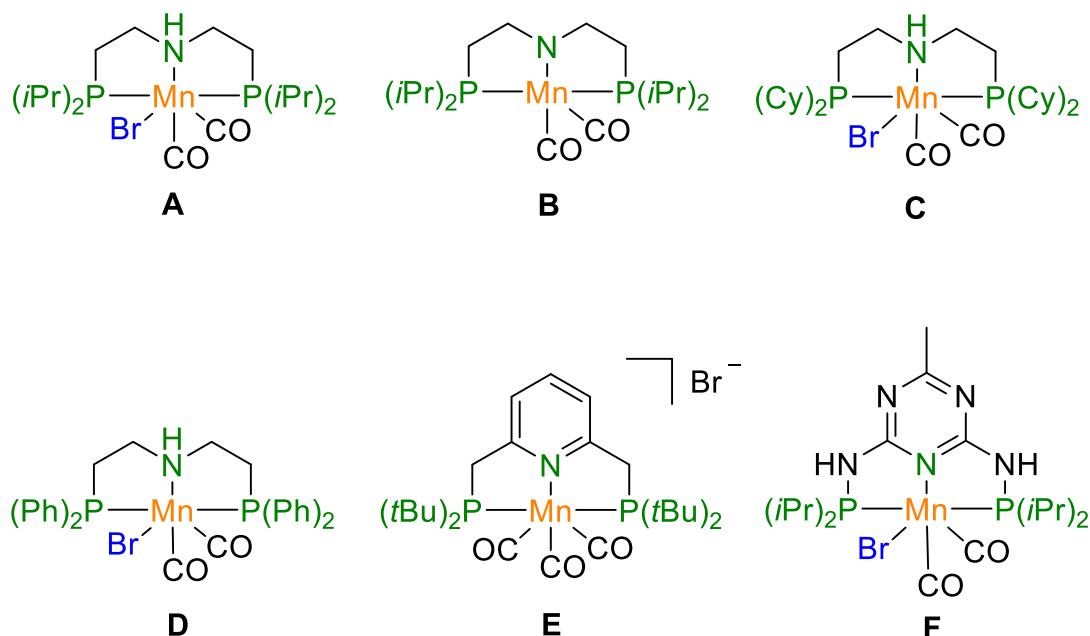
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1) General experimental information

All experiments were performed under inert argon atmosphere by using standard Schlenk techniques or a glove box, if not stated otherwise. $\text{PNP}^{(i\text{Pr})}$ and $\text{PNP}^{(t\text{Bu})}$ ligands were purchased from Strem as solutions in THF and $\text{PNP}^{(\text{Cy})}$ was purchased from Strem as a solid. The $\text{PNP}^{(\text{Ph})}$ ligand was purchased from abcr as a solid and all of these ligands were used as received. Dry and degassed THF, toluene, ethanol, acetonitrile, DMF, dichloromethane, heptane and hexane were taken from the solvents purification system. Isopropanol, methanol, chloroform, benzene, all the deuterated solvents and liquid substrates were degassed and stored in Schlenk flasks over 3Å molecular sieves. Solid starting materials were added to a Schlenk tube and stored under an argon atmosphere before use. Commercially available chemicals were purchased from Sigma, Alfa, Strem, abcr, Acros and TCI. ^1H NMR, ^{13}C NMR and ^{31}P NMR spectra were recorded at room temperature on 300 MHz spectrometers (Avance 300 or Fourier 300) or a 400 MHz spectrometer (Avance 400) from Bruker. The chemical shifts δ are given in ppm and referenced to the residual proton signal of the particular solvent. The coupling constants J are given in Hertz.

Electrospray ionization high resolution mass spectra were recorded on Agilent 6210. IR spectra were recorded on a Bruker Alpha FT-IR spectrometer and are reported in terms of frequency of absorption (cm^{-1}). For the quantification of C/H/N, a microanalyzer-TruSpec CHNS from the company Leco was used. The samples were catalytically combusted with pure oxygen in a helium stream. For the analysis of C and H contents an IR-detector was used, while for the analysis of N content a thermal conductivity detector was used.

2) Synthesis of the catalysts



Catalysts A,^[1] **B**,^[2] **C**,^[1] **E**^[2] and **F**^[3] were synthesized according to the literature procedures. The obtained analytical data were in agreement with the reported data in the literature.

Catalyst D

A suspension of HCl-PNP^(Ph) ligand (600 mg, 1.26 mmol) and NEt₃ (0.2 mL, 1.45 mmol) in THF (20 mL) was stirred for 15 minutes at room temperature. The liquid part of the resulting suspension was added dropwise through cannula filtration to a suspension of Mn(CO)₅Br (275 mg, 1.0 mmol) in THF (40 mL) (be aware of CO evolution). After one hour, the mixture was heated to 100 °C and stirred for 24 hours (a precipitate was formed during the course of the reaction). After this time, the mixture was allowed to cool to room temperature and the suspension was filtered. The resulting solid was washed with heptane (3 x 20 mL) and dried *in vacuo* to afford the title compound (388 mg, 61%). Single crystals suitable for X-ray diffraction measurement were obtained from slow diffusion of heptane into the solution of the title compound in toluene.

¹H NMR (400 MHz, CD₂Cl₂) δ_H: 8.16 – 6.76 (m, 20H), 3.39 (d, *J* = 155.2 Hz, 4H), 2.51 (d, *J* = 136.0 Hz, 4H) ppm.

³¹P NMR (162 MHz, CD₂Cl₂) δ_P: 69.7 ppm.

IR (FTIR): ν(N-H): 3190, ν(C-H): 3033, 2932, 2870, ν(CO): 1911, 1830, ν(C-C; C-H): 1574, 1482, 1462, 1434, 1406, 1330, 1304, 1206, 1167, 1097, 1068, 1021, 959, 830, 737, 695, 624, 579, 523, 473, 442 cm⁻¹.

Elemental analysis: Calculated for [C₃₀H₂₉BrMnNO₂P₂]: C, 56.98; H, 3.62; N, 2.22; found: C, 56.26; H, 3.46; N, 2.23. Carbon is slightly off, most likely due to the residues of the manganese precursor.

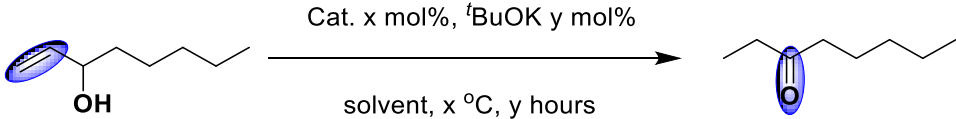
3) General procedure for the isomerization of allylic alcohols

An oven dried 10 mL pressure tube with a stirring bar was charged with complex **D** (0.01 mmol, 1 mol%), 0.01 mmol ^tBuOK and 1 mL toluene sequentially. Then 1 mmol of substrate was added immediately to the pressure tube. The solution was stirred for 1 hour at 120 °C. GC yields were determined with *n*-dodecane as internal standard. Isolated yields were obtained by using silica gel chromatography (Cyclohexane: Ethyl Acetate= 50:1) after rotary evaporation. For the neat reaction, base was added together with Complex **D**.

4) Computational procedure

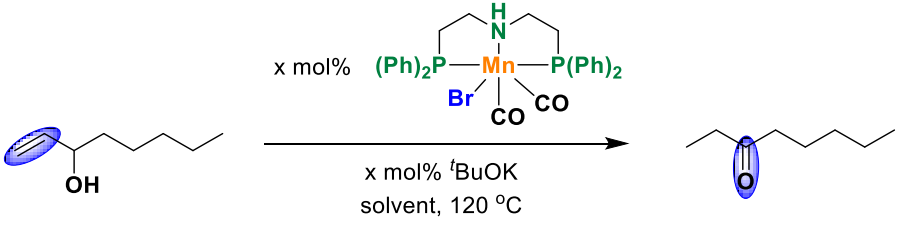
Structure optimizations have been carried out at the B3PW91^[4] density functional level of theory with the all-electron TZVP^[5] basis set (LANL2DZ^[6] for Mn) by using the Gaussian09 program package.^[7] The optimized geometries are characterized as energy minimums at the potential energy surface from frequency calculations at the same level of theory, i.e.; energy minimum structure has only real frequencies or transition state have only one imaginary vibration mode. The Gibbs free energies which are used for discussion and comparison are scaled with the thermal correction to Gibbs free energies at 298 K.

Table S1. Optimization of the isomerization of oct-1-en-3-ol with PNP pincer catalysts A, B and C. ^[a]

							
Entry	Cat. (%)	^t BuOK (%)	Solvent	Reaction Time (hour)	Temperature (°C)	Conversion (%) ^[b]	Yield (%) ^[b]
1	A (1)	1	Toluene	20	80	3	3
2	A (1)	1	MeOH	20	80	trace	trace
3	A (1)	1	EtOH	20	80	2	2
4	A (1)	1	ⁱ PrOH	20	80	18	15
5	A (1)	1	THF	20	80	17	17
6	B (1)	0	MeOH	16	80	0	0
7	B (1)	0	EtOH	16	80	trace	trace
8	B (1)	0	ⁱ PrOH	16	80	14	14
9	B (1)	0	Toluene	16	80	8	8
10	B (1)	0	THF	16	80	0	0
11	B (1)	0	Benzene	16	80	10	10
12	B (1)	0	Heptane	16	80	24	24
13	B (1)	0	DCM	16	80	10	10
14	B (1)	0	MeCN	16	80	0	0
15	B (5)	0	Toluene	1 & 9	120	19 & 82	19 & 82
16	B (5)	0	Benzene	1 & 9	120	14 & 65	14 & 63
17	B (5)	0	Heptane	1 & 9	120	30 & 90	30 & 88
18	B (5)	0	ⁱ PrOH	1 & 9	120	25 & 99	24 & 82
19 ^[c]	B (0.5)	0	Neat	1 & 9	120	19 & 70	19 & 69
20	C (5)	5	Toluene	2 & 16	120	33 & 97	33 & 94
21	C (5)	5	Benzene	2 & 16	120	22 & 91	22 & 91
22	C (5)	5	Heptane	2 & 16	120	45 & 98	44 & 88
23	C (5)	5	ⁱ PrOH	2 & 16	120	61 & 100	53 & 81
24 ^[c]	C (0.5)	0.5	Neat	2 & 16	120	52 & 92	51 & 90

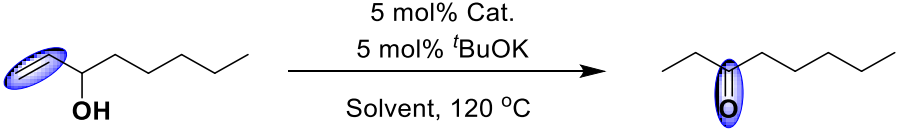
[a] General conditions: 1 mmol of substrate, catalyst, base (if used), 1 mL of solvent (if used). [b] Determined by GC with dodecane as an internal standard. [c] 10 mmol of substrate.

Table S2. Optimization of the isomerization reaction catalyzed by catalyst D. ^[a]

					
Entry	x (mol%)	Solvent	Time (hours)	Conversion (%) ^[b]	Yield (%) ^[b]
1	5	Toluene	2	100	93
2	5	1,4-Dioxane	2	100	98
3	5	Cyclohexane	2	100	93
4	5	Heptane	2	100	87
5	0.5	Neat	2	100	97
6	1	1,4-Dioxane	1	100	100
7 ^[c]	1	1,4-Dioxane	1 & 16	88 & 100	76 & 83
8 ^[d]	0.1	1,4-Dioxane	1	70	68
9 ^[d]	0.1	Cyclohexane	1	97	95
10 ^[d]	0.1	Toluene	1	100	99
11 ^[d]	0.1	Neat	1	94	94
12 ^[c]	0.1	Neat	16	6	6
13 ^[e]	0.01	Neat	16	3	3

[a] General conditions: 1 mmol of substrate, catalyst and base (the same loadings), 1 mL of solvent (if used). [b] Determined by GC with dodecane as an internal standard. [c] Room temperature. [d] 10 mmol of substrate. [e] 100 mmol of substrate.

Table 3.3.3 Optimization of the isomerization process with pincer catalyst E and F. ^[a]

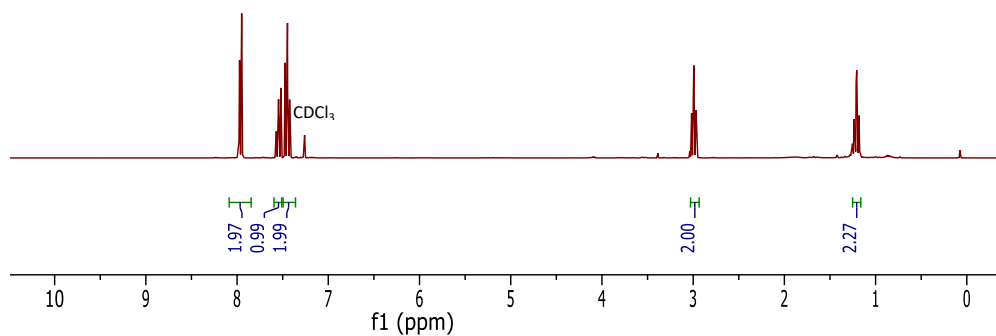
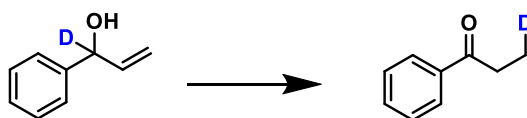
					
Entry	Catalyst	Solvent	Reaction Time (hours)	Conversion (%) ^[b]	Yield (%) ^[b]
1	E	Toluene	2; 6	13; 16	11; 12
2	E	1,4-Dioxane	2; 6	8; 9	7; 7
3	E	Cyclohexane	2; 6	27; 43	24; 39
4	E	Heptane	2; 6	17; 22	15; 18

5	E	Neat	2; 6	1; 1	1; 1
6	F	Toluene	2; 6	4; 11	2; 4
7	F	1,4-Dioxane	2; 6	5; 10	4; 6
8	F	Cyclohexane	2; 6	1; 7	0; 3
9	F	Heptane	2; 6	3; 9	2; 3
10	F	Neat	2; 6	22; 27	18; 21

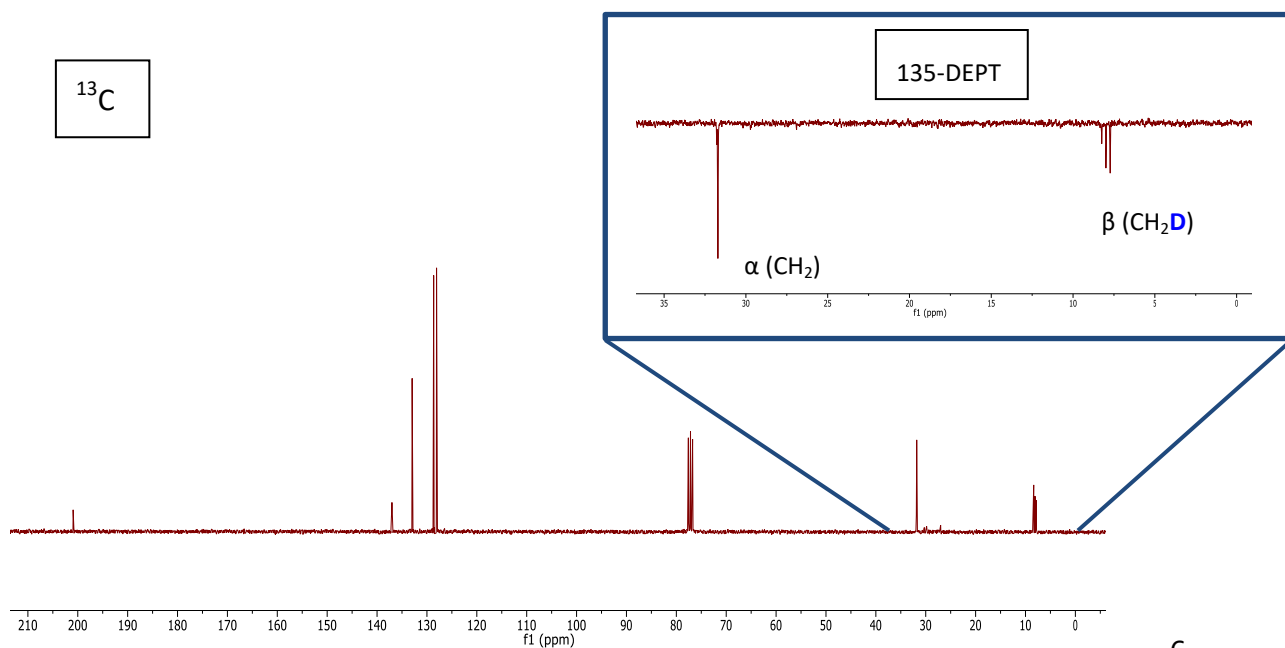
[a] General conditions: 1 mmol of substrate, 5 mol% catalyst, 5 mol% base, 1 mL of solvent (if used), 120 °C. [b] Determined by GC with dodecane as an internal standard.

