

Computational investigation of ligand effect on regioselectivity and reactivity of cobalt-catalysed hydroformylation

Pan Li,^a Chaoren Shen,^{*b} Jie Min,^a Jing-Yuan Mei,^a Huan Zheng,^{bc} Lin He,^b and Xinxin Tian^{*a}

^aInstitute of Molecular Science, Key Laboratory of Materials for Energy Conversion and Storage of Shanxi Province, Shanxi University, Taiyuan 030006 (P. R. China) E-mail: tianxx@sxu.edu.cn

^bState Key Laboratory for Oxo Synthesis and Selective Oxidation, Suzhou Research Institute of LICI, Lanzhou Institute of Chemical Physics (LICP), Chinese Academy of Sciences, Lanzhou 730000 (P. R. China) E-mail: shenchaoren@licp.cas.cn; shenchaoren@gmail.com

^c University of Chinese Academy of Sciences, Beijing 100039 (P. R. China)

Table of contents

Table S1 Reaction free energies for the coordination of HCo(CO) ₃ or HCo(CO) ₂ L with different alkene substrates	S3
Table S2 Free energy change for the conversion from HCo(CO) ₄ to HCo(CO) ₃ L via ligand exchange on equatorial site	S4
Table S3 Free energy change for the dissociation of equatorial carbonyl ligand in HCo(CO) ₃ L.	S4
Table S4 Relative free energies and enthalpies between the axial substitution and the equatorial substitution of phosphine ligand	S5
Table S5 Free energy changes of each step during the transformation from g or h to [Co]-H ₂ -a-ma or [Co]-H ₂ -a-(anti-ma)	S5
Table S6 Detailed relative free energies of each intermediate during hydrogen splitting and reductive elimination	S6
Table S7 Propene hydrogenation by unmodified or PBu ₃ -modified cobalt carbonyl catalyst	S6
Table S8 Reaction free energies (ΔG _R) for the coordination of HCo(CO) ₃ or HCo(CO) ₂ (PBu ₃) with <i>n</i> -PrCHO	S7
Figure S1 PES for Markovnikov/anti-Markovnikov propene hydroformylation pathway from a to k/l on unmodified cobalt carbonyl catalyst, transformation from propene to <i>n</i> -propane and H ₂ /CO additions along anti-Markovnikov pathway	S8
Figure S2 PES for Markovnikov and anti-Markovnikov isobutene hydroformylation pathway from a to i and j on unmodified cobalt carbonyl catalyst.	S9
Figure S3 PES for Markovnikov and anti-Markovnikov type propene hydroformylation processes and propene hydrogenation to <i>n</i> -propane by PBu ₃ -modified cobalt carbonyl catalyst and the formation of off-cycle species (η ¹ - <i>n</i> -C ₃ H ₇ CO)Co(CO) ₃ (PBu ₃) on anti-Markovnikov pathway	S10
Figure S4 PES for <i>n</i> -butyraldehyde hydrogenation to <i>n</i> -butanol and carbonylative reduction to <i>n</i> -butyl formate by unmodified cobalt carbonyl catalyst	S11
Figure S5 PES for <i>n</i> -butyraldehyde hydrogenation to <i>n</i> -butanol and carbonylative	

reduction to n-butyl formate by PBU_3 -modified cobalt carbonyl catalyst S12

Cartesian coordinates of all structures

1 Structures in Table 1	S13
2 Structures in Table 2	S27
3 Structures in Table 3	S51
4 Structures in Table 4	S126
5 Structures in Table 5	S130
6 Structures in Figure 6	S172
7 Structures in Figure S5	S184
8 Structures in Figure S6	S200
9 Structures in Table S1	S237
10 Structures in Table S2	S240
11 Structures in Table S4	S245
12 Structures in Figure S1	S271
13 Structures in Figure S2	S276

Table S1 Reaction free energies (ΔG_R) for the coordination of $\text{HCo}(\text{CO})_3$ or $\text{HCo}(\text{CO})_2\text{L}$ with different alkene substrates

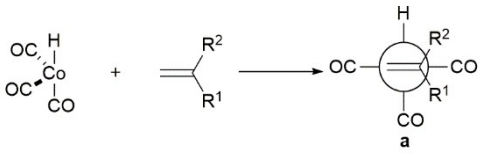
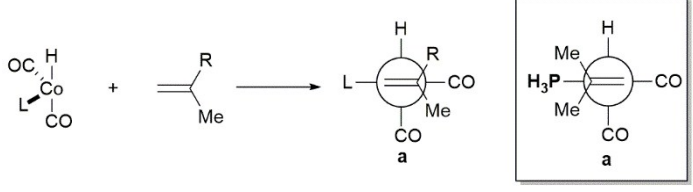
			
entry	L	R ¹ /R ²	ΔG_R
1	CO	CH ₃ /H	-3.3
2	CO	2,4-dimethylpentyl/H	-18.8
3	CO	CH ₃ /CH ₃	-1.4
4	CO	CH ₃ /CH ₂ C(CH ₃) ₂	-15.5
			
entry	L	R	ΔG_R
5	PH ₃	H	-2.7
6	PMe ₃	H	-1.8
7	PBu ₃	H	-1.7
8	a ₅ -PhobPC ₅	H	1.1
9	PH ₃	Me	-0.6
10	PMe ₃	Me	1.0
11	PBu ₃	Me	-1.1

Table S2 Free energy change for the conversion from $\text{HCo}(\text{CO})_4$ to $\text{HCo}(\text{CO})_3\text{L}$ via ligand exchange on equatorial site.

Entry	L	$\text{L} + \text{HCo}(\text{CO})_4 \rightarrow \text{HCo}(\text{CO})_3\text{L} + \text{CO}$	ΔG_R
1	PH_3		4.6
2	PMe_3		-4.1
3	PBu_3		-7.4
4	$\text{a}_5\text{-PhobPC}_5$		-3.0

Table S3 Free energy change for the dissociation of equatorial carbonyl ligand in $\text{HCo}(\text{CO})_3\text{L}$.

Entry	L	$\text{HCo}(\text{CO})_3\text{L} \rightarrow \text{HCo}(\text{CO})_2\text{L} + \text{CO}$	ΔG_R
1	CO		13.4
2	PH_3		15.0
3	PMe_3		15.0
4	PBu_3		16.3
5	$\text{a}_5\text{-PhobPC}_5$		11.2

Table S4 Relative free energies ($\Delta G = G(a) - G(e)$, kcal/mol) and enthalpies ($\Delta H = H(a) - H(e)$, kcal/mol) between the axial substitution (a) and the equatorial substitution (e) of monophosphine ligands in phosphine-modified cobalt carbonyl complexes.

entry	equatorial (e)	axial (a)	ΔG	ΔH
1			2.3	2.1
2			2.6	3.0
3			2.2	3.2
4			0.4	1.7

Table S5 Free energy changes (kcal/mol) of each step during the transformation from **g** or **h** to **[Co]-H₂-a-ma** or **[Co]-H₂-a-(anti-ma)**

ΔG_A (CO addition)	ΔG_R (CO addition)	ΔG_A (insertion)	ΔG_R (insertion)	ΔG_A (acyl-iso)	ΔG_R (acyl-iso)	ΔG_A (H ₂ addition)	ΔG_R (H ₂ addition)
10.1	-12.9	10.4	4.0	11.0	-2.7	10.1	9.5
ΔG_A (CO addition)	ΔG_R (CO addition)	ΔG_A (insertion)	ΔG_R (insertion)	ΔG_A (acyl-iso)	ΔG_R (acyl-iso)	ΔG_A (H ₂ addition)	ΔG_R (H ₂ addition)
8.6	-13.6	10.8	5.4	12.7	-1.5	9.4	8.3

Table S6 Detailed relative free energies (kcal/mol) of each intermediate during hydrogen splitting and reductive elimination

Reaction scheme showing the conversion of $[\text{Co}]\text{-H}_2\text{-a}$ (0.0 kcal/mol) to $[\text{Co}]\text{-H}_2\text{-b}$ via $\text{TS}_{\text{rotate}}$, then to $[\text{Co}]\text{-2H}$ via $\text{TS}_{\text{splitting}}$, and finally to $[\text{Co}]\text{-aldehyde}$ via $\text{TS}_{\text{eliminate}}$.

Entry	L	$\text{TS}_{\text{acyl-rotate}}$	$[\text{Co}]\text{-H}_2\text{-b}$	$\text{TS}_{\text{splitting}}$	$[\text{Co}]\text{-2H}$	$\text{TS}_{\text{eliminate}}$	$[\text{Co}]\text{-aldehyde}$
1	CO	5.8	1.6	9.8	9.0	11.0	-5.3
2	PH_3	6.7	3.2	8.3	7.2	9.8	-2.7
3	PMe_3	6.1	1.7	8.0	6.7	10.3	-4.2
4	PBu_3	7.4	3.0	8.5	6.6	9.8	-5.0
5	$\text{a}_5\text{-PhobPC}_5$	6.9	2.3	7.5	6.0	8.9	-7.8
6	$\text{PBu}_3^{[\text{a}]}$	6.7	3.0	7.4	5.9	9.7	-11.0

^[a] $i\text{-C}_3\text{H}_7$ instead of $n\text{-C}_3\text{H}_7$

Table S7 Propene hydrogenation by unmodified or PBu_3 -modified cobalt carbonyl catalyst.

on unmodified cobalt carbonyl catalyst			
$\text{f} \rightarrow \text{o}$		$\text{o} \rightarrow [\text{Co}]\text{-H}_2\text{-alkane}$	
ΔG_{A}	ΔG_{R}	ΔG_{A}	ΔG_{R}
2.9	1.0	-	7.5
$[\text{Co}]\text{-H}_2\text{-alkane} \rightarrow [\text{Co}]\text{-2H-alkane}$		$[\text{Co}]\text{-2H-alkane} \rightarrow [\text{Co}]\text{-alkane}$	
ΔG_{A}	ΔG_{R}	ΔG_{A}	ΔG_{R}
9.1	8.6	5.1	-28.3
on PBu_3 -modified cobalt carbonyl catalyst			
$\text{h} \rightarrow [\text{Co}]\text{-H}_2\text{-alkane}$		$[\text{Co}]\text{-H}_2\text{-alkane} \rightarrow [\text{Co}]\text{-2H-alkane}$	
ΔG_{A}	ΔG_{R}	ΔG_{A}	ΔG_{R}
7.7	6.8	5.8	8.0
$[\text{Co}]\text{-2H-alkane} \rightarrow [\text{Co}]\text{-alkane}$			
ΔG_{A}		ΔG_{R}	
6.5		-28.5	

Table S8 Reaction free energies (ΔG_R) for the coordination of $\text{HCo}(\text{CO})_3$ or $\text{HCo}(\text{CO})_2(\text{PBU}_3)$ with $n\text{-PrCHO}$

entry	$\text{HCo}(\text{CO})_3 + n\text{-PrCHO} \rightarrow \text{HCo}(\text{CO})_2\text{L} + \text{CO}$	ΔG_R
1		7.0
2		6.2
3		6.5
4		7.1
5		5.1
6		5.5

Figure S1 Potential energy surface for Markovnikov/anti-Markovnikov propene hydroformylation pathway from **a** to **k/l** on unmodified cobalt carbonyl catalyst, transformation from propene to propane and H₂/CO additions along anti-Markovnikov pathway (Unit: kcal/mol).

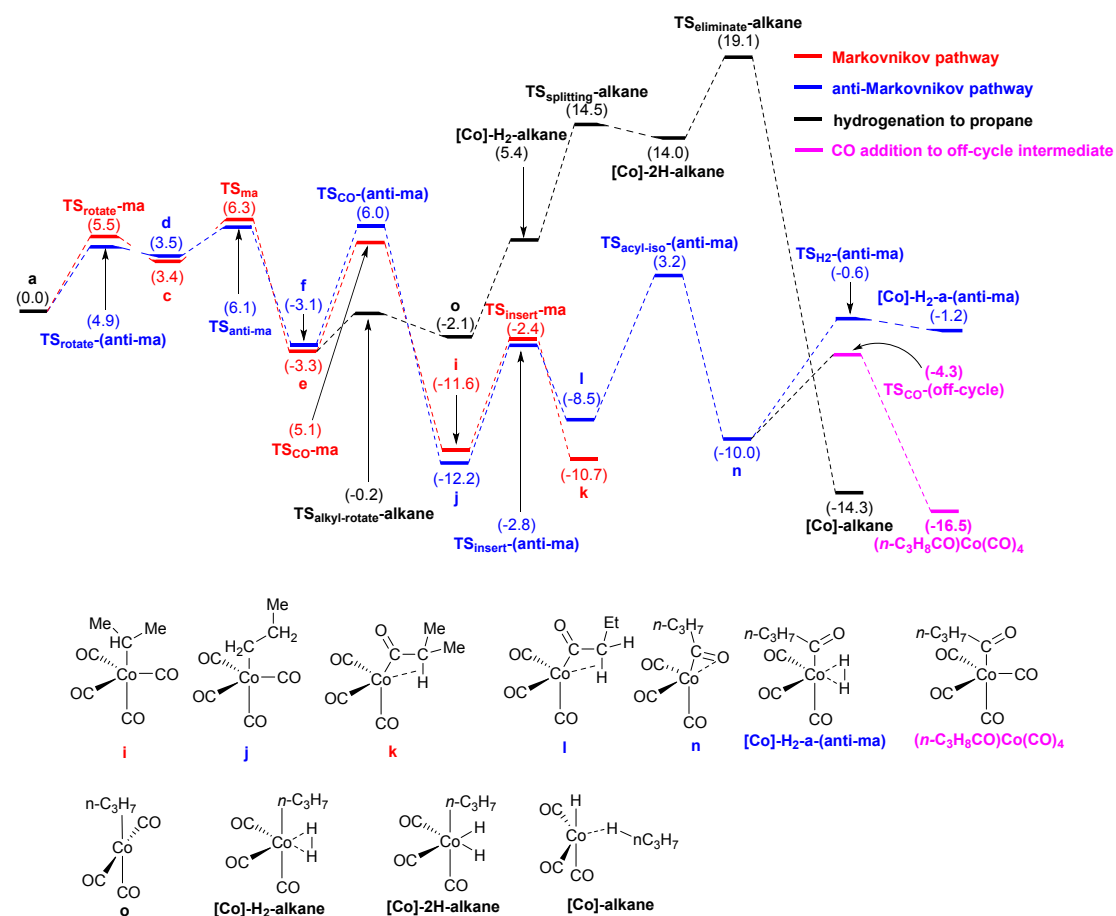


Figure S2 Potential energy surface for Markovnikov and anti-Markovnikov isobutene hydroformylation pathway from **a** to **i/j** on unmodified cobalt carbonyl catalyst (Unit: kcal/mol).

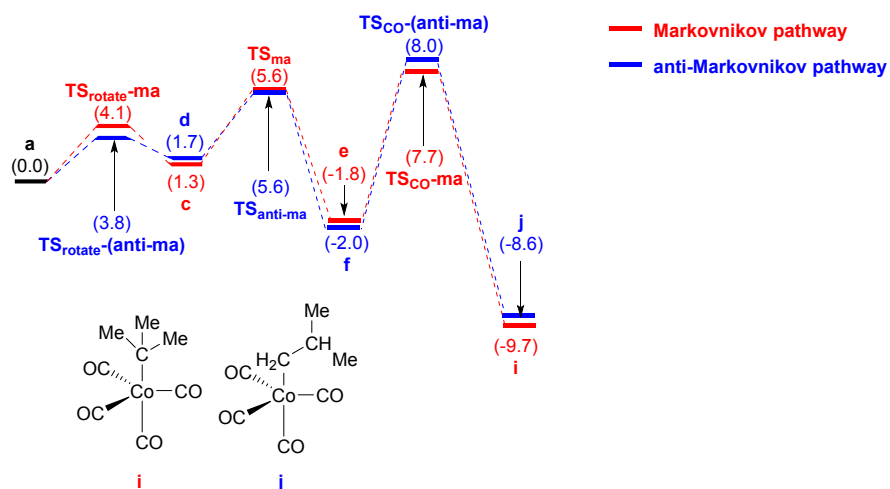


Figure S3 Potential energy surface for Markovnikov and anti-Markovnikov type propene hydroformylation pro, propene hydrogenation propane by PBU_3 -modified cobalt carbonyl catalyst and the formation of off-cycle species (η^1 - $n\text{-C}_3\text{H}_7\text{CO}$) $\text{Co}(\text{CO})_3(\text{PBU}_3)$ on anti-Markovnikov pathway.

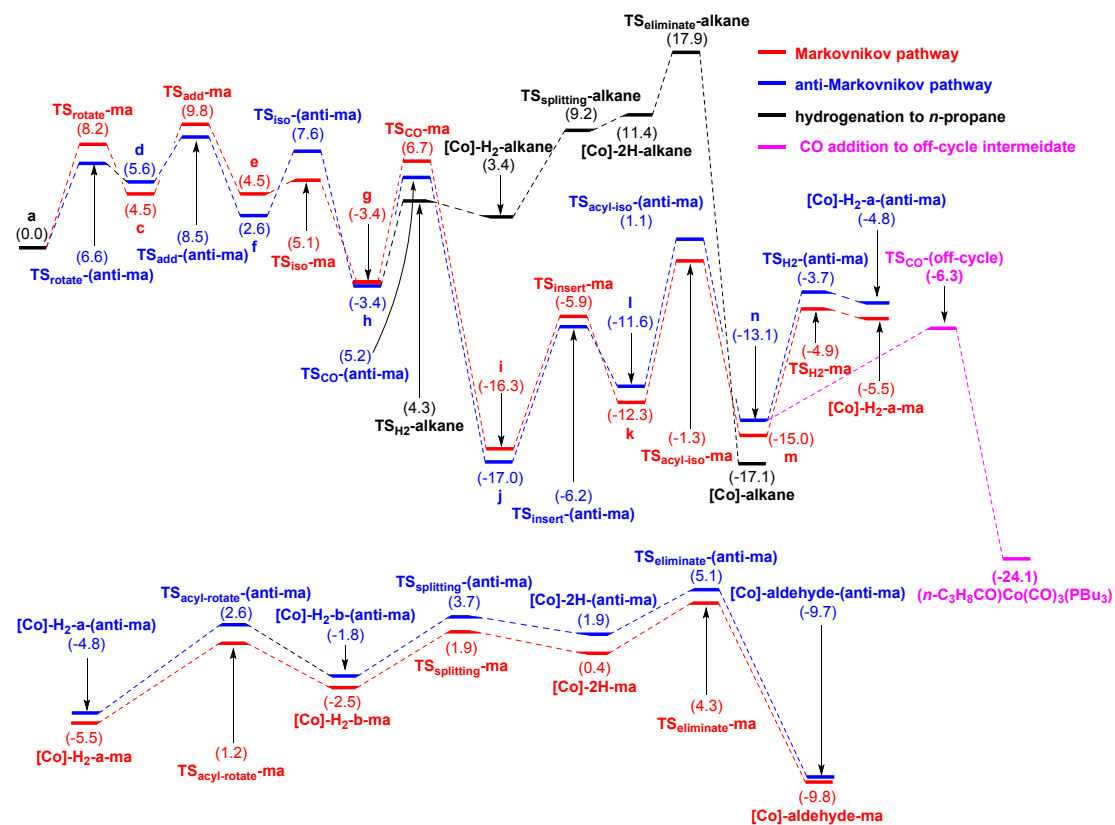


Figure S4 Potential energy surface for *n*-butyraldehyde hydrogenation to *n*-butanol and carbonylative reduction to *n*-butyl formate by unmodified cobalt carbonyl catalyst.

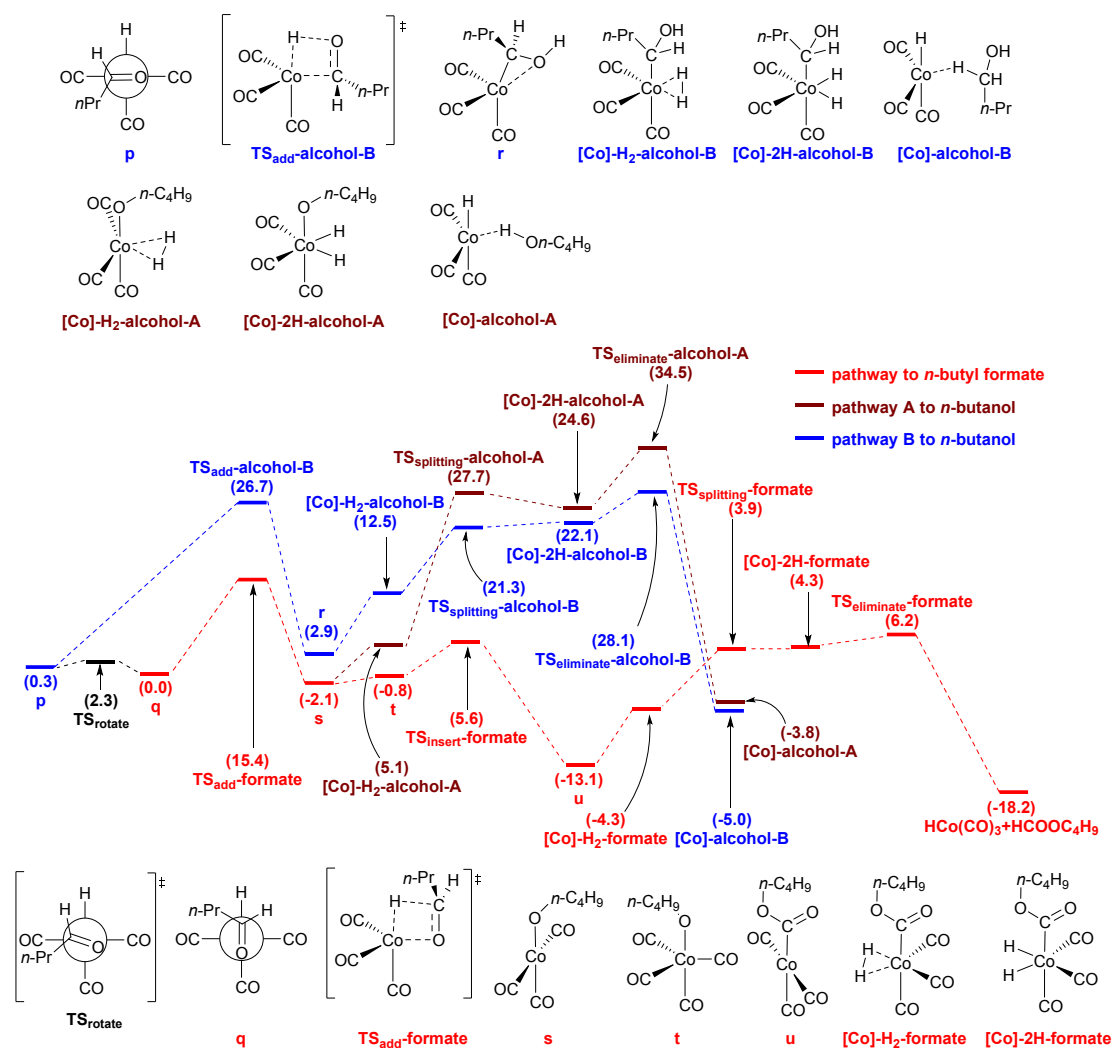
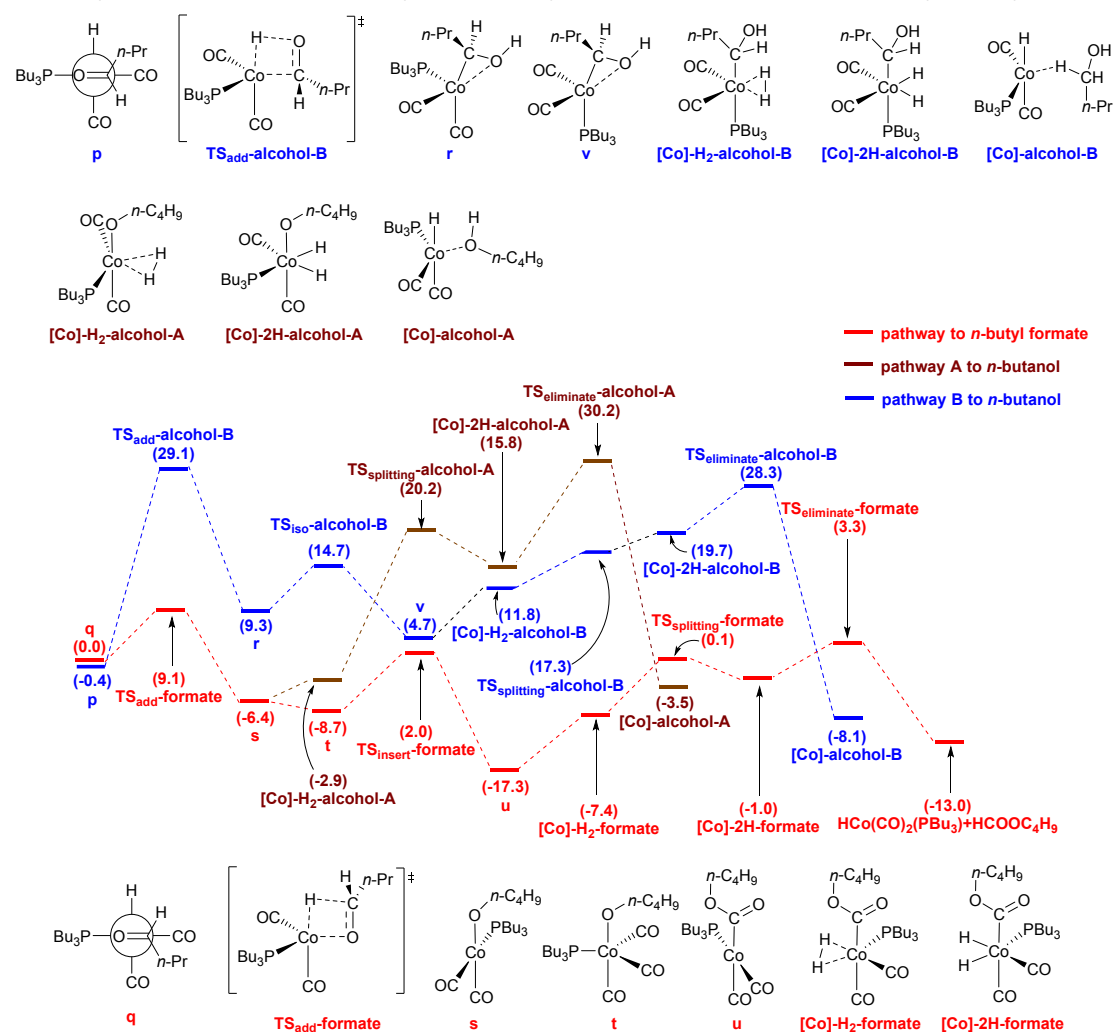


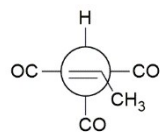
Figure S5 Potential energy surface for n-butyraldehyde hydrogenation to n-butanol and carbonylative reduction to n-butyl formate by PBU₃-modified cobalt carbonyl catalyst.