5) Deuterium labeling experiment

^1H

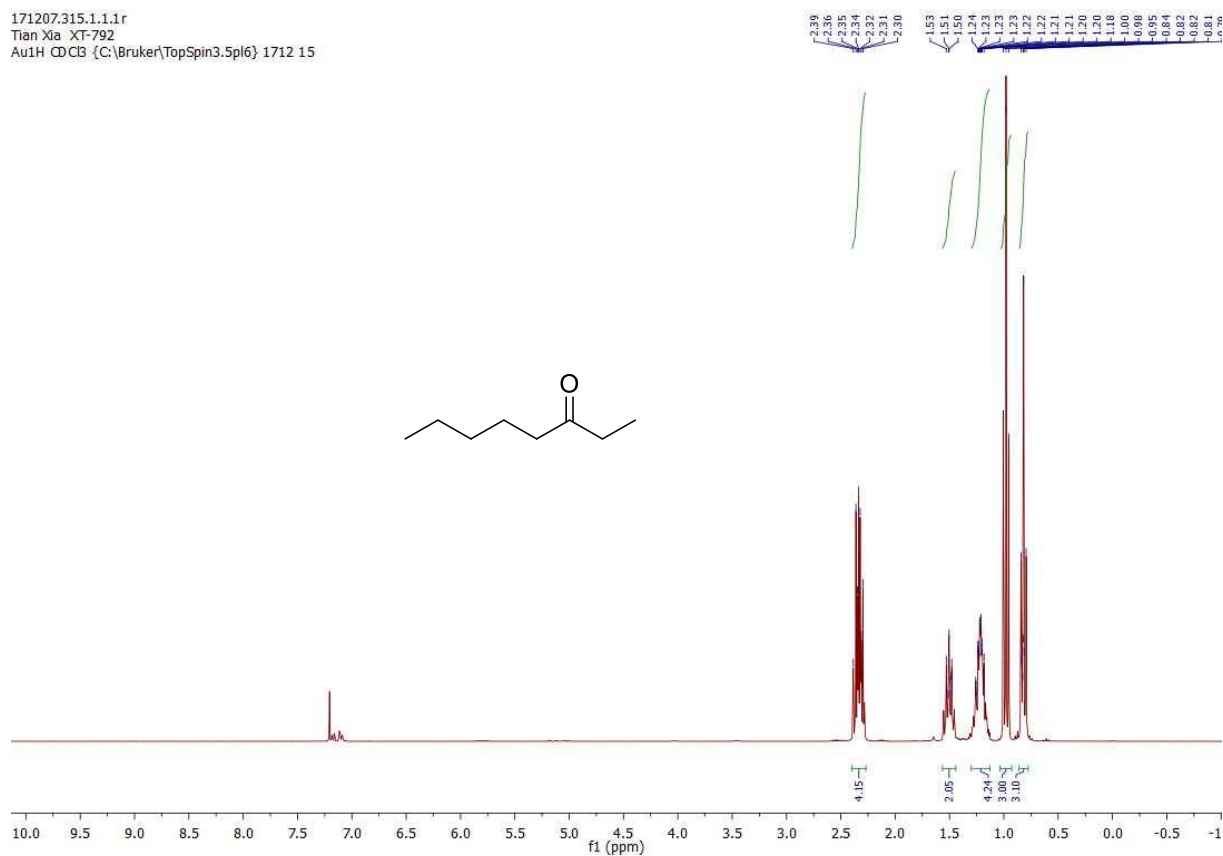


^{13}C

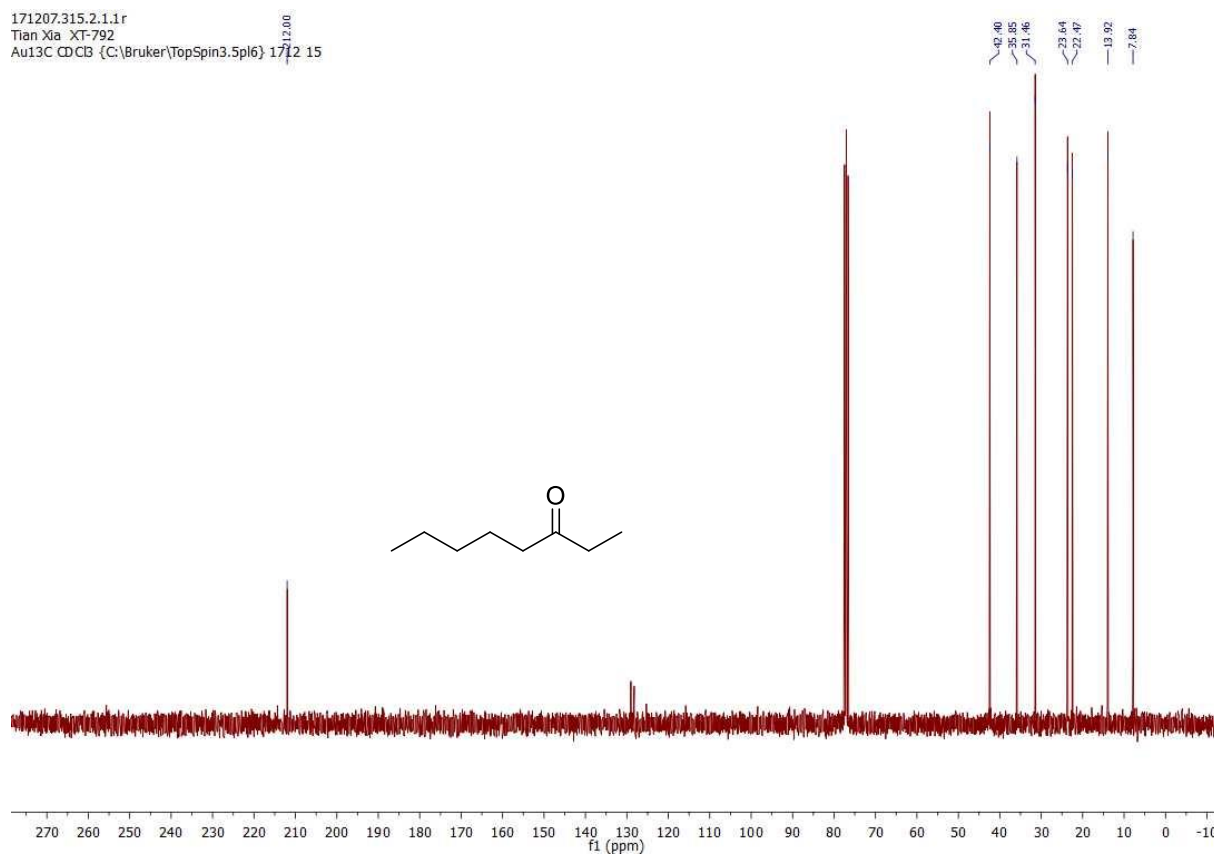


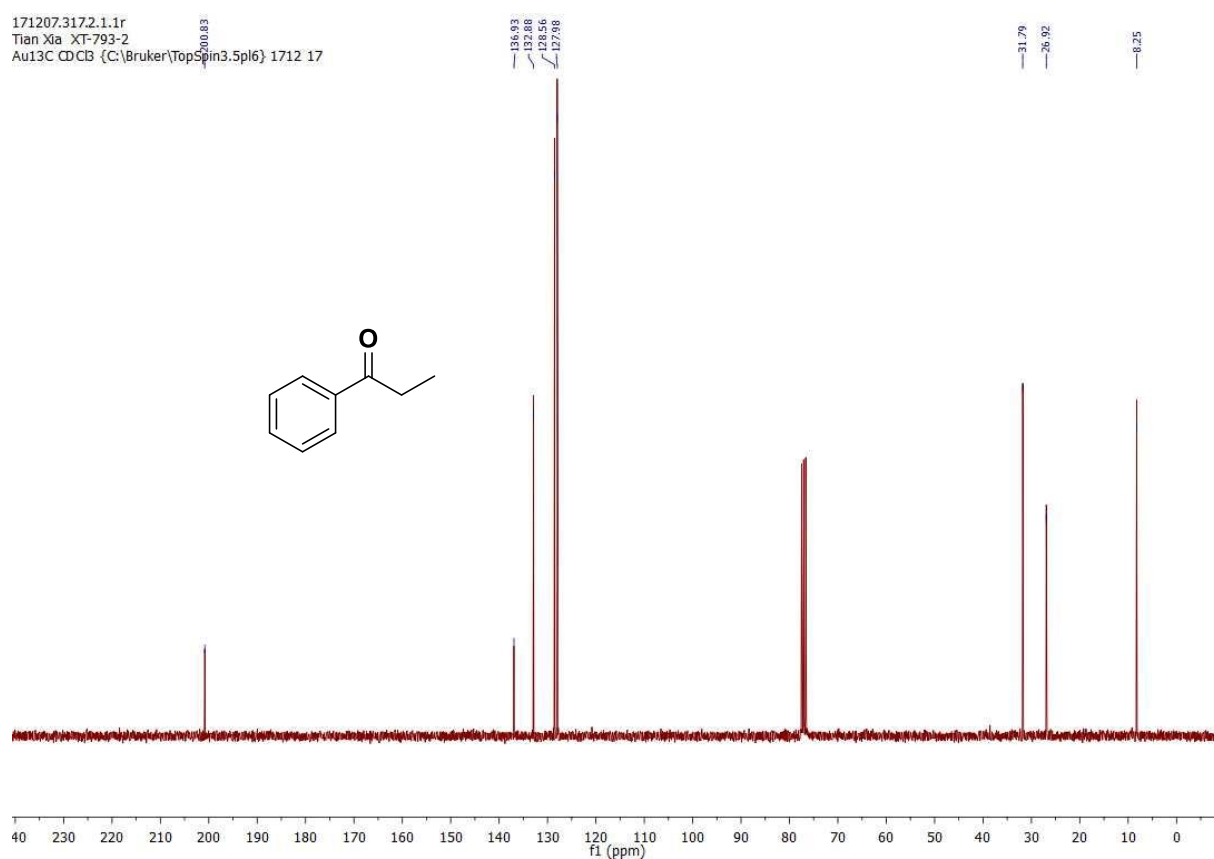
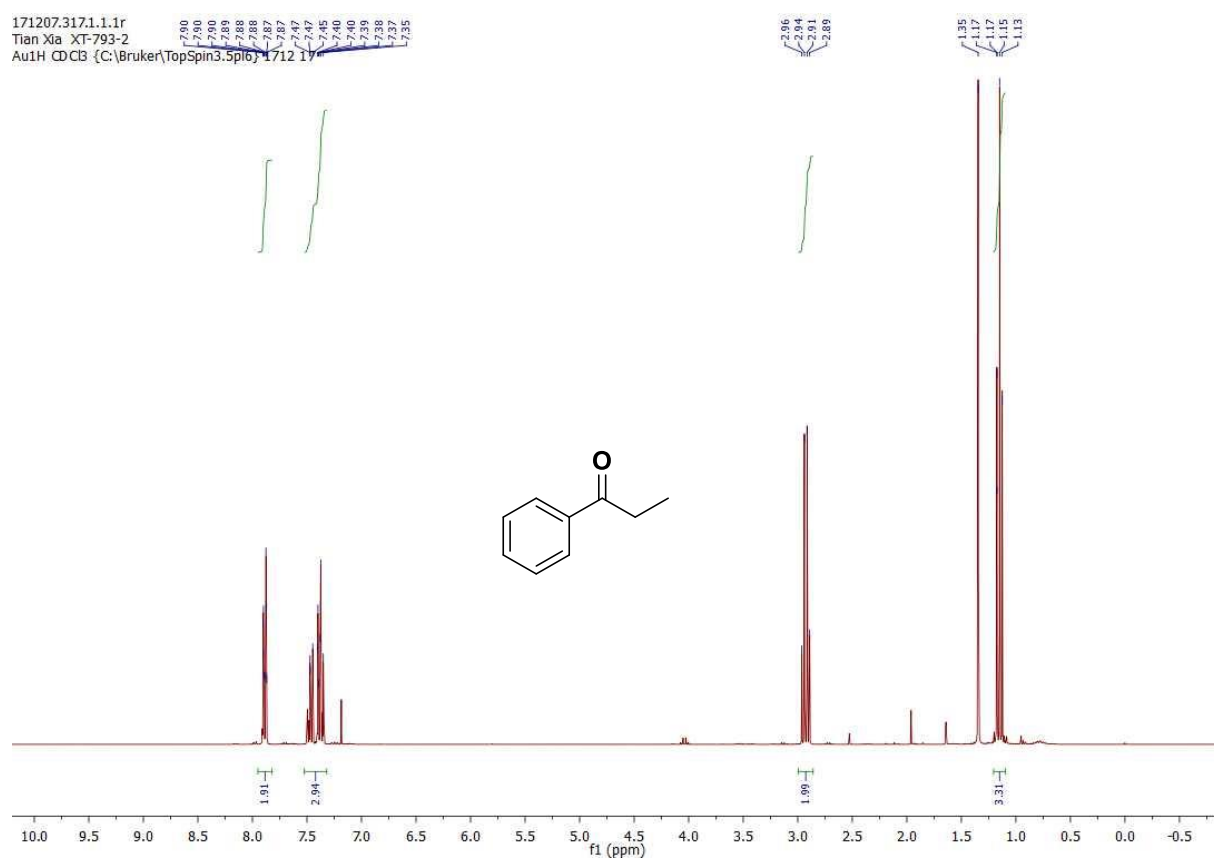
6) NMR data

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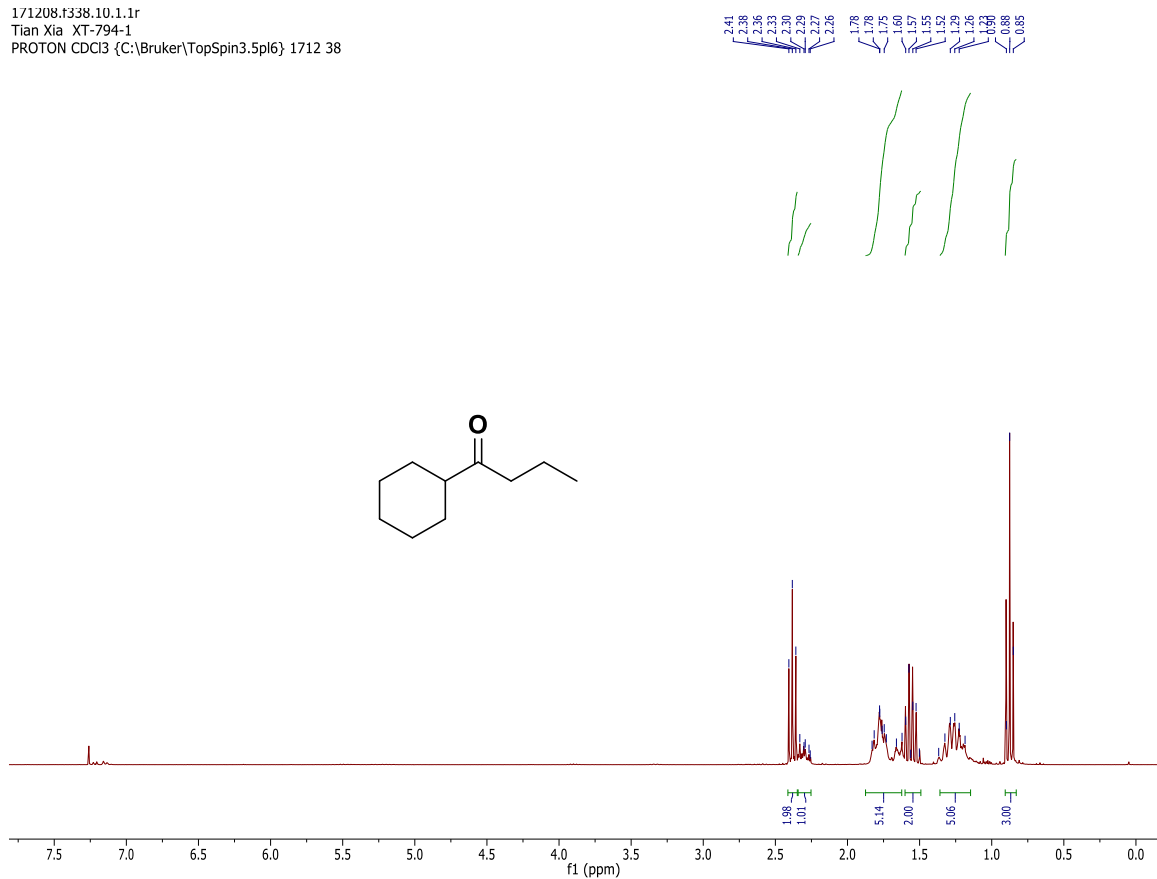


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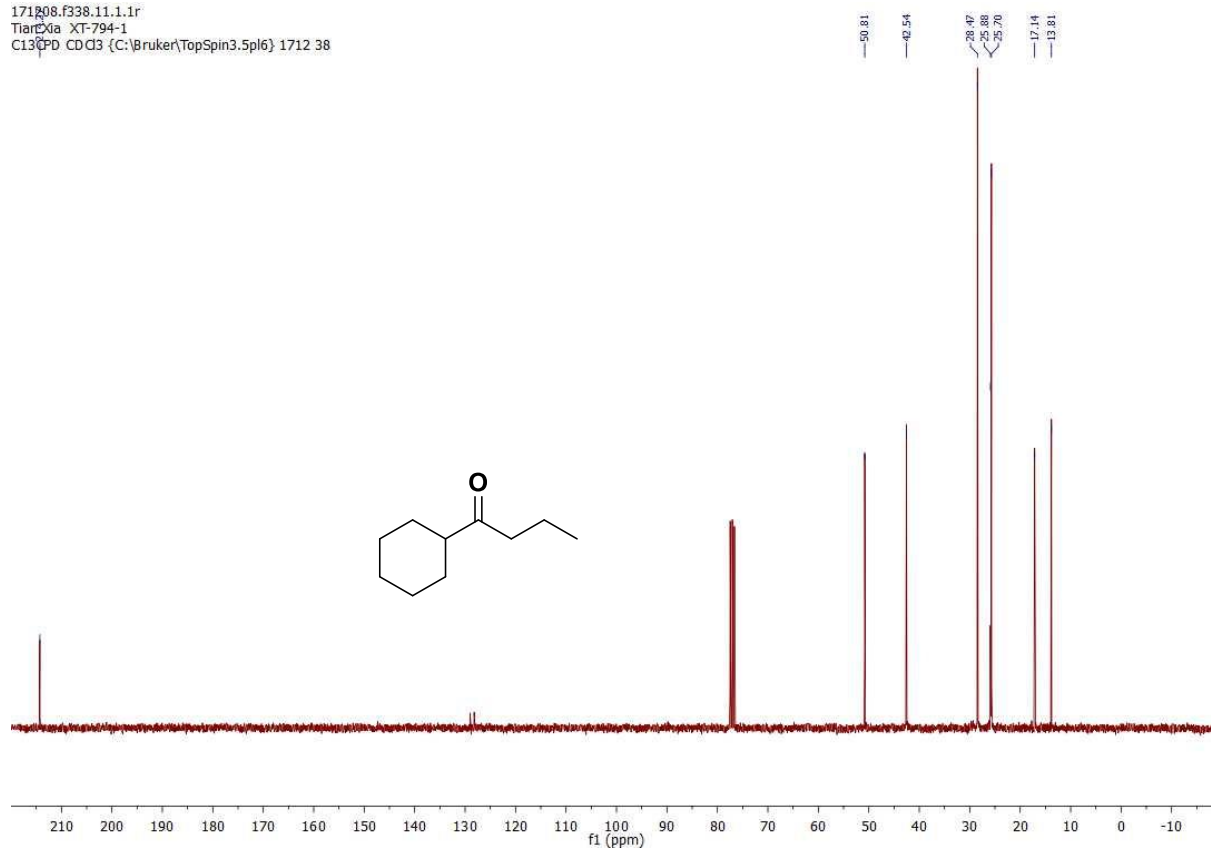


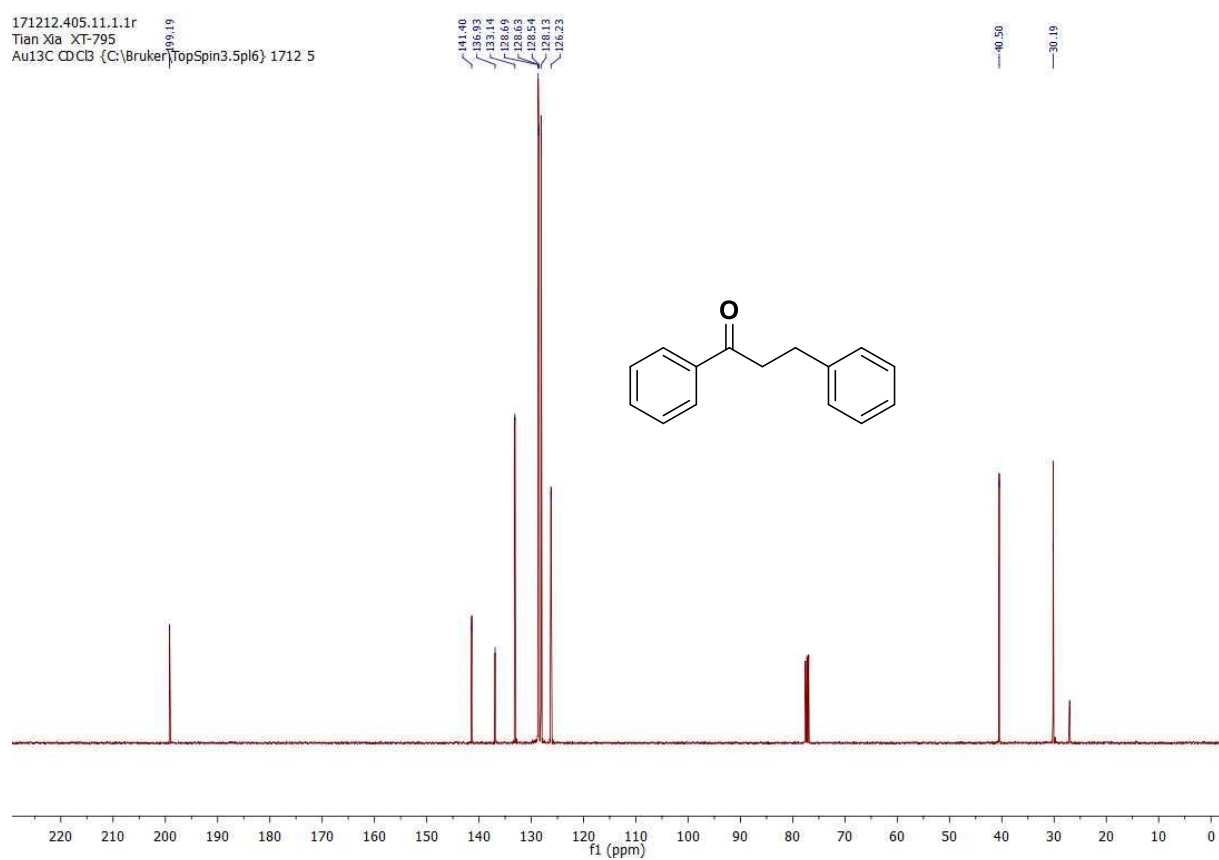
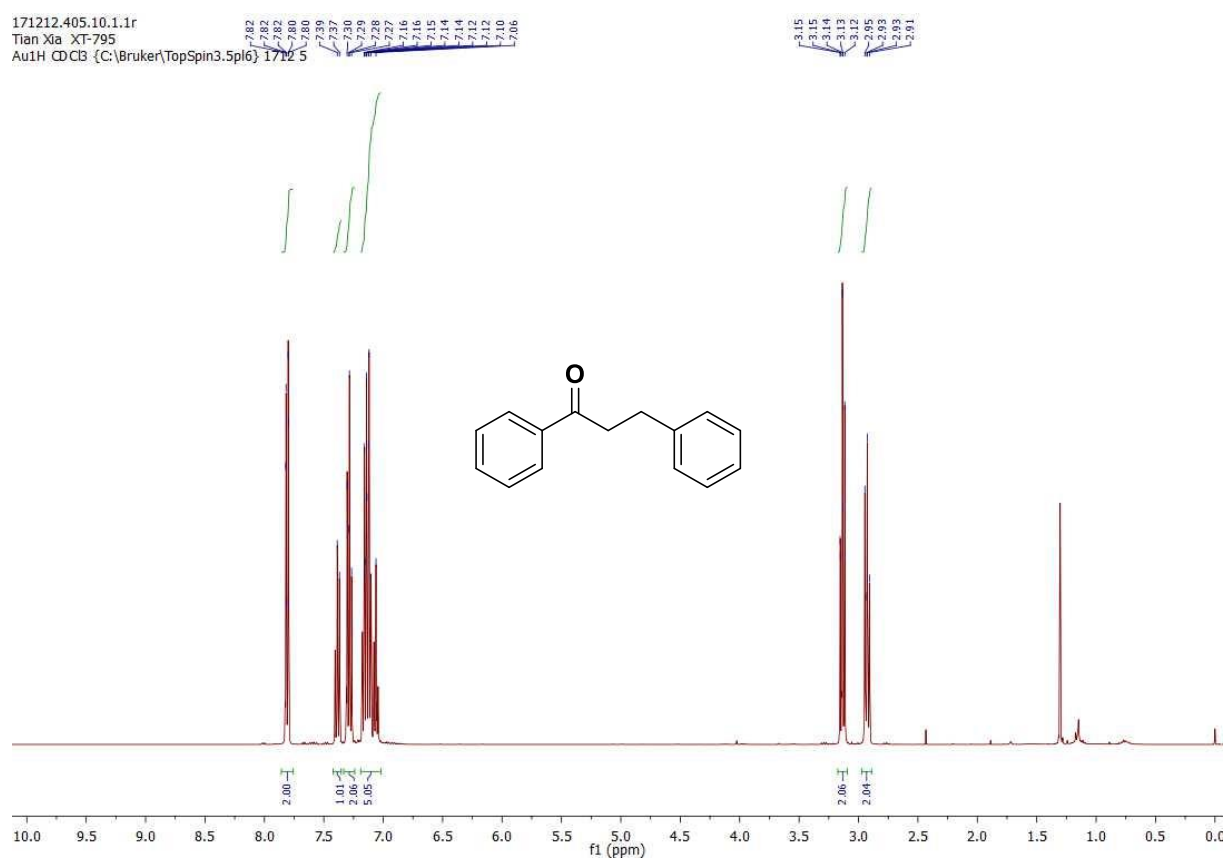


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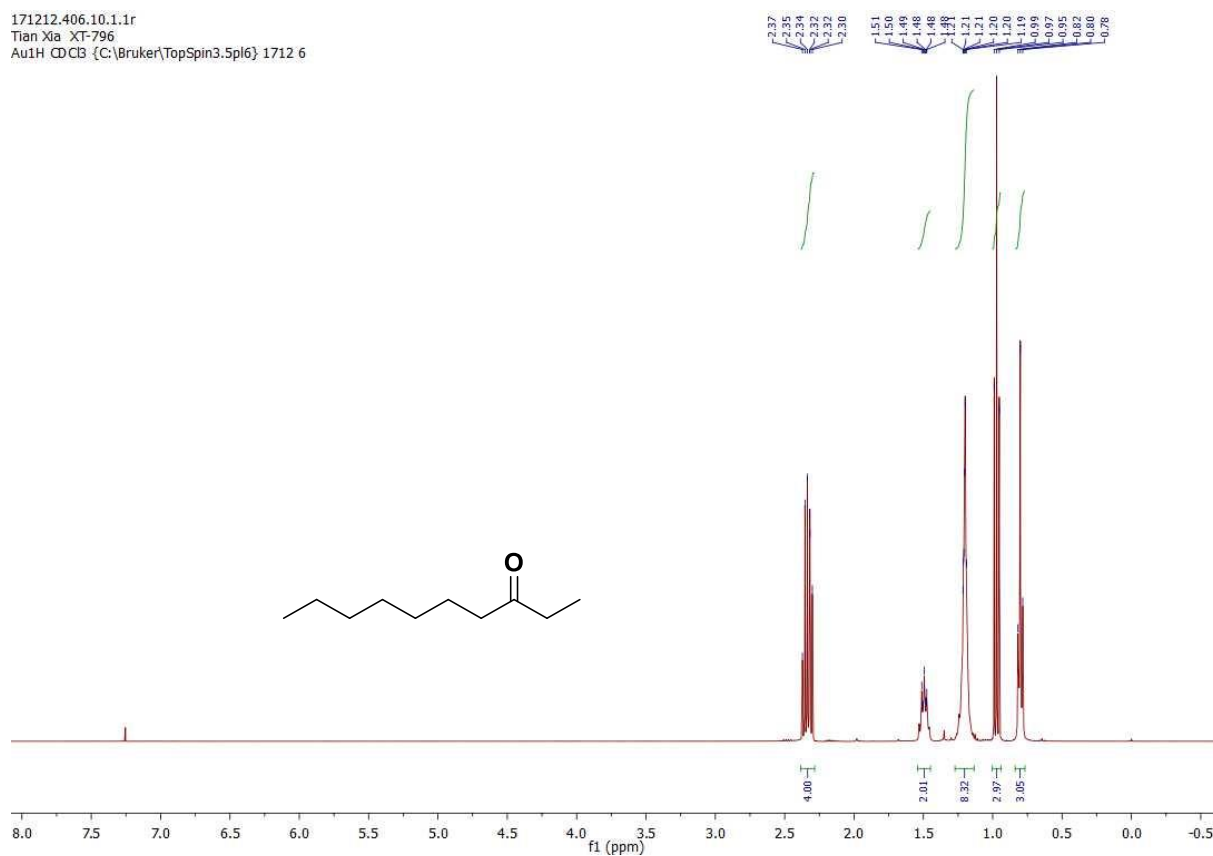


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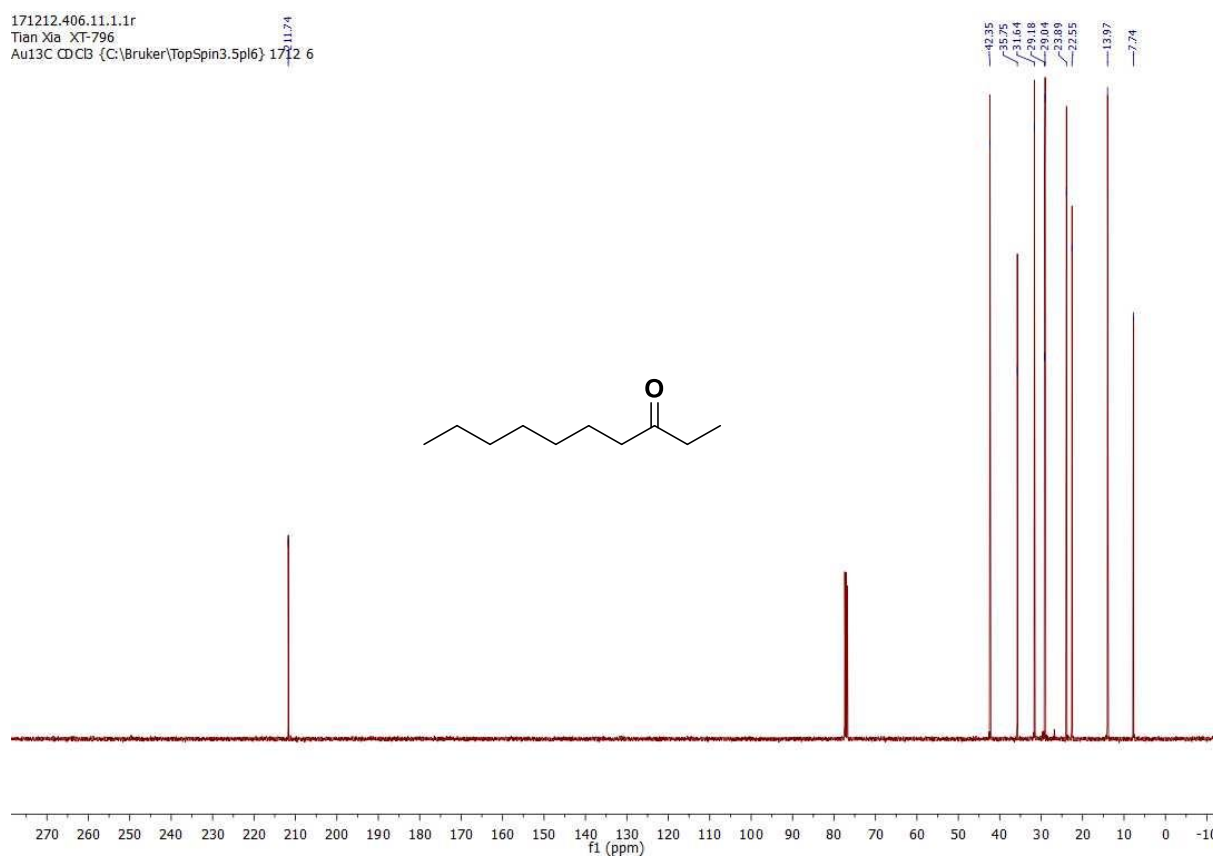