Cartesian coordinates of all structures

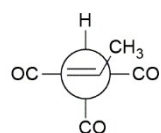
1. Structures in Table 1

a in entry 1



C	1.65892679	-0.53234159	-0.57011089
H	1.70829816	-1.46949584	-1.08411904
O	-0.64383177	1.18408215	-2.86005706
O	-1.64173056	0.76457960	2.29982515
C	-1.06327978	0.46613184	1.35773453
C	-0.44773022	0.72427575	-1.82989180
H	0.06828838	1.57634452	-0.00725144
Co	-0.21762557	0.11779164	-0.16944986
C	-0.90073487	-1.52807755	-0.42549961
O	-1.36633620	-2.55737438	-0.59356961
H	2.34365356	0.23293114	-0.87078831
H	2.00831929	0.08172044	1.36356339
C	1.46583578	-0.62892026	0.77568463
C	1.32879639	-2.06538974	1.31362110
H	1.29195962	-2.75143604	0.49332633
H	2.16978115	-2.29575854	1.93376209
H	0.42943271	-2.14704065	1.88753582

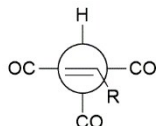
b in entry 1



C	-1.52910300	-0.95383800	0.64556600
H	-1.66595200	-0.52327100	1.63923100
O	-1.15568900	2.48697200	-0.96844500
O	2.65146400	-0.81893300	-1.52147400
C	1.72457600	-0.48056900	-0.95120900
C	-0.60226300	1.55554700	-0.61337500
H	-0.30657400	-0.34041200	-1.49752000
Co	0.20978200	0.03366100	-0.14964200
C	0.88208000	0.52584500	1.45468400
O	1.30469700	0.83422700	2.46493300
H	-0.50796500	-2.53825400	-0.37663300
C	-0.50138900	-1.86084400	0.47510700
C	-2.72965800	-0.89846100	-0.24593400
H	-3.11032500	0.11927000	-0.38160400

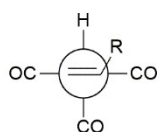
H	-2.51395000	-1.31241300	-1.23657700
H	-3.54712500	-1.48752500	0.19179700
H	0.11853700	-2.17044800	1.31247600

a in entry 2



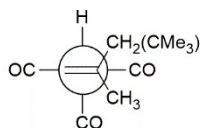
C	-0.94261600	-0.88570500	-1.39559200
H	-0.63157500	-1.85169500	-0.99759900
O	-4.78427400	-1.32384600	-0.89042900
O	-2.44044300	2.72778200	1.05948200
C	-2.39436000	1.66519200	0.64816900
C	-3.81916500	-0.82356100	-0.54671600
H	-2.77025800	0.83735200	-1.26852500
Co	-2.32391800	0.04149500	-0.09140200
C	-1.88685000	-0.93440300	1.36641900
O	-1.64050000	-1.55539900	2.28786300
H	-1.41657100	-0.91571100	-2.37222000
H	-0.44869800	1.17153900	-1.52661100
C	-0.36484000	0.27415700	-0.91331600
C	0.75266800	0.27089100	0.08821100
H	0.66165900	-0.61197300	0.73850600
H	0.68396800	1.14982800	0.74931500
C	2.14421000	0.25207100	-0.55738400
C	2.40779100	1.52252500	-1.34927700
C	3.18949200	0.04036400	0.53400200
H	2.16881100	-0.60869500	-1.24721600
H	1.65143500	1.69435400	-2.12241000
H	2.40755700	2.39805100	-0.68424000
H	3.37786500	1.49841200	-1.85664300
H	2.94877400	-0.88884700	1.07894300
H	3.08637900	0.85232800	1.27450500
C	4.64791800	-0.03708200	0.09325500
C	5.53729500	-0.25206600	1.30749700
C	4.87671300	-1.14119400	-0.92640400
H	4.93039000	0.92555500	-0.36322900
H	5.39628100	0.53273500	2.06019000
H	5.31119900	-1.21353300	1.78912400
H	6.59883400	-0.26532500	1.03421700
H	4.33697200	-0.97128600	-1.86469300
H	5.93996900	-1.23860900	-1.17524100
H	4.54498900	-2.11026600	-0.52683700

b in entry 2



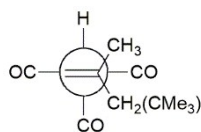
C	-0.86127700	-1.14484600	1.04245200
H	-1.36232700	-1.32764800	1.98955500
O	-3.99317500	-2.35098900	-0.88894900
O	-1.91648800	2.10532500	-2.06826200
C	-2.06950700	1.26231600	-1.31575800
C	-3.33216600	-1.47239400	-0.58760900
H	-1.49963000	-0.76588300	-1.33387000
Co	-2.22360700	-0.12546900	-0.20382700
C	-3.16878200	0.65581900	1.12649100
O	-3.76728800	1.14842700	1.95950600
H	-0.49331900	-2.03396200	0.53236700
C	-0.32004000	0.09284800	0.74229700
H	-0.45932400	0.89590900	1.46814700
C	0.84016000	0.26047500	-0.19553100
C	2.20126700	0.12962100	0.49901400
H	0.79532700	1.23963700	-0.69827200
H	2.20551000	-0.84180100	1.02220200
C	3.29636700	0.12219600	-0.56344400
C	4.73429900	-0.03227000	-0.07768300
H	3.08903300	-0.69239900	-1.27875800
H	4.98696600	0.83194700	0.55806900
H	0.77358100	-0.49573200	-0.99090900
C	5.67933100	-0.02229200	-1.26866000
H	5.56327100	0.88503300	-1.87336100
H	6.72780500	-0.08176500	-0.95404600
H	5.48536100	-0.88168200	-1.92546600
C	2.41507000	1.23586500	1.51953800
H	2.43017200	2.21797400	1.02538400
H	1.62454500	1.25874200	2.27734100
H	3.36332500	1.12614500	2.05611000
H	3.21859100	1.05532800	-1.14772500
C	4.92788700	-1.30266900	0.73462400
H	4.62290300	-2.18355700	0.15166600
H	5.97999500	-1.44255600	1.00933900
H	4.34557400	-1.30617900	1.66281100

a in entry 3



Co	-1.49953600	0.17935800	0.20059700
H	-0.86587500	1.20492600	1.07617200
C	-2.61877000	1.55214700	0.05674600
C	-1.21401700	-0.79262200	1.66333800
C	-2.44501600	-1.01236500	-0.76430200
O	-3.07281300	-1.75303700	-1.36033100
O	-0.98159100	-1.36747900	2.62223900
O	-3.30222500	2.46583400	0.02670600
C	-0.09194800	0.70227500	-1.33857500
C	0.58245800	-0.23643900	-0.58888300
C	0.64986000	-1.66638500	-1.04803800
H	1.55031500	-1.82899100	-1.65307900
C	1.59729200	0.20421800	0.44233100
H	1.53230000	-0.43788500	1.33464000
H	1.31963400	1.21245400	0.77717400
H	-0.20054400	-1.94628000	-1.67582000
H	0.70349700	-2.36731700	-0.20605400
H	-0.55440000	0.42638300	-2.28460500
H	0.11552700	1.76186100	-1.20901000
C	3.08613300	0.25914900	0.01853700
C	3.73700600	-1.12106400	-0.02684600
C	3.25432600	0.96043100	-1.32218600
C	3.80725700	1.07081500	1.09347900
H	3.57811000	-1.66734700	0.91194000
H	3.36711500	-1.74835700	-0.84270800
H	4.82092900	-1.02406300	-0.16858300
H	2.82363500	1.96998200	-1.30246700
H	4.31779200	1.06158800	-1.57333700
H	2.77322200	0.41423700	-2.14255700
H	4.88279500	1.13042400	0.88545800
H	3.42228900	2.09662600	1.14912800
H	3.68667900	0.61560600	2.08507000

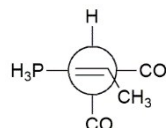
b in entry 3



Co	-1.58985100	0.10226000	-0.01133300
H	-1.94602900	1.31354300	-0.80270900

C	-3.08368000	-0.40146200	-0.83062800
C	-1.44247800	1.35726100	1.24190200
C	-1.36943200	-1.36531800	1.01138800
O	-1.27311000	-2.29218700	1.66670100
O	-1.33973000	2.21306500	1.99085600
O	-4.05562900	-0.64928100	-1.37540900
C	-0.16596100	-0.38066300	-1.54887700
C	0.54712100	0.42650500	-0.68988100
C	1.47644700	-0.18241100	0.33567200
C	0.74395700	1.88046500	-1.02020700
H	0.87247000	2.49711100	-0.12272500
H	1.64869500	2.00981500	-1.62734700
H	-0.09066200	2.28561900	-1.59760100
H	1.14181400	-1.21002900	0.53330600
H	1.38525400	0.35746600	1.29197200
H	-0.04084900	-1.46139100	-1.52264000
H	-0.57475800	0.02296400	-2.47254800
C	2.98406300	-0.27149500	-0.00845300
C	3.19458100	-0.84026700	-1.40486600
C	3.69883900	1.07042800	0.12619400
C	3.60205600	-1.22610400	1.01167000
H	2.71368000	-1.82112100	-1.51373400
H	2.78974000	-0.18736100	-2.18736800
H	4.26436800	-0.97403900	-1.60925500
H	3.51619900	1.52168300	1.11011500
H	4.78302000	0.93274700	0.02662200
H	3.40047800	1.79813100	-0.63326900
H	4.68391100	-1.32000500	0.85600600
H	3.44546100	-0.86958600	2.03804300
H	3.16784600	-2.23097700	0.93847000

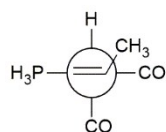
a in entry 4



Co	0.18060000	0.12799700	-0.17662700
C	-0.11813100	1.87000800	-0.07513200
O	-0.31954900	2.99580300	-0.06983400
H	0.54997800	0.54029100	-1.57276300
P	2.28272000	-0.48454400	-0.24894500
H	2.93089700	-1.17207200	0.80574800
H	2.67626100	-1.36107200	-1.28529100
H	3.29152800	0.48311100	-0.45393600

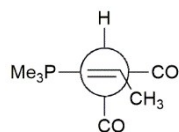
C	-0.15731600	-0.35124800	1.51501300
O	-0.33975500	-0.66339600	2.59859800
C	-0.62277100	-1.59859300	-1.03416300
C	-1.57570900	-0.58875100	-1.07408500
C	-2.78089900	-0.56255800	-0.18612500
H	-0.72269200	-2.40587200	-0.30809700
H	-0.03590900	-1.84067200	-1.91750600
H	-1.66937000	-0.01880200	-1.99859800
H	-2.63204900	-1.15870400	0.72147900
H	-3.05080200	0.45401500	0.12011000
H	-3.65146700	-0.98038000	-0.71121200

b in entry 4



Co	0.09509100	0.06584200	-0.07822000
C	-0.51491600	1.69103200	-0.42460400
O	-0.96587900	2.70580900	-0.69818100
H	-0.40882800	-0.12184000	-1.47901800
P	1.94017000	-0.50743000	-1.10793100
H	3.18291200	-0.68827600	-0.45355900
H	1.94652600	-1.73031300	-1.81563800
H	2.42670100	0.29838300	-2.16140900
C	0.76364700	0.31666800	1.56383600
O	1.19798700	0.47251800	2.60844300
C	-0.60761700	-1.86731400	0.27363200
C	-1.63433000	-0.96308200	0.51937100
H	-0.05150500	-2.31198100	1.09637900
H	-0.61120400	-2.44816100	-0.64886000
H	-1.81037400	-0.67031800	1.55636300
C	-2.80940000	-0.78886500	-0.39177800
H	-3.65766300	-1.39120500	-0.03673800
H	-3.15262300	0.25015100	-0.43918300
H	-2.57511100	-1.10996100	-1.41226900

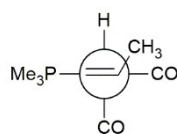
a in entry 5



Co	-0.47449700	0.18714900	-0.16185000
C	-0.97299800	1.88250300	-0.04525800

O	-1.27685600	2.98667900	-0.02533200
H	-0.05251800	0.65547700	-1.52945000
P	1.69657100	-0.10789600	-0.09938800
C	2.67934200	1.42152200	-0.30411000
C	2.45473700	-0.82642900	1.40766900
C	2.42111300	-1.17983000	-1.39301500
H	3.75721800	1.22025600	-0.27927000
H	2.42261500	1.89054300	-1.25918300
H	2.42944100	2.12886100	0.49295100
H	2.02823500	-1.81640400	1.60155800
H	3.54240500	-0.92287000	1.30605000
H	2.23643600	-0.19405700	2.27437700
H	2.02996900	-2.19745500	-1.29555900
H	2.14167900	-0.80218200	-2.38166400
H	3.51447500	-1.21311200	-1.31714600
C	-0.78316500	-0.37489700	1.49971000
O	-0.92435800	-0.73891200	2.57602700
C	-2.12572300	-0.68512100	-1.10544700
C	-1.05402000	-1.57388700	-1.10312900
C	-3.33403700	-0.86213700	-0.23846400
H	-3.11335400	-1.47523300	0.64341000
H	-3.74096700	0.09277000	0.11189000
H	-4.13644300	-1.36852000	-0.79401900
H	-0.45091100	-1.70734500	-1.99822100
H	-1.06255900	-2.42621500	-0.42202400
H	-2.28465800	-0.09158200	-2.00624000

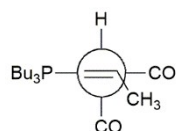
b in entry 5



Co	-0.51447600	-0.12513200	-0.02268600
C	-1.21835900	-1.30483900	1.09520300
O	-1.69286600	-2.00797600	1.86478200
H	-0.48151500	0.68844600	1.24289000
P	1.62844400	0.23306100	0.23975000
C	2.33048100	-0.44846900	1.78527400
C	2.79894700	-0.42165600	-1.00989200
C	2.16195200	1.98018000	0.33438300
H	3.40213100	-0.23375100	1.87618000
H	1.80293400	-0.01827200	2.64235300
H	2.17979400	-1.53234700	1.81007200
H	2.56158900	-0.00448100	-1.99436300

H	3.83792300	-0.17401500	-0.76116200
H	2.70110300	-1.51002300	-1.07725900
H	1.92695800	2.49019900	-0.60519000
H	1.61895500	2.48635500	1.13877300
H	3.23949400	2.06020400	0.52149800
C	-0.36158300	-1.09406800	-1.50962100
O	-0.21472900	-1.70974500	-2.46343100
C	-2.21357400	0.96115400	-0.58554400
C	-1.06085300	1.64675500	-0.96113900
H	-0.74385400	2.51408800	-0.38212400
H	-0.72260400	1.63818300	-1.99603900
C	-3.08745600	1.39684500	0.55044900
H	-2.52426300	1.98029300	1.28679900
H	-3.90948400	2.02735800	0.18195500
H	-3.54354800	0.55055400	1.07571500
H	-2.71800000	0.36621000	-1.34929100

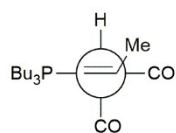
a in entry 6



Co	-1.47926100	-0.63150200	-0.69410100
C	-2.83159000	0.49772400	-0.84915500
O	-3.66579500	1.27010100	-0.99872500
H	-1.11324700	0.03030000	-1.99513800
P	0.40912600	0.38868100	-0.18813100
C	-1.75843700	-1.30221800	0.93093800
O	-1.88451000	-1.69921900	1.99871500
C	1.78305700	0.12824400	-1.39015600
C	3.11324400	0.81032100	-1.12078700
H	1.38005300	0.43463600	-2.36693400
H	1.92321800	-0.95995800	-1.46384500
C	4.15997300	0.45863800	-2.16643000
H	2.98743300	1.90305700	-1.09642200
H	3.49566400	0.53183100	-0.12665400
C	5.48738500	1.14578500	-1.91341500
H	4.29839100	-0.63288700	-2.18635300
H	3.78052900	0.72730200	-3.16359700
H	6.23615200	0.88434500	-2.66825800
H	5.37849400	2.23734300	-1.92323200
H	5.89793900	0.86999800	-0.93413700
C	0.23081400	2.22194400	-0.14136500
C	-0.66659400	2.71195300	0.98513300

H	-0.19397800	2.50477000	-1.11637500
H	1.21869400	2.69889800	-0.07013300
C	-1.10098600	4.15593800	0.79931300
H	-1.56068800	2.07410800	1.06274600
H	-0.14320900	2.61032900	1.94837300
C	-1.95692100	4.65417200	1.94676700
H	-0.21160800	4.79445800	0.68472900
H	-1.65541200	4.24194100	-0.14731200
H	-2.27452400	5.69201900	1.80231200
H	-2.86256600	4.04529500	2.05674400
H	-1.41457300	4.60547700	2.89927000
C	1.19687500	0.02751600	1.44074800
C	1.71237400	-1.39782600	1.55640100
H	0.42634900	0.20704900	2.20430700
H	2.00023700	0.75355500	1.63810700
C	2.07724500	-1.77425000	2.98238300
H	0.95455400	-2.10253000	1.17940000
H	2.59075000	-1.53566700	0.90634400
C	2.63058600	-3.18156600	3.08711200
H	2.80753100	-1.05061600	3.37557500
H	1.18386600	-1.67273300	3.61664600
H	2.88263100	-3.44864700	4.11858300
H	1.90511400	-3.92007300	2.72455500
H	3.54073800	-3.29797900	2.48554900
C	-0.76831700	-2.38863400	-1.54892900
C	-2.12157500	-2.25104300	-1.84689000
H	-0.45483300	-3.11942200	-0.80179400
H	-0.01418300	-2.13977100	-2.29208600
H	-2.38214500	-1.82518800	-2.81638200
C	-3.18571300	-3.09779300	-1.21838900
H	-4.11365400	-2.54192000	-1.04502700
H	-3.43717800	-3.94748000	-1.86950100
H	-2.85946900	-3.51200400	-0.25697700

b in entry 6

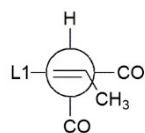


Co	-1.48332300	-0.89959300	-0.34064200
C	-3.02078100	-0.03262400	-0.44364800
O	-4.00953200	0.52891400	-0.58937400
H	-1.36333300	-0.32617700	-1.72637500
C	-1.49735600	-1.43252400	1.35781800

O	-1.46854800	-1.74149600	2.46088200
C	-2.01619300	-2.72377400	-1.22040000
C	-0.62996400	-2.62006600	-1.13898900
H	-0.05991000	-2.39800800	-2.04098100
H	-0.07757200	-3.15429200	-0.36768600
C	-2.76358600	-2.60807300	-2.51371800
H	-2.20726200	-2.00908800	-3.24300800
H	-2.92605200	-3.60317300	-2.95260900
H	-3.75040500	-2.14876700	-2.38987500
H	-2.52634900	-3.29954400	-0.44585100
P	0.31225700	0.36444300	-0.16826200
C	1.59428300	0.05422100	-1.45687500
C	-0.01655000	2.16923500	-0.34409100
C	1.27575500	0.29978100	1.40591700
C	2.84164600	0.92152500	-1.45333800
H	1.07089000	0.13181200	-2.42108000
H	1.86765200	-1.00671500	-1.36217300
C	-0.92113300	2.73655000	0.73720900
H	-0.47790400	2.30014400	-1.33467300
H	0.93766600	2.71572800	-0.35812900
C	1.98842300	-1.02454000	1.62784400
H	0.55357600	0.47278400	2.21668800
H	1.98816900	1.13769000	1.44547800
C	3.87828300	0.43674500	-2.45457200
H	2.58106400	1.96494600	-1.68461600
H	3.29850000	0.94322000	-0.45159800
C	-1.30247500	4.18469000	0.47829000
H	-1.83345400	2.12753600	0.82174900
H	-0.42308700	2.66623100	1.71699500
C	2.51944500	-1.17281100	3.04364200
H	1.30631700	-1.86121600	1.40974100
H	2.82068300	-1.12927700	0.91380400
C	5.11233700	1.31658600	-2.48604000
H	4.15958200	-0.59855600	-2.20858600
H	3.42248800	0.39002500	-3.45494800
C	-2.18733000	4.75304200	1.57018400
H	-0.38924000	4.79115300	0.37901000
H	-1.81355700	4.25382000	-0.49347200
C	3.26821100	-2.47478300	3.24840300
H	3.17350600	-0.31934200	3.27899100
H	1.67730900	-1.10802000	3.74878200
H	5.85651300	0.95596700	-3.20361700
H	4.85921000	2.34681500	-2.76521800
H	5.59693600	1.35729600	-1.50256700

H	-2.46259600	5.79484700	1.37574200
H	-3.11693100	4.17891500	1.66503400
H	-1.68571300	4.72192800	2.54543500
H	3.64035800	-2.57836100	4.27286500
H	2.62345800	-3.33841100	3.04433900
H	4.13192200	-2.54798400	2.57578600

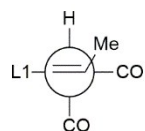
a in entry 7



O	-2.26619100	1.71693900	2.26868200
O	1.87917400	2.85943300	0.62585600
P	-0.17315500	-0.72841000	0.18639300
C	-1.59966200	1.63110500	1.34101400
C	0.90308400	2.31239800	0.37792100
C	-1.04033600	-1.86778000	1.37964000
C	-2.56531000	-1.72136600	1.36975500
C	-3.25546800	-1.52241300	0.02125100
C	-2.84583200	-2.45612900	-1.11557500
C	-1.60967700	-2.02602000	-1.90176400
C	-0.27476700	-2.00675300	-1.15937900
C	0.01748500	-3.32502100	-0.43913200
C	-0.55149400	-3.28434800	0.99740900
C	1.57548000	-0.92179900	0.77800500
C	2.64108800	-0.62396600	-0.26435300
C	4.01822200	-0.44717900	0.35144200
C	5.10339100	-0.19440400	-0.67927600
C	6.47024000	-0.00204300	-0.05199800
H	-0.68336000	-1.61304900	2.38757200
H	-2.84922500	-0.88293500	2.01829000
H	-2.98181900	-2.61697900	1.85666800
H	-3.11096800	-0.48528600	-0.31095700
H	-4.33534200	-1.62250500	0.19437200
H	-3.67479700	-2.51145900	-1.83384200
H	-2.72631900	-3.48485500	-0.74261700
H	-1.49311500	-2.71199500	-2.75473700
H	-1.79337000	-1.03525000	-2.33945800
H	0.51112000	-1.77170900	-1.89020400
H	1.09985600	-3.49686100	-0.40902800
H	-0.40071300	-4.16714100	-1.00692200
H	0.21288300	-3.61856200	1.70821300
H	-1.38072900	-3.99384900	1.10725700

H	1.66625300	-0.21776000	1.61815500
H	1.73105300	-1.92277500	1.20143400
H	2.67587400	-1.43720900	-1.00608000
H	2.37883000	0.28234100	-0.82955500
H	3.98795100	0.39251600	1.06441100
H	4.27656000	-1.33704800	0.94909200
H	5.13244400	-1.03307300	-1.39174800
H	4.83590100	0.69187800	-1.27410600
H	6.47315300	0.85122300	0.63729100
H	7.24677900	0.17956700	-0.80249100
H	6.77086300	-0.88547600	0.52514900
Co	-0.56675300	1.43692900	-0.09859400
H	0.26930700	1.08796100	-1.30098900
C	-1.40387300	2.91247900	-1.31394100
C	-2.11834700	1.72582500	-1.45595600
H	-3.10347600	1.64015000	-0.99510900
H	-1.96075800	1.08907100	-2.32262800
H	-0.64374200	3.13519900	-2.06352700
C	-1.94111600	4.10496800	-0.58358200
H	-1.15873100	4.65690400	-0.05084500
H	-2.40644200	4.80865700	-1.28869400
H	-2.70879000	3.82308900	0.14660200

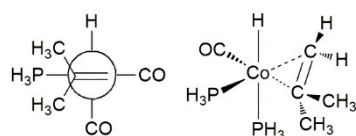
b in entry 7



O	-2.50008600	1.83132200	2.24572600
O	1.93380600	2.64250500	1.27950400
P	-0.29115400	-0.68598500	0.20053300
C	-1.71403600	1.70936300	1.42246100
C	0.95029600	2.21251000	0.87833500
C	-1.23991200	-1.86972600	1.28577900
C	-2.74447900	-1.58889900	1.33497900
C	-3.43639500	-1.18853500	0.03329700
C	-3.12983600	-2.03044700	-1.20326100
C	-1.87279500	-1.62942100	-1.97246700
C	-0.52576100	-1.80001300	-1.27030400
C	-0.33449200	-3.20693000	-0.70041600
C	-0.88875500	-3.27434800	0.74057600
C	1.43453100	-1.10033900	0.74675400
C	2.53356300	-0.79467700	-0.25636700
C	3.91836300	-0.89350200	0.36027900

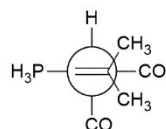
C	5.03460700	-0.63663700	-0.63574900
C	6.41045500	-0.72115700	-0.00426900
H	-0.84268500	-1.76020200	2.30455300
H	-2.93928000	-0.80232400	2.07491900
H	-3.23256000	-2.49054000	1.73679100
H	-3.20464100	-0.13887900	-0.19556300
H	-4.51792300	-1.20981700	0.22244800
H	-3.97085600	-1.93581700	-1.90323100
H	-3.09981600	-3.09912200	-0.94192400
H	-1.83204500	-2.23147400	-2.89317500
H	-1.97964700	-0.58736900	-2.30164200
H	0.26260600	-1.55516600	-1.99550800
H	0.73109700	-3.46518200	-0.70529100
H	-0.82270000	-3.94808900	-1.34764500
H	-0.15619300	-3.75689800	1.39764400
H	-1.78091200	-3.91080100	0.78395300
H	1.58787100	-0.50717400	1.66043900
H	1.49188200	-2.15224600	1.05597800
H	2.46573400	-1.48708000	-1.11022500
H	2.39594800	0.21178500	-0.67701000
H	3.99520200	-0.17325700	1.19093500
H	4.05346700	-1.88836800	0.81610000
H	4.95724800	-1.35792400	-1.46371200
H	4.89143500	0.35469900	-1.09122100
H	6.52182900	0.01339300	0.80274400
H	7.20957600	-0.53552000	-0.72964500
H	6.58699600	-1.71177900	0.43323600
Co	-0.50147900	1.52123000	0.12724200
H	0.47696900	1.24174400	-0.97710800
C	-1.12940000	3.15954700	-1.00124700
C	-1.78892500	2.00755400	-1.42737000
H	-1.66230100	3.82119200	-0.31518000
H	-2.82317000	1.82405900	-1.14037000
H	-1.48362100	1.54004800	-2.36294400
C	-0.05983600	3.82747900	-1.81026100
H	-0.49451200	4.61852200	-2.43829500
H	0.70704100	4.30023100	-1.18679600
H	0.44231200	3.11437900	-2.47312200

a in entry 8



Co	-0.42202400	-0.04778400	0.16185900
C	-2.03648200	0.02444000	0.89242100
O	-3.05253000	0.03214500	1.41685000
H	-0.30847000	-1.08896500	1.23592200
P	-0.05541700	-1.79979200	-1.08343800
H	-0.08195500	-1.74569800	-2.49801500
H	1.17275900	-2.49593700	-0.97476500
H	-0.89446200	-2.92742200	-0.94903000
C	-0.65361200	1.13576500	-1.15912400
O	-0.82755600	1.87234400	-2.01527900
C	0.75159000	1.16402700	1.36970600
C	1.63801200	0.39948500	0.61953500
H	0.56285500	2.20324200	1.10515100
H	0.55057200	0.90788800	2.40757800
C	2.37229100	-0.74698200	1.25743400
C	2.37926300	0.99904900	-0.54489700
H	3.35729100	-0.40193600	1.60663400
H	1.83675500	-1.16031900	2.11654000
H	2.57081400	-1.56520700	0.55344400
H	1.88269300	1.88218900	-0.95818800
H	3.38576400	1.30947100	-0.22542000
H	2.52559600	0.27911800	-1.36148500

b in entry 8

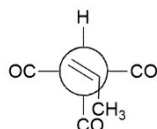


Co	0.31978600	0.17310300	-0.01025000
C	-0.13570200	1.47822000	1.09158000
O	-0.49416900	2.34473300	1.74769800
H	0.19340300	1.30658900	-0.98504000
P	2.30881900	0.21145500	-0.92152200
H	3.35709700	-0.66859000	-0.55715700
H	2.39635100	0.00118800	-2.31686600
H	3.07425300	1.39787500	-0.88252900
C	0.63713300	-1.13777000	1.16431100
O	0.88262900	-1.96721500	1.91131900
C	-1.62182000	-0.41734000	-0.69361900
C	-0.62367100	-1.01367300	-1.45519000
C	-2.40416000	0.75282100	-1.22140900
H	-2.64457900	1.47584600	-0.43265600
H	-1.87555500	1.28452100	-2.01730200
H	-3.36371100	0.39891000	-1.62830700

C	-2.35787200	-1.19334900	0.36230700
H	-3.32509900	-1.53521300	-0.03618300
H	-1.80970300	-2.07956000	0.69638300
H	-2.58049300	-0.57697300	1.24178100
H	-0.38868700	-0.62211000	-2.44410900
H	-0.37091700	-2.06168800	-1.29843400

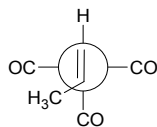
2 Structures in Table 2

TS_{rotate}-ma in entry 1



C	1.09179400	-0.26201200	-1.77248900
H	1.37290000	-1.31350800	-1.79534300
O	-1.27656100	-2.83239100	-0.05875300
O	-1.92673100	2.45720000	-0.28439300
C	-1.30512500	1.50283200	-0.20756400
C	-0.91190200	-1.75072400	-0.06516000
H	-1.32016500	-0.19452800	-1.34017400
Co	-0.43718600	-0.04443600	-0.13459600
C	0.20831100	0.09655400	1.52779200
O	0.57601100	0.18476000	2.60339300
H	0.52975300	0.10316900	-2.62491100
H	1.53223700	1.66189000	-1.03820000
C	1.68642500	0.59120900	-0.89988800
C	2.79542700	0.19016400	0.01805500
H	2.76592200	-0.88215000	0.24201400
H	3.76094000	0.40163500	-0.46040200
H	2.79110000	0.73858200	0.96465600

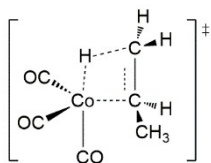
c in entry 1



C	-0.57537900	-1.24273200	-1.57821700
H	-1.11251100	-0.64865300	-2.31476800
O	-1.18951800	2.67074900	-0.44745000
O	3.19110500	-0.41031200	-0.37320800
C	2.07372400	-0.20436800	-0.26287900
C	-0.61694600	1.69331300	-0.30688200
H	0.73300600	0.71663600	-1.52266800
Co	0.34976800	0.20845600	-0.16224400

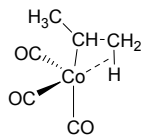
C	0.13039300	-0.07748700	1.58844700
O	-0.00922600	-0.24135100	2.70841700
H	0.28364600	-1.79605200	-1.94461500
H	-0.68267600	-2.30372800	0.23716400
C	-1.14402400	-1.52863100	-0.37623700
C	-2.52081800	-1.09936900	0.01544300
H	-2.86549200	-0.25471800	-0.59094400
H	-3.22772200	-1.92635000	-0.13355000
H	-2.59255500	-0.81250500	1.06984200

TS_{ma} in entry 1



C	-2.66692900	-0.66342300	-0.10380500
C	-1.34118900	-1.20989300	-0.53923400
C	-0.75803700	-0.85405000	-1.75306700
H	-1.05377100	-2.17224300	-0.11511900
H	-1.30364500	-0.17856900	-2.41227700
H	-0.09671900	-1.54952700	-2.26313100
O	-0.48078200	2.92438600	-0.00160900
O	3.13868500	-0.61931200	-0.40934900
C	2.03049600	-0.36652200	-0.30272200
C	-0.21058400	1.81722100	-0.05717600
H	0.42885000	0.35854600	-1.62542200
Co	0.30103900	0.08621500	-0.14875500
C	0.06010300	-0.39201600	1.54133800
O	-0.12111000	-0.70548200	2.62383000
H	-2.84071100	0.33600500	-0.51815500
H	-2.75678200	-0.59348100	0.98507100
H	-3.48278400	-1.31318600	-0.44956500

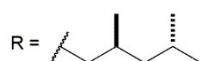
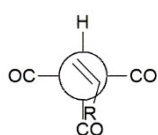
e in entry 1



C	-2.79131100	0.07811100	0.12301600
C	-1.58444100	-0.71968900	-0.29193200
C	-1.18318000	-0.62689300	-1.73163000
H	-1.66661300	-1.75235100	0.05730700
H	-1.80149900	0.07516300	-2.29980400
H	-1.13712900	-1.59012500	-2.24624000

O	-0.64683900	2.42467300	1.21853900
O	2.98271100	0.89827900	-0.74701400
C	1.92775300	0.54429800	-0.50235600
C	-0.31342100	1.50383400	0.63191900
Co	0.26551100	-0.01231500	-0.11925000
C	0.70625900	-1.50204700	0.75897100
O	0.95841200	-2.41199000	1.40060800
H	-2.76910800	1.09863200	-0.27810600
H	-2.88137500	0.15078800	1.21214900
H	-3.71417100	-0.39454500	-0.24494000
H	-0.12315000	-0.20844000	-1.88563500

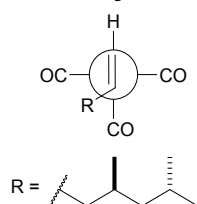
TS_{rotate}-ma in entry 2



Co	2.30930100	-0.22190500	-0.21953800
C	2.12878000	0.38715500	1.45445600
O	2.06743400	0.76442200	2.52841300
C	2.65956600	-1.91924800	0.16496300
O	2.94857200	-3.00616600	0.36113800
C	3.25376200	1.13260200	-0.86539700
O	3.90059100	1.95663400	-1.31903600
C	-0.01023100	-0.26457100	-0.37164300
C	0.53294900	0.04246000	-1.57869100
H	0.55058000	1.07494000	-1.92584300
H	2.83759300	-0.77326700	-1.51243500
H	0.72666700	-0.71807800	-2.32699600
C	-0.69236100	0.75685300	0.48907800
H	-0.62870400	0.48338700	1.55328100
H	-0.17766500	1.72363400	0.38369100
C	-2.17238800	0.94974200	0.13038700
H	-2.20988600	1.25789600	-0.92830000
C	-2.94886700	-0.35373300	0.29066500
H	-2.51856900	-1.11914500	-0.37632000
H	-2.78956000	-0.72720300	1.31765500
C	-2.74939800	2.06359000	0.98869400
H	-3.76507900	2.34059100	0.68815100
H	-2.79136600	1.75815400	2.04361400
H	-2.13502900	2.96993100	0.93452200
C	-4.44852300	-0.29704700	0.01532800

C	-5.06134900	-1.67057600	0.23644100
H	-4.64611100	-2.40029100	-0.47256500
H	-4.86458700	-2.04686000	1.24742900
H	-6.14781800	-1.65687300	0.09143000
C	-4.74760000	0.18907600	-1.39390300
H	-4.41489800	1.21826500	-1.56901500
H	-4.24658600	-0.44885000	-2.13600300
H	-5.82240300	0.15373400	-1.60687300
H	-4.91364400	0.39803300	0.73301100
H	-0.19287600	-1.31349500	-0.13728200

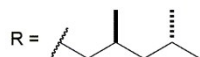
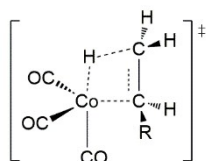
c in entry 2



C	-0.74549000	-0.03629400	0.21054000
C	0.37520300	-0.90019200	-0.28458800
C	0.89245800	-0.79440500	-1.53952300
H	0.59798100	-1.80171400	0.28752600
H	0.52683200	-0.02734500	-2.22038800
H	1.46998700	-1.59625800	-1.98872100
O	1.90827300	3.05339100	-0.54241400
O	4.75300000	-1.47814800	-0.49516600
C	3.80638300	-0.85590200	-0.35369000
C	2.05973800	1.93351000	-0.38081100
H	2.85796900	0.48035700	-1.60307700
Co	2.38089800	0.19422000	-0.20794100
C	2.16311700	0.06859000	1.56245000
O	2.03583600	0.00383200	2.69386700
H	-0.68544700	0.94795900	-0.27679400
H	-0.64967100	0.14719200	1.29219500
C	-2.13089500	-0.63771700	-0.05781000
C	-3.19409500	0.38650500	0.32667600
H	-2.19537400	-0.82952600	-1.14237300
C	-4.65033900	-0.00915800	0.10276200
H	-3.05761200	0.64566100	1.39073800
H	-3.00463800	1.31964600	-0.23149000
C	-5.56014200	1.13071800	0.53227000
H	-4.88102900	-0.88002900	0.73778100
H	-6.61849400	0.86320100	0.43242000
H	-5.38614500	1.42039900	1.57538700
H	-5.38748800	2.02057600	-0.08885600

C	-2.31666900	-1.95169200	0.68349400
H	-1.54832800	-2.68694000	0.42064200
H	-2.26629700	-1.79209400	1.77014800
H	-3.28458500	-2.41508300	0.46618500
C	-4.92389600	-0.38104100	-1.34568700
H	-4.64240900	0.44378200	-2.01588900
H	-4.36994400	-1.26966000	-1.66839200
H	-5.98867200	-0.58418900	-1.50943300

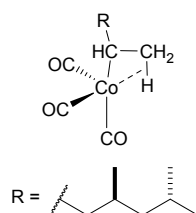
TS_{ma} in entry 2



C	-0.74467400	-0.03167700	0.28508400
C	0.39739900	-0.86284500	-0.22750400
C	0.85086900	-0.74218900	-1.53920300
H	0.57427300	-1.81556800	0.27214800
H	0.34880700	-0.03206100	-2.19760000
H	1.29392400	-1.59553500	-2.04597000
O	2.11191500	3.05678800	-0.37349100
O	4.85518600	-1.21446400	-0.65294100
C	3.84427300	-0.71729500	-0.46774500
C	2.14495700	1.91867200	-0.29652400
H	2.26437600	0.20146900	-1.70235400
Co	2.27919700	0.12146200	-0.19748700
C	2.17226300	-0.08583500	1.56036500
O	2.07983600	-0.22019000	2.69002200
H	-0.66971600	0.98084000	-0.13879700
H	-0.67456700	0.08971600	1.37744100
C	-2.12437900	-0.60972900	-0.05265600
C	-3.19444000	0.39755800	0.35691300
H	-2.16245800	-0.74350900	-1.14760300
C	-4.64581000	0.02249300	0.07377300
H	-3.08543800	0.59876700	1.43655900
H	-2.98633300	1.35844700	-0.14478300
C	-5.56263400	1.14137700	0.54179800
H	-4.89638900	-0.88097300	0.65325700
H	-6.61895700	0.88529400	0.39933100
H	-5.41534400	1.37170400	1.60365200
H	-5.37016700	2.06351600	-0.02395400
C	-2.33660800	-1.96046800	0.61131500

H	-1.56164100	-2.68346800	0.33445200
H	-2.31953700	-1.85877900	1.70589300
H	-3.29838000	-2.40820200	0.34001200
C	-4.88265900	-0.26746200	-1.39965700
H	-4.58169400	0.59225700	-2.01541100
H	-4.32261300	-1.13910200	-1.75650600
H	-5.94331400	-0.45696000	-1.60208600

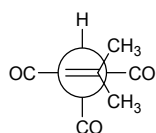
c in entry 2



C	-0.77185700	0.10401600	0.36678800
C	0.40705200	-0.65332600	-0.19170200
C	0.67099300	-0.48268900	-1.65656100
H	0.38049800	-1.70370700	0.10958400
H	0.00827600	0.25292300	-2.12403700
H	0.65956100	-1.41483000	-2.22788600
O	1.46105500	2.45434800	1.35373000
O	4.90312300	1.03418800	-0.97975600
C	3.87548600	0.66296000	-0.65659800
C	1.73665500	1.55757600	0.70333200
H	1.71671100	-0.06392900	-1.88619100
Co	2.25716800	0.07436500	-0.15192800
C	2.78494500	-1.44028500	0.62934100
O	3.09796600	-2.37022400	1.21309200
H	-0.74901600	1.13934700	-0.00809300
H	-0.69654700	0.17713900	1.46342100
C	-2.13273800	-0.51258700	0.01632300
C	-3.23160800	0.50040100	0.32583100
H	-2.13896700	-0.71748700	-1.06865000
C	-4.66960700	0.07297800	0.04996200
H	-3.14446000	0.78854600	1.38774000
H	-3.03454400	1.42311900	-0.24692800
C	-5.61896700	1.19884600	0.42764100
H	-4.90794900	-0.79515300	0.68590400
H	-6.66691900	0.90981600	0.28587900
H	-5.49499600	1.50238000	1.47394800
H	-5.43687400	2.08578000	-0.19510000
C	-2.35451100	-1.81978900	0.76092500
H	-1.53445300	-2.53017200	0.61055100

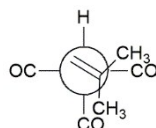
H	-2.43468700	-1.63546700	1.84162700
H	-3.27357700	-2.32609800	0.44718300
C	-4.87683500	-0.32121500	-1.40369900
H	-4.59030500	0.50396800	-2.07146800
H	-4.28768100	-1.19823000	-1.69439700
H	-5.92880600	-0.55361600	-1.60706700

a in entry 3



Co	-0.45586600	0.19093400	0.08283500
H	-0.29477100	1.66995800	-0.04107000
C	-2.07875600	0.68535200	-0.47067300
C	0.22744800	0.56789500	1.68398000
C	-0.78242700	-1.56839600	0.30477500
O	-1.01094000	-2.67434800	0.45069400
O	0.69752100	0.86682800	2.68014900
O	-3.09616200	1.07152100	-0.81217800
C	0.53340400	0.01987300	-1.80370400
C	1.55009000	0.04149800	-0.87258400
C	2.24237800	-1.21905600	-0.44038500
H	3.20816100	-1.30142500	-0.95996700
C	2.35447200	1.28716100	-0.63392800
H	2.65067200	1.39804500	0.41567400
H	3.28662000	1.22976200	-1.21506700
H	1.82395000	2.19353100	-0.93748900
H	1.66790000	-2.12107300	-0.67136600
H	2.46620300	-1.21826700	0.63325600
H	0.21251600	-0.92006400	-2.24859300
H	0.28414100	0.91636600	-2.36615000

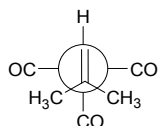
TS_{rotate}-ma, entry 3



Co	-0.57524300	0.24646500	-0.13926100
H	-1.02237400	0.88217200	-1.42448000
C	-2.08358200	-0.61855700	-0.48828500
C	-0.11909000	1.94555400	0.06810000
C	-0.34478200	-0.29804600	1.54800200
O	-0.23015000	-0.61165500	2.63891100

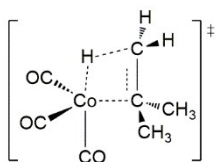
O	0.12335400	3.05794200	0.15963700
O	-3.07970000	-1.11174400	-0.74930800
C	0.75690800	-0.84265600	-1.60719600
C	1.63781200	-0.71702400	-0.58067800
C	1.91106200	-1.85426100	0.35616700
H	2.82930500	-2.36633000	0.03531700
C	2.62664600	0.40502000	-0.51445800
H	2.68511800	0.84129100	0.49019200
H	3.63105400	0.01977300	-0.74208900
H	2.40321900	1.20517900	-1.22620500
H	1.10276000	-2.59179500	0.36629200
H	2.09021000	-1.52019600	1.38416600
H	0.22364600	-1.77667200	-1.76801000
H	0.77076500	-0.14450100	-2.43896300

c in entry 3



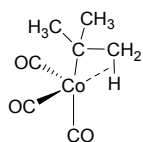
Co	-0.64013800	0.00125800	-0.13648000
H	-1.45101100	0.00360600	-1.40318200
C	-1.26878200	-1.65541400	-0.20764000
C	-1.26043100	1.66108200	-0.20749900
C	-0.10025300	-0.00000800	1.56473700
O	0.22845100	-0.00056900	2.65779300
O	-1.71401700	2.70529700	-0.29594700
O	-1.72752100	-2.69734100	-0.29633300
C	0.94805700	-0.00270900	-1.70949800
C	1.71998600	-0.00378800	-0.58799500
C	2.31013500	-1.27152000	-0.04838800
H	3.36455100	-1.33803300	-0.35250300
C	2.31519700	1.26209400	-0.04953800
H	2.30962800	1.29571600	1.04598500
H	3.36990300	1.32416900	-0.35356200
H	1.80533000	2.15412800	-0.42534700
H	1.79660100	-2.16181000	-0.42329300
H	2.30462300	-1.30402800	1.04716200
H	0.75073500	-0.92553900	-2.24921100
H	0.75461800	0.92032300	-2.25025400

TS_{ma} in entry 3



Co	0.49142000	0.00065800	-0.15023700
H	0.74260900	0.00197700	-1.63462000
C	1.36301000	1.57487800	-0.20205500
C	1.37110600	-1.56879000	-0.20421100
C	0.02557300	-0.00192400	1.55791500
O	-0.29622400	-0.00372100	2.65383900
O	1.96453700	-2.54353100	-0.24294100
O	1.95119100	2.55285000	-0.23907300
C	-0.93156000	-0.00170000	-1.74174300
C	-1.63231200	-0.00249500	-0.53172300
C	-2.29029800	1.26404000	-0.05684200
H	-3.31057200	1.32666800	-0.46454800
C	-2.28694600	-1.27062300	-0.05636600
H	-2.38502000	-1.30551600	1.03437000
H	-3.30717300	-1.33590200	-0.46377800
H	-1.74051900	-2.16331200	-0.37583600
H	-1.74597400	2.15800200	-0.37632300
H	-2.38878300	1.29891000	1.03385800
H	-0.90167400	0.91399400	-2.33090100
H	-0.89871200	-0.91768300	-2.33027900

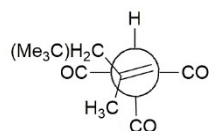
e in entry 3



Co	-0.41694700	0.00024000	0.14092400
C	-0.41521300	1.56210200	-0.72821200
C	-2.16345400	0.00038900	0.56546300
C	-0.41640200	-1.56148400	-0.72847600
O	-0.45488100	-2.49138300	-1.39051200
O	-3.26998700	0.00026400	0.83749300
O	-0.45297200	2.49214700	-1.39009200
C	2.34629600	1.23730700	-0.07786000
C	1.58375800	-0.00049800	0.33753100
C	2.34531200	-1.23882100	-0.07809000
H	3.37308200	-1.19958100	0.31744300
C	1.12828200	-0.00041700	1.76507400
H	-0.01576600	-0.00006900	1.89288700
H	1.42508000	-0.89808900	2.31611500

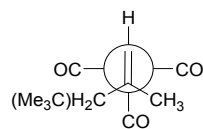
H	1.42565600	0.89700800	2.31619700
H	2.42963900	-1.31613100	-1.16839700
H	1.89234500	-2.16483100	0.29159900
H	2.43114000	1.31445500	-1.16814400
H	1.89377500	2.16365200	0.29152600
H	3.37386300	1.19741000	0.31812400

TS_{rotate}-ma in entry 4



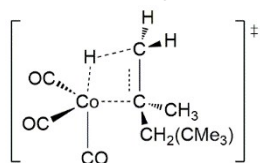
Co	-1.63705100	0.26628000	-0.19172300
C	-1.83607600	-0.29565400	1.49605400
O	-2.00126800	-0.61277100	2.57923000
C	-1.17813200	1.94140300	0.15033200
O	-0.92447500	3.04277200	0.31592400
C	-3.06113100	-0.51630600	-0.90351700
O	-3.99304800	-0.95154800	-1.39941500
C	0.61265900	-0.79190600	-0.15745700
C	-0.06739300	-0.94461100	-1.32398300
H	-1.71927100	0.92874300	-1.53777200
H	0.12130200	-0.28808000	-2.16854800
H	-0.60049000	-1.86800600	-1.53982100
C	1.57924100	0.34904800	0.02751300
H	1.43413800	0.80159300	1.02173900
H	1.32662500	1.12936600	-0.70397600
C	0.61377600	-1.89667900	0.85897400
H	-0.28693900	-2.51449200	0.79187700
H	1.46926000	-2.56135500	0.68489800
H	0.70853100	-1.52676700	1.88626300
C	3.08846600	0.04625700	-0.13428500
C	3.66437300	-0.71485400	1.05625700
C	3.35296200	-0.72166300	-1.42190400
C	3.79476100	1.39816000	-0.20868000
H	3.43820000	-0.20653600	2.00263300
H	3.29301000	-1.74087300	1.13218800
H	4.75669800	-0.77782500	0.97273400
H	2.96519200	-0.18246100	-2.29608500
H	4.43060100	-0.86227700	-1.57313000
H	2.88929200	-1.71567000	-1.41676800
H	4.88037200	1.26870500	-0.29882000
H	3.45694000	1.98192200	-1.07388000
H	3.60618600	1.99764800	0.69123800

c in entry 4



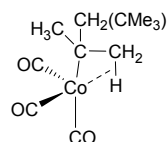
C	0.55870500	-0.70090500	-0.40226500
C	-0.05508800	-0.41643600	-1.58399200
H	-0.55523900	-1.19558600	-2.15474300
H	0.17219900	0.50059300	-2.12197000
O	-3.76982000	-1.71999300	-0.60814200
O	-1.53131300	3.15668500	-0.22069000
C	-1.54912200	2.01607300	-0.16656800
C	-2.92342900	-0.98046500	-0.40499700
H	-2.24508900	0.61835000	-1.49880600
Co	-1.66852200	0.24683800	-0.16044000
C	-1.35912200	-0.03473400	1.57704500
O	-1.18248200	-0.20426000	2.69177700
C	1.51861800	0.28617200	0.21358100
H	1.27107500	1.28583000	-0.17051000
H	1.36924100	0.33174000	1.30372500
C	0.50791100	-2.09512100	0.15464100
H	1.35625600	-2.68296400	-0.21830900
H	0.57117900	-2.11242400	1.24868500
H	-0.40286000	-2.62042800	-0.14751600
C	3.02961500	0.06064000	-0.03459400
C	3.58203600	-1.10871300	0.77515200
C	3.31539400	-0.15259500	-1.51445700
C	3.73952000	1.32971200	0.43114700
H	3.33871300	-1.00813300	1.84088800
H	3.20635200	-2.07907600	0.43739800
H	4.67558700	-1.14475800	0.69154200
H	2.94668000	0.68617800	-2.11928500
H	4.39528600	-0.23548300	-1.69029900
H	2.84815200	-1.06705500	-1.89975100
H	4.82599900	1.23791700	0.31052100
H	3.41479000	2.20653900	-0.14273400
H	3.54046200	1.53290200	1.49134200