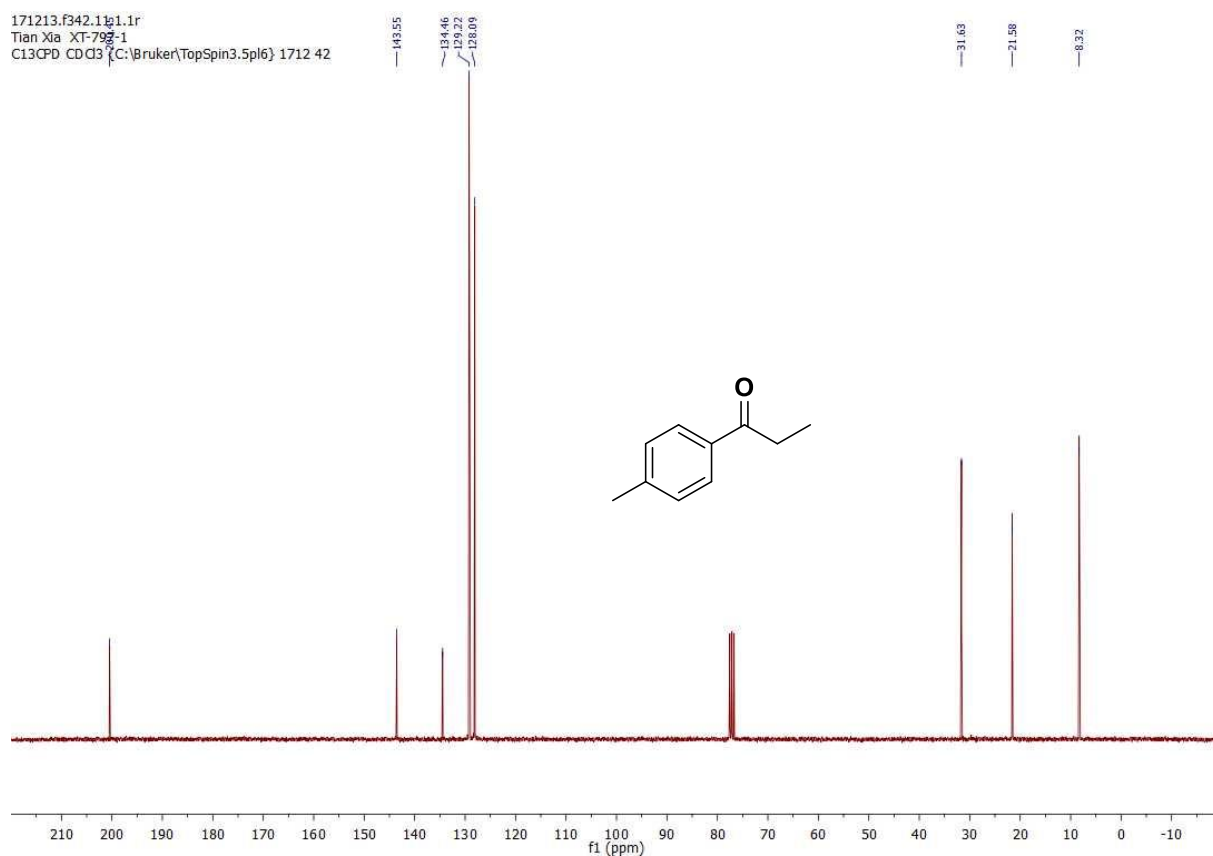
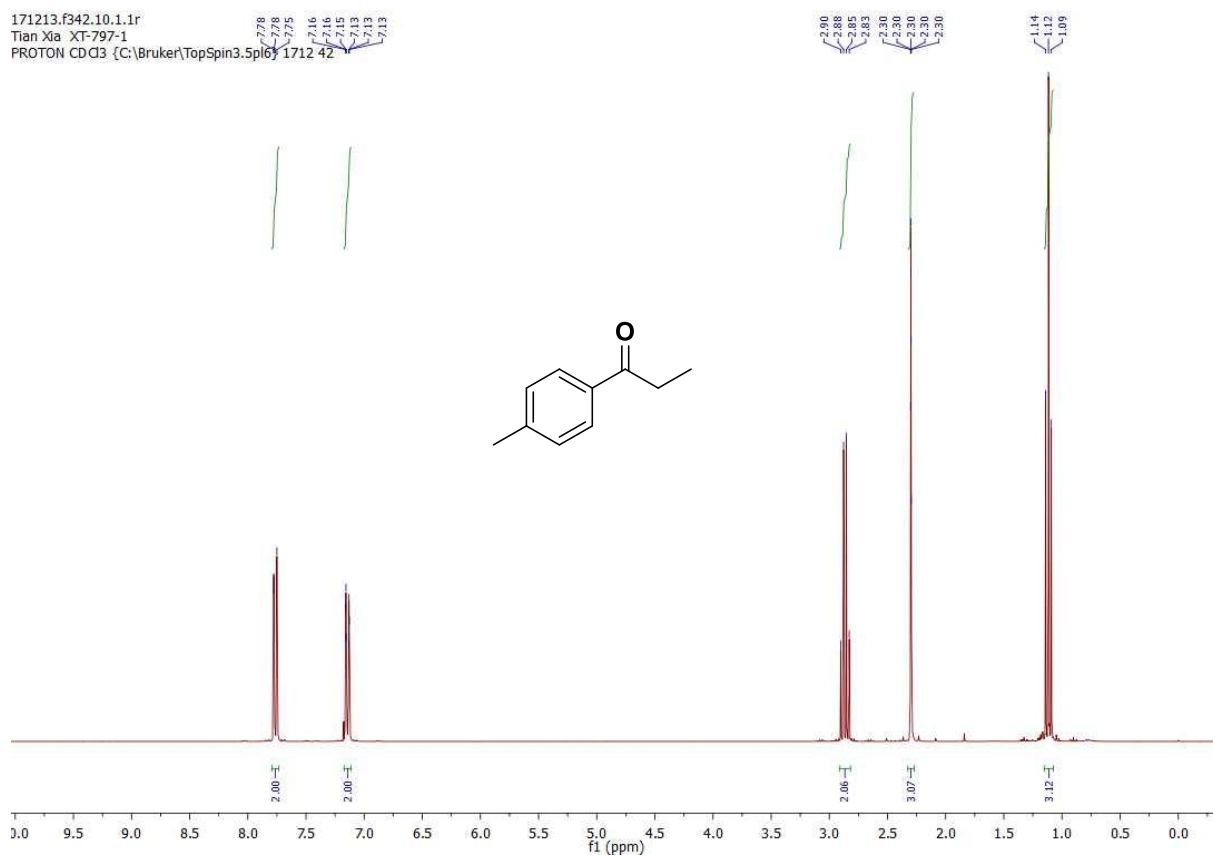


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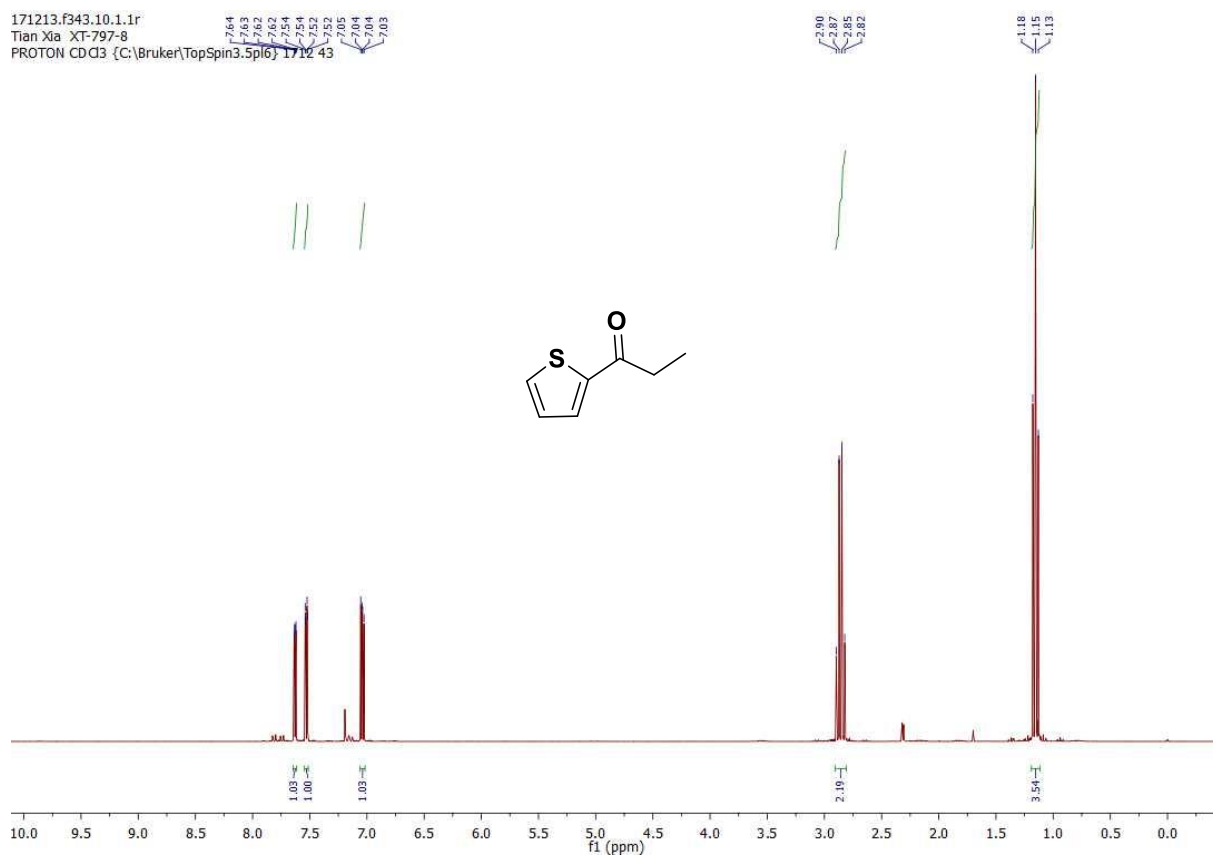


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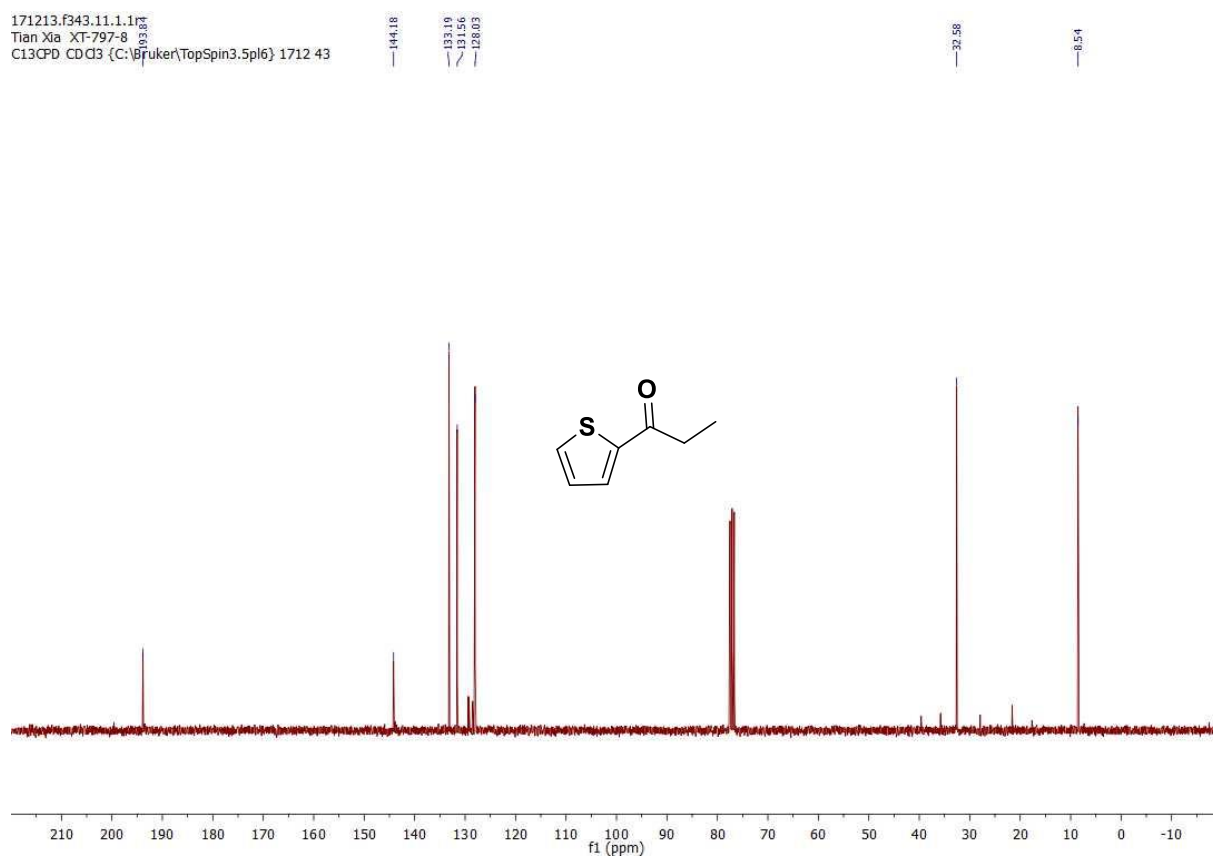




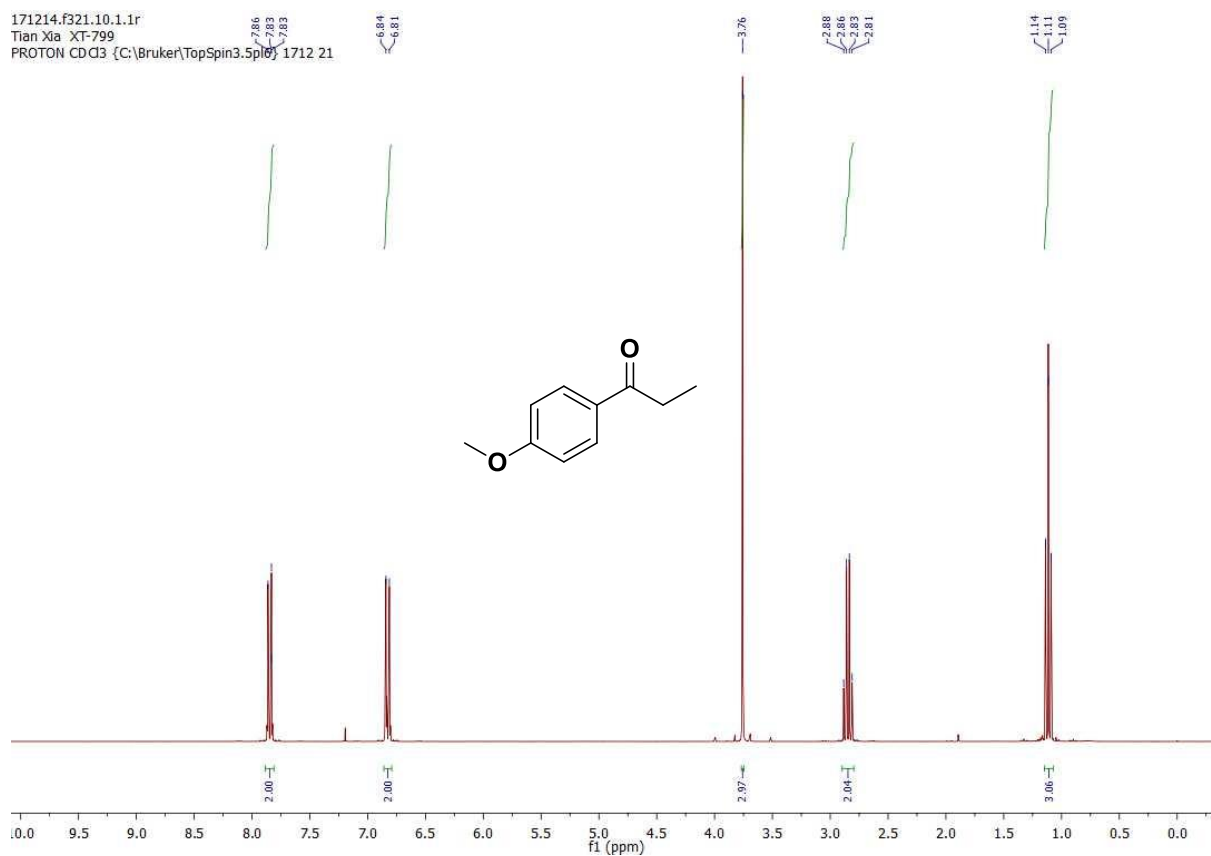
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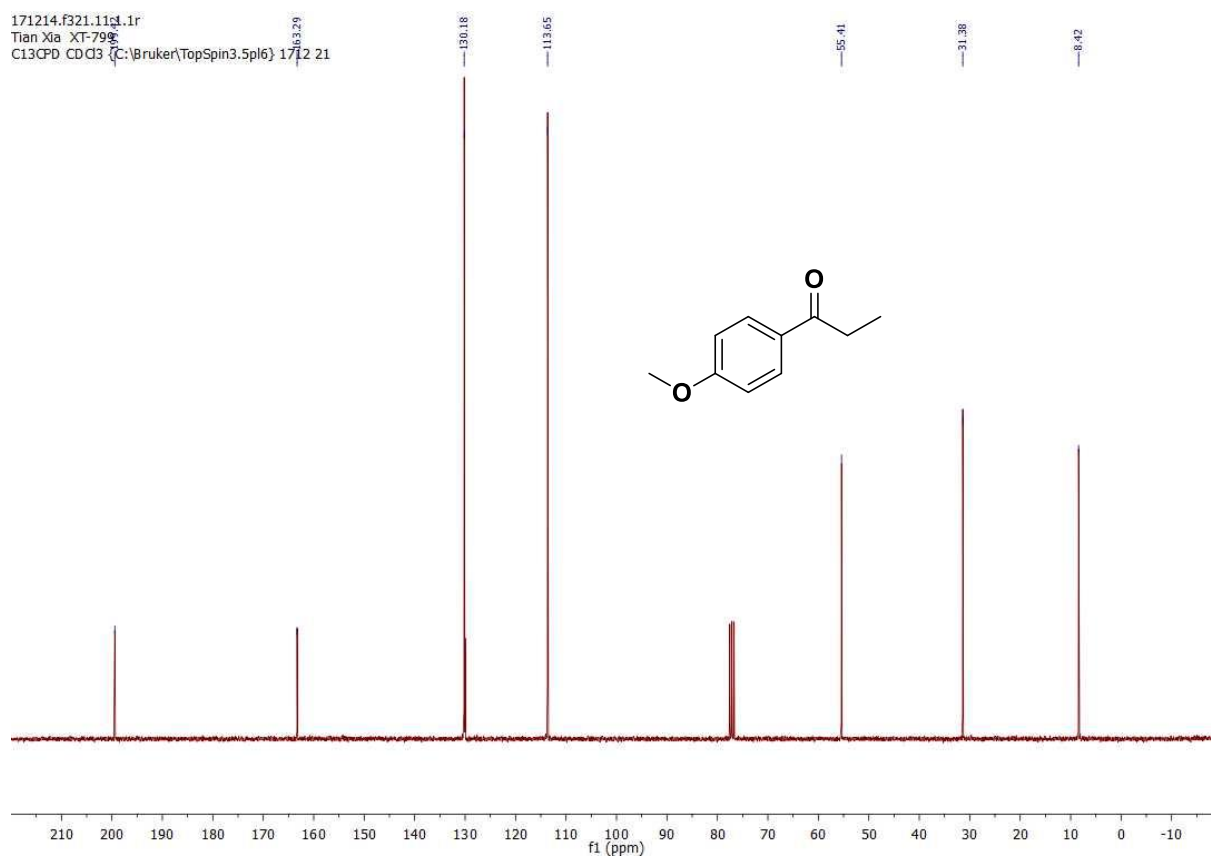
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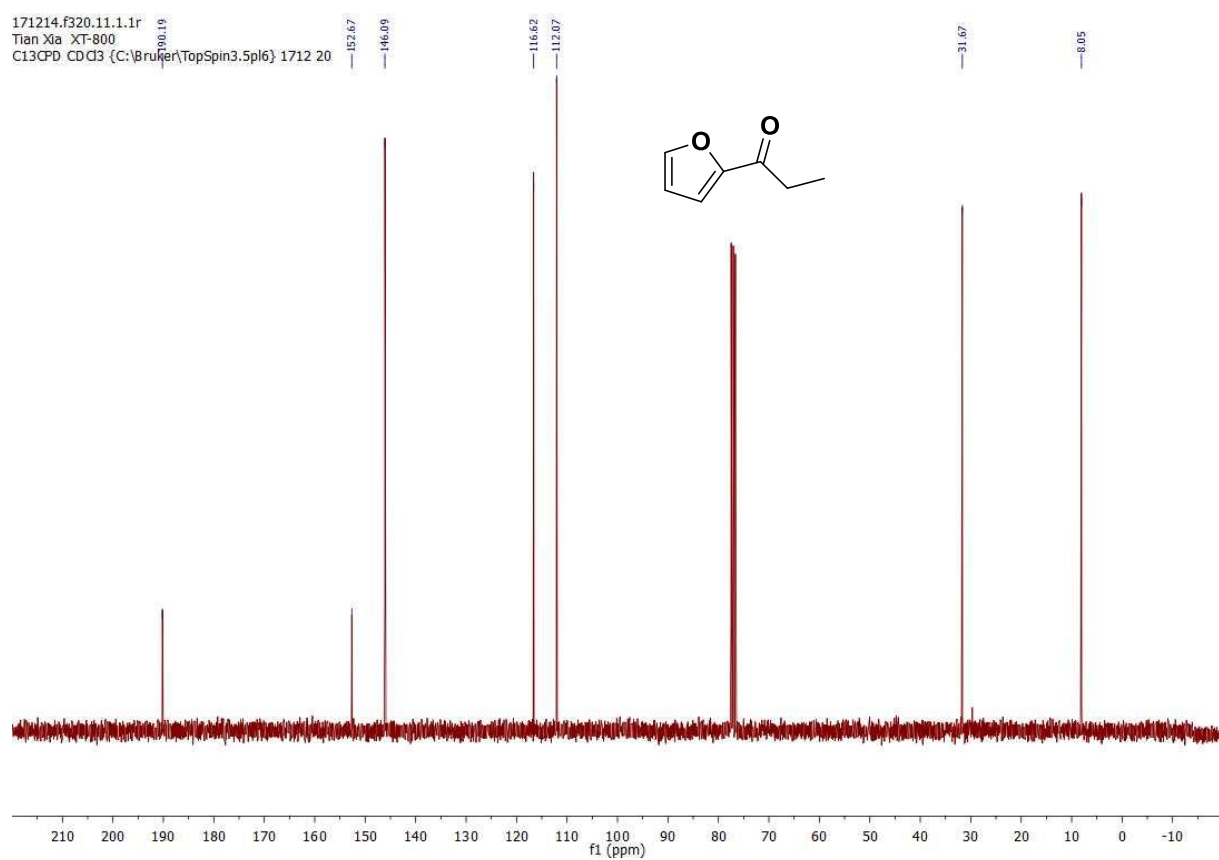
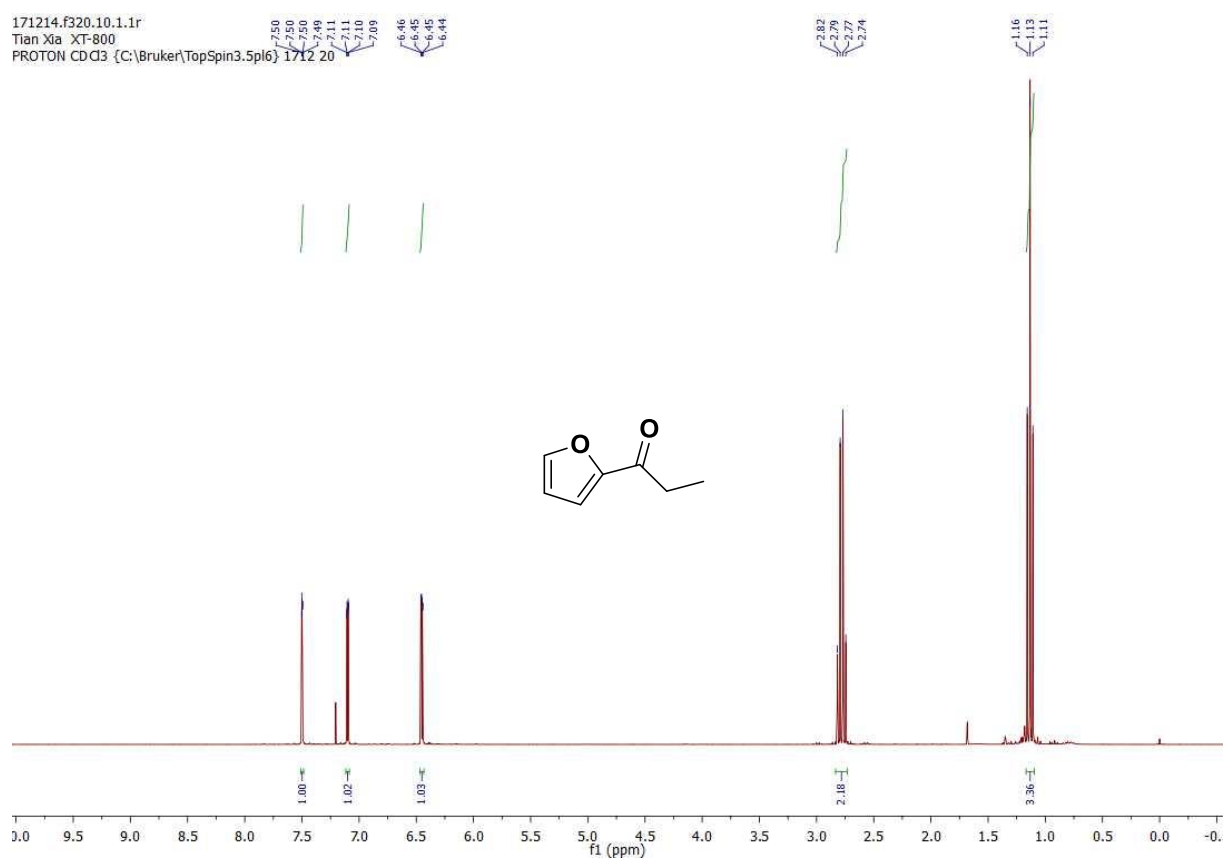