TS_{ma} in entry 4



C	0.49042200	-0.63144300	-0.35534900
C	-0.03477300	-0.33037300	-1.61748700
H	-0.34781000	-1.14937500	-2.26470300
H	0.34163900	0.54257800	-2.14861200
O	-3.85275300	-1.55995000	-0.62095000
O	-1.85715100	3.08501400	-0.13819400
C	-1.69757400	1.95435900	-0.13934500
C	-2.92981600	-0.91295700	-0.43607900
H	-1.56510700	0.32887900	-1.65120500
Co	-1.51676100	0.16153000	-0.15584900
C	-1.29832100	-0.12281500	1.57947900
O	-1.14125700	-0.31317000	2.69473000
C	1.48586800	0.32366200	0.26990500
H	1.22588900	1.34058900	-0.05762900
H	1.37234700	0.32446400	1.36491200
C	0.51740200	-2.07443500	0.08155100
H	1.36700400	-2.60317800	-0.37105300
H	0.62086100	-2.17643300	1.16790600
H	-0.38955900	-2.60542900	-0.22282000
C	2.98982700	0.11125300	-0.02996200
C	3.57027800	-1.07500300	0.73537900
C	3.24382000	-0.06187200	-1.52092300
C	3.70894500	1.37038000	0.44974700
H	3.35491300	-1.00054600	1.80918200
H	3.18978200	-2.03909800	0.38617000
H	4.66156000	-1.10275500	0.62228600
H	2.87844200	0.80018600	-2.09435900
H	4.31908300	-0.15286200	-1.71994400
H	2.76068800	-0.96007400	-1.92519100
H	4.79253300	1.28539700	0.30049700
H	3.36771800	2.26078300	-0.09299800
H	3.53537700	1.54588400	1.51930300

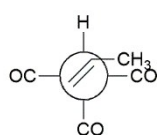
e in entry 4



Co	-1.47849000	-0.05668600	0.13900900
H	-1.08330700	-0.01543800	1.87163500
C	-3.17672700	-0.44623900	0.58213400
C	-1.11094100	-1.61798600	-0.68825000
C	-1.85072500	1.37724100	-0.84044300
O	-2.09887200	2.22787300	-1.56284900

O	-0.97477700	-2.54960900	-1.33416600
O	-4.25555800	-0.67822600	0.86750000
C	0.05505400	0.14582500	1.74767800
C	0.45516400	0.51850700	0.35665900
C	0.69763200	2.00300600	0.19011800
H	1.61031400	2.31522600	0.71639100
C	1.48887600	-0.37451400	-0.31401400
H	1.35139900	-0.31738400	-1.40570500
H	1.25631600	-1.41403800	-0.04200300
H	-0.11805200	2.59974600	0.61235900
H	0.81695200	2.28806500	-0.86163600
H	0.21928700	0.94742600	2.47752000
H	0.49362200	-0.78693400	2.10883200
C	3.00283500	-0.18659000	-0.03760600
C	3.60190200	0.99835000	-0.79274200
C	3.29923900	-0.06273300	1.45174500
C	3.68959400	-1.44808800	-0.56158800
H	3.36519500	0.94428900	-1.86329600
H	3.25857600	1.96933200	-0.42719200
H	4.69571700	0.99085600	-0.70081400
H	2.93916900	-0.93850600	2.00717300
H	4.38104100	0.00599800	1.62372800
H	2.84375800	0.82767600	1.90099000
H	4.77800900	-1.38358300	-0.43848000
H	3.34779700	-2.34457700	-0.02925000
H	3.48566700	-1.59861800	-1.62953000

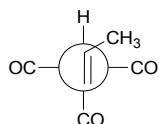
TS_{rotate}-(anti-ma) in entry 5



C	0.54576500	-1.62597700	1.03560400
H	0.79523400	-1.21766100	2.01365100
O	-2.80560600	-0.93412900	-1.24787500
O	1.36721200	2.26632700	-1.17753200
C	0.73511600	1.41277400	-0.75837400
C	-1.82392500	-0.57066000	-0.79323000
H	0.07076800	-0.36075500	-1.60836700
Co	-0.26199800	0.05512900	-0.20494000
C	-0.81881900	0.77820200	1.33538700
O	-1.18611800	1.25695400	2.30222900
H	-0.26972600	-2.34194400	1.00870800
H	1.25335000	-2.11586200	-0.88349900

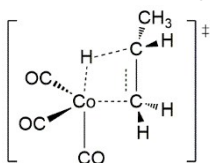
C	1.41618300	-1.49758500	-0.00165200
C	2.75567200	-0.84693600	0.10974200
H	2.80191300	-0.15867200	0.96083300
H	3.52916200	-1.61292000	0.25622900
H	3.02938600	-0.29280800	-0.79362700

d in entry 5



C	0.69679500	-0.78697300	1.66371700
H	1.08699100	0.06802400	2.21347600
O	-2.29384000	-1.78977800	-1.19922400
O	1.36812400	2.12482300	-1.43147300
C	0.73568100	1.32984600	-0.91077600
C	-1.50651200	-1.08720200	-0.76374700
H	0.40722000	-0.65773200	-1.37991600
Co	-0.23675600	0.02214000	-0.20380700
C	-1.24638100	1.02369600	0.88274100
O	-1.89982400	1.66995500	1.55680000
H	-0.13022500	-1.31988000	2.12349000
H	1.10141100	-2.30088800	0.25597900
C	1.40826300	-1.32731400	0.63824500
C	2.76674400	-0.85416600	0.23499100
H	2.96181300	0.16162000	0.59600900
H	3.53310100	-1.51309800	0.66386700
H	2.90888000	-0.86315900	-0.84997900

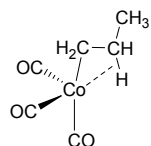
TS_{anti-ma} in entry 5



C	-2.86974800	0.60814400	0.11879800
C	-1.53102600	1.21871500	0.42493700
C	-0.80020100	0.82167100	1.54622600
H	-1.40782300	2.25545700	0.10608400
H	-1.18419100	0.01338600	2.16661800
H	-0.13304900	1.52089100	2.04239300
O	2.23119100	1.72560000	-1.38940400
O	-0.89959900	-2.30493900	-1.52941900
C	-0.47378300	-1.41482300	-0.95549500
C	1.44857700	1.08110500	-0.86568700

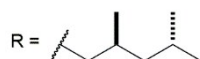
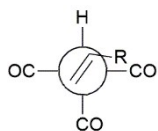
H	-0.75049200	0.79171700	-0.98791100
Co	0.20230800	0.02031300	-0.10625200
C	1.22775200	-0.81957600	1.06949400
O	1.87889300	-1.35306200	1.83929400
H	-2.91568400	-0.43160600	0.45952400
H	-3.10604300	0.62352700	-0.94962900
H	-3.65833200	1.16597500	0.63830700

f in entry 5



C	2.94931600	0.06726700	1.02227000
C	1.66879300	0.86253400	0.84792500
C	1.26751200	1.09489500	-0.57758900
H	1.68675700	1.80008800	1.41636700
H	1.94475500	0.65536000	-1.31341900
H	1.05089600	2.12962400	-0.84486000
O	-2.19529600	-1.58699100	1.53069500
O	0.65108500	-2.07619500	-1.85549300
C	0.31187000	-1.29788700	-1.09332300
C	-1.44973900	-0.97110900	0.92852900
Co	-0.27601100	-0.00204500	-0.01253800
C	-1.33591200	1.38924800	-0.36667800
O	-2.00663400	2.25561500	-0.68490400
H	3.80758200	0.63601300	0.64834200
H	3.14234200	-0.18365200	2.07040200
H	2.90437900	-0.87149200	0.45764400
H	0.85130800	0.28015000	1.41483800

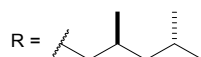
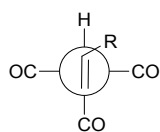
TS_{rotate}-(anti-ma) in entry 6



Co	2.32646900	0.07036800	0.14505100
C	2.80985800	0.86652200	-1.38459700
O	3.13749400	1.38314300	-2.34631500
C	1.83322200	1.52557400	1.03007200
O	1.53155200	2.43037900	1.65779400
C	3.72331500	-1.01896400	0.33748300

O	4.62367000	-1.68990800	0.54252400
C	0.89322500	-1.12157100	-1.10989300
C	0.29724800	-0.97833500	0.10494700
C	-0.82651500	-0.02033100	0.35695300
H	0.44963600	-1.76333300	0.84442300
H	2.13023300	-0.45948900	1.53595000
H	0.58703300	-0.49189000	-1.94458600
H	1.48190900	-1.99850900	-1.36088000
H	-0.71001600	0.85629300	-0.29729500
H	-0.78773200	0.35553800	1.39108400
C	-2.20825400	-0.64128500	0.11392200
C	-3.26573100	0.45134600	0.23791000
H	-2.21214800	-1.02675600	-0.91980400
C	-4.71566000	0.04380800	-0.00483300
H	-3.18729200	0.89706800	1.24438600
H	-3.01796900	1.26499600	-0.46549100
C	-5.61936600	1.25598800	0.15478200
H	-5.00737700	-0.69492800	0.75941600
H	-6.67634800	0.99105400	0.03541800
H	-5.50194500	1.72539900	1.13870800
H	-5.38525600	2.01726500	-0.60224900
C	-2.47388000	-1.79520600	1.06712000
H	-1.71189900	-2.57857700	0.99222400
H	-2.48549700	-1.44101000	2.10785600
H	-3.43921500	-2.27480200	0.87476200
C	-4.91121400	-0.57839800	-1.37807500
H	-4.56908800	0.10862200	-2.16532600
H	-4.36178500	-1.51840500	-1.50134100
H	-5.96910300	-0.79227300	-1.57040600

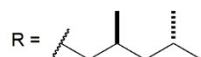
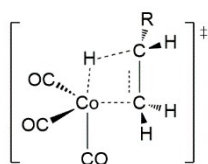
d in entry 6



C	0.84699500	-0.06911400	-0.32935500
C	-0.28869300	-0.89379300	0.19524500
C	-0.88330100	-0.65471700	1.39621900
H	-0.45015000	-1.86468200	-0.27288300
H	-0.58417600	0.20506100	1.99472200
H	-1.47313100	-1.41322900	1.90238400
O	-4.08761200	-2.04264800	-1.04032500
O	-1.51556600	2.62776800	-1.37940500

C	-1.82245900	1.65806200	-0.86092000
C	-3.39542100	-1.22219600	-0.65179200
H	-1.76280600	-0.30039400	-1.51223100
Co	-2.30444500	0.09580100	-0.16746500
C	-3.26414100	0.72491000	1.20611700
O	-3.88941900	1.13458700	2.06655200
H	0.75766000	0.95678200	0.05732500
H	0.79477600	0.00717300	-1.42624100
C	2.22205900	-0.62501800	0.06145100
C	3.29386200	0.37195100	-0.36869800
H	2.23591900	-0.71179200	1.16121400
C	4.74093100	0.02065500	-0.03722800
H	3.20749700	0.52528200	-1.45817100
H	3.06833700	1.35196200	0.08611400
C	5.66014200	1.12555600	-0.53302900
H	5.01099300	-0.90494000	-0.57128400
H	6.71469500	0.88444300	-0.35566700
H	5.53558300	1.30824500	-1.60699100
H	5.44821000	2.06985900	-0.01264400
C	2.45719000	-2.00077300	-0.54083700
H	1.68517300	-2.72008000	-0.24684000
H	2.45926300	-1.94563800	-1.63886100
H	3.41813900	-2.42636600	-0.23364600
C	4.94638700	-0.20338300	1.45231200
H	4.62634200	0.68003600	2.02322900
H	4.38375900	-1.06255500	1.83441900
H	6.00339900	-0.37630300	1.68613200

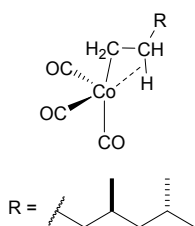
TS_{anti-ma} in entry 6



C	0.86808500	-0.12926200	-0.52426300
C	-0.30607900	-0.90157500	0.02168700
C	-0.81423500	-0.61730500	1.28842400
H	-0.39854400	-1.93301500	-0.32239300
H	-0.40710400	0.22806500	1.84229000
H	-1.27194000	-1.39873700	1.88849000
O	-4.20547300	-1.85459500	-1.14606000
O	-1.81248300	2.64190200	-1.43539800

C	-1.97063800	1.65316100	-0.88734100
C	-3.44157800	-1.12825300	-0.70828900
H	-1.38916200	-0.46649100	-1.20403800
Co	-2.24768900	0.06648600	-0.08308200
C	-3.14766600	0.63598200	1.33392500
O	-3.71375700	0.99700100	2.25618300
H	0.74202300	0.93228700	-0.26669900
H	0.88449000	-0.17842700	-1.62402300
C	2.21496500	-0.61793000	0.01522400
C	3.30896200	0.32740100	-0.47256100
H	2.16451200	-0.56565900	1.11587300
C	4.73329500	0.03824600	-0.00883100
H	3.29181200	0.33866500	-1.57598100
H	3.05185300	1.35501100	-0.16276000
C	5.67755500	1.08270100	-0.58251800
H	5.04091300	-0.94399700	-0.40302700
H	6.71969500	0.87846400	-0.31080100
H	5.62045400	1.12689200	-1.67663400
H	5.42944100	2.08250100	-0.20012100
C	2.48954500	-2.05657400	-0.39262900
H	1.70899500	-2.74293500	-0.04665900
H	2.54754200	-2.14316900	-1.48713400
H	3.43612900	-2.42677500	0.01436900
C	4.84420900	0.00705500	1.50699000
H	4.48313100	0.95090100	1.94001700
H	4.26349800	-0.80481000	1.95905500
H	5.88505300	-0.12025900	1.82667200

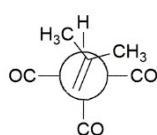
f in entry 6



C	-0.82942000	1.49400900	-0.75447100
C	0.12684500	0.40902400	-1.22610600
C	1.49309000	0.88634800	-1.60337200
H	-0.30667100	-0.22193500	-2.01160800
H	1.62966800	1.96822800	-1.54842800
H	1.88683900	0.50581100	-2.54613900
O	3.72996600	-1.78607900	-1.64578600
O	1.82170800	-1.88292400	2.37720900
C	1.87589900	-1.21243100	1.45762300

C	2.99846000	-1.19333900	-1.00113800
H	0.18427800	-0.35859900	-0.35925400
Co	1.95149900	-0.15960000	0.01176100
C	2.35679300	1.37230100	0.83854700
O	2.69269600	2.35145300	1.31905100
H	-0.25745800	2.23362100	-0.17344800
H	-1.21072100	2.03617500	-1.63528800
C	-2.00341000	1.01168900	0.09056100
C	-2.85492200	0.00337100	-0.67575400
H	-2.23400600	-0.86174700	-0.96242100
H	-3.16994800	0.47081900	-1.62551600
C	-4.08841600	-0.54016600	0.03910700
C	-4.82275800	-1.50976000	-0.87278900
H	-5.09872900	-1.04335700	-1.82610100
H	-4.19249800	-2.38016600	-1.10282200
H	-5.74117300	-1.88630800	-0.40767000
C	-2.82097200	2.20720400	0.55268600
H	-3.32455100	2.68510500	-0.29950600
H	-3.59466900	1.93392800	1.27755100
H	-2.18579700	2.96556800	1.02515700
C	-3.72834700	-1.22303600	1.34899100
H	-3.00093900	-2.02945200	1.17678200
H	-3.28851600	-0.53594600	2.08039000
H	-4.61024000	-1.67585500	1.81696900
H	-1.57835000	0.51341200	0.98066600
H	-4.76900200	0.29901500	0.25603400

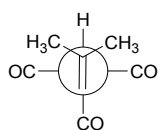
TS_{rotate}-(anti-ma) in entry 7



Co	0.46259600	-0.02604100	-0.21240600
H	-0.21616500	0.56775100	-1.41271700
C	1.47576900	1.38887000	-0.56767800
C	-0.03770100	-1.45887600	-1.12050400
C	1.52886200	-0.83636300	0.97840300
O	2.22424800	-1.35854600	1.71538000
O	-0.36994700	-2.34004700	-1.76751400
O	2.10720500	2.28810600	-0.87836900
C	-0.79735300	0.75514300	1.50113900
C	-1.76683600	0.50672300	0.58129600
C	-2.57138500	-0.75598400	0.60728500
H	-3.55273500	-0.55025200	1.05866200

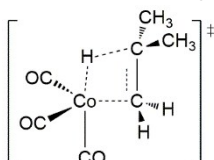
C	-2.33605100	1.59985200	-0.27014600
H	-2.54697000	1.26040300	-1.28981000
H	-3.29504900	1.92519700	0.15874500
H	-1.67701600	2.47099700	-0.32514500
H	-2.09128600	-1.54819500	1.18964000
H	-2.77112400	-1.13890600	-0.40023000
H	-0.59963000	0.04477700	2.30022400
H	-0.40399700	1.75904700	1.64083400

d in entry 7



Co	-0.44926600	0.00006900	-0.21444300
H	0.46074800	-0.00032700	-1.41335100
C	-0.61221800	-1.65683600	-0.82535000
C	-0.61157200	1.65725600	-0.82503600
C	-1.84554600	0.00011900	0.90606300
O	-2.74840200	0.00000600	1.60202500
O	-0.68245000	2.69717000	-1.29168800
O	-0.68327400	-2.69666000	-1.29220600
C	0.88526100	0.00031900	1.60652000
C	1.80573200	-0.00021900	0.60566700
C	2.47046400	1.26308400	0.15119400
H	3.49050500	1.30173900	0.55908300
C	2.46976300	-1.26420500	0.15201300
H	2.56674000	-1.30962500	-0.93825000
H	3.48954500	-1.30354900	0.56047900
H	1.94027900	-2.16053700	0.48845800
H	1.94191000	2.15995000	0.48768000
H	2.56687400	1.30808600	-0.93913200
H	0.60779100	0.92563800	2.10635700
H	0.60749200	-0.92446800	2.10716200

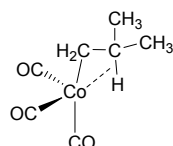
TS_{anti-ma} in entry 7



Co	0.38563500	0.00003500	0.10375600
H	-0.86668500	-0.00002500	0.95031100
C	0.71749800	-1.57622000	0.91270500
C	0.71694700	1.57661200	0.91243300

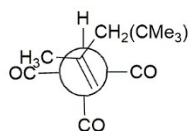
C	1.71592100	0.00007900	-1.06461900
O	2.55641700	0.00010500	-1.83612700
O	0.92262300	2.55704100	1.46000500
O	0.92344900	-2.55657700	1.46030500
C	-0.89834200	0.00023800	-1.53466500
C	-1.75362000	-0.00021100	-0.42327500
C	-2.50010200	1.26699600	-0.08408200
H	-3.43102900	1.30147100	-0.66525000
C	-2.49932600	-1.26797300	-0.08450700
H	-2.77461800	-1.31554000	0.97486500
H	-3.43020200	-1.30285500	-0.66573100
H	-1.91614600	-2.16125900	-0.32684900
H	-1.91749300	2.16071400	-0.32620700
H	-2.77537200	1.31407000	0.97531700
H	-0.75737300	0.92116300	-2.09740700
H	-0.75698900	-0.92036800	-2.09787500

f in entry 7



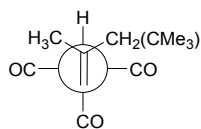
Co	-0.48246400	-0.00005400	0.05575200
C	-1.75379000	-0.00109000	-1.20293400
C	-0.79569900	1.62470600	0.72603100
C	-0.79352900	-1.62506500	0.72625400
O	-1.00601900	-2.62425000	1.23455700
O	-1.00977100	2.62371800	1.23400200
O	-2.55958600	-0.00171000	-2.00814000
C	2.57627700	1.26364600	-0.68824600
C	1.79525800	0.00068800	-0.36014300
C	2.57740200	-1.26175900	-0.68761000
C	1.23819900	0.00073500	1.03468600
H	1.46595200	-0.89234600	1.62083800
H	1.46496600	0.89437900	1.62036900
H	3.49833100	-1.29584900	-0.09215100
H	1.99814400	-2.16343700	-0.45971100
H	2.86138700	-1.30062900	-1.74562400
H	3.49691100	1.29915700	-0.09241100
H	2.86069200	1.30192300	-1.74616500
H	1.99606200	2.16496300	-0.46135600
H	0.92238800	0.00005900	-1.12066600

TS_{rotate}-(anti-ma) in entry 8



Co	-1.56677000	0.14032800	-0.22969300
C	-2.81114900	-0.00133900	1.05322400
O	-3.62523300	-0.08858400	1.84658200
C	-1.72951000	1.87197200	-0.58740700
O	-1.82876200	2.96499400	-0.90269400
C	-1.90853400	-1.36104900	-1.09623100
O	-2.10563400	-2.29722100	-1.72107400
C	0.06222800	0.21585000	1.39243500
C	0.70373900	-0.55954300	0.48011200
C	1.68575200	0.04409900	-0.49341400
H	-0.76188000	0.27895200	-1.49059900
H	0.25711400	1.28353400	1.45644300
H	-0.44842800	-0.23220400	2.24177700
H	1.34255300	1.05060100	-0.76821200
H	1.67853400	-0.54488400	-1.42352700
C	0.64079000	-2.05702700	0.56313500
H	-0.21027500	-2.39826700	1.16031800
H	0.57105700	-2.51723000	-0.42934400
H	1.55062800	-2.45859200	1.02387400
C	3.15443800	0.18648300	-0.02795200
C	3.25930800	1.14179000	1.15352500
C	3.78830300	-1.14795100	0.34721800
C	3.92585600	0.77299300	-1.20730400
H	2.84855000	2.13034900	0.90918400
H	2.72652200	0.76569900	2.03470100
H	4.30869900	1.28400500	1.44099000
H	3.64195900	-1.90359100	-0.43577900
H	4.86969900	-1.02779200	0.48943500
H	3.38930500	-1.54722700	1.28640500
H	4.97627100	0.94493800	-0.94170700
H	3.90898400	0.09770800	-2.07230600
H	3.50319600	1.73395100	-1.52650100

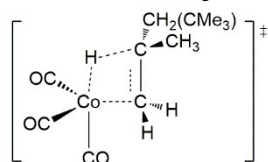
d in entry 8



Co	-1.56990600	-0.11308400	-0.20391000
C	-2.64429500	-0.70711900	1.09926800

O	-3.34440100	-1.09106000	1.91299000
C	-2.47070700	1.35392400	-0.62966600
O	-3.03321100	2.28184700	-0.98644600
C	-1.21617100	-1.67252700	-0.97097000
O	-0.98876500	-2.63612600	-1.54039900
C	-0.06695000	0.37936600	1.42458800
C	0.65371500	0.70564700	0.31760300
C	0.71367000	2.13016400	-0.15038700
H	-0.91630700	0.30501500	-1.49402300
H	-0.58875600	1.14406300	1.99642100
H	0.07360600	-0.58126600	1.91548200
H	-0.16904200	2.69909600	0.15467900
H	0.81415400	2.20399300	-1.23881000
H	1.58475100	2.63367400	0.28701200
C	1.62210900	-0.28450300	-0.27935700
H	1.32230400	-1.28993300	0.04793200
H	1.53026600	-0.28089200	-1.37633800
C	3.12107700	-0.12245200	0.06928600
C	3.77209400	1.03931400	-0.67598100
H	3.41644000	2.01848700	-0.34272800
H	4.85852100	1.02677000	-0.52207800
H	3.59431900	0.96958700	-1.75699600
C	3.31981300	0.04400000	1.56955000
H	2.87695900	-0.79167800	2.12710300
H	4.38862700	0.07438600	1.81599900
H	2.86844700	0.96843600	1.94983300
C	3.81025100	-1.40854200	-0.38189800
H	3.66689000	-1.58305800	-1.45604500
H	4.89024400	-1.36080500	-0.19542600
H	3.41942600	-2.28351700	0.15216900

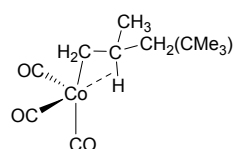
TS_{anti-ma} in entry 8



C	0.75074300	2.13565400	-0.13975300
C	0.58887900	0.66026300	0.15064400
C	-0.04622900	0.30373800	1.35174600
H	-0.40539600	1.08768700	2.01671300
H	0.21635600	-0.63470600	1.83546700
O	-1.33124400	-2.54986700	-1.69636900
O	-3.11941100	2.16203700	-1.08624700
C	-2.48231400	1.30563800	-0.68061100