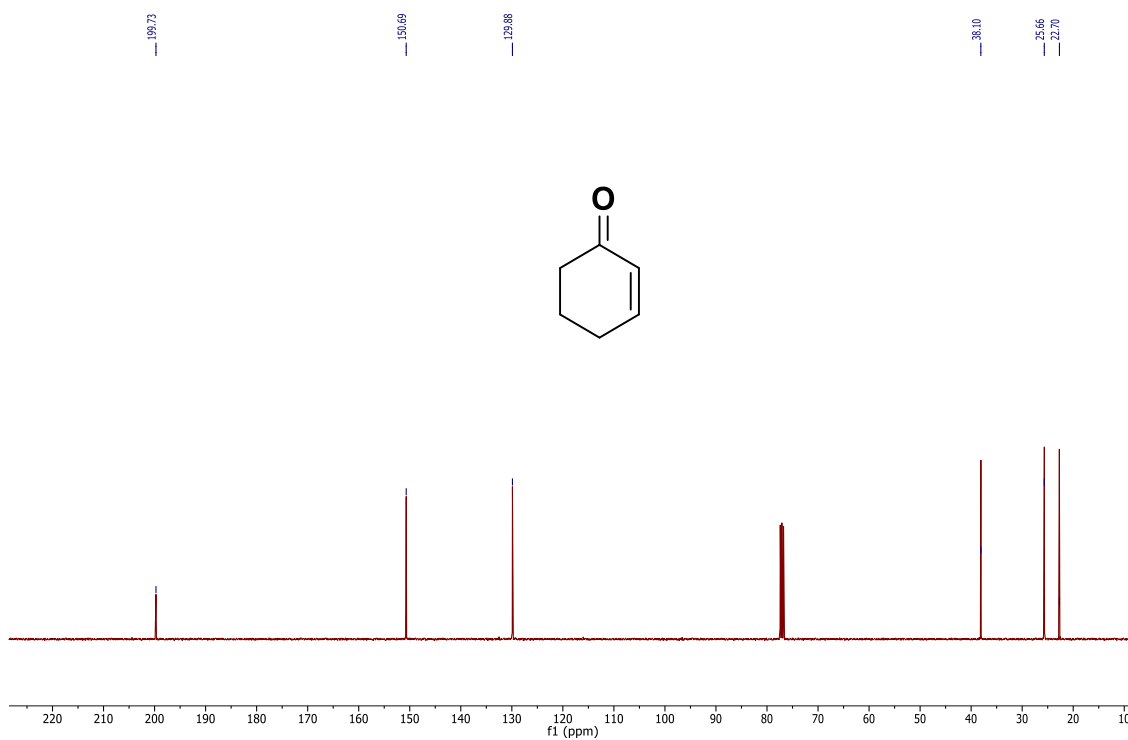
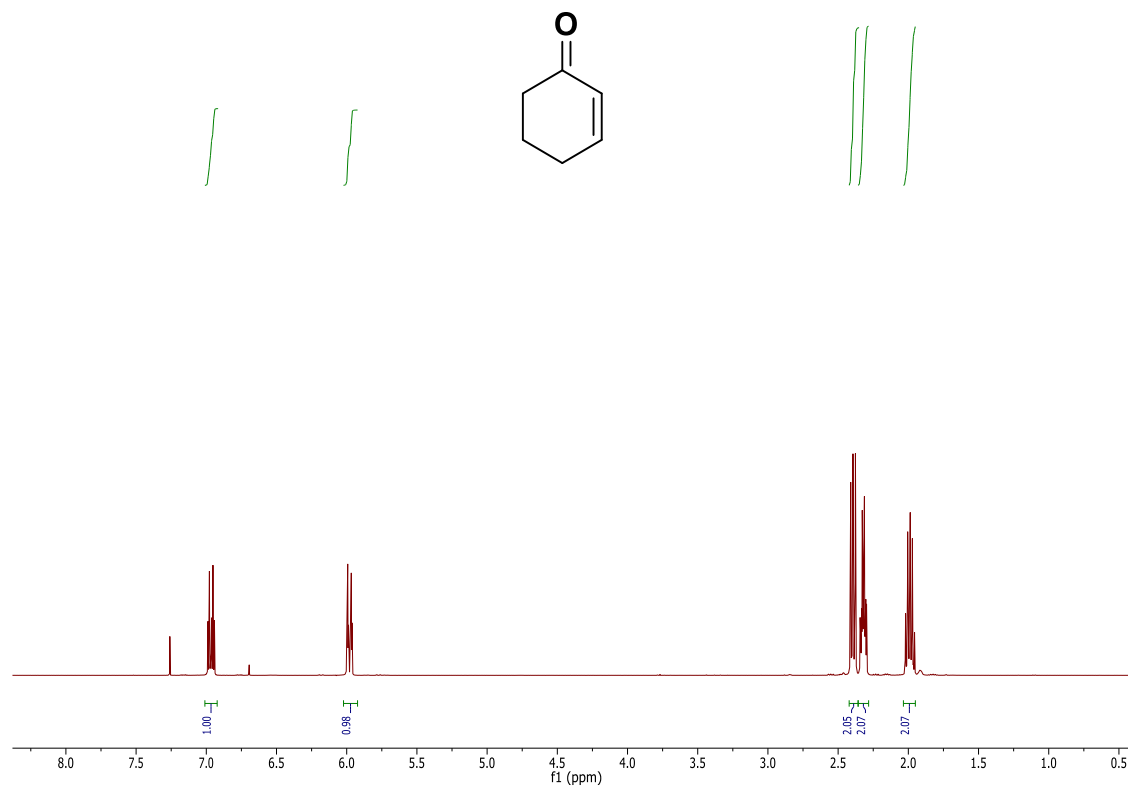
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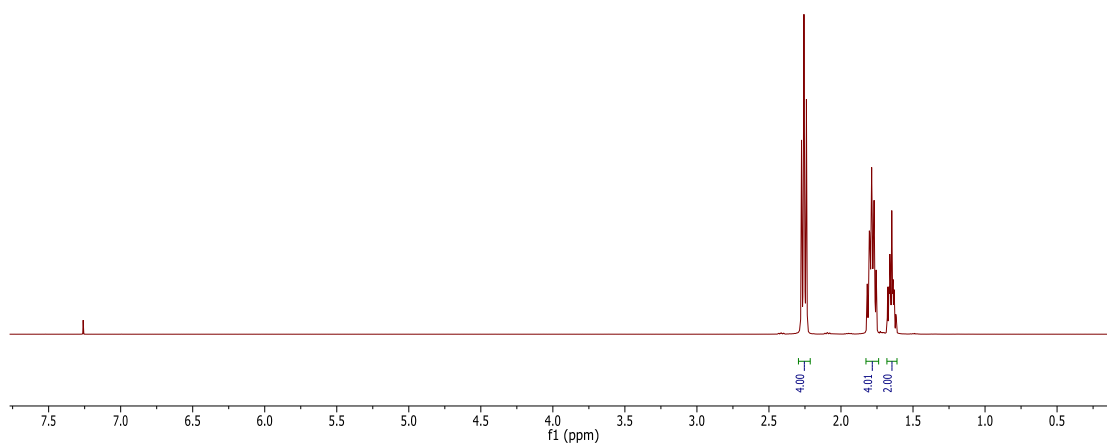
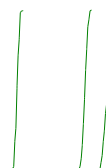
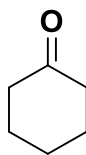


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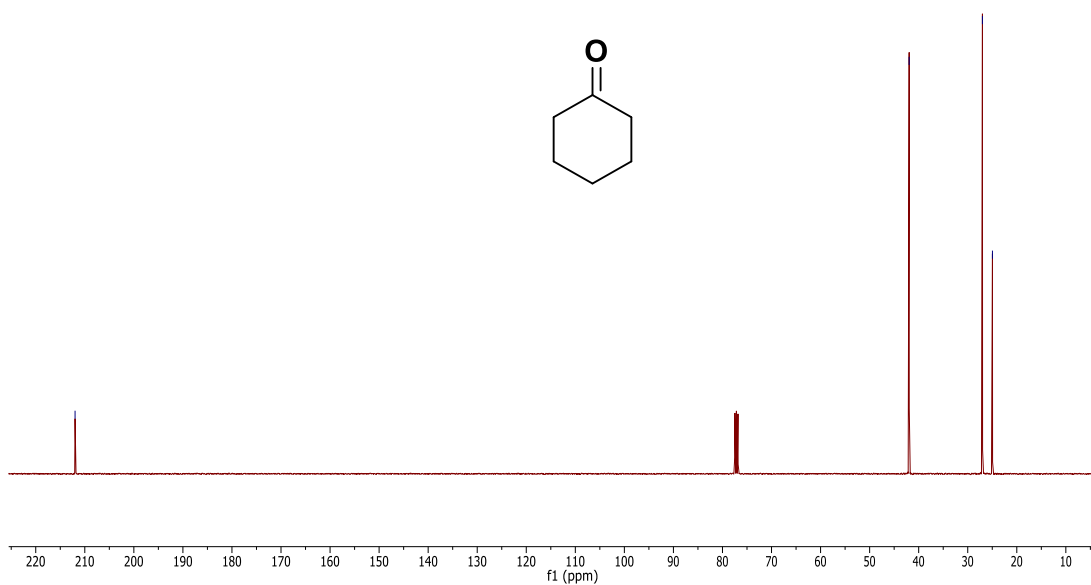
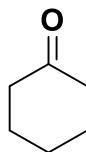
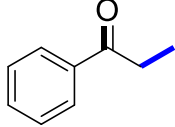
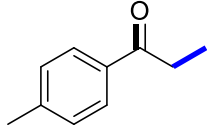
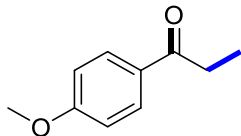
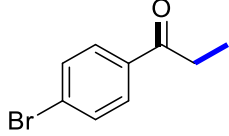
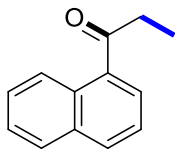
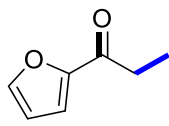
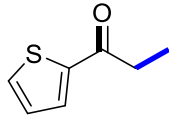
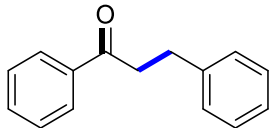
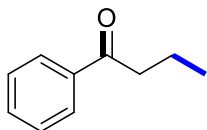
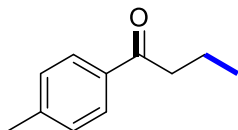
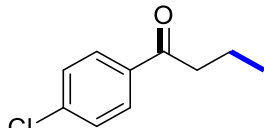
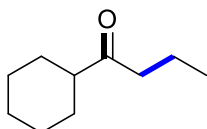
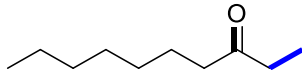
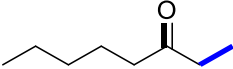
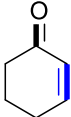
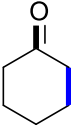


Table S3. Product data

	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.95 – 7.82 (m, 2H), 7.52 – 7.32 (m, 3H), 2.93 (q, J = 7.2 Hz, 2H), 1.15 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 200.8, 136.9, 132.9, 128.6, 128.0, 31.8, 8.3.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.79 – 7.73 (m, 2H), 7.14 (dt, J = 8.0, 0.7 Hz, 2H), 2.87 (q, J = 7.3 Hz, 2H), 2.33 – 2.27 (m, 3H), 1.12 (t, J = 7.3 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 200.5, 143.6, 133.5, 129.2, 128.1, 31.6, 21.6, 8.3.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.85 (d, J = 9.0 Hz, 2H), 6.83 (d, J = 8.9 Hz, 2H), 3.76 (s, 3H), 2.85 (q, J = 7.3 Hz, 2H), 1.11 (t, J = 7.3 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 199.4, 163.3, 130.2, 113.7, 55.4, 31.4, 8.4.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.87 – 7.81 (m, 2H), 7.64 – 7.58 (m, 2H), 2.99 (q, J = 7.2 Hz, 2H), 1.24 (t, J = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 199.7, 135.6, 131.9, 129.5, 128.0, 31.8, 8.1.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 8.50 – 8.44 (m, 1H), 7.87 – 7.81 (m, 1H), 7.77 – 7.68 (m, 2H), 7.50 – 7.32 (m, 3H), 2.95 (q, J = 7.3 Hz, 2H), 1.17 (t, J = 7.3 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 205.3, 136.2, 134.0, 132.3, 130.2, 128.4, 127.8, 127.2, 126.4, 125.9, 123.4, 35.4, 8.7.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.50 (dd, J = 1.7, 0.8 Hz, 1H), 7.10 (dd, J = 3.5, 0.8 Hz, 1H), 6.45 (dd, J = 3.6, 1.7 Hz, 1H), 2.78 (q, J = 7.4 Hz, 2H), 1.13 (t, J = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 190.2, 152.7, 146.1, 116.6, 112.1, 31.7, 8.1.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.63 (dd, J = 3.8, 1.1 Hz, 1H), 7.53 (dd, J = 5.0, 1.1 Hz, 1H), 7.04 (dd, J = 5.0, 3.8 Hz, 1H), 2.86 (q, J = 7.3 Hz, 2H), 1.15 (t, J = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 193.8, 144.2, 133.2, 131.6, 128.1,

	32.6, 8.5.
	^1H NMR (400 MHz, CDCl_3) δ_{H} 7.86 – 7.76 (m, 2H), 7.38 (d, J = 7.4 Hz, 1H), 7.29 (dd, J = 8.2, 6.9 Hz, 2H), 7.19 – 7.02 (m, 5H), 3.17 – 3.09 (m, 2H), 2.93 (dd, J = 8.5, 6.9 Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ_{C} 199.2, 141.4, 136.9, 133.1, 128.7, 128.6, 128.5, 128.1, 126.2, 40.5, 30.2.
	^1H NMR (400 MHz, CDCl_3) δ_{H} 7.89 – 7.84 (m, 2H), 7.47 – 7.41 (m, 1H), 7.38 – 7.32 (m, 2H), 2.88 – 2.81 (m, 2H), 1.74 – 1.62 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ_{C} 200.3, 137.1, 132.9, 132.8, 128.6, 128.5, 128.0, 40.5, 17.8, 13.9.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.81 – 7.76 (m, 2H), 7.20 – 7.14 (m, 2H), 2.84 (dd, J = 7.6, 7.0 Hz, 2H), 2.33 (p, J = 0.4 Hz, 3H), 1.76 – 1.59 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 200.13, 143.59, 133.67, 129.23, 128.18, 40.44, 21.62, 17.90, 13.93.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 7.83 – 7.78 (m, 1H), 7.35 – 7.30 (m, 1H), 2.82 (dd, J = 7.5, 7.0 Hz, 1H), 1.74 – 1.60 (m, 1H), 0.91 (t, J = 7.4 Hz, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 199.1, 139.3, 135.4, 129.5, 128.8, 40.5, 17.7, 13.8.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 2.33 (t, J = 7.3 Hz, 2H), 2.32 – 2.24 (m, 1H), 1.86 – 1.64 (m, 5H), 1.57 (sext, J = 7.3, 2H), 1.38 – 1.12 (m, 5H), 0.88 (t, J = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 213.3, 50.8, 42.5, 28.5, 25.9, 25.7, 17.1, 13.8.
	^1H NMR (400 MHz, CDCl_3) δ_{H} 2.38 – 2.28 (m, 4H), 1.54 – 1.45 (m, 2H), 1.20 (dt, J = 5.7, 2.4 Hz, 8H), 0.97 (t, J = 7.3 Hz, 3H), 0.84 – 0.77 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ_{C} 211.7, 42.4, 35.8, 31.6, 29.2, 29.0, 23.9, 22.5, 14.0, 7.7.

	^1H NMR (300 MHz, CDCl_3) δ_{H} 2.40 – 2.27 (m, 4H), 1.56-1.44 (m, 2H), 1.22 (dddd, J = 12.2, 6.4, 3.2, 1.7 Hz, 4H), 0.98 (t, J = 7.3 Hz, 3H), 0.86 -0.78 (m, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 212.0, 42.4, 35.9, 31.5, 23.6, 22.5, 13.9, 7.8.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 6.97 (dt, 1H), 5.98 (dt, 1H), 2.39 (t, 2H), 2.32 (tdd, 2H), 2.03-1.94 (m, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 199.7, 150.7, 129.9, 38.1, 25.7, 22.7.
	^1H NMR (300 MHz, CDCl_3) δ_{H} 2.26 (t, 4H), 1.79 (m, 4H), 1.65 (m, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ_{C} 212.0, 41.9, 27.0, 25.0.

7) Computational data

Table S4. The Cartesian Coordinates (xyz) for All Optimized Structures

C₅H₁₁CHOHCH₂	C₅H₁₁COCHCH₂
C 4.00191400 -0.99911000 0.36937500	C 1.88152600 0.15657200 0.00003300
H 4.86012000 -1.49044700 -0.07533600	C 0.55214400 -0.56645200 0.00025900
H 3.94347300 -1.00506200 1.45427000	H 0.54277400 -1.23782300 -0.86949700
C 3.06124300 -0.42530800 -0.37101200	H 0.54285900 -1.23723200 0.87048200
H 3.14213600 -0.42433400 -1.45679900	C -0.66355200 0.34400500 0.00003600
C 1.85366100 0.27160000 0.18111600	H -0.61628100 1.00441000 0.87131000
H 1.88464100 0.21489600 1.28000700	H -0.61614800 1.00413900 -0.87143800
C 0.55628300 -0.36055000 -0.30553900	C -1.98125700 -0.42385300 0.00006000
H 0.52692100 -0.28126300 -1.39827400	H -2.02174900 -1.08361000 0.87620200
H 0.58946200 -1.42864100 -0.06564000	H -2.02169100 -1.08375500 -0.87597600
C -0.69609600 0.26927800 0.29487800	C -3.20862900 0.48223600 -0.00005500
H -0.65800100 0.17660100 1.38764200	H -3.16894400 1.14094700 0.87494200
H -0.69717700 1.34092600 0.07677900	H -3.16882200 1.14089800 -0.87508300
C -1.98527100 -0.36283400 -0.21950900	C -4.52389100 -0.28687200 -0.00012500
H -1.97477700 -1.44019300 -0.01028800	H -5.38265200 0.38881700 -0.00017100
H -2.02390700 -0.26828200 -1.31191700	H -4.60759300 -0.92829500 -0.88225400
C -3.24592000 0.25179000 0.38080200	H -4.60768700 -0.92829400 0.88199600
H -3.20845200 0.15637100 1.47225700	O 1.96504300 1.36672500 0.00003500
H -3.25510900 1.32773700 0.17227900	C 3.09147200 -0.71782800 -0.00012700
C -4.53082700 -0.37946400 -0.14111000	H 2.93076500 -1.79251600 -0.00019500
H -5.41482400 0.08100700 0.30708400	C 4.32042100 -0.21138800 -0.00012700
H -4.61370100 -0.26808000 -1.22611600	H 5.20038300 -0.84414200 -0.00021300
H -4.56544400 -1.44966200 0.08280100	H 4.46504100 0.86413600 -0.00010900
O 1.83770000 1.64113300 -0.23215300	
H 1.81069994 1.65626187 -1.19378303	
C₅H₁₁COC₂H₅	C₅H₁₁CHOHC₂H₅
C 1.50316400 0.93567900 0.00000000	C 0.38961000 -0.52818800 0.18920100
C 0.00000000 0.72933600 0.00000000	H 0.36020500 -1.55062500 -0.20531400
H -0.40978300 1.25901800 0.86995000	H 0.35866100 -0.62623300 1.28383500
H -0.40978300 1.25901800 -0.86995000	C -0.83484700 0.24219000 -0.29169900
C -0.43642900 -0.72695300 0.00000000	H -0.77082700 1.27559000 0.06277100
H -0.00674700 -1.23026400 -0.87142300	H -0.81635500 0.29628400 -1.38721800
H -0.00674700 -1.23026400 0.87142300	C -2.15327100 -0.37688900 0.16060700
C -1.95255000 -0.89180700 0.00000000	H -2.17349700 -0.42750000 1.25674600
H -2.37702600 -0.38485800 -0.87603600	H -2.20976000 -1.41568000 -0.18904100
H -2.37702600 -0.38485800 0.87603600	C -3.38274000 0.38314600 -0.32745700
C -2.40254200 -2.34958900 0.00000000	H -3.32594300 1.42053400 0.02170100
H -1.97959700 -2.85616000 -0.87499600	H -3.36392600 0.43246100 -1.42233200
H -1.97959700 -2.85616000 0.87499600	C -4.69630000 -0.23800900 0.13137300
C -3.91756100 -2.51141400 0.00000000	H -5.55679000 0.32796300 -0.23398800
H -4.20760500 -3.56494700 0.00000000	H -4.79688000 -1.26478600 -0.23226600
H -4.36572700 -2.04493600 0.88211200	H -4.75963200 -0.26852600 1.22301000
H -4.36572700 -2.04493600 -0.88211200	C 2.91227200 -0.76585100 0.18441100
O 2.27925600 0.00784700 0.00000000	H 2.75553300 -1.76928500 -0.22607100
C 1.97788600 2.37788400 0.00000000	H 2.91655900 -0.88321200 1.27659300
H 1.53021900 2.87441100 0.86972700	C 4.25263300 -0.21616800 -0.28444000
H 1.53021900 2.87441100 -0.86972700	H 5.07804500 -0.84934600 0.04951500
C 3.48835600 2.53117600 0.00000000	H 4.29458100 -0.16335500 -1.37604700
H 3.76877700 3.58658100 0.00000000	H 4.41889400 0.79156200 0.10024900
H 3.93008000 2.05764800 0.87811100	C 1.72085700 0.10779100 -0.20295400
H 3.93008000 2.05764800 -0.87811100	H 1.73420000 0.25839800 -1.28845900
	O 1.84673100 1.42657700 0.33014100
	H 1.83380300 1.35500800 1.29094500

C₅H₁₁C(OH)=CHCH₃ H 4.88356700 -1.05879500 0.02457500 H 2.81658100 1.65971300 -0.20948900 C 4.13337200 -0.47386300 -0.51495100 H 4.24706600 -0.71276400 -1.57836500 C 2.75610800 -0.77920100 -0.01486100 H 2.50383200 -1.82480500 0.12058300 H 4.41929600 0.57641900 -0.39077800 C 1.80074900 0.10951800 0.27442400 O 1.94468600 1.46540400 0.15012500 C 0.43650300 -0.24455400 0.77347300 H 0.41092200 -1.31690800 0.98261900 H 0.27168300 0.27211900 1.72690600 C -0.68889400 0.12608000 -0.19706500 H -0.52763700 -0.39778700 -1.14615000 H -0.63238000 1.19576700 -0.41950500 C -2.07259700 -0.21315900 0.34603600 H -2.22610000 0.30895700 1.29881500 H -2.12255800 -1.28475100 0.57770800 C -3.20549200 0.14566100 -0.61059100 H -3.05176400 -0.37589300 -1.56238900 H -3.15530000 1.21592700 -0.84150400 C -4.58621400 -0.19289400 -0.06201000 H -4.78265000 0.34154500 0.87194600 H -5.37531300 0.07536400 -0.76888200 H -4.67794400 -1.26286200 0.14618500	H₂ H 0.00000000 0.00000000 0.37259400 H 0.00000000 0.00000000 -0.37259400
iPrOH C -0.00243400 0.04077500 0.36089000 H 0.00526000 0.08376300 1.46069100 C -1.32567300 -0.54428700 -0.08927600 H -2.15309900 0.08251200 0.24730200 H -1.36235800 -0.60296200 -1.17981800 H -1.46291400 -1.54830400 0.31814000 C 1.18837700 -0.78527300 -0.10226600 H 1.20751000 -0.84663100 -1.19323900 H 2.13155100 -0.34094600 0.23062100 H 1.14270100 -1.79969300 0.30232900 O 0.05393500 1.36877600 -0.16149200 H 0.89824900 1.75476300 0.08982600	CH₃COCH₃ C 0.00002000 -0.61117500 1.28460900 H 0.00094700 0.06104100 2.14079100 H -0.87890100 -1.26104400 1.32817900 H 0.87757900 -1.26288300 1.32747200 C 0.00002000 -0.61117500 -1.28460900 H -0.87890100 -1.26104400 -1.32817900 H 0.00094700 0.06104100 -2.14079100 H 0.87757900 -1.26288300 -1.32747200 C 0.00005800 0.18480000 0.00000000 O 0.00002000 1.39388400 0.00000000
1M-iPr C -2.46173700 -0.64027700 1.90985400 H -2.65684800 0.24940800 2.51158100 H -3.30929900 -1.31874500 2.03358000 C -1.14937200 -1.27172400 2.34588300 H -1.05401200 -1.17631300 3.43814400 H -1.16511100 -2.35448800 2.14421800 C 1.19290000 -1.00173100 2.46662400 H 1.39741500 -2.08152000 2.39234900 H 1.00503300 -0.81075700 3.53435400 C 2.41524700 -0.21056400 2.02923100 H 3.34930400 -0.71252400 2.29385200 H 2.41333200 0.76678800 2.51560200 C -3.28852000 1.49692000 0.05641900 H -3.12448700 1.84709000 -0.96816600	1M-Ph C 0.13805200 -2.11644600 0.12709500 O 0.24260000 -3.26995100 0.08485300 N 0.01164500 0.38352000 2.06222000 P -2.21887400 -0.15625600 0.51023100 P 2.24516500 -0.07303200 0.49671000 C 2.43865100 0.05798200 2.32584000 C -2.40525000 -0.02231800 2.33847400 H 3.36376300 0.55130800 2.63176400 H -3.33934600 0.44401000 2.65960700 H 2.42367700 -0.96266400 2.71693400 H -2.40465400 -1.05615300 2.69259700 C -1.17234300 0.70376500 2.85512600 C 1.20177800 0.80505700 2.80067600 H -1.34687100 1.79170300 2.86278100

C -4.78621600 1.30022600 0.27988700	H 1.36087200 1.89028200 2.69858200
H -4.99142500 0.87546800 1.26684600	H -1.00828700 0.42373100 3.90689000
H -5.24450800 0.65249100 -0.46886300	H 1.06706800 0.62131800 3.87680600
H -5.29802600 2.26630500 0.23138500	C 3.49614500 -1.28946500 -0.07831000
C -2.73808000 2.56366500 1.00315400	C -3.50264000 -1.37532200 -0.00678300
H -3.18604600 3.53350800 0.76981900	C 5.34615900 -3.14768500 -1.04265200
H -1.65561400 2.66451100 0.92556900	C -5.44266600 -3.22989000 -0.77436700
H -2.98105400 2.33684800 2.04464100	C 3.41722500 -1.75074800 -1.39406400
C -3.27017700 -1.31034300 -0.83486900	C -3.14713000 -2.50307000 -0.74166400
H -4.26633400 -1.30697100 -0.37897700	C 4.50888400 -1.77414900 0.74885700
C -3.39703400 -0.89245400 -2.29817600	C -4.84382700 -1.17857900 0.33214100
H -2.42291900 -0.85769500 -2.78855900	C 5.42773200 -2.70046900 0.26892300
H -3.86726700 0.08658200 -2.41225300	C -5.80670600 -2.10279300 -0.04447500
H -4.01288300 -1.61712100 -2.83929200	C 4.33993900 -2.66889700 -1.87370100
C -2.69456300 -2.71871100 -0.70451800	C -4.11460400 -3.42618200 -1.12452400
H -3.32844100 -3.42918000 -1.24372700	H 2.62805300 -1.39305800 -2.04606300
H -2.64347000 -3.04813800 0.33540800	H -2.11235200 -2.66247300 -1.01565600
H -1.69160700 -2.78010200 -1.12890200	H 4.58893500 -1.43347100 1.77455200
C 3.31332400 1.61240900 -0.10597900	H -5.14096400 -0.29264300 0.88319100
H 4.30316500 1.37427100 0.29869400	H 6.20769700 -3.07271000 0.92405100
C 3.44338700 1.87891100 -1.60567100	H -6.84444100 -1.94144500 0.22624000
H 2.47369700 2.10657900 -2.05190000	H 4.26648100 -3.01907800 -2.89721700
H 3.87209400 1.03308800 -2.14661400	H -3.82459000 -4.30027000 -1.69678000
H 4.09498600 2.74124900 -1.77472900	H 6.06219900 -3.87118200 -1.41626500
C 2.78565200 2.84781600 0.62070700	H -6.19627000 -3.95087000 -1.07149400
H 3.45175200 3.69491700 0.43121000	C 2.89864800 1.54095200 -0.12331100
H 2.73587600 2.70999000 1.70224800	C -2.91345400 1.41103000 -0.18120700
H 1.79107900 3.12418300 0.26893000	C 3.79809800 4.04832300 -0.95974400
C 3.22747100 -1.28767600 -0.60520800	C -3.89796800 3.76305400 -1.33709600
H 3.02593000 -1.14935500 -1.67259900	C 2.00234000 2.59905300 -0.27529300
C 2.66279300 -2.64931100 -0.19927200	C -3.28024800 2.49504900 0.61551100
H 3.06620000 -3.43003900 -0.85006900	C 4.24968700 1.74904300 -0.40240600
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H 2.94435900 -2.90154000 0.82632400	C 4.69566900 2.99650800 -0.81904300
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H 4.98710300 -1.30384000 0.68439600	C 2.45119300 3.84763500 -0.68636900
H 5.19965000 -0.34138300 -0.78275900	C -3.76850900 3.66371500 0.04078800
H 5.20829700 -2.09911200 -0.86959700	H 0.94792400 2.43414100 -0.07835400
N 0.00438100 -0.65790700 1.68808600	H -3.19193900 2.43918200 1.69346100
P -2.26358900 -0.07718600 0.15632100	H 4.95594100 0.93220000 -0.30539800
P 2.25313300 0.09806500 0.21357900	H -2.76062900 0.69602800 -2.20878000
Mn -0.00296600 0.07400800 -0.05535700	H 5.74707200 3.14553800 -1.03974800
C -0.10467900 1.59286400 -0.93996100	H -3.63121400 2.75556200 -3.21806100
C 0.11280100 -0.76504800 -1.58457600	H 1.74402700 4.66134200 -0.80375600
O 0.22271700 -1.35688100 -2.57946700	H -4.05031200 4.49645600 0.67607700
O -0.19673300 2.60182000 -1.50958500	H 4.14776800 5.02066100 -1.28896000
	H -4.28070900 4.67336000 -1.78496900
	C 0.02229300 -0.12272400 -1.42229800
	O 0.03427100 0.06178900 -2.56717900
	Mn 0.02292000 -0.38019000 0.32884500
2M-iPr	2M-Ph
P -2.21525100 0.08123500 -0.29325700	C 0.00019000 0.31834700 -1.52892300
P 2.21527800 0.08091500 -0.29346600	O 0.00044400 0.59022200 -2.65549300
C -2.42373900 -0.94789700 -1.84975100	N 0.00008100 -0.08856200 2.34445200
C 2.42363300 -0.94854300 -1.84976500	P 2.21219700 0.10213900 0.45448600
H -2.43921000 -0.25676000 -2.69880800	P -2.21220300 0.10333600 0.45423300

H	2.43949900	-0.25760600	-2.69897400	H	0.00018800	1.55048300	0.40978900
H	-3.36416000	-1.50091500	-1.87031600	C	-2.42898000	0.05918300	2.31183100
H	3.36388400	-1.50187500	-1.87001000	C	2.42930600	0.05551600	2.31207800
C	-1.23286500	-1.88284400	-1.97347600	H	-3.37365000	-0.38783700	2.62554200
C	1.23249100	-1.88315500	-1.97346200	H	3.37319900	-0.39377000	2.62489800
H	-1.22361100	-2.37491100	-2.95691800	H	-2.44614200	1.10396300	2.63526000
H	1.22310600	-2.37525700	-2.95688500	H	2.44861300	1.09985900	2.63678200
H	-1.26909100	-2.66214200	-1.20893600	C	1.23050200	-0.65750300	2.91358800
H	1.26850000	-2.66243000	-1.20888800	C	-1.23128600	-0.65542300	2.91367300
N	-0.00009200	-1.11284400	-1.76072900	H	1.24414400	-1.72188200	2.66555700
C	2.95955100	1.70959000	-0.88627700	H	-1.24658000	-1.71988200	2.66604700
C	-2.95954400	1.71002200	-0.88572900	H	1.23478200	-0.56735200	4.00917000
H	2.34159200	1.89023000	-1.77378800	H	-1.23545000	-0.56487300	4.00922000
H	-2.34078000	1.89145600	-1.77250500	H	0.00092100	0.91185100	2.52497200
C	3.50683000	-0.62882900	0.88102700	C	-3.22312200	1.58344900	-0.00922500
C	-3.50642800	-0.62844800	0.88171700	C	3.22355000	1.58254700	-0.00707500
C	3.45724800	-2.15383900	0.95621500	C	-4.70852900	3.86503900	-0.63047200
C	-3.45853200	-2.15359700	0.95521400	C	4.70977600	3.86429500	-0.62575700
H	-4.48185400	-0.33732600	0.47825800	C	-4.61737100	1.56492300	0.07453800
H	4.48212600	-0.33928700	0.47610300	C	2.58462300	2.75103900	-0.41362200
C	-3.34713500	-0.02891500	2.27833700	C	-2.58360800	2.75207300	-0.41455700
C	3.34985800	-0.02755800	2.27713200	C	4.61766700	1.56421700	0.07922300
H	-3.42364500	1.05895900	2.28230300	C	-3.32365300	3.88773000	-0.72422000
H	3.42857200	1.06016600	2.27987600	C	5.35551500	2.70000400	-0.22352900
H	-2.37757000	-0.29302400	2.70483800	C	-5.35482500	2.70064000	-0.22951200
H	2.38012900	-0.28930900	2.70473500	C	3.32508700	3.88678100	-0.72206100
H	-4.12412800	-0.41903800	2.94293800	H	-5.13123800	0.65532500	0.36605400
H	4.12663400	-0.41851200	2.94149800	H	1.50263200	2.75448500	-0.48085600
C	2.71655300	2.87532700	0.06656600	H	-1.50150100	2.75561700	-0.47997500
C	-2.71796900	2.87518900	0.06818100	H	5.13113100	0.65468600	0.37167900
H	3.30896400	2.78824500	0.98000700	H	-2.81480600	4.78990800	-1.04595600
H	-3.31163700	2.78734100	0.98073800	H	6.43753400	2.67462600	-0.15250900
H	1.66585300	2.94725800	0.34482500	H	-6.43696800	2.67509100	-0.16047500
H	-1.66766700	2.94721900	0.34793100	H	2.81668900	4.78887700	-1.04473300
H	3.00561000	3.81382000	-0.41686100	H	-5.28595700	4.75007900	-0.87459800
H	-3.00659400	3.81395500	-0.41497100	H	5.28753200	4.74939900	-0.86887500
C	4.42292400	1.63506500	-1.31464700	C	-3.27752000	-1.26285400	-0.19192100
C	-4.42249600	1.63531300	-1.31553800	C	3.27724100	-1.26337600	-0.19349100
H	4.62432700	0.80177800	-1.99231400	C	-4.75190000	-3.35546000	-1.32630700
H	-4.62302400	0.80245900	-1.99398000	C	4.75076400	-3.35520200	-1.33037700
H	5.09035400	1.53828600	-0.45469300	C	-3.49008400	-1.31969900	-1.57216200
H	-5.09069600	1.53772300	-0.45627600	C	3.79767700	-2.28101300	0.60287700
H	4.70529500	2.55569800	-1.83481800	C	-3.80225700	-2.27688500	0.60622000
H	-4.70468300	2.55623100	-1.83530600	C	3.49363600	-1.31618300	-1.57329100
H	0.00007400	1.27651100	-0.86338400	C	-4.53507500	-3.31657600	0.04312600
H	0.00000000	-0.33275200	-2.41241700	C	4.22838300	-2.34883100	-2.13542000
H	4.23353500	-2.50872100	1.64117400	C	-4.22529500	-2.35267200	-2.13307000
H	2.49882600	-2.50618700	1.33932500	C	4.53013800	-3.32027100	0.03856000
H	3.63958700	-2.63100200	-0.00900400	H	-3.07737400	-0.54898400	-2.21458700
H	-4.23396800	-2.50827200	1.64123900	H	3.63511100	-2.28231800	1.67449400
H	-3.64320900	-2.62951600	-0.01017000	H	-3.64287800	-2.27503200	1.67830800
H	-2.49983500	-2.50746800	1.33625800	H	3.08438900	-0.54253300	-2.21439500
Mn	0.00001600	-0.01612700	0.08687800	H	-4.93478300	-4.09793700	0.68036900
C	0.00018000	1.09435300	1.44576400	H	4.38828600	-2.37152900	-3.20774500
C	-0.00029600	-1.43593000	1.14443800	H	-4.38220200	-2.37848200	-3.20576700
O	0.00029600	1.84362900	2.33250500	H	4.92652900	-4.10443600	0.67442700
O	-0.00065200	-2.32937800	1.89330800	H	-5.32252800	-4.16598100	-1.76566500

	H 5.32107300 -4.16542200 -1.77070500 C -0.00039500 -1.80030200 -0.03074400 O -0.00056700 -2.94352400 -0.21598200 Mn -0.00004600 -0.03131900 0.19537000		
TS₁₋₄(3,4-H⁻)-iPr	TS₁₋₄(3,4-H⁻)-Ph		
P 0.36903900 2.31858000 0.05608200	P 1.40137800 1.60580300 -0.23740000		
P -2.20830100 -1.48826500 -0.29846600	P -2.49789100 -0.70331500 -0.38012800		
C 1.21384600 2.08855200 -1.59212600	C 1.81571100 1.36611200 -2.03161100		
C -1.72387000 -1.84259300 -2.06041900	C -2.39056700 -1.11167900 -2.18480700		
H 2.14012800 1.54423300 -1.39986300	H 2.38471300 0.43576600 -2.09766900		
H -0.88825800 -2.54268100 -1.99203900	H -1.82514800 -2.04456900 -2.25523500		
H 1.49166300 3.03446400 -2.06162100	H 2.43169200 2.16420200 -2.44918600		
H -2.52246300 -2.30564100 -2.64131000	H -3.36004000 -1.26075800 -2.66243400		
C 0.31308900 1.28076100 -2.50936700	C 0.50572400 1.21200200 -2.78638200		
C -1.24055400 -0.56249900 -2.70988300	C -1.59704300 -0.00192900 -2.85384700		
H 0.86454200 0.97125300 -3.40765100	H 0.70473300 0.91083000 -3.82366400		
H -0.78504500 -0.78332900 -3.68526600	H -1.38527400 -0.27181600 -3.89715600		
H -0.52528600 1.89735800 -2.84384800	H -0.04182300 2.15879200 -2.81712200		
H -2.06622600 0.13293700 -2.88089700	H -2.15777400 0.93757000 -2.86111300		
N -0.25962900 0.10361100 -1.83052000	N -0.33897300 0.20913700 -2.11818000		
C -1.89757500 -3.17236600 0.48321400	O -0.53542700 0.22081200 2.87893700		
C 1.83958200 2.51789400 1.21488200	H 0.39216100 -1.06657300 -0.02443900		
H -0.81124600 -3.24680500 0.40043900	H 0.17664400 -0.71007300 -2.16277800		
H 2.27030200 1.51658200 1.17723400	C 1.04394900 -2.29081700 -0.74280700		
C -4.09917000 -1.41448100 -0.28438300	O 0.82454400 -2.16352800 -1.99005500		
C -0.32612900 4.07476300 -0.01283000	C -0.53891400 0.31117700 1.72226700		
C -4.72640500 -0.80133500 -1.53543000	C 0.23581400 -3.33322100 -0.03315900		
C -0.94366300 4.45154900 -1.35894600	H -0.70952400 -3.54895400 -0.52098300		
O -1.51328900 0.50528600 3.00083000	C 0.59635800 -4.03262400 1.03753300		
H 0.54894500 4.71556300 0.13836000	H 1.53350400 -3.86584100 1.55656800		
H -4.40236000 -2.46563100 -0.25179600	H -0.04899200 -4.80598400 1.43834400		
C -1.31652800 4.34348400 1.12245700	C 2.48065100 -2.10424000 -0.26689500		
C -4.63077800 -0.73510400 0.97894800	H 2.83319600 -1.12890800 -0.60284400		
H -0.92792100 4.06066400 2.10028900	H 2.53423900 -2.09468200 0.82414300		
H -4.19077800 -1.13909200 1.89099800	C 3.39778700 -3.18579900 -0.84554400		
H -2.25106500 3.80551500 0.96764900	H 3.31395800 -3.16047500 -1.93633600		
H -4.43971700 0.33751900 0.96562100	H 3.04672700 -4.17522800 -0.53487400		
H -1.55205500 5.41181300 1.15570900	C 4.85504600 -3.01050700 -0.43146100		
H -5.71435800 -0.87666300 1.04226300	H 5.20434600 -2.01618600 -0.73608800		
C -2.30114000 -3.22389000 1.95472900	H 4.93151800 -3.03149800 0.66294600		
C 1.44192600 2.79169600 2.66397200	C 5.78161600 -4.07083600 -1.01917200		
H -3.38762300 -3.26137900 2.06838200	H 5.43237300 -5.06389000 -0.71344300		
H 1.09707500 3.81933700 2.79916400	H 5.70520500 -4.04861900 -2.11238500		
H -1.93532700 -2.36684500 2.52305600	C 7.23796900 -3.89444000 -0.60661400		
H 0.66162700 2.11746700 3.01753500	H 7.87579900 -4.66734100 -1.04308300		
H -1.89891700 -4.12903700 2.41933900	H 7.62554800 -2.92374700 -0.92959200		
H 2.31364300 2.66061400 3.31217900	H 7.35036700 -3.94726100 0.48030200		
C -2.49579300 -4.35282800 -0.28089000	C -3.05504000 -2.27092400 0.42491700		
C 2.90087600 3.51191600 0.74713800	C -3.94032100 -3.13646400 -0.22038800		
H -2.17463500 -4.38464800 -1.32289400	C -2.65386500 -2.56093400 1.72713600		
H 3.24941800 3.31490800 -0.26821900	C -4.40674400 -4.27490200 0.42179200		
H -3.58884500 -4.35428200 -0.25987600	H -4.27757100 -2.92386300 -1.22855400		
H 2.54318100 4.54396500 0.78803800	C -3.13524900 -3.69217600 2.37557900		
H -2.16838600 -5.28663900 0.18680500	H -1.95253400 -1.91092200 2.23449000		
H 3.77196400 3.45228200 1.40694000	C -4.00854700 -4.55252000 1.72452200		
H 0.53148600 -0.41758800 0.55661800	H -5.08866300 -4.94243900 -0.09348300		

H 0.47439500 -0.60315900 -1.64152800 C 1.50227600 -1.59163300 0.29633800 H -5.81653600 -0.85612500 -1.45353700 H -4.46537300 0.25041200 -1.65175100 H -4.44656800 -1.33211400 -2.44715500 H -1.27642200 5.49347300 -1.32231900 H -0.23471300 4.37120900 -2.18507100 H -1.81833500 3.84261600 -1.58908200 O 1.13714600 -2.15565300 -0.77525600 C -1.30114000 0.49927100 1.86210400 C 1.25927300 -2.29462100 1.64859900 H 0.19890100 -2.25420800 1.88199700 C 2.82945500 -0.82119700 0.22675700 H 2.76129300 -0.09587800 -0.58667400 H 3.00889200 -0.27259600 1.15518300 C 4.02294600 -1.73525300 -0.06626000 H 4.20142100 -2.40230900 0.78280500 H 3.77081000 -2.37237600 -0.91910800 C 5.30186900 -0.95617000 -0.35876000 H 5.13656300 -0.30035100 -1.22322600 H 5.53022800 -0.29221600 0.48491100 C 6.50838900 -1.84915100 -0.63258200 H 6.67798400 -2.50001400 0.23289700 H 6.27806500 -2.51636500 -1.47095600 C 7.78001100 -1.06676400 -0.93737400 H 8.62521100 -1.73302400 -1.12733300 H 7.65303900 -0.43366200 -1.82044000 H 8.05356500 -0.41505900 -0.10239600 H 1.76254200 -1.72997200 2.43883800 C 1.71771100 -3.75199700 1.65263000 H 2.80027600 -3.84997800 1.55704700 H 1.42340600 -4.24000800 2.58560100 H 1.26743900 -4.29760400 0.82093500 Mn -0.95601700 0.45034000 0.13297500 C -2.35279600 1.41583800 -0.28791900 O -3.26973800 2.08805900 -0.54101600	H -2.81689100 -3.90379800 3.39034100 H -4.37893000 -5.43808000 2.22906400 C -4.06094900 0.27634600 -0.19901300 C -4.83548700 0.69473100 -1.27816100 C -4.46188900 0.63086000 1.09101000 C -5.98935100 1.44418000 -1.07388500 H -4.55089800 0.44587400 -2.29342700 C -5.61467700 1.37309600 1.29529300 H -3.86884000 0.32487500 1.94629900 C -6.38361200 1.78279300 0.21193600 H -6.57941200 1.76264200 -1.92637900 H -5.91130500 1.63680700 2.30439600 H -7.28326700 2.36661000 0.37100000 C 2.98556700 1.28888500 0.66010900 C 2.96977600 0.63072400 1.88752300 C 4.19933600 1.76673500 0.16183600 C 4.14738000 0.45074300 2.60426100 H 2.03656100 0.24981900 2.28259900 C 5.37619800 1.57352100 0.87072800 H 4.23066100 2.30169800 -0.78098800 C 5.35176300 0.91687000 2.09620400 H 4.12044000 -0.06022300 3.56034200 H 6.31366300 1.94295400 0.46972100 H 6.27083200 0.77154900 2.65299100 C 1.30628400 3.44222100 -0.01126900 C 1.17327900 3.93173300 1.29010800 C 1.32465500 4.34913200 -1.06806600 C 1.07362700 5.29390500 1.52701300 H 1.14874800 3.24315700 2.12810900 C 1.22067100 5.71575900 -0.83087200 H 1.41648100 4.00516400 -2.09132800 C 1.09755800 6.19187700 0.46588700 H 0.97316200 5.65571500 2.54427900 H 1.23574100 6.40739800 -1.66615300 H 1.01626700 7.25712300 0.65065500 C -1.43615400 1.94694400 -0.03477000 O -2.01802400 2.94450400 -0.01065000 Mn -0.53442000 0.42478400 -0.03452500
TS₄₋₂(1,2-H⁻)_{1,2}-addition: H⁻ transfer to C₁-iPr P -0.70254700 2.29766400 -0.05088200 P -1.74541200 -2.10623400 -0.10197100 C 0.82008700 2.14997700 -1.12198300 C -0.26403600 -2.62605300 -1.11811100 H 1.67188700 2.02483200 -0.44822800 H 0.53859100 -2.85829200 -0.41186300 H 0.99903800 3.04175700 -1.72518000 H -0.44465900 -3.52329700 -1.71272100 C 0.68015800 0.92136200 -2.00103200 C 0.15475000 -1.46220400 -1.99705000 H 1.63426400 0.69395400 -2.49638200 H 1.12034700 -1.67050200 -2.47914400 H -0.06972900 1.07811000 -2.78023000 H -0.57854800 -1.29071500 -2.78831400 N 0.23308900 -0.23022400 -1.19414800 C -1.45687800 -3.14813300 1.44382000 C 0.06394500 3.04010000 1.50224300	TS₄₋₂(1,2-H⁻)_{1,2}-addition: H⁻ transfer to C₁-Ph P -0.57863600 2.27765800 -0.18398700 P -1.09050500 -2.16467200 -0.20428200 C 0.91368200 2.31405500 -1.29607400 C 0.33678300 -2.52600900 -1.35301300 H 1.80878700 2.20593900 -0.68086200 H 1.22519000 -2.65445900 -0.72927500 H 0.98795600 3.24529300 -1.85821900 H 0.19924800 -3.43467900 -1.94018600 C 0.81737600 1.11756800 -2.22697100 C 0.52538900 -1.31905900 -2.25588000 H 1.74942800 1.00857900 -2.79686900 H 1.45468100 -1.41772300 -2.83351500 H -0.00218200 1.23313300 -2.94042900 H -0.29983200 -1.22864000 -2.96594300 N 0.55079400 -0.09766200 -1.43497200 O -3.13199500 0.38720000 1.94248600 H -0.00889500 -0.07106500 1.02357200