C	-1.38380200	-1.60463300	-1.05788100
H	-0.44746500	0.43644800	-1.07725100
Co	-1.48438800	-0.08059900	-0.10189700
C	-2.51677900	-0.64711300	1.21925200
O	-3.16373600	-1.00643800	2.08808400
H	-0.15059500	2.69231900	0.13169700
H	0.96730700	2.32856500	-1.19649100
H	1.57658300	2.54816100	0.45045500
C	1.62692600	-0.29314200	-0.42457700
H	1.29740000	-1.31317000	-0.18179000
H	1.61899900	-0.23152500	-1.52393600
C	3.09280600	-0.14979700	0.04125000
C	3.79741400	1.03287700	-0.61942300
C	3.19900900	-0.03768100	1.55636900
C	3.81075000	-1.42221000	-0.40667900
H	3.70665000	0.98950400	-1.71257100
H	3.41259100	2.00287100	-0.29268000
H	4.86826200	1.01748200	-0.38047000
H	2.74072400	-0.90022400	2.05678400
H	4.25198400	-0.00351700	1.86330900
H	2.71517000	0.86568300	1.94663500
H	4.87566900	-1.38361700	-0.14624400
H	3.38422500	-2.31385800	0.06928600
H	3.74071200	-1.55935400	-1.49347000

f in entry 8

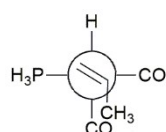


Co	1.43596400	-0.12828100	-0.05373700
H	-0.20113400	0.36435300	0.55627500
C	1.84965600	-1.03620700	1.43290300
C	2.65404300	1.16976300	0.08467300
C	1.34888800	-1.51243800	-1.17881900
O	1.35454300	-2.35763900	-1.94575000
O	3.46233700	1.97538300	0.09479700
O	2.09496200	-1.61161000	2.38523000
C	0.49998300	0.96639900	-1.41111000
C	-0.56857900	0.97908700	-0.35180900
C	-0.79579600	2.37640400	0.21101800
H	-1.40377100	2.97157800	-0.48223900
C	-1.82231000	0.23996800	-0.83052500
H	-2.28625500	0.85002600	-1.62373500

H	-1.47495600	-0.67698700	-1.33191500
H	0.15751700	2.89792000	0.35166400
H	-1.30403900	2.36685500	1.17943300
H	0.93672400	1.94139600	-1.63661900
H	0.22645100	0.46111100	-2.33968200
C	-2.91434000	-0.17713600	0.16946800
C	-3.82257900	-1.16456600	-0.56150000
C	-2.31651200	-0.87569700	1.38569900
C	-3.77673900	0.99932500	0.61975700
H	-4.24715400	-0.71752800	-1.46989200
H	-3.27610500	-2.06804800	-0.86007900
H	-4.65951500	-1.47755400	0.07498000
H	-1.73214300	-0.19452100	2.01714300
H	-3.10990500	-1.29289100	2.01848400
H	-1.66008200	-1.70591700	1.09084200
H	-4.61908200	0.64425300	1.22713800
H	-3.22905800	1.72553500	1.22723100
H	-4.19754800	1.53552000	-0.24087400

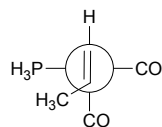
3 Structures in Table 3

TS_{rotate}-ma in entry 1



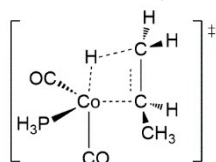
Co	0.36025600	0.04075900	-0.17004100
C	1.48856200	1.38585300	-0.22661700
O	2.26346800	2.22756200	-0.28903300
H	1.17648400	-0.21399900	-1.41278100
P	0.79754900	-2.08540600	0.01482700
H	0.43094200	-2.85107800	1.14843400
H	0.30984300	-2.99027700	-0.95849500
H	2.14492700	-2.50563700	-0.03131600
C	-0.23432900	0.25138200	1.48252000
O	-0.57594300	0.36978900	2.56928600
C	-1.15667000	-0.14161000	-1.76157300
C	-1.66848700	0.75557300	-0.87078800
C	-2.80669900	0.43076500	0.04487000
H	-1.53296800	-1.16426900	-1.78432000
H	-0.62255500	0.18608800	-2.64631300
H	-1.45994800	1.81427900	-1.02614900
H	-2.83427900	-0.63801900	0.28831300
H	-2.77979600	0.99142300	0.98388700
H	-3.75726800	0.68148600	-0.44508000

c in entry 1



Co	-0.38860400	-0.07975300	0.15868100
C	-2.10834000	0.24891000	0.28529900
O	-3.23513800	0.42487000	0.39673800
H	-0.75302300	-0.70827500	1.47992400
P	0.68572200	-1.98166000	0.07343000
H	1.55033500	-2.34412100	-0.98974700
H	1.57686200	-2.31475700	1.12310400
H	-0.05295700	-3.18471500	0.09820100
C	-0.16229500	0.38503900	-1.53364600
O	0.00072000	0.66034800	-2.63356700
C	0.65666800	1.04296300	1.70945900
C	1.21807500	1.44148800	0.52962700
C	2.57419100	1.00760500	0.06912500
H	1.18395500	0.34418800	2.35758200
H	-0.14204200	1.60944000	2.17760200
H	3.30975100	1.80121200	0.25781100
H	2.91766300	0.11685200	0.60866100
H	2.61335000	0.79445400	-1.00520300
H	0.80814700	2.32618000	0.04167300

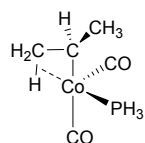
TS_{ma} in entry 1



Co	-0.34706700	-0.00825500	-0.18074800
C	-2.09648000	-0.12133500	-0.39516300
O	-3.22932700	-0.18988000	-0.55201100
H	-0.47341700	0.71733900	-1.49668500
P	0.46089600	1.93546900	0.58298800
H	1.29446400	2.00212400	1.72793000
H	1.29537500	2.73304800	-0.24140000
H	-0.40308500	2.98629200	0.97027000
C	-0.19388900	-0.98258700	1.27935000
O	-0.05285600	-1.61102800	2.22678200
C	0.78803200	-0.42091000	-1.91341400
C	1.37743300	-1.04055600	-0.81176200
C	2.67389100	-0.57203100	-0.22204500

H	1.30043800	0.42713500	-2.37071300
H	0.17330800	-0.99561400	-2.60109900
H	1.14805500	-2.09576600	-0.66009400
H	2.86517800	0.48244900	-0.45637700
H	2.70307500	-0.68472700	0.86791200
H	3.51752000	-1.14964000	-0.62433300

e in entry 1



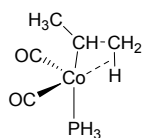
Co	0.28005000	0.10441900	-0.18024400
C	1.97786000	-0.32518600	-0.47884100
O	3.07520800	-0.58607900	-0.67360900
P	-0.26326900	-1.77934700	0.87116400
H	-1.10571200	-1.70996100	2.00560300
H	-0.93082600	-2.87931700	0.26943700
H	0.76247700	-2.54485900	1.47158100
C	0.56083400	1.60251100	0.67909000
O	0.70821300	2.56578300	1.28324300
C	-1.23801500	0.19842700	-1.81468400
C	-1.58905400	0.70359800	-0.45365800
C	-2.77459700	0.07733200	0.23068100
H	-2.81170300	-1.01194100	0.09578500
H	-2.77833600	0.27899100	1.30837000
H	-3.72101100	0.47179200	-0.16896600
H	-1.82539100	-0.67795000	-2.11087700
H	-1.27145100	0.95562900	-2.60301400
H	-1.66867100	1.79407600	-0.42536300
H	-0.15122300	-0.18329500	-1.89602400

TS_{iso}-ma in entry 1

Co	0.21633000	-0.10869100	0.10966000
C	1.55237800	-1.35257600	-0.00262800
O	2.37383900	-2.11191800	-0.24446000
P	1.01797200	1.92258800	0.50903400
H	0.85126200	2.93618200	-0.46209400
H	0.52588600	2.67874200	1.60283900
H	2.38633300	2.18692700	0.76466200
C	-0.27426200	0.18938600	-1.51153200
O	-0.61225800	0.37647900	-2.59452700
C	-1.07929900	-0.70865600	1.75374600
C	-1.60432900	-0.85082800	0.38596100

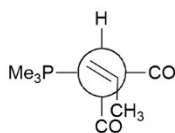
C	-2.81776500	-0.03684500	0.02773300
H	-2.69776100	1.01194800	0.32783300
H	-3.02319700	-0.05020400	-1.04747300
H	-3.71854400	-0.42190700	0.52933500
H	-1.61604500	0.02646600	2.36236000
H	-0.95162900	-1.64768700	2.29928500
H	-1.65019100	-1.88030900	0.02297000
H	0.03041100	-0.30368100	1.79616300

g in entry 1



Co	-0.16143500	-0.04271300	-0.08016800
C	-0.59674300	-1.52281600	0.77792500
O	-0.85253800	-2.43065300	1.43137800
P	-2.22616200	0.57442500	-0.56188800
H	-2.65595600	1.90679500	-0.37070600
H	-2.70954200	0.43178600	-1.88423100
H	-3.31547700	-0.05282500	0.08251300
C	0.34350800	1.48979600	0.65083100
O	0.62495300	2.43117300	1.24323600
C	1.28212200	-0.60249700	-1.74064900
C	1.68165000	-0.70427600	-0.29786700
C	2.87256300	0.11402400	0.12332600
H	2.82158100	1.14081400	-0.25967000
H	2.96364000	0.17194900	1.21347800
H	3.80726500	-0.32747500	-0.25576000
H	1.89454300	0.11209500	-2.30089000
H	1.25518700	-1.56046400	-2.26737100
H	1.79126000	-1.74067700	0.03452300
H	0.22073800	-0.19467400	-1.87734200

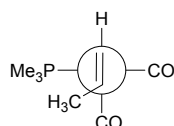
TS_{rotate}-ma in entry 2



Co	-0.58563300	0.38775100	-0.15768700
C	-1.74708800	1.69925700	-0.20417000
O	-2.45640100	2.59961700	-0.25540000
H	-0.14993000	1.24667700	-1.32667000
P	1.58156500	0.14162400	-0.09512300

C	2.44222300	1.32079200	1.00635000
C	2.23313900	-1.46058300	0.52116100
C	2.52622900	0.33466100	-1.64883300
H	3.52833700	1.16688000	0.99836500
H	2.22008100	2.34357900	0.68735100
H	2.07151100	1.20205000	2.02979200
H	1.91716400	-2.27310700	-0.14231400
H	3.32860900	-1.45973400	0.57442700
H	1.82973200	-1.66337600	1.51923000
H	2.16958900	-0.37352800	-2.40290500
H	2.37444500	1.34483100	-2.04087300
H	3.59756500	0.16862100	-1.48488200
C	-0.73398000	-0.09047200	1.52762300
O	-0.76020400	-0.38019900	2.63991400
C	-1.74477400	-1.43170700	-0.77422800
C	-0.87875200	-1.08076900	-1.76993300
C	-1.54227200	-2.62888800	0.10106500
H	-0.47875600	-2.87262300	0.21095100
H	-1.96235500	-2.50096700	1.10346200
H	-2.03600900	-3.50562900	-0.34055700
H	-1.19116400	-0.45923000	-2.60219900
H	0.02901600	-1.66437800	-1.92806700
H	-2.75474200	-1.02279600	-0.80104600

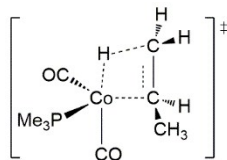
c in entry 2



Co	-0.69062000	-0.25932400	0.14290100
C	-1.95303900	-1.48320800	0.24256900
O	-2.72825000	-2.32389100	0.33126400
H	-0.31470900	-0.97750200	1.42181200
P	1.48901500	-0.36076500	0.09069900
C	2.12621300	-2.07558300	0.03907200
C	2.39683000	0.38536100	-1.31906200
C	2.43463800	0.31667800	1.50803600
H	3.22184100	-2.09989800	-0.01109500
H	1.79196100	-2.61368300	0.93128300
H	1.71531100	-2.59099900	-0.83436800
H	2.20902000	1.46314400	-1.36426600
H	3.47735400	0.21877200	-1.23436400
H	2.04495300	-0.05344700	-2.25836100
H	2.29680000	1.40006700	1.58402800

H	2.07695500	-0.13731800	2.43761900
H	3.50625700	0.11068100	1.39977300
C	-0.84404700	0.15995900	-1.55877800
O	-0.88963900	0.43525400	-2.67318500
C	-1.17408200	1.18520200	1.70848800
C	-1.30879200	1.85720400	0.52677800
H	-0.29949600	1.34389400	2.33709000
H	-2.02807500	0.73055800	2.20045400
C	-0.33118300	2.87888900	0.03690200
H	0.64670700	2.76722400	0.52039700
H	-0.18373500	2.84210700	-1.04807100
H	-0.69150000	3.89043200	0.26962200
H	-2.29424200	1.88128900	0.06097200

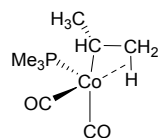
TS_{ma} in entry 2



Co	-0.73867100	0.21495500	-0.17156300
C	-1.55781700	1.78372500	-0.30099900
O	-2.06295000	2.81125600	-0.38011400
H	-0.45962500	0.42314900	-1.64652200
P	1.48461100	0.24830000	-0.02238100
C	2.20058400	1.93362300	0.06435200
C	2.29256400	-0.54221200	1.42405100
C	2.47749400	-0.45858300	-1.39738500
H	3.29492200	1.91381200	0.14300900
H	1.91443800	2.49626600	-0.83021000
H	1.78892600	2.46025400	0.93116500
H	2.02665400	-1.60366100	1.46735500
H	3.38489800	-0.44978200	1.38256200
H	1.93595200	-0.07321300	2.34705800
H	2.28375000	-1.53095600	-1.50421600
H	2.20045500	0.02931200	-2.33798300
H	3.55198800	-0.31540300	-1.22975000
C	-1.06931700	-0.15338400	1.50716100
O	-1.24368700	-0.44111800	2.60545700
C	-1.38317400	-1.73651800	-0.55202300
C	-1.19675900	-1.07686500	-1.77301700
C	-0.47450900	-2.83857500	-0.09329100
H	0.54558500	-2.70113400	-0.47198000
H	-0.41620400	-2.90484100	0.99919800
H	-0.82620600	-3.81626200	-0.45265000

H	-2.05869900	-0.70538600	-2.32191900
H	-0.36889400	-1.39363400	-2.41044000
H	-2.40427400	-1.78519300	-0.17259000

e in entry 2



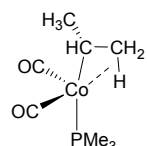
Co	-0.75735600	0.23371600	-0.23121600
C	-0.67590000	1.95528700	-0.63328200
O	-0.63665900	3.07119300	-0.89519900
P	1.44694500	0.04136900	0.18892700
C	2.29026400	1.65852300	0.40299100
C	1.91912300	-0.75663700	1.77298600
C	2.62554200	-0.74956700	-0.98485800
H	3.34107500	1.52989600	0.68900600
H	2.24614700	2.23349600	-0.52769200
H	1.78097900	2.24131600	1.17753600
H	1.63106800	-1.81037200	1.78255900
H	2.99969800	-0.68297700	1.94767100
H	1.39304100	-0.25728100	2.59297600
H	2.37945100	-1.80313000	-1.14711200
H	2.56789800	-0.24037500	-1.95292000
H	3.65694900	-0.68536200	-0.61642700
C	-1.96044700	0.34990100	1.02675200
O	-2.70444400	0.39392800	1.90067900
C	-1.20405800	-1.69474500	-0.35124100
C	-1.11167500	-1.32769500	-1.79882900
C	-0.33884400	-2.82930000	0.12514200
H	-2.04307800	-1.45581400	-2.35833700
H	-0.29377300	-1.83974400	-2.31882600
H	-2.24027000	-1.87081700	-0.04555500
H	-0.87115000	-0.21404400	-1.97300700
H	-0.35734500	-2.91839200	1.21736000
H	-0.68901700	-3.79302600	-0.27671800
H	0.70755500	-2.71981400	-0.18337300

TS_{iso}-ma in entry 2

Co	-0.58399500	0.37721300	-0.11777000
C	-0.73307100	2.18447000	-0.21558400
O	-0.81518500	3.32507000	-0.12201500
P	1.54900400	-0.25168700	-0.10843400
C	2.62120400	0.68142400	1.04530600

C	1.92098900	-1.97742000	0.39499100
C	2.50594700	-0.14262700	-1.67040600
H	3.65770800	0.32282700	1.02145300
H	2.60176400	1.74464100	0.78619700
H	2.23427300	0.57948500	2.06493900
H	1.45333200	-2.67597500	-0.30757700
H	3.00020400	-2.17505600	0.42346600
H	1.49747200	-2.16907600	1.38724000
H	2.04159000	-0.77612000	-2.43435000
H	2.49561200	0.88877500	-2.03695200
H	3.54619900	-0.46353100	-1.53425400
C	-0.83835200	-0.00928400	1.53156000
O	-0.98646700	-0.29654600	2.63828800
C	-2.14508100	-0.78204200	-0.53225300
C	-1.52515000	-0.53448100	-1.84307700
C	-2.16551600	-2.20183500	-0.03493200
H	-2.14645000	0.01850400	-2.55307600
H	-1.09971000	-1.42823200	-2.31385500
H	-3.08463000	-0.24961600	-0.36764100
H	-0.58546600	0.19271300	-1.80036900
H	-2.46251800	-2.26584700	1.01708600
H	-2.87366400	-2.82212300	-0.60558600
H	-1.17551700	-2.66823300	-0.12422700

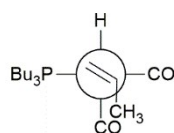
g in entry 2



Co	-0.48561700	0.13418200	0.01589600
C	-0.38765300	1.70651600	0.79606400
O	-0.32770000	2.68079000	1.40378800
P	1.69968300	-0.14687700	-0.19129500
C	2.79122000	1.11599400	0.55988200
C	2.42560700	-1.68746600	0.47905700
C	2.32278500	-0.17721800	-1.91659700
H	3.84926500	0.87658200	0.39984400
H	2.57850900	2.09804100	0.12557500
H	2.60048000	1.18004900	1.63587700
H	1.96403200	-2.55581900	-0.00192100
H	3.50922500	-1.72304300	0.31609200
H	2.22542300	-1.75684700	1.55298700
H	1.84745300	-0.99436200	-2.46857500
H	2.07081700	0.76266700	-2.41808200

H	3.41045500	-0.31426800	-1.94690800
C	-0.79086400	-1.42280400	0.78436700
O	-0.95138600	-2.37639000	1.40638500
C	-2.37645900	0.44688300	-0.45725000
C	-1.78785500	0.34491800	-1.83479700
C	-3.45377500	-0.55017900	-0.12118600
H	-1.86144800	1.26331200	-2.42441300
H	-2.19374400	-0.49489400	-2.40934400
H	-2.70479000	1.46268400	-0.21852500
H	-0.66168000	0.12900200	-1.81929500
H	-3.67165300	-0.56862300	0.95248000
H	-4.39641900	-0.30967400	-0.63772000
H	-3.17486700	-1.56962400	-0.41647700

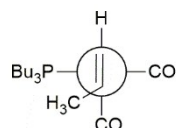
TS_{rotate}-ma in entry 3



Co	-1.39937700	-0.71212700	-0.81892000
C	-3.04496400	-0.25689300	-1.24680600
O	-4.09270400	0.12374800	-1.52086300
H	-1.18087200	0.32053000	-1.90755700
P	0.28907600	0.49766400	-0.12672900
C	-1.68936600	-1.43109700	0.75850000
O	-1.86099500	-1.84991800	1.81552600
C	1.73402200	0.62143500	-1.26765500
C	2.88844400	1.52011900	-0.86012200
H	1.31790700	0.93748600	-2.23564400
H	2.09721900	-0.40352700	-1.42958800
C	4.01985600	1.50100600	-1.87614800
H	2.54112700	2.55625200	-0.73266900
H	3.28594900	1.21383700	0.11970700
C	5.17491900	2.39731000	-1.47490100
H	4.37389600	0.46706200	-2.00519500
H	3.62987500	1.80567400	-2.85870200
H	5.98562800	2.37706000	-2.21046300
H	4.85165600	3.44042100	-1.37079200
H	5.59869000	2.09163500	-0.51027200
C	-0.16404200	2.26485000	0.13623900
C	-1.41825800	2.45474200	0.97236700
H	-0.30876500	2.70228400	-0.86346800
H	0.68435600	2.79196600	0.59758300
C	-1.76626200	3.91958000	1.17717400

H	-2.25880800	1.93712800	0.48858500
H	-1.29948100	1.96947100	1.95513000
C	-3.03446200	4.10373500	1.98734700
H	-0.92605000	4.43216500	1.67010300
H	-1.87482200	4.40358000	0.19474000
H	-3.28254000	5.16085000	2.12929800
H	-3.89095300	3.62683400	1.49568600
H	-2.93980100	3.65120900	2.98231800
C	1.07209600	0.07382400	1.49123200
C	1.74105800	-1.28936100	1.49407800
H	0.27002800	0.09608800	2.24254900
H	1.78378200	0.86088600	1.77948400
C	2.12173600	-1.76456400	2.88560100
H	1.06772200	-2.03096900	1.03706200
H	2.63972800	-1.27082100	0.85624400
C	2.78002700	-3.12985600	2.86614800
H	2.78985300	-1.02722800	3.35594700
H	1.21763200	-1.79274800	3.51212900
H	3.04297200	-3.47506600	3.87138700
H	2.11417200	-3.88208400	2.42425700
H	3.70123900	-3.12105200	2.27003900
C	-0.41939300	-1.94098600	-2.38221000
C	-1.16501700	-2.81758500	-1.65236300
H	-0.80631700	-1.48783000	-3.28846300
H	-2.19388300	-3.00461900	-1.95957600
H	0.66259000	-1.91453600	-2.25950800
C	-0.56635400	-3.81980600	-0.71719800
H	-1.17982200	-4.00552400	0.17005600
H	-0.45222500	-4.78460800	-1.23016100
H	0.43070000	-3.50868600	-0.38344900

c in entry 3

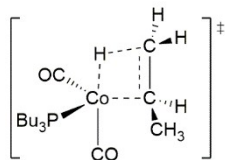


Co	-1.36574900	-0.96900300	-0.74378800
C	-3.10322800	-0.81128700	-0.99692800
O	-4.22478200	-0.62347400	-1.15309600
H	-1.41474800	0.13228600	-1.78295300
P	0.15400900	0.48690700	-0.12593500
C	-1.38101400	-1.82836600	0.78957900
O	-1.36574200	-2.35024800	1.81410400
C	1.56591800	0.73410300	-1.29151000

C	2.60086700	1.79201400	-0.94778400
H	1.10402500	0.95369200	-2.26577300
H	2.05271400	-0.24508200	-1.41325300
C	3.73167800	1.84070800	-1.96312600
H	2.12709800	2.78333500	-0.89215900
H	3.02588700	1.60668500	0.05084100
C	4.75965200	2.90612500	-1.63670600
H	4.21544900	0.85350300	-2.01342200
H	3.31194200	2.01648500	-2.96494500
H	5.57210900	2.93227700	-2.37017700
H	4.30476900	3.90411800	-1.61464000
H	5.21150000	2.73432600	-0.65185800
C	-0.51478700	2.19880300	0.03662900
C	-1.75903300	2.29102700	0.90264000
H	-0.73928900	2.54302200	-0.98440000
H	0.27202200	2.85745700	0.43292100
C	-2.29652000	3.70875900	1.00234600
H	-2.53586500	1.62648900	0.49812500
H	-1.54467000	1.91392300	1.91564400
C	-3.54386800	3.79418500	1.86001300
H	-1.51546900	4.37071000	1.40673300
H	-2.51031500	4.08464700	-0.00964500
H	-3.93020100	4.81683000	1.92391000
H	-4.34521000	3.16306700	1.45727700
H	-3.34650000	3.45242000	2.88364800
C	0.98252700	0.27872100	1.51347300
C	1.89414600	-0.93219000	1.60255800
H	0.17431900	0.18854300	2.25369500
H	1.52963400	1.19842600	1.76820800
C	2.33641600	-1.23328200	3.02429200
H	1.38214400	-1.81664200	1.19783700
H	2.78170100	-0.78703200	0.96548300
C	3.26132200	-2.43212300	3.09722300
H	2.82876000	-0.34712800	3.45298600
H	1.44329000	-1.40950000	3.64246600
H	3.56555600	-2.65622800	4.12483000
H	2.77544100	-3.32994100	2.69490700
H	4.17481800	-2.26748900	2.51213500
C	-0.56836500	-1.89353000	-2.57231800
C	-0.55311700	-2.88305100	-1.63286000
H	-1.40008700	-1.78138100	-3.25988200
H	-1.43166000	-3.52292300	-1.54734500
H	0.35614200	-1.39608600	-2.86192600
C	0.70010500	-3.40559100	-1.00602600