H	-0.44987100	-2.82026300	1.71961500	H	1.30431300	-0.20019500	-0.75099500
H	0.90162700	2.35309100	1.65885200	C	1.46414100	-0.29959900	1.92195500
C	-3.20762900	-2.95226300	-0.93961200	H	0.84859200	-0.87943600	2.59658700
C	-1.67227400	3.72526400	-0.80807400	H	1.47043100	0.77250800	2.07275100
C	-3.18303000	-2.83671400	-2.46299200	C	2.51411800	-0.89602300	1.27915500
C	-1.77940000	3.65246000	-2.33027700	H	2.62619600	-1.97487800	1.32663700
O	-3.55676500	0.62650000	1.98863600	C	3.55891100	-0.13989700	0.61541500
H	-1.09844300	4.62317100	-0.55979300	C	-2.35425700	0.26278600	1.09040400
H	-3.11699000	-4.01283900	-0.68505200	C	4.82456400	-0.90979300	0.26398600
C	-3.05738200	3.84114100	-0.17342300	H	5.32344600	-1.15329400	1.21173600
C	-4.53115300	-2.42705100	-0.38340700	H	4.54003100	-1.87878900	-0.16369600
H	-3.01367200	3.94068700	0.91206400	C	5.78118900	-0.16861800	-0.65636000
H	-4.59925500	-2.52064000	0.70103300	H	5.27377000	0.05553300	-1.60118300
H	-3.66870700	2.96639900	-0.40139900	H	6.01977900	0.80261100	-0.21433400
H	-4.67168300	-1.37474400	-0.63410000	C	7.06301000	-0.94664100	-0.93477600
H	-3.57490700	4.72168000	-0.56642300	H	6.81473100	-1.92278600	-1.37127800
H	-5.36447700	-2.98779800	-0.81771900	H	7.57154000	-1.16269600	0.01342500
C	-2.38730200	-2.79980700	2.60185000	C	8.02721300	-0.21523900	-1.86371400
C	-0.84206200	2.97479200	2.72745800	H	7.51998500	0.00029500	-2.81132600
H	-3.40814200	-3.14170400	2.41778100	H	8.27646200	0.75875300	-1.42746500
H	-1.68445000	3.66624600	2.65217400	C	9.30782300	-0.99421000	-2.13749200
H	-2.42183400	-1.72705700	2.79029000	H	9.97639700	-0.44503300	-2.80507000
H	-1.24507600	1.97372800	2.88023500	H	9.85522200	-1.19348700	-1.21166500
H	-2.04422800	-3.29501400	3.51566500	H	9.09205900	-1.95913000	-2.60560400
H	-0.27562900	3.25397600	3.62147000	O	3.47125300	1.06340600	0.36485800
C	-1.40920500	-4.65667300	1.20916200	C	-0.70025300	-3.16668900	1.30369500
C	0.65637000	4.43603300	1.32124800	C	0.14062300	-4.27970500	1.27677400
H	-0.75943500	-4.93568200	0.37659400	C	-1.31311200	-2.81767500	2.50785700
H	1.29470700	4.50968600	0.43790900	C	0.36843400	-5.02388600	2.42813600
H	-2.40248400	-5.06858600	1.01559600	H	0.62827700	-4.57975000	0.35617500
H	-0.11880200	5.20324200	1.24944500	C	-1.09183300	-3.56641500	3.65634700
H	-1.02689700	-5.15721200	2.10419300	H	-1.96382200	-1.95259800	2.55180600
H	1.27509400	4.68463800	2.18871400	C	-0.24814400	-4.66962300	3.62084500
H	-0.47891900	-0.13200300	1.25403400	H	1.02906400	-5.88331200	2.39089100
H	0.92043300	-0.38561600	-0.45237700	H	-1.57674700	-3.28090000	4.58330600
C	0.92274800	-0.52146400	2.28157100	H	-0.07145300	-5.25067200	4.51908900
H	-4.04291400	-3.37113100	-2.87844900	C	-0.07124700	3.14050100	1.37252500
H	-3.25648300	-1.80022200	-2.79275200	C	1.25557000	3.37395900	1.73328000
H	-2.28769800	-3.27967900	-2.90389800	C	-1.08706300	3.54101100	2.24525500
H	-2.31097500	4.53660400	-2.69589600	C	1.55518100	4.00730900	2.93597200
H	-0.80304000	3.64155200	-2.81887300	H	2.07235600	3.04989300	1.10065400
H	-2.34056800	2.77808700	-2.65895200	C	-0.78451400	4.16891000	3.44372200
H	0.22904500	-1.12032700	2.85503900	H	-2.12547800	3.36736300	1.98554600
H	0.95787300	0.52989100	2.53019600	C	0.54018500	4.40779300	3.79231200
C	2.00389300	-1.09308200	1.67382400	H	2.59257500	4.18217600	3.19946600
H	2.08969600	-2.17417700	1.61373600	H	-1.58670300	4.47259200	4.10727900
C	3.10940500	-0.29712000	1.16837900	H	0.77775400	4.90120900	4.72828500
C	-2.74978600	0.44192400	1.17625600	C	-1.70187900	3.57371800	-0.88748000
C	4.37231400	-1.05936800	0.79320400	C	-3.06648100	3.32710100	-1.01021400
H	4.77146600	-1.49774900	1.71769400	C	-1.20961600	4.83135300	-1.24601100
H	4.08963800	-1.91824700	0.17168000	C	-3.92226100	4.30970900	-1.49672400
C	5.43696400	-0.21952600	0.10645900	H	-3.46372600	2.36155700	-0.72484200
H	5.02569300	0.20141500	-0.81727400	C	-2.06041500	5.80892400	-1.73969300
H	5.67526300	0.64037000	0.73871300	H	-0.15604000	5.05984600	-1.12485100
C	6.70555800	-1.00604300	-0.20662400	C	-3.42088300	5.54857800	-1.86827300
H	6.45800400	-1.86958200	-0.83755300	H	-4.98216400	4.10012100	-1.58842400
H	7.11629600	-1.42123900	0.72252700	H	-1.66303300	6.77889000	-2.01821700

C 7.77998700 -0.17342400 -0.89940600	H -4.08674700 6.31340300 -2.25257700
H 7.37092500 0.24077200 -1.82823900	C -2.50635500 -3.15567300 -0.87742600
H 8.02798600 0.68822800 -0.26924000	C -2.34131500 -4.44067600 -1.39728800
C 9.04718800 -0.96130700 -1.20778000	C -3.79141900 -2.62274300 -0.80171700
H 9.79616700 -0.33837500 -1.70295900	C -3.43398900 -5.16758000 -1.84816900
H 9.49870200 -1.35791100 -0.29379800	H -1.35693300 -4.89311200 -1.44535000
H 8.83592400 -1.81009500 -1.86480000	C -4.88779800 -3.35367000 -1.24315900
O 3.06002800 0.92778300 1.06771100	H -3.93371800 -1.62727800 -0.39963500
Mn -1.50734800 0.15599200 -0.03431900	C -4.71145600 -4.62442200 -1.77215400
C -2.63308200 0.43741700 -1.35707100	H -3.28863300 -6.16230100 -2.25525400
O -3.43446100 0.62415200 -2.18205100	H -5.88060100 -2.92259900 -1.17882200
	H -5.56577200 -5.19280000 -2.12279900
	C -2.27553200 0.20066400 -1.53271800
	O -3.00881200 0.25677900 -2.42988000
	Mn -1.14296200 0.08804400 -0.17413400
Interm(1,2)-iPr	Interm(1,2)-Ph
P -0.25120100 2.29609500 -0.05904200	P 0.83854200 2.13142700 -0.07928300
P -1.95353600 -1.98492300 -0.09426300	P -2.05318500 -1.39686100 -0.20372500
C 1.33494000 1.84755200 -0.91840200	C 2.20930000 1.24392900 -0.95312800
C -0.45754200 -2.73716700 -0.91132700	C -0.95523900 -2.49459000 -1.22929200
H 2.06323200 1.64766500 -0.12376500	H 2.80380900 0.71373500 -0.20023000
H 0.20809700 -3.05876500 -0.10591000	H -0.36168000 -3.08682500 -0.52951700
H 1.71910700 2.65713800 -1.54123600	H 2.86695800 1.92150300 -1.49806000
H -0.69493400 -3.61459800 -1.51516600	H -1.50759500 -3.17651900 -1.87646000
C 1.11357400 0.59259600 -1.73949200	C 1.57679800 0.22858300 -1.88802500
C 0.23901000 -1.67216700 -1.73767000	C -0.02292500 -1.60877800 -2.03878600
H 2.07653400 0.19183200 -2.08107300	H 2.35456700 -0.41780100 -2.31256200
H 1.22237500 -2.03322700 -2.06644900	H 0.76139500 -2.22141300 -2.50173900
H 0.50966500 0.80055900 -2.62681200	H 1.06039500 0.71823300 -2.71840000
H -0.33855400 -1.43136400 -2.63344900	H -0.56053800 -1.09792200 -2.84104500
N 0.39522100 -0.43260100 -0.94914500	N 0.58225900 -0.58925000 -1.15899100
C -2.01942900 -2.99039900 1.49738900	O -2.54192800 1.99800500 1.76415000
C 0.41023600 3.01564900 1.54520500	H 0.08676700 -0.29864200 1.33636900
H -1.02952900 -2.78402100 1.91560800	H 1.09048400 -1.12372100 -0.40965100
H 1.10543100 2.22339900 1.84855800	C 0.77351300 -0.96525600 2.01763000
C -3.43437900 -2.59308000 -1.08482100	H 0.03837400 -1.36065400 2.71855900
C -0.94707000 3.76869700 -1.00209900	H 1.39518300 -0.21379500 2.50409000
C -3.20778900 -2.57745500 -2.59589900	C 1.55732900 -1.99713000 1.34283000
C -0.85433300 3.63524000 -2.52120200	H 1.14893000 -3.00151500 1.29874700
O -3.59189700 1.12723000 1.63885100	C 2.91998100 -1.82648000 1.04705200
H -0.30396400 4.60288500 -0.70590700	C -1.86080500 1.40714300 1.04014200
H -3.56369800 -3.63610900 -0.77973000	C 3.71923100 -3.06032800 0.63630300
C -2.37746800 4.08366000 -0.56664500	H 4.38762400 -3.29200400 1.47527400
C -4.70146300 -1.81968500 -0.71882700	H 3.05763500 -3.92384700 0.51267900
H -2.46778600 4.21285400 0.51259400	C 4.56251500 -2.84437300 -0.61669400
H -4.90107600 -1.81902800 0.35310000	H 3.89965600 -2.67625400 -1.47626300
H -3.06629000 3.29195700 -0.86562200	H 5.13723000 -1.92298500 -0.48538300
H -4.63877400 -0.78099300 -1.04536100	C 5.49916100 -4.00636900 -0.92847400
H -2.71340200 5.01093000 -1.04049500	H 4.91840100 -4.93215200 -1.03266300
H -5.56459600 -2.27168700 -1.21640600	H 6.16843400 -4.16651800 -0.07385800
C -3.05847400 -2.49239700 2.49801100	C 6.33552100 -3.79652300 -2.18712600
C -0.64352700 3.19371100 2.63310700	H 5.66703200 -3.64001000 -3.04227100
H -4.07589700 -2.71912800 2.17172600	H 6.91321800 -2.87089400 -2.08319300
H -1.34451800 4.00013600 2.40362100	C 7.27907400 -4.95528200 -2.48604200
H -2.98883200 -1.41765300 2.66597300	H 7.86259100 -4.77591400 -3.39278400
H -1.22169000 2.28453500 2.80001700	H 7.98400400 -5.11214300 -1.66446300

H -2.91168000 -2.99204000 3.46004200	H 6.72676300 -5.88914900 -2.62676900
H -0.15223500 3.45296600 3.57564600	O 3.53426100 -0.73014000 1.11284300
C -2.13142600 -4.49962300 1.28898800	C -2.44560900 -2.40352700 1.29565700
C 1.23967600 4.28459700 1.35978000	C -2.33272000 -3.79345000 1.31980000
H -1.39982800 -4.88396100 0.57534000	C -2.91644200 -1.74400500 2.43153800
H 1.99014100 4.18193800 0.57340100	C -2.67967700 -4.50892600 2.45896600
H -3.12709800 -4.79095100 0.94609600	H -1.97214800 -4.33343400 0.45197800
H 0.61935700 5.15720000 1.13739200	C -3.26921600 -2.46077900 3.56688900
H -1.95960800 -5.01285900 2.23975500	H -3.00424900 -0.66396100 2.43462800
H 1.77752200 4.49797600 2.28783700	C -3.14882200 -3.84459200 3.58448000
H -0.37908700 -0.20150900 1.52703700	H -2.58048700 -5.58875800 2.46574400
H 0.99943600 -0.68643200 -0.12711200	H -3.63097900 -1.93369700 4.44258800
C 0.43608500 -0.53224400 2.29679800	H -3.41761200 -4.40365000 4.47366500
H -4.09151800 -2.98709200 -3.09411100	C 1.54771900 2.78428800 1.49526900
H -3.06251800 -1.56634200 -2.97658200	C 2.61320000 2.15755500 2.14405800
H -2.35631000 -3.18903300 -2.89952200	C 0.95870200 3.90999800 2.07752300
H -1.20672700 4.56229400 -2.98376200	C 3.08744200 2.67112700 3.34704000
H 0.16905800 3.47446000 -2.86468900	H 3.06919300 1.25632900 1.74293600
H -1.47826800 2.82704300 -2.90217400	C 1.43384900 4.41019400 3.28070300
H -0.14751900 -1.15389800 2.97721800	H 0.13248300 4.41077000 1.58586300
H 0.68534700 0.40717000 2.78961800	C 2.50487900 3.79402400 3.91733700
C 1.62353400 -1.18841700 1.75026900	H 3.91939300 2.17803500 3.83767900
H 1.66605900 -2.27291200 1.73572100	H 0.96829000 5.28644900 3.71831900
C 2.81381200 -0.46619800 1.56472800	H 2.88056300 4.18779100 4.85543600
C -2.70186300 0.78005400 0.98787000	C 0.57624400 3.70281100 -1.01744700
C 4.09313700 -1.25100300 1.28863100	C -0.70449500 4.23542200 -1.15134900
H 4.70924000 -1.17279200 2.19339200	C 1.65900200 4.41877900 -1.53295800
H 3.86856300 -2.31378300 1.15045500	C -0.90325500 5.44860900 -1.79997600
C 4.89060500 -0.71240200 0.10485800	H -1.55531200 3.70239000 -0.74634200
H 4.30581500 -0.84105600 -0.81584200	C 1.46042800 5.62493500 -2.18898900
H 5.01783100 0.36545400 0.24150100	H 2.66973400 4.04643000 -1.41142800
C 6.24924100 -1.38219700 -0.06944800	C 0.17718800 6.14194200 -2.32619200
H 6.11554200 -2.46626000 -0.17949600	H -1.90712000 5.84646600 -1.89724600
H 6.83751900 -1.24377700 0.84636400	H 2.31115100 6.16597600 -2.58836000
C 7.04357800 -0.85324000 -1.25979700	H 0.02265900 7.08525300 -2.83809300
H 6.45713300 -0.99403900 -2.17572500	C -3.69934800 -1.38901800 -1.04634000
H 7.17548300 0.22931500 -1.15010000	C -4.21067500 -2.52309600 -1.67893300
C 8.40497500 -1.51868100 -1.42173600	C -4.48757600 -0.24155900 -0.98151100
H 8.94859300 -1.11971300 -2.28206400	C -5.47522800 -2.50303100 -2.25007900
H 9.02771900 -1.36384200 -0.53589000	H -3.63152200 -3.43849600 -1.72280800
H 8.30295800 -2.59838000 -1.56592200	C -5.75735500 -0.22419300 -1.54473600
O 2.89275400 0.78751000 1.62980100	H -4.10726600 0.64596400 -0.49111700
Mn -1.35417900 0.24691300 -0.03154400	C -6.25155800 -1.35207100 -2.18483100
C -2.26651200 0.62179200 -1.46555400	H -5.85670600 -3.39007700 -2.74359300
O -2.89830800 0.87303200 -2.40761800	H -6.35679800 0.67735100 -1.48762400
	H -7.24002100 -1.33704000 -2.63013400
	C -1.58471700 1.17135000 -1.51508300
	O -2.07633400 1.56233900 -2.48633800
	Mn -0.81078100 0.52271000 -0.08172100
TS2(1,2-H⁺)_1,2-addition: H⁺ transfer to C₁-iPr	TS2(1,2-H⁺)_1,2-addition: H⁺ transfer to C₁-Ph
P -0.15790600 2.24512100 -0.04743000	P 0.65497800 2.10909300 -0.03789600
P -2.17627300 -1.89076200 -0.09117700	P -2.07597600 -1.53300800 -0.19642500
C 1.38383100 1.69185700 -0.92286000	C 2.06037700 1.30058200 -0.92893700
C -0.74631900 -2.75240500 -0.91101400	C -0.94453500 -2.58548200 -1.22926100
H 2.11809400 1.47919200 -0.14209800	H 2.70554100 0.83385800 -0.18140200
H -0.12372500 -3.14946000 -0.10601200	H -0.38492100 -3.20303100 -0.52483100

H	1.80037700	2.46735500	-1.56806900	H	2.66378500	2.01103400	-1.49455800
H	-1.05449300	-3.59509100	-1.53233100	H	-1.48682900	-3.25395200	-1.90013200
C	1.07182100	0.43041100	-1.70870000	C	1.47083600	0.23050600	-1.83388000
C	0.04456500	-1.72843700	-1.70629500	C	0.00579200	-1.66596600	-1.98307600
H	2.01268900	-0.06671600	-1.98896200	H	2.28386400	-0.40468100	-2.21506800
H	1.02300800	-2.15358200	-1.97680500	H	0.85556400	-2.25483500	-2.35934400
H	0.55643000	0.67679100	-2.64507300	H	0.98826400	0.68661000	-2.70729800
H	-0.46722100	-1.49506700	-2.64769800	H	-0.48867400	-1.23219400	-2.86093100
N	0.23411400	-0.49496000	-0.92891800	N	0.49151700	-0.59093600	-1.10626500
C	-2.32843100	-2.89136600	1.49946100	O	-2.65403600	1.70816700	1.92895900
C	0.56944500	2.90400800	1.55891400	H	0.15754000	-0.42641400	1.48683300
H	-1.34660100	-2.71851900	1.95119300	H	1.19797300	-1.23726800	-0.21757800
H	1.20366200	2.06256300	1.85784200	C	0.98663600	-1.06649200	1.93560800
C	-3.70370200	-2.37329800	-1.07981200	H	0.45754100	-1.68861900	2.65867400
C	-0.74864000	3.77340700	-0.97167500	C	1.74943900	-1.85161300	0.92357400
C	-3.47621800	-2.36402600	-2.59100200	H	1.45155600	-2.89526800	0.82598300
C	-0.70363900	3.62764900	-2.49201100	H	1.62184800	-0.35461500	2.46259300
O	-3.49180700	1.28877700	1.76591100	C	3.17402400	-1.65276800	0.81746000
H	-0.02990400	4.55042500	-0.69392000	C	-1.95647200	1.18765700	1.16747600
H	-3.91247600	-3.40554000	-0.78090200	O	3.75239500	-0.61327300	1.15917600
C	-2.13689900	4.20883800	-0.50464600	C	3.99002800	-2.79628000	0.22196200
C	-4.90857200	-1.50793900	-0.70858500	H	4.32881400	-3.40428500	1.07218700
H	-2.18797600	4.35876100	0.57444800	H	3.34045600	-3.44735600	-0.37216100
H	-5.10097100	-1.48836700	0.36427600	C	5.19843800	-2.34406300	-0.58718900
H	-2.89526000	3.47215200	-0.77430000	H	5.77277800	-1.63446400	0.01423600
H	-4.77283800	-0.47821200	-1.04036900	H	4.85640600	-1.78509500	-1.46691900
H	-2.40871900	5.15441100	-0.98344700	C	6.08866300	-3.49790900	-1.03567400
H	-5.80520100	-1.89804500	-1.19951000	H	5.49923200	-4.21406100	-1.62293600
C	-3.38272000	-2.36373500	2.46890100	H	6.43795200	-4.04903900	-0.15321900
C	-0.45322900	3.15175200	2.66287200	C	7.29492800	-3.05237500	-1.85669000
H	-4.39478800	-2.57438200	2.11614100	H	7.88301900	-2.33706200	-1.27053900
H	-1.10337400	4.00162100	2.44222700	H	6.94662300	-2.50372000	-2.73965900
H	-3.29729700	-1.28986600	2.63342200	C	8.18644900	-4.20785100	-2.29503000
H	-1.08664100	2.28280800	2.84082100	H	7.63334400	-4.92295700	-2.91114400
H	-3.27225600	-2.86038300	3.43742300	H	9.03987600	-3.85715100	-2.88089800
H	0.06895500	3.37997300	3.59688200	H	8.57930400	-4.75335000	-1.43206100
C	-2.48731100	-4.39566900	1.28419800	C	-2.48450000	-2.59646800	1.25571000
C	1.48889200	4.10925200	1.37133800	C	-2.85005200	-3.93353900	1.08076200
H	-1.73705300	-4.80835500	0.60710400	C	-2.45254900	-2.06528600	2.54270000
H	2.21873000	3.95789900	0.57340200	C	-3.16483700	-4.72469900	2.17558800
H	-3.47505700	-4.64766800	0.89065700	H	-2.89965800	-4.35921000	0.08429900
H	0.92986000	5.02492900	1.16085900	C	-2.77702500	-2.85687000	3.63935400
H	-2.38456800	-4.91518600	2.24167100	H	-2.17158600	-1.02963200	2.68985100
H	2.05228600	4.27860300	2.29329600	C	-3.12902900	-4.18668400	3.45796000
H	-0.35220600	-0.26183000	1.65399200	H	-3.44343900	-5.76235700	2.02851600
H	0.99925400	-0.87666000	0.06454300	H	-2.74989900	-2.43053400	4.63588200
C	0.54586900	-0.69695100	2.19852100	H	-3.37817900	-4.80514600	4.31305300
H	-4.39137200	-2.69215600	-3.09300000	C	1.34223300	2.78847000	1.53823300
H	-3.24407400	-1.36545000	-2.96177000	C	2.48390100	2.26516100	2.14640600
H	-2.67864300	-3.04185800	-2.89958300	C	0.65456400	3.83066400	2.16621100
H	-0.98640200	4.58005200	-2.95089300	C	2.93340600	2.79404800	3.35216700
H	0.29341300	3.37748500	-2.85835700	H	3.02808800	1.43372900	1.71137300
H	-1.40250500	2.87364100	-2.85286600	C	1.10534900	4.34890100	3.37099000
H	0.11062600	-1.42930100	2.88079400	H	-0.23329200	4.25207600	1.70875600
H	0.93982400	0.13417700	2.78419700	C	2.25088300	3.83405100	3.96663100
C	1.58662700	-1.26405900	1.29146600	H	3.82548200	2.38004600	3.80911100
H	1.61517600	-2.35184000	1.22839800	H	0.56117700	5.15964100	3.84282000

C 2.89435600 -0.65387300 1.31478900 C -2.65189200 0.88852000 1.07728800 C 4.06871600 -1.50512500 0.84197900 H 4.49161000 -1.97002000 1.74326500 H 3.70446200 -2.32978000 0.22052600 C 5.15795000 -0.71944300 0.12335800 H 4.74999700 -0.30126500 -0.80508100 H 5.43356200 0.13775100 0.74343700 C 6.39141500 -1.55601400 -0.19860700 H 6.10207200 -2.42443000 -0.80464200 H 6.80458100 -1.96403000 0.73266700 C 7.48052500 -0.77737300 -0.93024300 H 7.06859800 -0.37115500 -1.86153400 H 7.76909000 0.08975700 -0.32531900 C 8.71466600 -1.61472900 -1.24291000 H 9.47487700 -1.02989200 -1.76694700 H 9.16984600 -2.00479500 -0.32789700 H 8.46216000 -2.47138900 -1.87477900 O 3.09520100 0.51236600 1.67444400 Mn -1.39600200 0.28261500 -0.02134500 C -2.34269700 0.75477600 -1.39413600 O -2.97316000 1.06357300 -2.32031400	H 2.60694200 4.24168900 4.90639800 C 0.29741000 3.67472000 -0.95381100 C -1.00947500 4.15123300 -1.03963000 C 1.32963200 4.44103700 -1.49917500 C -1.28257200 5.35982600 -1.66937300 H -1.82253500 3.57747000 -0.61315500 C 1.05644100 5.64284900 -2.13624900 H 2.35910100 4.11186400 -1.41715600 C -0.25190300 6.10440000 -2.22474700 H -2.30579600 5.71314900 -1.72974100 H 1.86870900 6.22365500 -2.55922600 H -0.46476600 7.04410300 -2.72219300 C -3.69112600 -1.50822500 -1.08698800 C -3.77277600 -1.68620200 -2.46699600 C -4.85808100 -1.23367600 -0.37144600 C -4.99813200 -1.60610800 -3.11737800 H -2.88097200 -1.88035500 -3.05136100 C -6.08054200 -1.15285300 -1.02239600 H -4.81524000 -1.09039300 0.70259600 C -6.15469900 -1.34189100 -2.39728300 H -5.04518800 -1.74794300 -4.19136000 H -6.97873500 -0.94296800 -0.45230800 H -7.11042900 -1.27913000 -2.90531600 C -1.78933400 1.06236200 -1.38287200 O -2.35632300 1.44745700 -2.31393600 Mn -0.89693300 0.41022500 -0.03119400
TS₄₋₂(1,4-H⁻)_{1,4}-addition: H⁻ transfer to C₁-iPr P 1.89694000 -2.08756200 -0.04978700 P 0.69735000 2.27226400 -0.05424000 C 0.74919100 -2.58012400 -1.44004500 C -0.48204000 2.14000600 -1.49743200 H -0.20909200 -2.85280500 -0.98692700 H -1.46895100 1.91743400 -1.08422100 H 1.09918500 -3.44999100 -1.99871300 H -0.56643900 3.06693500 -2.06681900 C 0.54904900 -1.38179800 -2.35136300 C -0.04256100 0.98620500 -2.38108400 H -0.23018000 -1.59494200 -3.09561200 H -0.80470900 0.78025500 -3.14452100 H 1.47032100 -1.14719300 -2.89003900 H 0.89346500 1.22058300 -2.89403200 N 0.18263400 -0.20616100 -1.54637200 C -0.46219100 2.88238300 1.29226800 C 1.33502300 -3.26143000 1.31687100 H -1.15504800 2.03664800 1.35576400 H 0.32400500 -2.90100800 1.52268000 C 1.77244700 3.77478400 -0.43650700 C 3.58007800 -2.79825200 -0.52671300 C 2.19657800 3.86965200 -1.90134400 C 3.90083900 -2.67154900 -2.01514500 O 2.97346100 0.53939000 2.58558500 H 3.52022900 -3.86511600 -0.28786900 H 1.14493600 4.64369100 -0.21201600 C 4.69868100 -2.17627000 0.31081600 C 2.99961400 3.81164500 0.47515100 H 4.50976900 -2.23621100 1.38262600	TS₄₋₂(1,4-H⁻)_{1,4}-addition: H⁻ transfer to C₁-Ph P 2.29501600 -1.28377900 -0.35021700 P -0.73852300 1.98070500 0.00345200 C 1.45652600 -2.19347800 -1.74731800 C -1.91971500 1.27661300 -1.24999000 H 0.77781400 -2.92998600 -1.30946000 H -2.56281200 0.58602100 -0.69904300 H 2.15919500 -2.72059300 -2.39384100 H -2.56170900 2.02963600 -1.71047600 C 0.64025800 -1.18017100 -2.53156300 C -1.10668600 0.51240900 -2.28214700 H 0.01268200 -1.69610700 -3.27013900 H -1.77228600 -0.04152000 -2.95661800 H 1.28947400 -0.48227000 -3.06630900 H -0.50403500 1.19357300 -2.88900000 N -0.19226500 -0.41245500 -1.59211800 O 2.32780600 1.57681900 2.30241100 H 0.03387300 -0.35830100 0.99109800 H -0.78714900 -1.09779000 -1.10986600 C -0.83625200 -1.68769500 1.64518100 H -0.38451600 -1.45576500 2.60107000 C -2.19498000 -1.64648900 1.49384500 H -2.82066100 -1.21779700 2.26854400 H -0.25664100 -2.33892600 1.00568600 C -2.82832600 -2.17396900 0.31184600 C 1.80192900 1.16805300 1.35125500 O -2.20664800 -2.39827400 -0.73656900 C -4.31263200 -2.48474300 0.39930100 H -4.40429200 -3.42795600 0.95513900 H -4.79490000 -1.73069500 1.03113700

H	2.74276700	3.74982000	1.53297000	C	-5.01658700	-2.60543000	-0.94429900
H	4.83876000	-1.12487200	0.05876700	H	-4.48106300	-3.33169300	-1.56163600
H	3.67713400	2.98646500	0.25166600	H	-4.94406300	-1.65050500	-1.47735400
H	5.64097000	-2.69522900	0.10906800	C	-6.48221200	-3.00633100	-0.81477700
H	3.54870900	4.74552500	0.31953700	H	-7.00958300	-2.27829500	-0.18516200
C	0.20880300	3.02919100	2.65502800	H	-6.55129700	-3.96584400	-0.28659000
C	2.14262100	-3.11157800	2.60447400	C	-7.20099200	-3.12069600	-2.15556100
H	0.87036400	3.89832700	2.68859300	H	-6.67408200	-3.84735900	-2.78455200
H	3.14198500	-3.54097800	2.50202400	H	-7.13417900	-2.16166100	-2.68243800
H	0.79004400	2.14724000	2.92347100	C	-8.66351900	-3.52715000	-2.02266300
H	2.24885400	-2.06989500	2.90857200	H	-9.22361900	-2.80076600	-1.42658900
H	-0.55266600	3.17804100	3.42709200	H	-9.15015900	-3.59968800	-2.99851200
H	1.64551100	-3.65035400	3.41695900	H	-8.76068500	-4.49962300	-1.53134500
C	-1.26008800	4.13520700	0.93748700	C	-1.79848900	2.25700900	1.49114300
C	1.23289400	-4.72935700	0.90573800	C	-2.97019600	3.01238400	1.40294100
H	-1.76731500	4.05556500	-0.02614200	C	-1.42319600	1.73081800	2.72348800
H	0.62073700	-4.87746400	0.01422900	C	-3.75953400	3.21995400	2.52463800
H	-0.62906500	5.02746900	0.91381300	H	-3.26309900	3.45350400	0.45603800
H	2.21496000	-5.17063100	0.71839600	C	-2.20824300	1.94869700	3.85064300
H	-2.02830500	4.31034800	1.69736800	H	-0.51493600	1.14553700	2.79250000
H	0.77486500	-5.30619000	1.71532300	C	-3.37832300	2.68857300	3.75248600
H	0.20741200	-0.09350300	1.06675600	H	-4.66931300	3.80477200	2.44360600
H	-0.71853200	-0.41773200	-1.10497400	H	-1.90162300	1.53908200	4.80685300
C	-1.33764300	-0.83779500	1.65523800	H	-3.99136900	2.85742600	4.63100800
H	2.79750100	4.77294000	-2.04535900	C	-0.45375900	3.73033800	-0.52477400
H	2.81320700	3.02095600	-2.19938400	C	-0.76352700	4.20233200	-1.79829900
H	1.34685700	3.93751300	-2.58314500	C	0.16538600	4.59680900	0.37950000
H	4.87724600	-3.12430500	-2.21332400	C	-0.47288800	5.51384000	-2.15839800
H	3.17460800	-3.18419400	-2.64865600	H	-1.23064000	3.55294100	-2.52941100
H	3.96046500	-1.62836400	-2.32810400	C	0.45262000	5.90524500	0.02148000
H	-0.85438200	-0.93270100	2.61867800	H	0.42238100	4.24780500	1.37406800
C	-2.48042800	-0.10873300	1.50797000	C	0.13281900	6.36911900	-1.24966800
H	-2.86203900	0.49546400	2.32359700	H	-0.72083200	5.86408600	-3.15444500
H	-1.13017500	-1.60702700	0.92600400	H	0.93067200	6.56487900	0.73726900
C	-3.21412300	-0.14023600	0.26363900	H	0.35991000	7.39144600	-1.53048900
C	2.41772800	0.39772000	1.57650400	C	4.06099100	-1.11621400	-0.89015200
O	-2.72170100	-0.57671000	-0.78427200	C	4.74703200	-2.16842800	-1.50015300
C	-4.64440900	0.36244700	0.25483900	C	4.74483100	0.06795400	-0.62597500
H	-4.88288200	0.85687800	1.20078400	C	6.08042300	-2.03046400	-1.85736400
H	-4.73139300	1.10810400	-0.54313900	H	4.24761700	-3.11229000	-1.69024500
C	-5.63812200	-0.77231900	-0.01270600	C	6.08363700	0.20392600	-0.97470400
H	-5.55697700	-1.51861600	0.78605800	H	4.22693700	0.89022100	-0.14876500
H	-5.34673700	-1.27525100	-0.93960900	C	6.75227100	-0.84142200	-1.59545700
C	-7.08104000	-0.29029300	-0.11353200	H	6.59838300	-2.85467700	-2.33561900
H	-7.15808100	0.45594200	-0.91415600	H	6.60011800	1.13376100	-0.76430200
H	-7.36033200	0.22886600	0.81189700	H	7.79505400	-0.73372000	-1.87284500
C	-8.07716400	-1.41538700	-0.37756000	C	2.50231600	-2.57200400	0.96521200
H	-7.99986400	-2.15998200	0.42313200	C	2.38741500	-3.94095900	0.72338000
H	-7.79612700	-1.93468900	-1.30088800	C	2.82781800	-2.14308500	2.25353100
C	-9.51766300	-0.93005500	-0.48388500	C	2.58835300	-4.86029300	1.74674900
H	-9.63351200	-0.21045800	-1.29949200	H	2.13689200	-4.30764900	-0.26524300
H	-10.20617300	-1.75741900	-0.67255100	C	3.03779800	-3.06176600	3.27243100
H	-9.83812100	-0.43636200	0.43811900	H	2.91708500	-1.08359600	2.46348100
Mn	1.53609900	0.16365400	0.07552800	C	2.91529100	-4.42352100	3.02302000
C	2.93404300	0.54788600	-0.92339500	H	2.48853600	-5.92079900	1.54266600
O	3.88777400	0.82632500	-1.53247700	H	3.29248100	-2.71093700	4.26649700
				H	3.07314000	-5.14078500	3.82073500

	C 1.87440400 1.54909900 -1.20451500
	O 2.44910900 2.24749600 -1.92801200
	Mn 0.97485000 0.53018700 -0.06156800
Interm(1,4)-iPr	Interm(1,4)-Ph
P 2.63409300 -1.47430900 -0.16406500	P 2.43636000 -1.04800100 -0.35786100
P -0.40131100 1.99726400 0.05853300	P -1.13175100 1.78504800 0.00880700
C 1.63207600 -2.43245500 -1.40551300	C 1.66662200 -2.09124300 -1.68428200
C -1.49773900 1.32352500 -1.28329400	C -2.17596400 0.80851400 -1.16558600
H 0.93370700 -3.05438100 -0.83739700	H 1.05852800 -2.85455200 -1.19067700
H -2.24355100 0.69378700 -0.79228400	H -2.61515500 -0.00221000 -0.57523800
H 2.23852600 -3.09858700 -2.02180900	H 2.39968700 -2.58107300 -2.32558300
H -2.02238100 2.10375000 -1.83649400	H -2.98225100 1.38231600 -1.62363900
C 0.84100000 -1.45285000 -2.25440500	C 0.72693500 -1.19612200 -2.47521400
C -0.66441500 0.44813500 -2.20209600	C -1.24796100 0.21051600 -2.20999000
H 0.13369300 -1.99972400 -2.89076200	H 0.15277800 -1.80640600 -3.18323600
H -1.32392300 -0.09619000 -2.88935300	H -1.81554500 -0.46177700 -2.86479800
H 1.50577000 -0.88433200 -2.91147500	H 1.27439900 -0.44071500 -3.04694400
H 0.02772000 1.04555200 -2.80302800	H -0.80054000 0.99033700 -2.83466400
N 0.11021600 -0.51102400 -1.39157700	N -0.18411100 -0.53883900 -1.52532500
C -1.57575900 2.07110200 1.51685400	O 2.16874100 1.93857100 2.17076000
C 2.85731600 -2.73384000 1.22153800	H -0.26113700 -0.33933500 1.19330200
H -1.84007400 1.01028200 1.63785300	H -0.67737600 -1.35441100 -1.03608700
H 1.84077000 -2.84325200 1.60687300	C -0.44438500 -1.36729100 1.69450900
C -0.06947900 3.79894700 -0.37909000	H -0.16751900 -1.16286900 2.72945000
C 4.37199400 -1.33893300 -0.88345800	C -1.82953100 -1.84323000 1.53972900
C 0.12032300 4.05189600 -1.87390800	H -2.52420000 -1.70150900 2.35846300
C 4.40416800 -1.14116800 -2.39797800	H 0.27544700 -2.06336100 1.26848800
O 2.76150500 1.51745200 2.36971100	C -2.21351300 -2.54872700 0.42304100
H 4.83051300 -2.30908400 -0.66608000	C 1.62703200 1.39307100 1.30535300
H -0.97765600 4.32340900 -0.06451800	O -1.48605300 -2.67244500 -0.63394500
C 5.19141300 -0.25379400 -0.18280700	C -3.55556400 -3.25894300 0.41051500
C 1.11033700 4.35745200 0.41695600	H -3.34733800 -4.33662600 0.39160500
H 5.17734700 -0.34526000 0.90305800	H -4.09704700 -3.05638200 1.33994300
H 1.01303900 4.19036800 1.48987200	C -4.42029300 -2.90962000 -0.79879700
H 4.82891000 0.74207900 -0.43728000	H -3.81946400 -3.05341300 -1.70195000
H 2.05121800 3.90901900 0.09502600	H -4.67983500 -1.84321300 -0.76305200
H 6.23425500 -0.31760000 -0.50785600	C -5.70079700 -3.73240500 -0.88884500
H 1.18637900 5.43675700 0.25414700	H -6.28720100 -3.60324500 0.03006700
C -0.91792000 2.54369100 2.81028600	H -5.44069500 -4.79762100 -0.93148100
C 3.73060100 -2.21902300 2.36387200	C -6.57171400 -3.38091600 -2.09122300
H -0.71041700 3.61674200 2.79357700	H -5.98486300 -3.50792900 -3.00841700
H 4.78431900 -2.17935600 2.07816100	H -6.83484700 -2.31721200 -2.04681500
H 0.01559800 2.01990300 3.01864400	C -7.84412600 -4.21485000 -2.18138100
H 3.43121400 -1.22687000 2.70417800	H -8.46717500 -4.08277100 -1.29186700
H -1.59433400 2.36032300 3.65011200	H -8.44619300 -3.93927500 -3.05123400
H 3.65551700 -2.89967000 3.21675600	H -7.61225600 -5.28074200 -2.26337200
C -2.86332600 2.84452800 1.24116200	C -2.12643000 1.92702900 1.55584000
C 3.32652100 -4.10880600 0.74882800	C -3.48269600 1.60923900 1.60505600
H -3.36880900 2.51039800 0.33348500	C -1.50009500 2.40525600 2.70756600
H 2.68075000 -4.53186800 -0.02214100	C -4.19967600 1.77027400 2.78423300
H -2.68885000 3.92083400 1.15894500	H -3.99162900 1.22590000 0.72954600
H 4.34848500 -4.08535000 0.36194900	C -2.21870100 2.56845300 3.88348700
H -3.55901100 2.69591500 2.07236200	H -0.44494400 2.65197100 2.69203300
H 3.32194000 -4.80361000 1.59400300	C -3.57058900 2.25001800 3.92479900
H 0.04144000 -0.29897600 1.38767900	H -5.25278500 1.51319300 2.80997200
H -0.63332900 -1.07939600 -0.88174800	H -1.71829700 2.93959300 4.77091500

C -0.33142200 -1.30866600 1.80081500	H -4.13114000 2.37277700 4.84479200
H 0.25431800 5.12484500 -2.04162900	C -1.16047500 3.53496900 -0.58654400
H 1.00767800 3.55120900 -2.26241100	C -2.28373700 4.08537900 -1.20506000
H -0.74082500 3.73850700 -2.46596800	C -0.05828500 4.35269200 -0.34204000
H 5.44499700 -1.12587200 -2.73488800	C -2.29653600 5.42018900 -1.58533300
H 3.90210000 -1.94532800 -2.93823600	H -3.16425200 3.48036000 -1.38744600
H 3.95640800 -0.19166600 -2.69349200	C -0.07492300 5.69107700 -0.71297000
H 0.16250000 -1.38101700 2.77093000	H 0.82167100 3.94264400 0.13851500
C -1.80148900 -1.39445200 1.87742300	C -1.19144000 6.22629600 -1.34035100
H -2.29103900 -1.28291700 2.83735200	H -3.17443000 5.83229400 -2.07053200
H 0.05782500 -2.07765800 1.13504400	H 0.79143700 6.31284000 -0.51730900
C -2.52201500 -1.74195400 0.75701800	H -1.20272100 7.26930200 -1.63638500
C 2.17245400 1.08004700 1.47645700	C 2.91377500 -2.22245000 0.98606500
O -2.01047300 -1.83260200 -0.41911300	C 3.42838000 -1.68539900 2.16813400
C -3.99924900 -2.06834000 0.88651000	C 2.80520100 -3.60671100 0.86391700
H -4.11517700 -3.13405600 0.65091500	C 3.83117700 -2.51672000 3.20257800
H -4.32396000 -1.93417100 1.92327200	H 3.51651100 -0.61099600 2.28459700
C -4.88777800 -1.26079200 -0.05707000	C 3.20488600 -4.43776300 1.90423800
H -4.49565700 -1.36703600 -1.07316600	H 2.40153400 -4.05288400 -0.03651800
H -4.81209900 -0.19583600 0.19830100	C 3.71876900 -3.89623800 3.07385700
C -6.35285700 -1.68165400 -0.01854100	H 4.22801100 -2.08488000 4.11457700
H -6.73322200 -1.59574000 1.00753200	H 3.10824600 -5.51245500 1.79739200
H -6.42835300 -2.74507700 -0.27865800	H 4.02768900 -4.54600200 3.88496000
C -7.24783600 -0.87268000 -0.95246200	C 4.10871600 -0.57659500 -0.99006700
H -6.86738200 -0.95795100 -1.97704600	C 4.62563200 0.68673700 -0.71178300
H -7.17422800 0.18969800 -0.69097000	C 4.90367800 -1.49334800 -1.68096700
C -8.70887000 -1.30454600 -0.91420800	C 5.90631100 1.03316200 -1.12567900
H -9.12599100 -1.19878700 0.09161000	H 4.02643900 1.40744400 -0.17003300
H -9.32391100 -0.70689700 -1.59212700	C 6.17868300 -1.14487600 -2.10196300
H -8.81824800 -2.35328000 -1.20550000	H 4.53797700 -2.49363500 -1.88401900
Mn 1.28730000 0.40959400 0.09453100	C 6.68265700 0.12119000 -1.82619700
C 2.25966100 1.33978500 -1.01106800	H 6.29254700 2.02150800 -0.90334700
O 2.90315400 1.97583700 -1.73878700	H 6.78257100 -1.86567500 -2.64205200
	H 7.67972600 0.39279200 -2.15445400
	C 1.55120200 1.63712800 -1.22911500
	O 2.00440600 2.33543400 -2.03026000
	Mn 0.82060700 0.57100600 -0.03896000
TS2(1,4-H⁺)_1,4-addition: H⁺ transfer to C₁-iPr	TS2(1,4-H⁺)_1,4-addition: H⁺ transfer to C₁-Ph
P 2.54329000 -1.54108900 -0.15246500	P 2.35539500 -1.23344900 -0.29434900
P -0.34606800 2.06527100 0.04888400	P -0.99836200 1.88036300 0.06507400
C 1.43018300 -2.52871800 -1.26266400	C 1.55148000 -2.17753900 -1.66757900
C -1.55151800 1.35485100 -1.17049500	C -2.04787700 1.09671100 -1.24145400
H 0.76360600 -3.10277200 -0.61201300	H 0.93077300 -2.94364300 -1.19571000
H -2.30189500 0.81731500 -0.58579000	H -2.66811000 0.35281800 -0.73642800
H 1.97180000 -3.23907700 -1.89009500	H 2.26525000 -2.67780700 -2.32436100
H -2.06748300 2.11759700 -1.75580800	H -2.71714700 1.79924700 -1.73892000
C 0.60205800 -1.55656000 -2.08539500	C 0.65465000 -1.20422700 -2.41749800
C -0.80731100 0.36546100 -2.05052700	C -1.10868200 0.39791200 -2.20930300
H -0.18237600 -2.11475300 -2.61731300	H 0.03035500 -1.76854400 -3.12455500
H -1.53768900 -0.20992100 -2.63750600	H -1.70357800 -0.19475100 -2.91821600
H 1.22720300 -1.08121700 -2.85443900	H 1.25676100 -0.50167800 -3.01120600
H -0.16747100 0.89551700 -2.76987400	H -0.54643500 1.13682600 -2.79783300
N -0.00965000 -0.54428200 -1.21927900	N -0.19683000 -0.48099600 -1.46801800
C -1.43411300 2.31055900 1.56362000	O 1.99233900 1.50436700 2.54645000
C 2.81784700 -2.72523600 1.29189400	H -0.56263000 -0.55562800 1.29968700
H -1.76106100 1.28263400 1.76452700	H -1.01080400 -1.42936200 -1.04234400

H	1.81946400	-2.79599200	1.73169800	C	-0.62394100	-1.62851700	1.62456400
C	0.04344700	3.81713800	-0.52363900	H	-0.36911500	-1.60285900	2.68466700
C	4.23572500	-1.50430400	-0.98330600	C	-1.97546500	-2.22060000	1.38890200
C	0.14075400	3.96725100	-2.04125600	H	-2.57281700	-2.47715100	2.25576700
C	4.17637500	-1.38834700	-2.50556500	H	0.15408900	-2.19828400	1.11560300
O	2.92970900	1.57423100	2.20107400	C	-2.43662400	-2.56168700	0.16351300
H	4.67434100	-2.47809100	-0.74271700	C	1.51390200	1.05767600	1.59268200
H	-0.81399500	4.40808900	-0.18607200	O	-1.82341100	-2.29857900	-0.97673600
C	5.13485100	-0.41604000	-0.39425100	C	-3.72872400	-3.32323600	0.00019500
C	1.30014500	4.36209300	0.15583900	H	-3.48948600	-4.27730600	-0.48644200
H	5.18588200	-0.45018600	0.69389100	H	-4.14183800	-3.56184800	0.98462900
H	1.27344900	4.25768900	1.24077400	C	-4.77101200	-2.58995600	-0.84442900
H	4.79227400	0.57850000	-0.67954300	H	-4.31920700	-2.32713200	-1.80560700
H	2.19578400	3.85431600	-0.20409900	H	-5.03274800	-1.64479500	-0.35260000
H	6.15233600	-0.53645800	-0.77850800	C	-6.03822800	-3.40600200	-1.07533600
H	1.40951200	5.42642700	-0.07337100	H	-6.47786700	-3.68260300	-0.10839700
C	-0.67685600	2.81973100	2.78701500	H	-5.77422200	-4.35092000	-1.56690900
C	3.75400600	-2.16938800	2.36258000	C	-7.08771900	-2.68147300	-1.91263200
H	-0.39419800	3.86995000	2.67976500	H	-6.64858200	-2.40571700	-2.87845000
H	4.79270400	-2.16406300	2.02414400	H	-7.35172600	-1.73773900	-1.42101400
H	0.22839700	2.24483300	2.98597100	C	-8.34934400	-3.50454300	-2.14342400
H	3.48836200	-1.15528400	2.66337300	H	-8.82927800	-3.76647400	-1.19589200
H	-1.31724400	2.74878500	3.67113000	H	-9.08103400	-2.95944800	-2.74534300
H	3.71102000	-2.80357000	3.25289200	H	-8.12164100	-4.43885200	-2.66484300
C	-2.68365400	3.14956100	1.30255700	C	-2.14093400	2.15688300	1.49345300
C	3.23763800	-4.13341200	0.87307600	C	-2.88900000	1.08617000	1.98881700
H	-3.25213700	2.79875100	0.43942500	C	-2.24944100	3.40090200	2.11610300
H	2.55395500	-4.57732700	0.14784200	C	-3.73591100	1.26447100	3.07412900
H	-2.44529400	4.20513500	1.14808800	H	-2.81777500	0.09767200	1.54293700
H	4.24435500	-4.15307300	0.44812400	C	-3.09302200	3.57230100	3.20673800
H	-3.34559500	3.09598400	2.17212500	H	-1.68075400	4.24595600	1.74875400
H	3.25034100	-4.78544200	1.75173300	C	-3.84149900	2.50668700	3.68715900
H	-0.00049300	-0.08486800	1.63558500	H	-4.31325300	0.42315100	3.44149200
H	-0.97896700	-1.23546500	-0.57733500	H	-3.16650700	4.54666300	3.67720500
C	-0.34310200	-1.08513700	2.00632600	H	-4.50201700	2.64237100	4.53639600
H	0.32312800	5.01825200	-2.28538100	C	2.85738000	-2.51063700	0.94156900
H	0.96714700	3.38995500	-2.45629400	C	3.29327700	-3.77171400	0.53080300
H	-0.77677800	3.67153000	-2.55193400	C	2.84789800	-2.20721200	2.30195000
H	5.19359600	-1.42819000	-2.90691900	C	3.70478400	-4.71179500	1.46488000
H	3.61392900	-2.20145100	-2.96676600	H	3.31757000	-4.02552000	-0.52289100
H	3.73958200	-0.44176900	-2.82488900	C	3.26959200	-3.14613300	3.23573200
H	0.07196000	-1.15991000	3.01356300	H	2.50333000	-1.23637600	2.63703600
C	-1.82622700	-1.24534100	1.98672100	C	3.69568900	-4.39989600	2.81949700
H	-2.37398100	-1.11863400	2.91296200	H	4.03602900	-5.68978900	1.13367300
H	0.11901200	-1.85282100	1.38733900	H	3.25698600	-2.89689300	4.29090300
C	-2.48875900	-1.67743400	0.88871100	H	4.01863400	-5.13485800	3.54833800
C	2.26415100	1.10570900	1.37843500	C	4.00498100	-0.70038900	-0.93111700
O	-1.93490800	-1.85474000	-0.30012700	C	4.92975300	-0.17747900	-0.02477300
C	-3.94962400	-2.04597300	0.94521700	C	4.34303700	-0.75555200	-2.28134900
H	-4.02861700	-3.11006600	0.68855500	C	6.16965000	0.26585400	-0.45937800
H	-4.31552200	-1.93747300	1.97039200	H	4.68507400	-0.12151700	1.03039000
C	-4.82827300	-1.24534700	-0.01612900	C	5.58533100	-0.30759600	-2.71620900
H	-4.41034900	-1.32935000	-1.02377000	H	3.64155300	-1.14212500	-3.01053600
H	-4.78372300	-0.18313300	0.25510700	C	6.50186400	0.20123600	-1.80770600
C	-6.28300200	-1.70241600	-0.02148400	H	6.87850000	0.66457500	0.25778800
H	-6.69291600	-1.63509300	0.99444100	H	5.83317600	-0.35697700	-3.77075100
H	-6.32568000	-2.76461100	-0.29341700	H	7.47052800	0.54986700	-2.14771500