H	0.56493400	-3.70254600	0.03989800
H	1.04109200	-4.30104600	-1.54385100
H	1.51175500	-2.67012200	-1.05104800

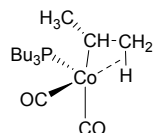
TS_{ma} in entry 3



Co	-1.30465000	-1.11015200	-0.77902600
C	-2.98725400	-0.53658700	-0.94054900
O	-4.04796400	-0.10030300	-1.00376100
H	-1.08647300	-0.43046600	-2.11581800
P	0.14435300	0.45671800	-0.16213600
C	-1.37227600	-1.91651000	0.76817400
O	-1.35979600	-2.43168500	1.79637400
C	1.55740000	0.78030600	-1.30995300
C	2.59513800	1.81638300	-0.91166600
H	1.09143200	1.05442400	-2.26965100
H	2.04691100	-0.18783100	-1.49222600
C	3.67643700	1.97931300	-1.96771100
H	2.11826700	2.79162700	-0.73332300
H	3.06568200	1.53619300	0.04322300
C	4.71948800	3.00900100	-1.57961800
H	4.15690400	1.00541900	-2.14593600
H	3.20946800	2.25879900	-2.92401100
H	5.49262200	3.12133800	-2.34684300
H	4.26555100	3.99563700	-1.42421100
H	5.2232300	2.73323800	-0.64434100
C	-0.65458000	2.11693700	-0.06167800
C	-1.71459500	2.21160900	1.02542500
H	-1.11223000	2.28381200	-1.04872300
H	0.10170600	2.90307100	0.07685600
C	-2.64078800	3.40120300	0.83730300
H	-2.31571800	1.28930000	1.04689600
H	-1.23195500	2.27744100	2.01277500
C	-3.68253900	3.50165700	1.93352200
H	-2.04660500	4.32696200	0.79183600
H	-3.13532900	3.31410000	-0.14185400
H	-4.35432100	4.35367600	1.78613500
H	-4.30176400	2.59701200	1.97122900
H	-3.21524200	3.61748100	2.91950600
C	0.94897900	0.32848600	1.49365100

C	1.94114000	-0.81614600	1.61021000
H	0.13325900	0.17960200	2.21614900
H	1.42295200	1.28699600	1.75520100
C	2.39567500	-1.05144300	3.04086100
H	1.49253700	-1.74231200	1.22121500
H	2.82127700	-0.62583600	0.97494800
C	3.40866700	-2.17384100	3.14926300
H	2.81744600	-0.12036800	3.44931800
H	1.51480200	-1.27794700	3.66013600
H	3.72222700	-2.34697200	4.18396200
H	2.99682600	-3.11673400	2.76852200
H	4.31074000	-1.95404000	2.56460800
C	-0.64172000	-1.97091500	-2.58816100
C	-0.56844900	-2.91326400	-1.55539400
H	0.29187100	-1.58277300	-3.00024100
H	-1.45310100	-2.02655000	-3.31032500
H	-1.39864900	-3.61514700	-1.47096400
C	0.74728000	-3.41048700	-1.03377900
H	0.69161900	-3.74163700	0.00924100
H	1.09512900	-4.27313200	-1.62017200
H	1.52415400	-2.63938700	-1.09765100

e in entry 3



Co	-1.44273700	-1.17069700	-0.76835400
C	-2.83622100	-0.07606300	-0.85704400
O	-3.76163700	0.59851100	-0.93951700
P	0.16100400	0.40056200	-0.25660500
C	-1.97036400	-2.15081600	0.55989900
O	-2.22760600	-2.80161200	1.47305500
C	1.64066200	0.69089500	-1.34519400
C	2.77033900	1.55794000	-0.81476600
H	1.22599200	1.12778500	-2.26830500
H	2.03886200	-0.28693200	-1.64672400
C	3.85190900	1.80078100	-1.85579800
H	2.38751100	2.52909000	-0.46602600
H	3.22535400	1.08448200	0.06912300
C	4.99186600	2.64570900	-1.32183700
H	4.23580300	0.83312500	-2.21251600
H	3.40471200	2.28523600	-2.73678900
H	5.76540900	2.81787200	-2.07737100

H	4.63587600	3.62771000	-0.98645700
H	5.47398800	2.16497600	-0.46165600
C	-0.52732800	2.12143500	-0.20216400
C	-1.50002100	2.37215900	0.94124400
H	-1.03393400	2.27299000	-1.16720900
H	0.28959400	2.85610500	-0.16232800
C	-2.37797300	3.58968400	0.70689700
H	-2.14396200	1.49398600	1.10208000
H	-0.94209100	2.50188300	1.88072200
C	-3.33489100	3.83929200	1.85549500
H	-1.74222300	4.47303400	0.54105100
H	-2.94422700	3.44648000	-0.22521100
H	-3.96538000	4.71766400	1.68251900
H	-4.00114900	2.98052300	2.00441100
H	-2.79602500	4.00082400	2.79756100
C	0.87824800	0.28289200	1.44377400
C	1.67069500	-0.98182700	1.71545100
H	0.02207300	0.32625500	2.13202600
H	1.48439600	1.17947000	1.64707000
C	2.28315100	-1.00180800	3.10524200
H	1.01158800	-1.85338200	1.59196100
H	2.47230000	-1.10891200	0.96991200
C	3.04158600	-2.28537200	3.38103000
H	2.95262700	-0.13527400	3.22028300
H	1.48817800	-0.86517400	3.85359100
H	3.48461300	-2.29644400	4.38232900
H	2.38242800	-3.15873400	3.30315000
H	3.85562700	-2.42867200	2.65934800
C	1.03192000	-3.06347500	-1.00686900
C	-0.39800900	-2.75218500	-1.35133200
C	-0.66905400	-2.06011400	-2.63976700
H	-1.01693300	-3.64732600	-1.23258000
H	0.23955600	-1.69655200	-3.13285600
H	-1.27963700	-2.62934300	-3.34673700
H	-1.29063800	-1.08512500	-2.52150800
H	1.12846800	-3.43811800	0.01820400
H	1.43494100	-3.84567200	-1.66916300
H	1.68997500	-2.19338900	-1.10115500

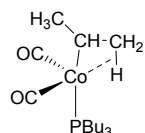
TS_{iso}-ma in entry 3

Co	-1.28102300	-1.11283300	-0.81026500
C	-2.90272800	-0.36210900	-1.09472600
O	-3.94129100	0.12488900	-1.15252800
P	0.16551700	0.48806800	-0.16538700

C	-1.45294900	-1.86981700	0.71878500
O	-1.51843700	-2.38227700	1.74939200
C	1.60719000	0.80410100	-1.28287400
C	2.64878200	1.82762300	-0.86171700
H	1.16692900	1.08739000	-2.25227100
H	2.08915400	-0.16944800	-1.45762100
C	3.74687900	1.98887000	-1.90068100
H	2.17773300	2.80563400	-0.68362700
H	3.10325500	1.53711200	0.09772900
C	4.79606600	3.00204300	-1.48624900
H	4.21872500	1.01152000	-2.08295400
H	3.29696100	2.28457500	-2.86029600
H	5.58072600	3.11463900	-2.24165900
H	4.35096400	3.99179900	-1.32525900
H	5.28283200	2.70944400	-0.54767400
C	-0.58907200	2.16732400	-0.02360200
C	-1.67449400	2.24510200	1.03988300
H	-1.01703300	2.38661300	-1.01385300
H	0.18181000	2.92812900	0.16673600
C	-2.56209900	3.46827100	0.88418200
H	-2.30199000	1.34061900	1.00739600
H	-1.21518300	2.25323600	2.04033000
C	-3.61735600	3.55783800	1.96838100
H	-1.93982800	4.37657300	0.88389100
H	-3.04329800	3.43445600	-0.10483500
H	-4.26365700	4.43267900	1.84251100
H	-4.26096500	2.66958500	1.96522400
H	-3.16160300	3.62566700	2.96415200
C	0.93532100	0.29392900	1.50048300
C	1.84215400	-0.91823400	1.61997700
H	0.09822700	0.19141900	2.20658300
H	1.46622700	1.21675000	1.78024200
C	2.28903500	-1.18152200	3.04795100
H	1.31832600	-1.80800200	1.24104400
H	2.72915900	-0.79940700	0.97693500
C	3.21214100	-2.37986900	3.14905400
H	2.78616400	-0.28570900	3.45034000
H	1.39887200	-1.33843200	3.67525800
H	3.51627700	-2.58026800	4.18167500
H	2.72559000	-3.28624900	2.76742100
H	4.12574900	-2.22927200	2.56041000
C	0.58243100	-3.51612400	-0.95221400
C	-0.67645800	-2.88826800	-1.48349400
C	-0.56158100	-1.99557300	-2.64324600

H	-1.51877400	-3.58197000	-1.53037200
H	0.45820700	-1.89356800	-3.03250100
H	-1.26851600	-2.18847900	-3.45344300
H	-0.80544500	-0.85013600	-2.40164100
H	0.43756400	-3.94540600	0.04598700
H	0.93174700	-4.33323200	-1.60208000
H	1.39821600	-2.78518000	-0.88008100

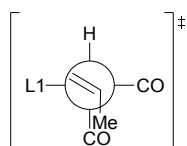
g in entry 3



Co	-1.46166800	-0.49235100	-0.71614900
C	-1.73149900	0.80698100	-1.86725900
O	-1.95289600	1.73231000	-2.51584900
P	0.48618600	0.31436400	-0.04180900
C	-2.14022000	-0.65920200	0.89799100
O	-2.60253400	-0.63071900	1.95200000
C	1.83420300	0.08868400	-1.28327400
C	3.23180400	0.55408900	-0.91237300
H	1.47955200	0.60881900	-2.18641800
H	1.84455700	-0.97782100	-1.55177100
C	4.22805000	0.34406100	-2.04181000
H	3.22028500	1.62000100	-0.63894800
H	3.58723500	0.01864000	-0.01835800
C	5.62574900	0.80232900	-1.67489200
H	4.24134700	-0.72059200	-2.31964900
H	3.87858400	0.87970800	-2.93693200
H	6.33685400	0.64744000	-2.49281700
H	5.64122200	1.87015700	-1.42413100
H	6.00629900	0.25861000	-0.80134700
C	0.52651000	2.12828700	0.27188000
C	-0.58830600	2.61332400	1.18442400
H	0.44783200	2.61765600	-0.71113700
H	1.50773400	2.40342000	0.68591000
C	-0.54603400	4.11657900	1.40125200
H	-1.56199900	2.32754200	0.76028600
H	-0.53026600	2.10589600	2.16047700
C	-1.66093600	4.60060200	2.30740600
H	0.43105300	4.39865700	1.82259100
H	-0.60759600	4.62255400	0.42605400
H	-1.62681600	5.68470700	2.45754100
H	-2.64492000	4.35603400	1.88975200

H	-1.60320700	4.12879700	3.29604600
C	1.18296700	-0.37891100	1.51583300
C	1.38314200	-1.88361600	1.46028900
H	0.47158700	-0.12738500	2.31573000
H	2.12392600	0.13544800	1.76133300
C	1.88607300	-2.45854500	2.77381700
H	0.43277400	-2.36906500	1.18675700
H	2.09286200	-2.14321800	0.65782000
C	2.08181100	-3.96049800	2.71110100
H	2.83138100	-1.96637200	3.04872000
H	1.17440000	-2.20441300	3.57317900
H	2.44277700	-4.36807500	3.66099300
H	1.14263200	-4.47279800	2.46921300
H	2.80987100	-4.23532300	1.93765700
C	-3.90197100	-2.31829700	-0.80646500
C	-2.79365300	-1.65950900	-1.58531800
C	-1.55991600	-2.48781100	-1.80510100
H	-3.17838100	-1.23157600	-2.51560600
H	-3.52617900	-2.81682300	0.09625200
H	-4.66184800	-1.59573500	-0.48833600
H	-4.41664300	-3.08378700	-1.40869700
H	-1.59973600	-3.45484800	-1.29131900
H	-1.30270800	-2.64199700	-2.85740900
H	-0.61544300	-2.00024000	-1.37448800

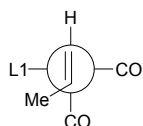
TS_{rotate}-ma in entry 4



O	-1.69096700	1.60608100	2.63160700
O	1.83797000	3.06734900	0.23992000
P	-0.18817800	-0.73455100	0.17394100
C	-1.26562500	1.55089200	1.56548600
C	0.85976700	2.47466000	0.13712400
C	-1.08105200	-1.85745600	1.35916700
C	-2.60045000	-1.66310000	1.34484800
C	-3.27779800	-1.43780100	-0.00591000
C	-2.88644900	-2.37446900	-1.14801300
C	-1.62847500	-1.99177100	-1.92601100
C	-0.29954500	-2.00777600	-1.17439500
C	-0.03780200	-3.33133500	-0.45275900
C	-0.63015500	-3.28555100	0.97450700
C	1.55318800	-0.94237500	0.77682100

C	2.62158700	-0.67334200	-0.26971500
C	4.00053300	-0.49647700	0.34167400
C	5.08706300	-0.27329500	-0.69456000
C	6.45582700	-0.08047100	-0.07159300
H	-0.72027000	-1.61352100	2.36842800
H	-2.85746700	-0.81457600	1.99207600
H	-3.04972400	-2.54473800	1.82800400
H	-3.10946000	-0.39814400	-0.32118100
H	-4.36091800	-1.51386000	0.15894900
H	-3.71127800	-2.39836300	-1.87288800
H	-2.80564500	-3.40824600	-0.77845700
H	-1.53008200	-2.69032600	-2.77093200
H	-1.76825300	-1.00012400	-2.37798800
H	0.49628500	-1.78772800	-1.89907000
H	1.04263700	-3.51312300	-0.40272000
H	-0.45429500	-4.16881600	-1.02890500
H	0.11143100	-3.64920900	1.69500000
H	-1.48192100	-3.97059900	1.06524500
H	1.64688200	-0.21926800	1.60019600
H	1.69738900	-1.93697300	1.22024600
H	2.64767400	-1.50054800	-0.99625400
H	2.36649200	0.22622800	-0.84909800
H	3.97831700	0.35692800	1.03848300
H	4.25200200	-1.37649800	0.95659300
H	5.10800300	-1.12626400	-1.39001500
H	4.82629500	0.60343300	-1.30622300
H	6.46622200	0.78629000	0.60059400
H	7.23384300	0.07941700	-0.82559700
H	6.74884000	-0.95481900	0.52313400
Co	-0.55216100	1.42620600	-0.04255700
H	0.21631500	1.11045700	-1.30330200
C	-1.93036300	1.79139300	-1.69528600
C	-2.21433000	2.70725100	-0.71818500
H	-2.53160700	0.89467400	-1.81236700
H	-3.03764500	2.47726700	-0.03928700
H	-1.34926700	2.08497700	-2.56644400
C	-1.79734500	4.14230800	-0.77118200
H	-2.62482100	4.76574400	-1.13895000
H	-1.51690700	4.53115600	0.21336200
H	-0.94553100	4.28471500	-1.44503200

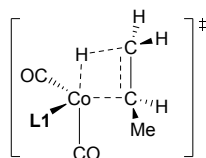
c in entry 4



O	1.09705300	-1.70281800	2.67473600
O	-1.43102200	-3.44477900	-0.64244900
P	0.11584400	0.72080700	0.15675900
C	0.90601800	-1.61320500	1.54438100
C	-0.59979900	-2.67713500	-0.44710600
C	0.97341900	1.82324100	1.38478100
C	2.49650700	1.68067100	1.33117900
C	3.15301100	1.58899100	-0.04638600
C	2.69614800	2.57878800	-1.11623300
C	1.44982800	2.16613800	-1.89745300
C	0.13704600	2.06728500	-1.12182300
C	-0.17300500	3.33690700	-0.32686700
C	0.46232700	3.24969500	1.07983500
C	-1.62068800	0.80632300	0.80139000
C	-2.68916200	0.48313800	-0.22865100
C	-4.05951900	0.28995500	0.39700500
C	-5.14802100	0.01358400	-0.62438000
C	-6.50694500	-0.19657700	0.01436300
H	0.64131600	1.51322500	2.38578400
H	2.78535600	0.78420500	1.89787100
H	2.93002300	2.52905400	1.88308300
H	3.01375000	0.57307300	-0.43961100
H	4.23596300	1.69494900	0.10125100
H	3.50627200	2.69308000	-1.84913600
H	2.56339200	3.58235700	-0.68461700
H	1.29489100	2.90025200	-2.70270800
H	1.64080400	1.20895000	-2.40448600
H	-0.66107300	1.84637600	-1.84361800
H	-1.25927900	3.45852600	-0.24149900
H	0.18379000	4.22280900	-0.86958300
H	-0.26858100	3.55447900	1.83737400
H	1.29385900	3.95890400	1.17435600
H	-1.65208700	0.06911400	1.61715000
H	-1.81692500	1.78446400	1.26186800
H	-2.74401800	1.29016200	-0.97649600
H	-2.41037100	-0.42382700	-0.78528200
H	-4.01418100	-0.54144900	1.11858300
H	-4.32778400	1.18105900	0.98853400
H	-5.19551300	0.84827400	-1.34035800
H	-4.87109000	-0.87087800	-1.21740500

H	-6.49205300	-1.04723500	0.70683300
H	-7.28658800	-0.39239600	-0.72933300
H	-6.81600100	0.68436800	0.59093700
Co	0.58762300	-1.40075000	-0.17306200
H	0.02862000	-0.97967000	-1.51468300
C	2.21049400	-1.71221700	-1.60884200
C	2.67942100	-2.16037900	-0.40627700
H	2.47421100	-0.72908100	-1.98793700
H	3.28673300	-1.48144700	0.19625400
H	1.83869900	-2.41715600	-2.34966100
C	2.76255200	-3.61032000	-0.04485400
H	3.76992000	-3.99512400	-0.25606900
H	2.56854600	-3.79424800	1.01696700
H	2.04988600	-4.20554400	-0.62575600

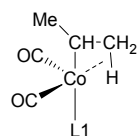
TS_{ma} in entry 4



O	1.30105000	-1.82590400	2.63963700
O	-1.97751600	-2.94008000	-0.26825400
P	0.17967500	0.72570400	0.17638400
C	0.99107100	-1.68165400	1.54152800
C	-0.96790500	-2.39341900	-0.24038600
C	1.12874400	1.76430700	1.39153000
C	2.64066900	1.53087800	1.31070200
C	3.27151900	1.39058500	-0.07471200
C	2.86563800	2.40988900	-1.13661100
C	1.57945500	2.08929200	-1.89495100
C	0.27507300	2.07721500	-1.09904800
C	0.06373100	3.36202700	-0.29400000
C	0.70100800	3.22162700	1.10697100
C	-1.54425400	0.93398200	0.82797800
C	-2.62031800	0.71262100	-0.22275100
C	-3.98900800	0.46252300	0.38497000
C	-5.06906600	0.23130200	-0.65593400
C	-6.43358600	-0.00237600	-0.03768600
H	0.79775800	1.46612000	2.39667300
H	2.89119500	0.62694700	1.88267900
H	3.13185500	2.35880700	1.84547200
H	3.06760300	0.38269400	-0.46307600
H	4.36065800	1.43062700	0.06026400
H	3.66821600	2.46928100	-1.88420600

H	2.81283300	3.41862400	-0.70023900
H	1.46235000	2.83525500	-2.69594200
H	1.69840200	1.12360700	-2.40791600
H	-0.54711400	1.91762300	-1.81014500
H	-1.01069800	3.55999000	-0.19853200
H	0.47812800	4.22372100	-0.83509600
H	-0.00770800	3.55821600	1.87225800
H	1.57121000	3.88228100	1.20586700
H	-1.63453500	0.17674500	1.62068100
H	-1.67627100	1.90976200	1.31431500
H	-2.67189200	1.58610400	-0.89138700
H	-2.34963300	-0.13930500	-0.86499400
H	-3.93384900	-0.41208600	1.05308900
H	-4.27015200	1.31164200	1.02981900
H	-5.10916200	1.09393200	-1.33867700
H	-4.78641300	-0.63057600	-1.27924500
H	-6.42332200	-0.87628200	0.62524500
H	-7.20622600	-0.17369600	-0.79469400
H	-6.74930600	0.85803600	0.56568500
Co	0.54553500	-1.44451500	-0.13152200
H	0.31454200	-1.12613700	-1.59647300
C	2.34490500	-2.41170100	-0.57057500
C	1.83158300	-1.86799100	-1.75309100
H	3.14766400	-1.85881300	-0.07802900
H	2.28894600	-0.97792500	-2.18063500
H	1.41473800	-2.54861400	-2.49590600
C	2.31673800	-3.88769000	-0.30277600
H	3.21291600	-4.37622600	-0.71201800
H	2.28779100	-4.11828200	0.76750200
H	1.44066000	-4.35635000	-0.76501300

g in entry 4

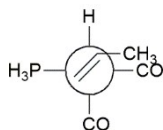


O	-2.16267700	1.57661300	2.60524400
O	2.00602500	2.50361700	0.11457500
P	-0.20727600	-0.75105600	0.22732400
C	-1.64009300	1.47548300	1.58441100
C	0.95364800	2.05247700	-0.00062500
C	-1.18183600	-1.94263600	1.27209100
C	-2.69681600	-1.71487300	1.21030400
C	-3.31145400	-1.35276400	-0.13980200

C	-2.90193000	-2.20826100	-1.33564500
C	-1.61072100	-1.78477900	-2.03163700
C	-0.31057400	-1.89991500	-1.23722200
C	-0.11710800	-3.28906000	-0.62449100
C	-0.74305800	-3.34401700	0.78733400
C	1.50964000	-1.04830600	0.85552800
C	2.60040400	-0.83234500	-0.18344400
C	3.97009500	-0.63947500	0.44317300
C	5.05957100	-0.38336400	-0.58184500
C	6.42258500	-0.18950700	0.05311400
H	-0.86301600	-1.79555400	2.31352600
H	-2.97082500	-0.92991900	1.92543000
H	-3.17865200	-2.63021700	1.58770700
H	-3.09623300	-0.29724100	-0.36542200
H	-4.40201400	-1.40237900	-0.02142300
H	-3.69905100	-2.15886700	-2.08937200
H	-2.85003700	-3.26950100	-1.04758600
H	-1.49096500	-2.40352100	-2.93388300
H	-1.72702500	-0.75404600	-2.39831700
H	0.51781400	-1.65052700	-1.91366800
H	0.95251200	-3.52174500	-0.56824800
H	-0.55122600	-4.05503800	-1.28134100
H	-0.02374200	-3.77386900	1.49383400
H	-1.60650900	-4.02025700	0.80512200
H	1.63275300	-0.33151400	1.68019800
H	1.59594600	-2.04825100	1.30069800
H	2.63412600	-1.68695500	-0.87592100
H	2.36790300	0.04341800	-0.80662100
H	3.93034100	0.20511500	1.14878000
H	4.22923400	-1.52261300	1.05029900
H	5.09374800	-1.21888800	-1.29778900
H	4.79116100	0.50605700	-1.17218200
H	6.41843100	0.66100700	0.74574400
H	7.20231700	-0.00204500	-0.69262000
H	6.72331600	-1.07419600	0.62832800
Co	-0.69816800	1.42898600	0.11019000
H	-1.45420300	1.21221300	-1.55399600
C	-1.51621900	3.13279500	-0.46955600
C	-1.90981200	2.26117000	-1.62422600
H	-2.37084600	3.41190400	0.15399600
H	-2.98527900	2.07695100	-1.70890300
H	-1.52086000	2.62436800	-2.58237300
C	-0.68845900	4.34490200	-0.80586100
H	-1.30045400	5.12129700	-1.29116500

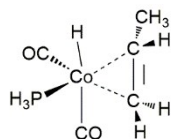
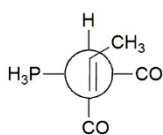
H	-0.24456900	4.79805700	0.08761200
H	0.13161900	4.10300900	-1.49358300

TS_{rotate}-(anti-ma) in entry 5



Co	0.11972400	0.10709200	-0.15468100
C	-0.82937600	1.45122000	-0.76044800
O	-1.46795400	2.29892600	-1.19282300
H	-0.27908400	-0.37326800	-1.52618400
P	2.01076300	-0.69200800	-0.92024200
H	3.23083600	-0.62894600	-0.20316700
H	2.08123400	-2.07518800	-1.22203900
H	2.52288500	-0.23327200	-2.15361700
C	0.74809200	0.88695300	1.30896000
O	1.17458300	1.39616600	2.24098000
C	-0.47847700	-1.54795100	1.15464900
C	-1.33628500	-1.54678000	0.08919400
C	-2.72821400	-1.00429400	0.14597900
H	-0.78588500	-1.11427300	2.10470800
H	0.36373700	-2.23403000	1.20214500
H	-1.12789700	-2.23748100	-0.72799600
H	-2.83675100	-0.26410900	0.94613000
H	-3.02710800	-0.53043100	-0.79430500
H	-3.44343600	-1.81599100	0.33908100

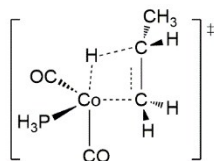
d in entry 5



Co	0.11494200	0.11159400	-0.15650900
C	-0.83395300	1.43030200	-0.81700200
O	-1.47349900	2.25781000	-1.28561800
H	-0.45448700	-0.49382200	-1.41522000
P	1.83617300	-0.99393400	-0.94299600
H	3.13364600	-0.91985300	-0.38006000
H	1.76077500	-2.40952300	-0.97933500
H	2.23337700	-0.82049700	-2.28626800
C	0.98246300	1.02529500	1.08926300
O	1.56176400	1.61577300	1.88041700
C	-0.56182200	-1.17826600	1.48209900

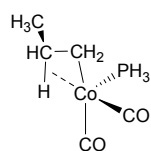
C	-1.33660800	-1.47554600	0.39555800
C	-2.74376500	-0.99629400	0.23146400
H	-2.92800800	-0.09017700	0.81872500
H	-2.99002200	-0.77690800	-0.81204300
H	-3.44800900	-1.76636700	0.57501200
H	-1.05114500	-2.33434900	-0.21346800
H	0.29534300	-1.79007300	1.75166000
H	-0.94151500	-0.52404800	2.26500800