C -7.17023700 -0.90544900 -0.97287500 H -6.75947000 -0.97177900 -1.98701700 H -7.12935900 0.15562800 -0.69968600 C -8.62078000 -1.37256300 -0.97954300 H -9.06859600 -1.28629300 0.01480700 H -9.23012600 -0.78285400 -1.66922500 H -8.69683700 -2.42054400 -1.28368000 Mn 1.27402000 0.40019100 0.08291500 C 2.21153300 1.22833900 -1.11737500 O 2.82293700 1.78337900 -1.93393700	C -0.65072800 3.60533800 -0.49098900 C -1.46467400 4.28007200 -1.40049800 C 0.44434600 4.27662300 0.05618500 C -1.18380100 5.59144100 -1.76275800 H -2.32974300 3.79280000 -1.83286600 C 0.71758100 5.59121300 -0.29593200 H 1.09167400 3.76906400 0.76179200 C -0.09327600 6.25041000 -1.21065900 H -1.82241000 6.09886300 -2.47733100 H 1.57284000 6.09595000 0.13892800 H 0.12465800 7.27416200 -1.49370300 C 1.74279700 1.50291100 -0.88610400 O 2.36454900 2.19684900 -1.56697300 Mn 0.79315600 0.41388100 0.10127000
TS₁₋₃(1,2-H⁻)_{1,2}-addition: H⁻ transfer to C₁-iPr P -0.16457000 2.23862000 0.04964900 P -2.23542500 -1.80640100 -0.20527300 C 1.36142800 1.71406100 -0.88883900 C -0.87538900 -2.64599900 -1.16976900 H 2.08920200 1.37461000 -0.14704200 H -0.21310700 -3.11638700 -0.43806800 H 1.82294400 2.53049300 -1.44686900 H -1.24203500 -3.43257400 -1.83145300 C 0.99660400 0.56246000 -1.80572400 C -0.10433400 -1.59404200 -1.94423400 H 1.90408900 0.10358700 -2.22140000 H 0.82321800 -2.02308800 -2.34761100 H 0.39143300 0.91165100 -2.64563100 H -0.69144000 -1.22355800 -2.78777700 N 0.20575500 -0.44443500 -1.07099700 C -2.32079100 -2.94921900 1.29517100 C 0.62123200 2.80570800 1.66802000 H -1.28281400 -2.91639700 1.64034000 H 1.16562400 1.90184900 1.95844400 C -3.81836300 -2.20223300 -1.14877600 C -0.70831600 3.84658400 -0.76902000 C -3.67742400 -2.06198700 -2.66383600 C -0.65762800 3.80046300 -2.29542800 O -3.40607500 1.21455000 1.93686300 H 0.01632000 4.59559500 -0.43516000 H -4.02387900 -3.25482400 -0.93185300 C -2.09783200 4.26413100 -0.28737700 C -4.98774200 -1.36228700 -0.63487200 H -2.16347400 4.33377400 0.79894800 H -5.13322000 -1.45706300 0.44177800 H -2.85858800 3.55704700 -0.62048500 H -4.84047100 -0.30468600 -0.85697600 H -2.35223000 5.24566000 -0.69873300 H -5.91371200 -1.67964900 -1.12394300 C -3.19953900 -2.42052500 2.42498500 C -0.38507000 3.11088500 2.77344900 H -4.26031800 -2.46990700 2.16957400 H -0.93639600 4.03291400 2.57624900 H -2.96429100 -1.38754900 2.68064700 H -1.10895300 2.30705700 2.90444900 H -3.05697700 -3.03173800 3.32144200	TS₁₋₃(1,2-H⁻)_{1,2}-addition: H⁻ transfer to C₁-Ph P 0.84914900 1.94822700 0.07029900 P -2.34511500 -1.20689900 -0.35189200 C 2.10004700 1.10355700 -1.01397100 C -1.40145000 -2.28568100 -1.53837600 H 2.69247500 0.46893700 -0.35089500 H -0.85768300 -3.01867300 -0.93934100 H 2.78324200 1.79856900 -1.50517200 H -2.04229100 -2.82437500 -2.23735200 C 1.34841200 0.24130700 -2.01242000 C -0.40442000 -1.40937400 -2.27554500 H 2.04615400 -0.43076600 -2.52943300 H 0.31078900 -2.04142800 -2.81947800 H 0.86024100 0.85476900 -2.77481500 H -0.90849500 -0.77335600 -3.00788700 N 0.31142300 -0.54582000 -1.31616300 O -2.39819700 1.81152700 2.12279000 H 0.00723100 -0.52964100 1.11453800 H 0.84535500 -1.22667500 -0.64755900 C 0.64975500 -1.49187100 1.61409200 H -0.19420100 -2.00182300 2.07699200 H 1.20936200 -0.92370600 2.36002700 C 1.44718400 -2.25402700 0.69733900 H 1.03932100 -3.20916500 0.36548200 C 2.93858300 -2.22164700 0.77730400 H 3.26386600 -1.19673700 1.02335600 C -1.81044600 1.29892600 1.26266800 C 3.64561300 -2.66424500 -0.49941200 H 3.29181200 -3.67198000 -0.74837500 H 3.32721600 -2.00843300 -1.31743000 C 5.16755900 -2.66261200 -0.40783700 H 5.51380100 -1.65092500 -0.15890100 H 5.47186100 -3.30171700 0.42544300 C 5.84803200 -3.12591600 -1.69176600 H 5.53050900 -2.48886700 -2.52810800 H 5.50365600 -4.13839200 -1.93817400 C 7.37157700 -3.12221700 -1.61260800 H 7.71680700 -2.11108800 -1.36673100 H 7.68835000 -3.75896900 -0.77879000 C 8.04469700 -3.59139100 -2.89672900 H 9.13407900 -3.57750200 -2.80835200 H 7.74624900 -4.61325000 -3.14868700

H 0.14135600 3.24945000 3.72272800	H 7.77313200 -2.95252800 -3.74244600
C -2.65058400 -4.40604500 0.97435000	O 3.44846700 -3.08607700 1.83185100
C 1.64140900 3.93340300 1.52306200	H 2.72785000 -3.17980800 2.46102000
H -2.04641900 -4.80695600 0.15756400	C -2.80465300 -2.35340700 1.02862500
H 2.36727000 3.74811100 0.72840400	C -2.82171500 -3.74081800 0.88395800
H -3.70348100 -4.53647600 0.71342100	C -3.19101500 -1.80006000 2.25031500
H 1.15945100 4.89394400 1.32568400	C -3.21157000 -4.55724600 1.93857600
H -2.46189000 -5.02750200 1.85503400	H -2.53026900 -4.20152400 -0.05275600
H 2.20148900 4.04357000 2.45649500	C -3.58715500 -2.61628300 3.30133100
H -0.40794800 -0.22145300 1.31008900	H -3.18035200 -0.72524600 2.38600200
H 0.81197900 -0.81504600 -0.29457100	C -3.59578700 -3.99719200 3.14963000
C 0.50886100 -0.86125500 2.09498300	H -3.21386600 -5.63425200 1.81129400
H -4.62178400 -2.34411200 -3.13934000	H -3.88392100 -2.16976300 4.24388600
H -3.46041400 -1.03574900 -2.95996900	H -3.89957000 -4.63460000 3.97245800
H -2.90458400 -2.71384800 -3.07574200	C 1.77961700 2.29031800 1.62785900
H -0.94958300 4.77689300 -2.69397100	C 3.00574300 2.95908100 1.59305400
H 0.34271700 3.58547600 -2.67615000	C 1.26082300 1.88889900 2.85587200
H -1.35031800 3.06438800 -2.70350900	C 3.70471600 3.20570500 2.76523700
H -0.23208900 -1.48902700 2.58163200	H 3.41379500 3.29941200 0.64726400
H 0.74452600 0.00244600 2.71555700	C 1.95749700 2.14543500 4.03199600
C 1.59249500 -1.48933100 1.45328900	H 0.30897100 1.37341500 2.88971000
H 1.50597500 -2.54183400 1.18792000	C 3.18064600 2.79895800 3.98798300
C 2.97977300 -0.94303800 1.49619800	H 4.65834200 3.72054400 2.72637900
H 2.93257800 0.15770800 1.55136600	H 1.54139200 1.83079300 4.98255500
C -2.62188900 0.86739700 1.15538900	H 3.72627000 2.99500900 4.90429700
C 3.84968400 -1.33241700 0.30512500	C 0.66906100 3.65530600 -0.60965500
H 3.86485700 -2.42713900 0.24384900	C 0.08674500 4.63571400 0.19676100
H 3.36725800 -0.97286800 -0.61093200	C 1.02490900 3.98392900 -1.91604700
C 5.27775100 -0.80261900 0.37132200	C -0.12052500 5.91759200 -0.29034400
H 5.25526400 0.29368000 0.42707900	H -0.20134500 4.39896200 1.21535400
H 5.73815800 -1.14531100 1.30190900	C 0.81615600 5.26894100 -2.40376800
C 6.13303700 -1.22819500 -0.81760900	H 1.46477000 3.24134000 -2.57146000
H 5.66053900 -0.89340900 -1.75067200	C 0.24559600 6.23901900 -1.59236000
H 6.15858300 -2.32400200 -0.87030600	H -0.57031000 6.66849500 0.34974000
C 7.56227700 -0.69732400 -0.76369200	H 1.10002900 5.50868300 -3.42255600
H 7.53804100 0.39753100 -0.71164900	H 0.08250500 7.24102900 -1.97295400
H 8.03378700 -1.03219900 0.16719100	C -4.01010300 -0.94693800 -1.11825600
C 8.41305900 -1.13141400 -1.95103600	C -4.66411100 -1.95508700 -1.82834900
H 9.42961400 -0.73566000 -1.88330200	C -4.66218200 0.26852200 -0.92066700
H 8.48554200 -2.22145300 -2.00770900	C -5.93437000 -1.74447200 -2.34577300
H 7.98397500 -0.78162500 -2.89474200	H -4.19249400 -2.92038900 -1.97498300
O 3.69381700 -1.39018200 2.68094000	C -5.93822300 0.47629900 -1.42985800
H 3.01188800 -1.66135600 3.30249100	H -4.16898600 1.05952600 -0.36954400
Mn -1.43023200 0.33453100 -0.02826300	C -6.57446700 -0.52651100 -2.14783500
C -2.38628300 0.90702700 -1.37757500	H -6.42747700 -2.53505100 -2.90073600
O -3.05404000 1.31017800 -2.24307200	H -6.43026600 1.42900800 -1.26953100
	H -7.56755000 -0.36238900 -2.55109400
	C -1.66862200 1.52035300 -1.30131400
	O -2.14081300 2.17479500 -2.13104600
	Mn -0.91517600 0.53752800 -0.05328900
TS₂₋₃(3,4-H)-iPr	TS₂₋₃(3,4-H)-Ph
P 0.36903900 2.31858000 0.05608200	P -1.38961200 1.63432700 0.25530400
P -2.20830100 -1.48826500 -0.29846600	P 2.48677700 -0.71061400 0.39202100
C 1.21384600 2.08855200 -1.59212600	C -1.79206400 1.42524700 2.05704300
C -1.72387000 -1.84259300 -2.06041900	C 2.35425700 -1.14569200 2.18596500
H 2.14012800 1.54423300 -1.39986300	H -2.38702000 0.51296800 2.13930900

H	-0.88825800	-2.54268100	-1.99203900	H	1.74786200	-2.05468200	2.23615200
H	1.49166300	3.03446400	-2.06162100	H	-2.38254400	2.24481700	2.46981200
H	-2.52246300	-2.30564100	-2.64131000	H	3.31128800	-1.33950600	2.67201100
C	0.31308900	1.28076100	-2.50936700	N	0.33815100	0.22157800	2.13643000
C	-1.24055400	-0.56249900	-2.70988300	O	0.56408000	0.29897800	-2.86856600
H	0.86454200	0.97125300	-3.40765100	H	-0.39386700	-1.04119900	0.03151900
H	-0.78504500	-0.78332900	-3.68526600	H	-0.18892800	-0.68686500	2.18136600
H	-0.52528600	1.89735800	-2.84384800	C	-1.05849700	-2.28937200	0.77002900
H	-2.06622600	0.13293700	-2.88089700	O	-0.78254300	-2.18532900	2.00188200
N	-0.25962900	0.10361100	-1.83052000	C	0.55352500	0.36278700	-1.70919300
C	-1.89757500	-3.17236600	0.48321400	C	-2.50881200	-2.04712300	0.36270300
C	1.83958200	2.51789400	1.21488200	H	-2.85892500	-1.13553100	0.84909500
H	-0.81124600	-3.24680500	0.40043900	H	-2.59835200	-1.89077000	-0.71329400
H	2.27030200	1.51658200	1.17723400	C	-3.39879200	-3.21389700	0.80441200
C	-4.09917000	-1.41448100	-0.28438300	H	-3.24906300	-3.38259000	1.87569500
C	-0.32612900	4.07476300	-0.01283000	H	-3.08381800	-4.13436200	0.29940400
C	-4.72640500	-0.80133500	-1.53543000	C	-4.87786000	-2.97262600	0.52024700
C	-0.94366300	4.45154900	-1.35894600	H	-5.20018000	-2.05633900	1.02992400
O	-1.51328900	0.50528600	3.00083000	H	-5.01944600	-2.78476300	-0.55112400
H	0.54894500	4.71556300	0.13836000	C	-5.77404700	-4.12981400	0.95137200
H	-4.40236000	-2.46563100	-0.25179600	H	-5.45410500	-5.04407300	0.43795900
C	-1.31652800	4.34348400	1.12245700	H	-5.62823800	-4.31851400	2.02124200
C	-4.63077800	-0.73510400	0.97894800	C	-7.25206700	-3.88245500	0.67461200
H	-0.92792100	4.06066400	2.10028900	H	-7.86746800	-4.72776900	0.99300600
H	-4.19077800	-1.13909200	1.89099800	H	-7.60999200	-2.99436300	1.20365800
H	-2.25106500	3.80551500	0.96764900	H	-7.43342700	-3.72397500	-0.39249000
H	-4.43971700	0.33751900	0.96562100	C	-0.33546600	-3.38466500	-0.01362200
H	-1.55205500	5.41181300	1.15570900	H	0.73024400	-3.30426800	0.19846700
H	-5.71435800	-0.87666300	1.04226300	H	-0.65969500	-4.32329300	0.45374300
C	-2.30114000	-3.22389000	1.95472900	C	-0.58203600	-3.44417100	-1.51211000
C	1.44192600	2.79169600	2.66397200	H	0.04655200	-4.20956200	-1.97251100
H	-3.38762300	-3.26137900	2.06838200	H	-1.62065500	-3.69031600	-1.74603000
H	1.09707500	3.81933700	2.79916400	H	-0.34733500	-2.49051500	-1.98921100
H	-1.93532700	-2.36684500	2.52305600	C	1.59638100	-0.01616700	2.86308700
H	0.66162700	2.11746700	3.01753500	H	2.18071700	0.90901500	2.86513600
H	-1.89891700	-4.12903700	2.41933900	H	1.38675000	-0.28148300	3.90796900
H	2.31364300	2.66061400	3.31217900	C	-0.48051900	1.24535400	2.80388100
C	-2.49579300	-4.35282800	-0.28089000	H	-0.67932800	0.95531100	3.84447500
C	2.90087600	3.51191600	0.74713800	H	0.08760800	2.18012200	2.82547100
H	-2.17463500	-4.38464800	-1.32289400	C	-2.98109800	1.31214800	-0.62619400
H	3.24941800	3.31490800	-0.26821900	C	-4.19338500	1.78234400	-0.11773600
H	-3.58884500	-4.35428200	-0.25987600	C	-2.97117800	0.65751800	-1.85547800
H	2.54318100	4.54396500	0.78803800	C	-5.37438400	1.58574800	-0.81893900
H	-2.16838600	-5.28663900	0.18680500	H	-4.22070900	2.31415000	0.82701200
H	3.77196400	3.45228200	1.40694000	C	-4.15271200	0.47472900	-2.56505800
H	0.53148600	-0.41758800	0.55661800	H	-2.03851200	0.28238500	-2.25772900
H	0.47439500	-0.60315900	-1.64152800	C	-5.35564000	0.93354000	-2.04684900
C	1.50227600	-1.59163300	0.29633800	H	-6.31074500	1.94926400	-0.41000100
H	-5.81653600	-0.85612500	-1.45353700	H	-4.13005600	-0.03331800	-3.52281500
H	-4.46537300	0.25041200	-1.65175100	H	-6.27792800	0.78615200	-2.59776700
H	-4.44656800	-1.33211400	-2.44715500	C	-1.28718100	3.46712000	0.00134600
H	-1.27642200	5.49347300	-1.32231900	C	-1.18189000	3.93885700	-1.30908700
H	-0.23471300	4.37120900	-2.18507100	C	-1.26814800	4.38751200	1.04641900
H	-1.81833500	3.84261600	-1.58908200	C	-1.07347800	5.29683200	-1.56593000
O	1.13714600	-2.15565300	-0.77525600	H	-1.18710300	3.23985700	-2.13869800
C	-1.30114000	0.49927100	1.86210400	C	-1.15567000	5.74976600	0.78920000
C	1.25927300	-2.29462100	1.64859900	H	-1.33556300	4.05753700	2.07618300

H	0.19890100	-2.25420800	1.88199700	C	-1.06081600	6.20832400	-0.51624100
C	2.82945500	-0.82119700	0.22675700	H	-0.99540400	5.64466800	-2.59003900
H	2.76129300	-0.09587800	-0.58667400	H	-1.14146400	6.45185400	1.61572900
H	3.00889200	-0.27259600	1.15518300	H	-0.97292400	7.27022300	-0.71663000
C	4.02294600	-1.73525300	-0.06626000	C	4.06300500	0.25568000	0.23800400
H	4.20142100	-2.40230900	0.78280500	C	4.92133200	0.50572100	1.30598200
H	3.77081000	-2.37237600	-0.91910800	C	4.39841400	0.75745900	-1.02131800
C	5.30186900	-0.95617000	-0.35876000	C	6.09108700	1.23484300	1.11989800
H	5.13656300	-0.30035100	-1.22322600	H	4.69136600	0.13893800	2.29893100
H	5.53022800	-0.29221600	0.48491100	C	5.56879400	1.47617100	-1.20955900
C	6.50838900	-1.84915100	-0.63258200	H	3.73633600	0.59259600	-1.86448400
H	6.67798400	-2.50001400	0.23289700	C	6.42012100	1.71838700	-0.13776400
H	6.27806500	-2.51636500	-1.47095600	H	6.74533200	1.42276200	1.96430600
C	7.78001100	-1.06676400	-0.93737400	H	5.81228400	1.85631900	-2.19543800
H	8.62521100	-1.73302400	-1.12733300	H	7.33270900	2.28554900	-0.28294200
H	7.65303900	-0.43366200	-1.82044000	C	3.03752000	-2.27116300	-0.43424600
H	8.05356500	-0.41505900	-0.10239600	C	2.82208500	-2.43236300	-1.80262500
H	1.76254200	-1.72997200	2.43883800	C	3.73874000	-3.25847500	0.25967300
C	1.71771100	-3.75199700	1.65263000	C	3.30221600	-3.55580100	-2.46394900
H	2.80027600	-3.84997800	1.55704700	H	2.26939800	-1.68405100	-2.35737100
H	1.42340600	-4.24000800	2.58560100	C	4.20567000	-4.38742800	-0.39972800
H	1.26743900	-4.29760400	0.82093500	H	3.92547300	-3.15498800	1.32208500
Mn	-0.95601700	0.45034000	0.13297500	C	3.99162800	-4.53721100	-1.76444500
C	-2.35279600	1.41583800	-0.28791900	H	3.12735200	-3.66624800	-3.52842500
O	-3.26973800	2.08805900	-0.54101600	H	4.74214100	-5.14984800	0.15441400
				H	4.36061700	-5.41692800	-2.27994300
				C	1.44441100	1.95976000	0.08478000
				O	2.02779700	2.95702100	0.08777900
				Mn	0.53515500	0.44196000	0.04750900

Table S5. Computed Energetic Data for All Optimized Structures

C₅H₁₁CHOHCH=CH₂ HF= -389.680399 ZPE= 0.226459 NImag= 0 Htot = -389.441216 Gtot = -389.492268	C₅H₁₁COCH=CH₂ HF= -388.476190 ZPE= 0.203059 NImag= 0 Htot = -388.260985 Gtot = -388.31121
C₅H₁₁COC₂H₅ HF= -389.715165 ZPE= 0.226005 NImag= 0 Htot = -389.477144 Gtot = -389.52683	C₅H₁₁CHOHC₂H₅ HF= -390.921835 ZPE= 0.2501 NImag= 0 Htot = -390.658582 Gtot = -390.710348
C₅H₁₁C(OH)=CHCH₃ HF= -389.696458 ZPE= 0.22649 NImag= 0 Htot = -389.457083 Gtot = -389.508978	H₂ HF= -1.178636 ZPE= 0.010066 NImag= 0 Htot = -1.165265 Gtot = -1.180063
<i>i</i>PrOH HF= -194.360750 ZPE= 0.107927 NImag= 0 Htot = -194.246425 Gtot = -194.280211	CH₃COCH₃ HF= -193.152623 ZPE= 0.083336 NImag= 0 Htot = -193.063758 Gtot = -193.096232
1M-<i>i</i>Pr HF= -1699.453006 ZPE= 0.518844 NImag= 0 Htot = -1698.901598 Gtot = -1698.994510	1M-Ph HF= -2151.821244 ZPE= 0.504289 NImag= 0 Htot = -2151.282227 Gtot = -2151.387599
2M-<i>i</i>Pr HF= -1700.652679 ZPE= 0.539668 NImag= 0 Htot = -1700.080142 Gtot = -1700.174062	2M-Ph HF= -2153.024518 ZPE= 0.525246 NImag= 0 Htot = -2152.464306 Gtot = -2152.568924
TS₁₋₄(3,4-H⁻)-<i>i</i>Pr HF= -2089.106108 ZPE= 0.744077 NImag= 1(-520.5498) Htot = -2088.317552 Gtot = -2088.437778 E(strain/sub) = -389.457658 E(strain/cat) = -1699.420275	TS₁₋₄(3,4-H⁻)-Ph HF= -2541.479601 ZPE= 0.728434 NImag= 1(-443.8322) Htot = -2540.704374 Gtot = -2540.835086 E(strain/sub) = -389.4828634 E(strain/cat) = -2151.794057
TS₄₋₂(1,2-H⁻)_1,2-addition: H⁻ transfer to C₁-<i>i</i>Pr HF= -2089.120876 ZPE= 0.743426 NImag= 1(-280.8458)	TS₄₋₂(1,2-H⁻)_1,2-addition: H⁻ transfer to C₁-Ph HF= -2541.492392 ZPE= 0.72907 NImag= 1(-286.5826)

Htot = -2088.332491 Gtot = -2088.456246	Htot = -2540.716322 Gtot = -2540.849672
Interm(1,2)-iPr HF= -2089.137764 ZPE= 0.746837 NImag= 0 Htot = -2088.345715 Gtot = -2088.468016	Interm(1,2)-Ph HF= -2541.506847 ZPE= 0.732295 NImag= 0 Htot = -2540.727424 Gtot = -2540.859043
TS2(1,2-H⁺)_1,2-addition: H⁺ transfer to C₁-iPr HF= -2089.130009 ZPE= 0.742122 NImag= 1(-1166.4034) Htot = -2088.342841 Gtot = -2088.465427	TS2(1,2-H⁺)_1,2-addition: H⁺ transfer to C₁-Ph HF= -2541.500565 ZPE= 0.727518 NImag= 1(-1144.3631) Htot = -2540.72602 Gtot = -2540.858037
TS₄₋₂(1,4-H⁻)_1,4-addition: H⁻ transfer to C₁-iPr HF= -2089.121894 ZPE= 0.744097 NImag= 1(-266.9345) Htot = -2088.333033 Gtot = -2088.455664	TS₄₋₂(1,4-H⁻)_1,4-addition: H⁻ transfer to C₁-Ph HF= -2541.494581 ZPE= 0.728845 NImag= 1(-327.1052) Htot = -2540.718671 Gtot = -2540.852566
Interm(1,4)-iPr HF= -2089.141476 ZPE= 0.747638 NImag= 0 Htot = -2088.348871 Gtot = -2088.469959	Interm(1,4)-Ph HF= -2541.508163 ZPE= 0.732058 NImag= 0 Htot = -2540.728803 Gtot = -2540.862149
TS2(1,4-H⁺)_1,4-addition: H⁺ transfer to C₁-iPr HF= -2089.135692 ZPE= 0.742826 NImag= 1(-865.8345) Htot = -2088.347874 Gtot = -2088.46969	TS2(1,4-H⁺)_1,4-addition: H⁺ transfer to C₁-Ph HF= -2541.505551 ZPE= 0.728171 NImag= 1(-904.1865) Htot = -2540.730326 Gtot = -2540.862644
TS₁₋₃(1,2-H⁻)_1,2-addition: H⁻ transfer to C₁-iPr HF= -2090.302907 ZPE= 0.765585 NImag= 1(-242.4623) Htot = -2089.491741 Gtot = -2089.61564	TS₁₋₃(1,2-H⁻)_1,2-addition: H⁻ transfer to C₁-Ph HF= -2542.675384 ZPE= 0.750558 NImag= 1(-169.243) Htot = -2541.877189 Gtot = -2542.01151
TS₂₋₃(3,4-H⁻)-iPr HF= -2090.338713 ZPE= 0.767823 NImag= 1(-431.8926) Htot = -2089.525704 Gtot = -2089.646889	TS₂₋₃(3,4-H⁻)-Ph HF= -2542.717581 ZPE= 0.752253 NImag= 1(-435.9) Htot = -2541.918125 Gtot = -2542.049229

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