TS_{anti-ma} in entry 5



Co	0.08285800	0.09443300	-0.07108000
C	-0.42773400	1.60609000	-0.82203500
O	-0.78819100	2.57432100	-1.31777800
H	-0.71087200	-0.47569500	-1.22195100
P	1.77754900	-1.04357000	-0.99408600
H	3.09597100	-1.00963800	-0.47938100
H	1.68436100	-2.45960300	-1.05083800
H	2.14601700	-0.87087900	-2.34872300
C	0.88900300	0.77832900	1.33989700
O	1.41304800	1.20371400	2.26450900
C	-0.72071200	-1.32337700	1.22134500
C	-1.51792900	-1.32224900	0.07556900
C	-2.87311100	-0.67683800	0.05973000
H	-1.08567000	-0.82310400	2.11702000
H	-0.01798600	-2.13475500	1.40092500
H	-1.40874700	-2.17934900	-0.59323700
H	-3.14826900	-0.30847200	-0.93338200
H	-3.63918000	-1.40089600	0.36700200
H	-2.91199200	0.17024500	0.75211900

f in entry 5



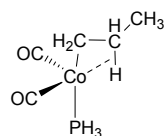
Co	0.20972600	0.10550300	0.01012100
C	1.43648200	0.82951500	-1.04169100
O	2.22733600	1.29990000	-1.72199200
P	1.28498000	-1.74234600	0.53474200
H	1.50356500	-1.97911700	1.91039100

H	0.65742900	-2.98478400	0.26205300
H	2.57969600	-2.10454100	0.09360900
C	-0.13285000	1.51692500	0.99512000
O	-0.34924200	2.40450600	1.68618200
C	-1.40818300	-0.74211900	0.75547500
C	-1.74109800	-0.83905000	-0.70384200
C	-2.95737000	-0.04046300	-1.13417500
H	-2.86746500	1.00084000	-0.80393500
H	-3.08858800	-0.03564500	-2.22150400
H	-3.86816300	-0.45301400	-0.68586100
H	-2.08599600	-0.09951300	1.32285300
H	-1.30990200	-1.70114000	1.27459800
H	-1.79954200	-1.88492300	-1.03482100
H	-0.86495900	-0.45565600	-1.35063500

TS_{iso}-(anti-ma) in entry 5

Co	0.13456900	0.03447900	-0.00381100
C	-0.28658100	1.50907100	-0.99619400
O	-0.45290100	2.50631500	-1.53231900
P	1.61250600	-1.28164900	-1.01882900
H	2.90005300	-1.44079900	-0.45716100
H	1.34101700	-2.66520700	-1.16760300
H	2.05648100	-1.08478700	-2.34957500
C	1.19036100	0.60736100	1.22941000
O	1.87718700	0.98461300	2.06933600
C	-1.72673100	-1.07110800	0.32247100
C	-1.09439700	-0.41703000	1.47299500
H	-1.69064800	-2.16559600	0.38269600
H	-1.62459100	0.44190700	1.88859300
H	-1.08688400	-0.90887900	-0.67741000
H	-0.67702700	-1.06321100	2.24457200
C	-3.09619800	-0.54882400	-0.07370900
H	-3.42751200	-0.93926700	-1.04174500
H	-3.84274100	-0.82937800	0.67649500
H	-3.08213000	0.54477100	-0.13950700

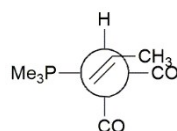
h in entry 5



Co	-0.20543200	0.05941900	0.07305100
C	0.31715000	-1.23584600	1.15911400
O	0.61191900	-2.01708400	1.94480500

P	-1.68840300	-1.09816100	-1.06907100
H	-3.04032000	-0.68987200	-1.09446100
H	-1.52685200	-1.23928600	-2.46762100
H	-1.92348400	-2.46225100	-0.78686400
C	-1.22805900	1.46654300	0.38159300
O	-1.89072100	2.35019200	0.68968800
C	1.77045400	0.81069100	-0.86750900
C	1.38360200	1.10367500	0.55397100
H	1.83629000	1.72915400	-1.46398400
H	2.05441600	0.66631000	1.29804700
H	0.92333500	0.25178400	-1.40405300
H	1.21279700	2.15631300	0.78514800
C	3.01430500	-0.04550000	-1.01696900
H	3.19840500	-0.33571800	-2.05720800
H	3.89814700	0.49346200	-0.65780500
H	2.92567400	-0.96403300	-0.42463300

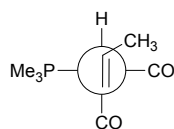
TS_{rotate}-(anti-ma) in entry 6



Co	-0.48889200	0.19329500	-0.08717700
C	-1.62025300	1.07727900	-1.09852900
O	-2.34511100	1.62350500	-1.80022200
H	-0.35276100	-0.56745200	-1.38742600
P	1.65202100	-0.19491900	-0.25937900
C	2.48824400	0.58751900	-1.68484000
C	2.74113000	0.30790700	1.12727800
C	2.14513800	-1.94757600	-0.47213600
H	3.55840200	0.34779200	-1.71066300
H	2.01828000	0.24463100	-2.61171600
H	2.36583900	1.67346100	-1.63043500
H	2.41658300	-0.18842300	2.04880100
H	3.79042100	0.05268400	0.93725600
H	2.66023100	1.38783000	1.28795500
H	1.79924000	-2.54731300	0.37669600
H	1.68107500	-2.34739900	-1.37942800
H	3.23363100	-2.05345700	-0.55186200
C	-0.33511900	1.35483000	1.23248200
O	-0.17852000	2.11006000	2.08240200
C	-1.61186500	-1.68967900	0.27504100
C	-0.97661000	-1.32066600	1.42844300
C	-3.07619300	-1.49895700	0.03901200

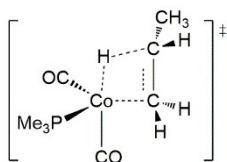
H	-3.47787900	-0.68732800	0.65544000
H	-3.30264200	-1.27036000	-1.00742300
H	-3.62474700	-2.41702700	0.29322800
H	-0.03320300	-1.77123100	1.72915000
H	-1.52927700	-0.82119400	2.22224100
H	-1.12119900	-2.42286400	-0.36530000

d in entry 6



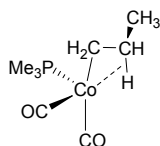
Co	0.49654700	0.23796900	0.10265500
C	1.78288100	0.87814500	1.11218400
O	2.60645000	1.25418100	1.81637200
H	0.42476800	-0.69419300	1.29710600
P	-1.62277000	-0.25536400	0.26028500
C	-2.44395300	0.21127000	1.82545800
C	-2.77881300	0.44794200	-0.97810500
C	-2.04561400	-2.03518800	0.14858400
H	-3.50395100	-0.07109000	1.82639900
H	-1.93668100	-0.28057300	2.66097500
H	-2.36035300	1.29197900	1.97445800
H	-2.46495400	0.15706600	-1.98673800
H	-3.80702800	0.10377400	-0.81456000
H	-2.75976000	1.54112200	-0.92768500
H	-1.70528500	-2.44832800	-0.80704500
H	-1.54576100	-2.58231100	0.95425400
H	-3.12761900	-2.19249400	0.23025700
C	0.23569700	1.65534200	-0.91493800
O	0.02490900	2.57866400	-1.56350400
C	1.43002400	-1.64544000	-0.63842100
C	1.02825000	-0.89219000	-1.70528700
H	0.75813400	-2.42528100	-0.27955600
H	1.74658800	-0.28921800	-2.25773000
H	0.08625000	-1.08434800	-2.21535200
C	2.85402000	-1.76460900	-0.19809200
H	3.30216100	-2.68157500	-0.60543700
H	3.45349400	-0.91691900	-0.54783700
H	2.94895800	-1.81669700	0.89129300

TS_{anti-ma} in entry 6



Co	-0.56370700	0.20124800	-0.00379600
C	-1.40122300	1.12538600	-1.25645800
O	-1.94158200	1.71081500	-2.08279200
H	-0.73213800	-0.94406100	-0.98417600
P	1.61768400	-0.23064500	-0.22790300
C	2.45027300	0.32646900	-1.76178300
C	2.74419100	0.44018500	1.05574000
C	2.10893400	-2.00035400	-0.19819400
H	3.51478900	0.06054200	-1.77246800
H	1.95857600	-0.12894000	-2.62751500
H	2.35189700	1.41213300	-1.85863600
H	2.42076500	0.09164700	2.04330400
H	3.78387200	0.13046000	0.89319000
H	2.69922400	1.53409900	1.06039700
H	1.77963100	-2.46810900	0.73643200
H	1.63396900	-2.53206700	-1.02956700
H	3.19615300	-2.12001100	-0.28147700
C	-0.43740100	1.45809200	1.21114000
O	-0.31842300	2.25648100	2.02689800
C	-1.49963500	-1.68953100	0.29965900
C	-1.11968600	-1.08649000	1.50848000
C	-2.93804200	-1.72309800	-0.13516200
H	-3.47974000	-0.84796700	0.23758300
H	-3.04314800	-1.73942300	-1.22468700
H	-3.43201700	-2.62150500	0.25782900
H	-0.25802800	-1.46223500	2.05932400
H	-1.88661900	-0.61785000	2.12310800
H	-0.91679100	-2.56305300	-0.00498900

f in entry 6



Co	0.49457000	0.36345300	0.04845900
C	0.07246500	1.77882200	1.00636200
O	-0.22641600	2.69584600	1.62780300
P	-1.57877700	-0.35888100	-0.13670500
C	-2.93172100	0.71853100	0.46980200
C	-2.09994700	-0.62270400	-1.87161400

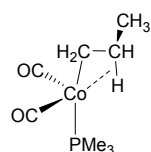
C	-2.05126700	-1.95306900	0.64223000
H	-3.91670100	0.28144200	0.26729500
H	-2.83094100	0.87787700	1.54837700
H	-2.87289700	1.69698500	-0.01788200
H	-1.44466100	-1.35331600	-2.35385800
H	-3.13752100	-0.97378500	-1.93229600
H	-2.00869200	0.31979900	-2.42037700
H	-1.39515500	-2.76188600	0.30661000
H	-1.95805200	-1.87086800	1.72998500
H	-3.08640600	-2.21938100	0.39708100
C	1.59043500	1.13615800	-1.08936300
O	2.25102000	1.62441500	-1.88942400
C	1.56139200	-1.54429100	0.80272900
C	1.10327900	-1.38918500	-0.62380000
C	3.06357000	-1.68065800	0.97112900
H	0.36156900	-2.12565800	-0.94855700
H	1.92636900	-1.38875600	-1.34386900
H	3.36686100	-1.67729300	2.02384300
H	3.42051500	-2.61357300	0.51993600
H	3.58165400	-0.85310800	0.47237100
H	1.25140900	-0.63525300	1.43068700
H	1.02484300	-2.35695500	1.31096300

TS_{iso}-(anti-ma) in entry 6

Co	-0.52968100	0.26402400	0.02437700
C	-1.16147400	0.92632400	-1.53953900
O	-1.51633500	1.44899200	-2.49684100
P	1.59719600	-0.40869300	-0.12208900
C	2.35603200	-0.49065800	-1.79065200
C	2.84876600	0.58832500	0.77240000
C	1.98893100	-2.09030800	0.50707200
H	3.39922800	-0.82965900	-1.75520500
H	1.77905000	-1.17423600	-2.42197600
H	2.31823000	0.49902300	-2.25723400
H	2.60202200	0.62440100	1.83849000
H	3.85769900	0.17526600	0.65168000
H	2.84138700	1.61701900	0.39735900
H	1.70821000	-2.16773200	1.56304400
H	1.41736800	-2.84038000	-0.05011200
H	3.05702800	-2.32070100	0.40830400
C	-0.22285800	1.67086800	0.95956000
O	-0.00378800	2.59232000	1.61291200
C	-1.73135600	-1.45631400	0.60076100
C	-1.70573200	-0.30973300	1.51068700

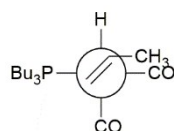
C	-3.06401100	-1.76579500	-0.05611700
H	-1.20683000	-0.44350300	2.47059800
H	-2.63348100	0.25885700	1.59418600
H	-2.96791500	-2.48979300	-0.87238300
H	-3.76492300	-2.17679400	0.67819900
H	-3.50601100	-0.85205800	-0.46815500
H	-0.99269500	-1.29576300	-0.34246600
H	-1.25374800	-2.34892700	1.02521600

h in entry 6



Co	0.47089300	0.34720000	0.19328700
C	0.70950700	-0.71272300	1.57686100
O	0.84319800	-1.32047600	2.54345800
P	-1.56613900	-0.35363500	-0.26278600
C	-2.43996900	-1.26373400	1.06166600
C	-2.82737600	0.87630000	-0.75410800
C	-1.65897200	-1.55196700	-1.64820600
H	-3.44388100	-1.56999500	0.74478200
H	-1.86480300	-2.15301700	1.33859600
H	-2.52262000	-0.63197200	1.95161100
H	-2.48402500	1.42770100	-1.63514400
H	-3.78694200	0.39771400	-0.98277800
H	-2.97524200	1.59978000	0.05400200
H	-1.30936300	-1.08062500	-2.57239800
H	-1.00780300	-2.40683700	-1.43710600
H	-2.68350800	-1.91286300	-1.80073300
C	0.12235500	2.07393100	0.13268200
O	-0.12395500	3.19421800	0.19970600
C	2.21903000	-0.12299700	-1.22246400
C	2.40864100	0.64864800	0.05069300
C	2.89006700	-1.48351100	-1.25136500
H	2.72625100	1.68490300	-0.07318600
H	3.04522500	0.14722700	0.78415800
H	2.61059700	-2.06815700	-2.13560500
H	3.98087200	-1.37769500	-1.25189100
H	2.61686000	-2.06796700	-0.36462300
H	1.09881700	-0.30849300	-1.41383000
H	2.48389700	0.47680400	-2.10267300

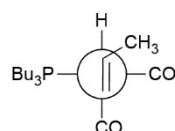
TS_{rotate}-(anti-ma) in entry 7



Co	-1.49784800	-0.77132700	-0.36339200
C	-3.16294100	-0.25707800	-0.58180300
O	-4.23277200	0.11900400	-0.76064600
H	-1.36636500	0.04410500	-1.63184700
P	0.34479600	0.39382300	-0.11914100
C	-1.59489400	-1.28107500	1.32203500
O	-1.61810100	-1.55945900	2.43640800
C	1.61760600	0.12138900	-1.43017700
C	2.90951100	0.91661900	-1.35041600
H	1.09874700	0.32658400	-2.37878100
H	1.83827600	-0.95601100	-1.44863800
C	3.87224300	0.56991400	-2.47564200
H	2.69507800	1.99529500	-1.38514600
H	3.41242100	0.74266000	-0.38632400
C	5.15303500	1.37825000	-2.41277000
H	4.10294100	-0.50538200	-2.43641200
H	3.37285300	0.73072700	-3.44291500
H	5.84304900	1.11857500	-3.22219600
H	4.94887500	2.45349600	-2.48740500
H	5.68114700	1.21366300	-1.46526200
C	0.09290900	2.21713100	-0.20009300
C	-0.99122000	2.72959700	0.73209700
H	-0.17023000	2.44474600	-1.24445300
H	1.04564600	2.72554500	0.00968700
C	-1.20202300	4.22960600	0.60981400
H	-1.93338100	2.20290100	0.52171100
H	-0.74057900	2.48429200	1.77665100
C	-2.28440500	4.73911000	1.54111300
H	-0.25440900	4.75165200	0.81293800
H	-1.45811600	4.47311300	-0.43237600
H	-2.43641000	5.81913100	1.44320500
H	-3.24487300	4.25075500	1.33671400
H	-2.03470500	4.53544900	2.58982300
C	1.29628800	0.21885500	1.45331100
C	1.88897800	-1.16363200	1.66771700
H	0.59006800	0.44470500	2.26554400
H	2.07950200	0.99013700	1.49961400
C	2.49743800	-1.32920700	3.05012300
H	1.11273500	-1.93048200	1.52382500
H	2.65730300	-1.36995400	0.90544800

C	3.12066100	-2.69660800	3.24912700
H	3.25074500	-0.54353200	3.21412000
H	1.71630300	-1.15774400	3.80588600
H	3.55275000	-2.81035200	4.24875400
H	2.37749800	-3.49288200	3.11963000
H	3.92200100	-2.87832000	2.52194800
C	-0.67199700	-2.75034700	-0.86433300
C	-1.34234700	-2.30905600	-1.97007000
H	-1.13596600	-3.47144300	-0.19320900
H	0.40790300	-2.66073300	-0.78279900
H	-0.76361100	-1.81871500	-2.75286600
C	-2.69116300	-2.80916400	-2.37823300
H	-3.30377300	-2.02944000	-2.84214800
H	-2.58658500	-3.61573300	-3.11793000
H	-3.24595100	-3.21049900	-1.52299600

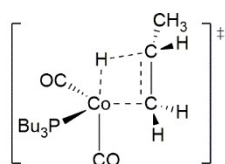
d in entry 7



Co	-1.48241300	-0.85801700	-0.28286700
C	-3.19411800	-0.60489900	-0.59070100
O	-4.29462400	-0.38910500	-0.83494400
H	-1.43094100	-0.08122400	-1.58601500
P	0.30905700	0.39596500	-0.11754000
C	-1.57743100	-1.17597900	1.44645600
O	-1.61693600	-1.33282300	2.58416300
C	1.58125100	0.13343000	-1.43167400
C	2.86194900	0.94686100	-1.35487700
H	1.05726100	0.33318900	-2.37877000
H	1.81536200	-0.94141000	-1.44911200
C	3.79173800	0.67919000	-2.52832700
H	2.63008400	2.02224200	-1.32263000
H	3.40060400	0.72918900	-0.41954500
C	5.06684400	1.49549700	-2.45300900
H	4.03232500	-0.39401600	-2.56352800
H	3.26170400	0.89540200	-3.46801800
H	5.73191700	1.29838200	-3.30002600
H	4.85020600	2.57088800	-2.44820900
H	5.62780000	1.27397700	-1.53651400
C	-0.04508800	2.19823900	-0.26597400
C	-1.17904500	2.66602500	0.63016100
H	-0.30333000	2.37525500	-1.32116700

H	0.87029500	2.77137800	-0.05728100
C	-1.47455600	4.14822100	0.47497500
H	-2.08152500	2.07922200	0.40547500
H	-0.94313500	2.45252800	1.68538100
C	-2.62433800	4.60126000	1.35331000
H	-0.57031400	4.73101100	0.70829700
H	-1.70205500	4.36159900	-0.58046200
H	-2.83478800	5.66964500	1.23731800
H	-3.54481500	4.05548600	1.11319500
H	-2.40895100	4.42117900	2.41387600
C	1.29622000	0.34165000	1.44255800
C	1.91007700	-1.01569800	1.73943600
H	0.61598300	0.62626500	2.25817700
H	2.07402100	1.11883700	1.40532500
C	2.72548400	-1.01841000	3.02185400
H	1.11636500	-1.77350100	1.81417200
H	2.55272300	-1.33683900	0.90358100
C	3.33563100	-2.37412700	3.31785000
H	3.51621100	-0.25602600	2.95035500
H	2.08210000	-0.70397200	3.85699700
H	3.92208200	-2.36836300	4.24248500
H	2.56048000	-3.14259700	3.42534700
H	4.00222500	-2.69613700	2.50795300
C	-0.97634700	-2.38828500	-1.83691900
C	-0.73317900	-2.90298000	-0.59601700
H	-0.14267000	-1.94592300	-2.38315700
H	0.26648000	-2.90976900	-0.16912600
H	-1.45397100	-3.56988900	-0.12602800
C	-2.17110500	-2.74770500	-2.66153000
H	-2.55730800	-1.89514100	-3.22941100
H	-1.90884200	-3.52858000	-3.38873400
H	-2.98572700	-3.13360400	-2.03888400

TS_{anti-ma} in entry 7

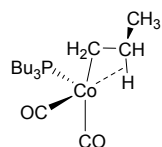


Co	-1.46519900	-0.92725000	-0.38191500
C	-3.10291700	-0.24056500	-0.41430000
O	-4.15561400	0.21795600	-0.43844600
H	-1.36423500	-0.40141500	-1.80534800
P	0.32073800	0.38463700	-0.09412000

C	-1.46891100	-1.59813400	1.23119200
O	-1.42575600	-2.03143200	2.29471200
C	1.64020900	0.22154900	-1.38007300
C	2.87538900	1.09874600	-1.26546100
H	1.13598100	0.40641200	-2.34147800
H	1.93034300	-0.84000400	-1.40283200
C	3.89448200	0.80770900	-2.35578900
H	2.59172300	2.16032100	-1.31780600
H	3.35464400	0.96602900	-0.28299500
C	5.11463100	1.70267700	-2.26346700
H	4.19644700	-0.24893400	-2.29761900
H	3.41546400	0.92542300	-3.33956000
H	5.84452000	1.48695800	-3.05054700
H	4.83842400	2.76062500	-2.35218800
H	5.62481100	1.58113900	-1.29980800
C	-0.00554600	2.20103000	-0.11919200
C	-1.07063500	2.64468400	0.86844400
H	-0.31849200	2.44522100	-1.14627600
H	0.93274400	2.74475500	0.06655300
C	-1.36176100	4.13391200	0.78550200
H	-1.99629000	2.07828800	0.69150600
H	-0.76045600	2.39526000	1.89571700
C	-2.43421500	4.56869200	1.76496200
H	-0.43502000	4.69971400	0.96612000
H	-1.66794900	4.38422100	-0.24142900
H	-2.64237700	5.64167500	1.69727600
H	-3.37620700	4.03763100	1.58207300
H	-2.13811000	4.35565800	2.79963900
C	1.24258800	0.19200900	1.49346600
C	1.92700900	-1.15839000	1.63779600
H	0.49307600	0.30989900	2.28987100
H	1.96242900	1.01360300	1.62469200
C	2.34423900	-1.45417400	3.06859100
H	1.25510500	-1.95909600	1.29083900
H	2.81104800	-1.20724000	0.98235400
C	3.06959000	-2.77857900	3.19884900
H	2.97920900	-0.63600900	3.44147700
H	1.44663600	-1.45376400	3.70471500
H	3.35568400	-2.99058800	4.23427000
H	2.43998700	-3.60877700	2.85574100
H	3.98576300	-2.79373200	2.59501900
C	-0.88080900	-2.77112800	-1.10469500
C	-1.15419000	-1.96819000	-2.22329900
H	-1.61212800	-3.52207200	-0.80920400

H	0.14894100	-3.00088000	-0.83778900
H	-0.28631500	-1.63453500	-2.79831500
C	-2.39427000	-2.19217100	-3.04524000
H	-2.73138300	-1.28200400	-3.55209800
H	-2.20520400	-2.95058800	-3.81564900
H	-3.21785200	-2.54725800	-2.41725000

f in entry 7



Co	-1.59165600	-0.79448000	-0.38661400
C	-2.59771100	0.57443700	-0.85188900
O	-3.25017100	1.45845000	-1.18568900
P	0.29701500	0.36722000	-0.22495000
C	-2.60058600	-1.44974800	0.89654700
O	-3.19445400	-1.86213500	1.78780700
C	1.66561600	-0.06368500	-1.39420600
C	3.04902200	0.50702800	-1.12734100
H	1.30313600	0.26121800	-2.38248100
H	1.72259600	-1.15930700	-1.45376800
C	4.04159900	0.14872600	-2.22215600
H	3.00599400	1.60238200	-1.03094200
H	3.43275800	0.13893700	-0.16340800
C	5.42556900	0.70783300	-1.95632400
H	4.09079800	-0.94584800	-2.32318600
H	3.66513800	0.51903900	-3.18749500
H	6.13356900	0.44779300	-2.74994000
H	5.40444000	1.80196100	-1.88025900
H	5.83476300	0.32546200	-1.01294100
C	0.16587900	2.19158700	-0.48407300
C	-0.62902000	2.91691900	0.59196800
H	-0.31602400	2.32637700	-1.46406500
H	1.16973800	2.63219700	-0.56558600
C	-1.03529500	4.31929100	0.17180100
H	-1.53168300	2.34473700	0.85689400
H	-0.03481500	2.97379000	1.51632500
C	-1.78756800	5.05315200	1.26408400
H	-0.13844800	4.88792100	-0.11854100
H	-1.65633100	4.25500600	-0.73376400
H	-2.08284000	6.06105400	0.95440800
H	-2.70098200	4.51424100	1.54383500
H	-1.17803600	5.15268900	2.17087600

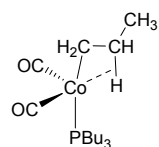
C	1.08464600	0.31515900	1.44400700
C	1.50909200	-1.05586000	1.93907100
H	0.33956700	0.73258900	2.13595400
H	1.93649900	1.01377000	1.45088100
C	2.15525000	-0.99615800	3.31338400
H	0.63373200	-1.72079100	1.97194300
H	2.21331800	-1.52413500	1.23261500
C	2.56744100	-2.36509500	3.81799800
H	3.03045500	-0.32917800	3.27808500
H	1.45466900	-0.52943900	4.02196000
H	3.02759400	-2.31676300	4.81042500
H	1.70414200	-3.03804100	3.88722000
H	3.29185600	-2.83626600	3.14199200
C	-0.57869000	-2.48606900	-0.40373300
C	-1.09133500	-2.50690200	-1.81549800
C	-2.06916400	-3.62633100	-2.12098400
H	0.50921500	-2.45215100	-0.31533600
H	-0.95857600	-3.30670900	0.21180000
H	-1.57055700	-4.60091300	-2.06697800
H	-2.88545200	-3.63071000	-1.38945700
H	-2.51491800	-3.53038100	-3.11716500
H	-1.63860800	-1.52505500	-2.06716400
H	-0.26866900	-2.47903100	-2.54279700

TS_{iso}-(anti-ma) in entry 7

Co	-1.41137200	-1.07871700	-0.32638000
C	-2.80161000	-0.38314500	-1.23761100
O	-3.71805700	0.09849600	-1.73426000
P	0.27545100	0.40921700	-0.12793900
C	-1.96517700	-0.99110900	1.29750400
O	-2.27984500	-0.93858400	2.40353600
C	1.62643900	0.24836700	-1.38624100
C	2.85548600	1.13142900	-1.25763700
H	1.13212000	0.41904500	-2.35561200
H	1.92715300	-0.80954200	-1.40029900
C	3.83292900	0.92976800	-2.40480900
H	2.56468700	2.19192100	-1.21626200
H	3.37403700	0.92556000	-0.30808500
C	5.06247800	1.80808600	-2.28216900
H	4.12911700	-0.12928600	-2.44657200
H	3.32035600	1.13176000	-3.35731600
H	5.76101400	1.65723700	-3.11171400
H	4.79142900	2.87095800	-2.26975800
H	5.60766000	1.60226200	-1.35256300

C	-0.21012000	2.18039400	-0.31336500
C	-1.36866700	2.58170200	0.58445000
H	-0.49069500	2.31722700	-1.36895800
H	0.65781700	2.83022800	-0.12497500
C	-1.77284300	4.03564100	0.40555800
H	-2.23244600	1.93232200	0.38006400
H	-1.10954300	2.40750800	1.64121200
C	-2.94260300	4.42311000	1.28860500
H	-0.90925500	4.68415900	0.61789400
H	-2.02568800	4.21204400	-0.65084600
H	-3.22603800	5.47278200	1.15798500
H	-3.82619900	3.81298300	1.06592000
H	-2.70627000	4.27526200	2.34964500
C	1.19998400	0.45468300	1.46942700
C	1.84676100	-0.87583200	1.81346300
H	0.47920900	0.72929300	2.25289300
H	1.94828800	1.26134000	1.44412000
C	2.69924800	-0.81181000	3.06913700
H	1.06266900	-1.63745600	1.93869000
H	2.47002500	-1.22689700	0.97400100
C	3.32240800	-2.14942100	3.41638900
H	3.48598900	-0.05342600	2.93470400
H	2.08191700	-0.45443900	3.90672300
H	3.93780200	-2.09510700	4.32042600
H	2.55362100	-2.91280600	3.58765000
H	3.96396500	-2.51213800	2.60343800
C	-1.00138400	-2.98265900	0.03554100
C	-0.59510900	-2.80272600	-1.35978100
H	-1.88085700	-3.60697000	0.20161700
H	0.48878900	-2.90804700	-1.50156200
H	-0.69820000	-1.64970600	-1.71326100
H	-0.21270200	-3.16783600	0.76521300
C	-1.39505300	-3.56021000	-2.40306000
H	-1.18782400	-3.21139900	-3.42048100
H	-1.16438900	-4.62999800	-2.35998100
H	-2.46807100	-3.43866300	-2.21922400

h in entry 7

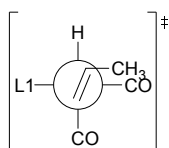


Co	-1.25510600	-1.16346800	-0.36012300
C	-1.91532300	-0.41197200	-1.80260900

O	-2.42218800	0.14669900	-2.67244900
P	0.20028900	0.45383800	-0.01164800
C	-1.89340700	-1.22078600	1.28044200
O	-2.37202200	-1.16287200	2.32495000
C	1.57593900	0.42163000	-1.24239200
C	2.68209800	1.45325500	-1.10344500
H	1.08289400	0.51043400	-2.22288800
H	1.99366400	-0.59610300	-1.22400200
C	3.73005400	1.32559500	-2.19772600
H	2.26120900	2.46992900	-1.12739000
H	3.17456900	1.35503700	-0.12346000
C	4.83693000	2.35276800	-2.06369600
H	4.15350000	0.31016600	-2.17647200
H	3.24223400	1.42278900	-3.17896400
H	5.58753200	2.25343600	-2.85451100
H	4.44000600	3.37417500	-2.11424400
H	5.35713700	2.25432900	-1.10281700
C	-0.45305400	2.16775800	-0.16459100
C	-1.71430900	2.40591500	0.65035100
H	-0.65828400	2.33299800	-1.23347900
H	0.33180400	2.88291000	0.12292400
C	-2.23948900	3.82411500	0.50524600
H	-2.49017900	1.68949400	0.34297800
H	-1.52564800	2.19685900	1.71558200
C	-3.50375300	4.05636400	1.30909200
H	-1.46003900	4.53719600	0.81464100
H	-2.42733400	4.03102300	-0.55907100
H	-3.87893800	5.07906400	1.19834200
H	-4.30369000	3.37551000	0.99442100
H	-3.33282000	3.88181300	2.37851100
C	1.04708000	0.49186100	1.62308900
C	1.80496000	-0.78718100	1.93394100
H	0.26204400	0.65176100	2.37649200
H	1.71223400	1.36669000	1.67385500
C	2.43193300	-0.77680000	3.31803600
H	1.12259100	-1.64737900	1.84665000
H	2.59355400	-0.95369900	1.18205100
C	3.18710200	-2.05590400	3.62086600
H	3.10598300	0.08876800	3.40632300
H	1.64342500	-0.61827300	4.06848500
H	3.63458500	-2.04224100	4.62000600
H	2.52504400	-2.92882200	3.56912900
H	3.99768500	-2.22007900	2.89991400
C	-1.97969300	-2.92465200	-0.84506300

C	-0.52023000	-3.24384200	-0.99291500
C	-0.06388800	-3.52387400	-2.41267800
H	-2.54559200	-2.98887200	-1.77781900
H	-2.49790700	-3.46756600	-0.05337500
H	0.12259500	-2.36605400	-0.61429100
H	-0.20734400	-4.03903200	-0.30347200
H	1.02641300	-3.60906300	-2.49053300
H	-0.49984800	-4.45787800	-2.78520400
H	-0.38357900	-2.71939300	-3.08598400

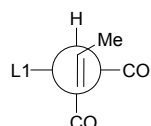
TS_{rotate}-(anti-ma) in entry 8



O	2.89663000	1.84251800	-1.95789800
O	-1.21712600	3.41156700	-1.52880200
P	0.23793700	-0.55629900	-0.28958800
C	2.00283000	1.75117300	-1.24409900
C	-0.45770200	2.74134900	-0.98765400
C	1.12016800	-1.73534100	-1.43587700
C	2.64483700	-1.58978900	-1.42190100
C	3.32817900	-1.35204200	-0.07727400
C	2.90948600	-2.25511200	1.07993900
C	1.66398900	-1.81080300	1.84419600
C	0.33173400	-1.80684500	1.09475800
C	0.04385500	-3.14379700	0.40819900
C	0.62926600	-3.14216800	-1.02161000
C	-1.50185700	-0.80162200	-0.89802200
C	-2.59855800	-0.56239600	0.12496300
C	-3.98591900	-0.61479100	-0.49268300
C	-5.09793600	-0.41343500	0.52102400
C	-6.47715500	-0.48154500	-0.10510300
H	0.77065400	-1.50781500	-2.45257200
H	2.93574600	-0.77457800	-2.09515800
H	3.06419500	-2.50117500	-1.87608100
H	3.18737000	-0.30454000	0.22404500
H	4.40888100	-1.45796200	-0.24067500
H	3.73088800	-2.28993500	1.80823600
H	2.79598300	-3.29331600	0.73303700
H	1.54333900	-2.47819100	2.71123400
H	1.84681000	-0.81175900	2.26531200
H	-0.45682900	-1.55995600	1.81921400
H	-1.03875200	-3.31327600	0.36805000

H	0.45117200	-3.97265300	1.00330700
H	-0.12667500	-3.49731200	-1.73132100
H	1.46022200	-3.85321400	-1.10434900
H	-1.60944000	-0.08950700	-1.72887300
H	-1.61301700	-1.80320600	-1.33376100
H	-2.53738200	-1.31163000	0.92945900
H	-2.45439800	0.41431400	0.61290800
H	-4.06412200	0.15032800	-1.28144500
H	-4.12638200	-1.58192300	-1.00307000
H	-5.00869000	-1.17238400	1.31333900
H	-4.96045900	0.55669200	1.02190100
H	-6.60031300	0.28593000	-0.87917200
H	-7.27300800	-0.33437700	0.63264000
H	-6.64802700	-1.45391900	-0.58383900
Co	0.61696500	1.62895400	-0.15316400
H	-0.66938800	1.43023000	0.58689600
C	0.77253600	2.47933400	1.89435700
C	2.01600500	2.10210500	1.46682400
H	0.45647000	3.50624800	1.71203100
H	2.69621300	2.82199900	1.02154400
H	2.47542400	1.19251800	1.84883400
C	0.02332300	1.74640200	2.96518600
H	0.27999300	2.15931100	3.95051000
H	-1.06197600	1.83003000	2.85113200
H	0.27984800	0.68101400	2.97820100

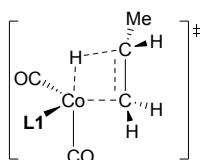
d in entry 8



O	3.06501300	1.81737800	-1.72599600
O	-0.92985300	3.59258000	-1.59634700
P	0.21565400	-0.54082600	-0.29270800
C	2.11318800	1.72815800	-1.09107300
C	-0.27730100	2.84846800	-1.01367800
C	1.09374500	-1.69090700	-1.47074300
C	2.61960900	-1.56137000	-1.44546700
C	3.30864300	-1.40763200	-0.09090700
C	2.86260400	-2.34577600	1.02612100
C	1.62528200	-1.89566800	1.79939300
C	0.29328900	-1.84230200	1.04871800
C	-0.00958300	-3.15052000	0.31450900
C	0.58544300	-3.10619300	-1.11044000

C	-1.52184500	-0.75588900	-0.91964000
C	-2.62164800	-0.52411200	0.10095200
C	-4.00656100	-0.56331200	-0.52300400
C	-5.12193500	-0.35003100	0.48455900
C	-6.49821400	-0.40337200	-0.14945100
H	0.75437500	-1.42400500	-2.48137700
H	2.91770800	-0.71129800	-2.07107100
H	3.02891400	-2.44992800	-1.95091000
H	3.20385400	-0.37240900	0.26346500
H	4.38561300	-1.53896100	-0.26054600
H	3.67835800	-2.42673200	1.75731500
H	2.72793400	-3.36747900	0.64103000
H	1.48682000	-2.58327500	2.64781800
H	1.83597400	-0.91379600	2.24794100
H	-0.49363600	-1.61547900	1.78133700
H	-1.09418400	-3.30262200	0.26266500
H	0.38196200	-4.00532500	0.88290000
H	-0.16885200	-3.42827000	-1.83733900
H	1.40992800	-3.82236500	-1.21168900
H	-1.61453500	-0.02440700	-1.73523900
H	-1.64144600	-1.74665200	-1.37710100
H	-2.56661500	-1.28135600	0.89866200
H	-2.47398000	0.44766000	0.59714600
H	-4.07358200	0.20189800	-1.31267300
H	-4.15380100	-1.52918100	-1.03382800
H	-5.04517900	-1.10936900	1.27774700
H	-4.97707000	0.61893400	0.98567000
H	-6.60862200	0.36536800	-0.92422800
H	-7.29669300	-0.24754800	0.58364000
H	-6.67681500	-1.37380900	-0.62925700
Co	0.63848500	1.64645400	-0.12396900
H	-0.73299800	1.54492900	0.47924800
C	0.64429900	2.33402400	1.99692900
C	1.93009200	2.12139700	1.58294000
H	0.23290300	3.33728600	1.88638500
H	2.54033500	2.94041200	1.21417100
H	2.47235800	1.23096200	1.89713700
C	-0.06280800	1.44893000	2.97560900
H	0.09412100	1.82387500	3.99627200
H	-1.14368600	1.41552200	2.80695600
H	0.31756400	0.42251500	2.94234300

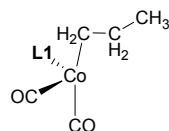
TS_{anti-ma} in entry 8



O	3.20587400	2.01462900	-1.40096400
O	-0.99996500	3.19599500	-1.96245500
P	0.24857700	-0.53629700	-0.28113200
C	2.18777500	1.86222600	-0.89344300
C	-0.33277400	2.62430000	-1.22286900
C	1.15662800	-1.64051700	-1.47871300
C	2.67712300	-1.46183000	-1.44210600
C	3.35581000	-1.32101900	-0.08052400
C	2.93012700	-2.29277000	1.01576500
C	1.67735800	-1.88929900	1.78986500
C	0.34957000	-1.86892200	1.03025200
C	0.09292500	-3.17139500	0.26981200
C	0.69055100	-3.07813000	-1.15116500
C	-1.48047800	-0.78066900	-0.91996600
C	-2.58378300	-0.49480800	0.08244200
C	-3.96970100	-0.60788200	-0.52947900
C	-5.08594700	-0.36147300	0.46954700
C	-6.46301000	-0.47391600	-0.15490700
H	0.81422700	-1.36357800	-2.48567700
H	2.94727800	-0.58391600	-2.04247900
H	3.11866100	-2.32088400	-1.97104500
H	3.22105200	-0.29751900	0.29617900
H	4.43668800	-1.41907600	-0.24755800
H	3.74485300	-2.36547400	1.74889900
H	2.82327500	-3.31040200	0.61142800
H	1.55686600	-2.59041500	2.63002800
H	1.85567100	-0.90494100	2.24905800
H	-0.44964600	-1.68458900	1.76145900
H	-0.98680700	-3.35478100	0.21232900
H	0.50938300	-4.02508600	0.82226700
H	-0.05105800	-3.40641000	-1.88835900
H	1.53650800	-3.76724200	-1.26432100
H	-1.56671400	-0.09196900	-1.77317400
H	-1.60239400	-1.79206000	-1.32914100
H	-2.51053600	-1.18817900	0.93591800
H	-2.45423000	0.51486400	0.50279800
H	-4.05865800	0.10465300	-1.36503500
H	-4.09438100	-1.60701000	-0.97847200
H	-4.99253800	-1.07635500	1.30137000
H	-4.95805000	0.63509700	0.91868800

H	-6.59280800	0.25601200	-0.96338600
H	-7.26203100	-0.30218200	0.57402100
H	-6.62189000	-1.46893700	-0.58909500
Co	0.63805500	1.68887600	-0.08515900
H	-0.68183500	1.66130600	0.63992600
C	0.29399600	2.28862600	1.95718000
C	1.65358100	2.22663200	1.66047800
H	-0.17923100	3.26969600	1.90125200
H	2.20411200	3.13695300	1.43911800
H	2.25011400	1.40677300	2.06049900
C	-0.33220400	1.34163800	2.94325200
H	-0.19131400	1.72387200	3.96217700
H	-1.40860700	1.21432400	2.78557500
H	0.13535500	0.35251200	2.89587100

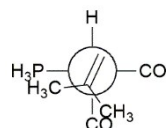
f in entry 8



O	1.10867900	4.35654100	-0.06647800
O	1.64037400	1.25311900	-3.11683000
P	0.49712200	-0.69727500	-0.21781300
C	0.91309100	3.24096800	-0.22485100
C	1.30076800	1.35852100	-2.02428100
C	1.76076100	-1.78989700	-1.02404700
C	3.17992000	-1.22348600	-0.88843000
C	3.54799300	-0.54857000	0.43108400
C	3.22444600	-1.31723600	1.71052400
C	1.81162100	-1.11216900	2.24978500
C	0.65141600	-1.61333100	1.38874500
C	0.79783500	-3.07582600	0.96286200
C	1.56859100	-3.17748700	-0.37254100
C	-1.07629900	-1.33045000	-0.95317000
C	-2.31392100	-0.94519200	-0.16099800
C	-3.61043800	-1.33837800	-0.84396100
C	-4.83285500	-0.90500100	-0.05398600
C	-6.13440500	-1.28260300	-0.73296900
H	1.51689900	-1.84354500	-2.09425500
H	3.34947900	-0.49708300	-1.69378500
H	3.88544500	-2.04591400	-1.08211600
H	3.06550700	0.44212900	0.48135600
H	4.62511100	-0.33809000	0.39791000
H	3.91508500	-0.98958400	2.49862800

H	3.43491000	-2.38955900	1.57715000
H	1.73599100	-1.62407800	3.22098900
H	1.66554500	-0.04320000	2.46146900
H	-0.27251800	-1.47396400	1.96304100
H	-0.19755600	-3.52392400	0.85595600
H	1.29709800	-3.64900900	1.75555500
H	1.02921300	-3.83853600	-1.06058700
H	2.54800800	-3.64797800	-0.22311100
H	-1.12197100	-0.89506600	-1.96275100
H	-1.02141700	-2.41955500	-1.08769800
H	-2.28010600	-1.40718200	0.83871100
H	-2.31793400	0.13929900	0.01441600
H	-3.64627200	-0.89102400	-1.85027500
H	-3.63654900	-2.42887300	-1.00263900
H	-4.79114500	-1.34947400	0.95235200
H	-4.79034600	0.18400600	0.10404900
H	-6.21282500	-0.82249300	-1.72570500
H	-7.00837200	-0.96533900	-0.15458000
H	-6.20953800	-2.36820200	-0.87290300
Co	0.67032700	1.51194100	-0.39376900
C	-1.64668300	2.47461700	1.09774100
C	-0.35517100	1.69621600	1.34475600
H	0.24282600	2.20973900	2.11340700
H	-0.61281100	0.72474800	1.78928200
C	-2.68185200	2.25429800	2.18919000
H	-3.58739900	2.85325400	2.03196400
H	-2.98841400	1.19972400	2.23542300
H	-2.27511100	2.51480500	3.17441600
H	-1.42618600	3.54840800	1.01145500
H	-2.09163400	2.20502400	0.12558900

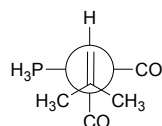
TS_{rotate}-ma in entry 9



Co	-0.53716900	0.05863500	-0.17984400
C	-2.02733200	-0.82177500	-0.47429200
O	-3.01527500	-1.35856700	-0.69547100
H	-0.99375100	0.62677900	-1.49906000
P	-0.32626200	2.20310000	0.12114400
H	0.20352900	2.76230700	1.31138600
H	0.43217400	2.99902300	-0.77089500
H	-1.49731600	2.99089500	0.08083800

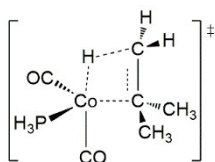
C	-0.27298000	-0.41422800	1.50698000
O	-0.13310300	-0.66818800	2.61551800
C	0.87156900	-0.83166500	-1.61006700
C	1.70116500	-0.59329200	-0.55264300
H	0.45417000	-1.82224800	-1.77456300
H	0.86155000	-0.16384300	-2.46661800
C	2.60390000	0.60247100	-0.51152800
C	2.09892200	-1.69947300	0.38097100
H	3.63610700	0.29252500	-0.73325700
H	2.32552200	1.36494400	-1.24554400
H	2.63279700	1.06472000	0.48387500
H	1.36397300	-2.50983100	0.40318200
H	3.05681100	-2.12231000	0.04456800
H	2.25747600	-1.35081500	1.40780200

c in entry 9



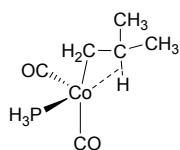
Co	0.56841300	0.02405800	0.14823400
C	1.70968100	-1.30201900	0.24337300
O	2.48449500	-2.14161300	0.33706800
H	1.30021000	0.28815600	1.44318400
P	0.76399500	2.19437100	0.13357000
H	0.31551900	3.01130300	-0.93383800
H	0.14665900	2.93572800	1.17200700
H	2.04518600	2.77437100	0.25543000
C	0.08117700	-0.15415500	-1.54025900
O	-0.22977100	-0.24700300	-2.63988300
C	-0.94572300	-0.25943700	1.71282100
H	-0.57733800	-1.12125900	2.26330300
H	-0.98037000	0.67670300	2.26661300
C	-1.68168000	-0.42082100	0.57371200
C	-2.55220400	0.68085500	0.04499500
C	-2.00366400	-1.78840900	0.04648200
H	-3.59996300	0.47885300	0.31179600
H	-2.29128200	1.65819700	0.46454900
H	-2.52212800	0.75310200	-1.04860700
H	-2.02789500	-1.82006800	-1.04863800
H	-1.29256300	-2.54306200	0.39524500
H	-3.00640400	-2.08430300	0.38887700

TS_{ma} in entry 9



Co	-0.45315800	-0.05248300	-0.15664900
C	-1.82398000	-1.15917900	-0.32608200
O	-2.70800200	-1.87852400	-0.44617600
H	-0.74764100	0.18171000	-1.61751800
P	-0.86486500	2.13368700	0.03574900
H	-0.47950900	2.88476700	1.17383000
H	-0.31336600	3.02837600	-0.91802700
H	-2.18264100	2.64428500	-0.03469800
C	-0.02921100	-0.38574500	1.51580100
O	0.27981100	-0.58288900	2.60205100
C	0.92493000	-0.12787000	-1.74799600
C	1.62292500	-0.29092700	-0.54461900
H	0.75835600	-0.99507700	-2.38526000
H	1.03482200	0.80971200	-2.29481000
C	2.47077800	0.83366800	-0.01339100
C	2.11100800	-1.66319800	-0.16039200
H	3.51106600	0.71436300	-0.35317600
H	2.12698500	1.81550000	-0.35717100
H	2.50143800	0.84946200	1.08282300
H	1.43433500	-2.45070700	-0.50638800
H	3.10069700	-1.84569800	-0.60662400
H	2.23052500	-1.77414600	0.92338900

e in entry 9



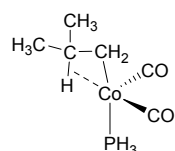
Co	0.38207800	0.11640000	-0.17490900
C	2.08087300	0.42133500	-0.61018100
O	3.16592900	0.64296900	-0.89967000
P	0.72249700	-1.87825100	0.79872000
H	0.04000600	-2.17770100	2.00182300
H	0.47836000	-3.13880700	0.18918700
H	2.01924200	-2.19859100	1.26402700
C	0.17775900	1.49759400	0.87322000
O	0.04457000	2.36697100	1.61005700
C	-2.39839600	1.24269200	-0.33575200
C	-1.60113500	-0.04430900	-0.36691800
C	-1.10561400	-0.40751600	-1.72890100

C	-2.34107600	-1.13039400	0.37579100
H	-1.47723600	0.25027900	-2.52205200
H	0.03994800	-0.29214500	-1.85728600
H	-1.27562000	-1.45534800	-1.99808800
H	-3.37748300	1.09975700	-0.82180600
H	-2.60050200	1.57193400	0.69039500
H	-1.89010400	2.06296000	-0.85472100
H	-1.90742000	-2.12723200	0.23321600
H	-2.37302000	-0.92821900	1.45395100
H	-3.38820400	-1.19185000	0.03642400

TS_{iso}-ma in entry 9

Co	-0.34916400	-0.11433300	-0.11105900
C	-0.87127700	-1.86222100	-0.07478700
O	-1.17798200	-2.94954600	0.11206800
P	-2.08156600	1.25736800	-0.38085700
H	-2.34671700	2.25545300	0.58556100
H	-2.12643700	2.12209900	-1.50400900
H	-3.42070800	0.80968400	-0.49818700
C	0.00690400	0.28429000	1.52448400
O	0.27753700	0.53527000	2.61429200
C	2.48808100	-0.94542500	-0.05036700
C	1.59436700	0.20040500	-0.44844100
C	1.00234700	0.13501800	-1.79913600
C	2.16363500	1.54209000	-0.05551700
H	1.36961000	-0.69531500	-2.41118300
H	-0.15210500	-0.11039700	-1.80569300
H	1.04291000	1.07620800	-2.35618100
H	3.48824200	-0.83764000	-0.50250200
H	2.63280900	-0.97711400	1.03607600
H	2.08273500	-1.91407400	-0.36057600
H	1.48664400	2.36717800	-0.30453300
H	2.37395200	1.59536600	1.01856400
H	3.11919300	1.72428600	-0.57417400

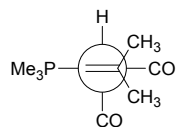
g in entry 9



Co	0.30892200	0.00054700	-0.09488900
C	0.34164100	1.55990500	0.73908200
O	0.41137800	2.49975700	1.39447600
P	2.45876600	0.00603800	-0.62003800

H	3.31119000	-1.02129700	-0.15744600
H	2.84848900	-0.05176400	-1.97936900
H	3.28484600	1.09302200	-0.25556900
C	0.35074400	-1.56134700	0.73584500
O	0.42723800	-2.50104400	1.39063700
C	-2.43264700	-1.23706600	0.09152200
C	-1.66706500	-0.00240400	-0.32767200
H	-1.97568700	-2.16516900	-0.26834200
H	-3.45993200	-1.20332200	-0.30801800
C	-2.43321100	1.23723800	0.07594900
C	-1.21708300	-0.01038300	-1.76115400
H	-2.51954400	-1.30649700	1.18239700
H	-3.45918100	1.19978700	-0.32654500
H	-2.52341300	1.31875300	1.16571800
H	-1.97426900	2.16094300	-0.29267900
H	-1.52596600	0.87995100	-2.31873800
H	-0.07691900	-0.00291800	-1.87538000
H	-1.51518700	-0.91218100	-2.30579500

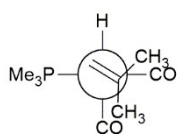
a in entry 10



Co	0.30019400	-0.04478000	0.18415900
C	0.92069200	-0.73663500	1.68913000
O	1.35835200	-1.24354600	2.61903800
H	0.10118000	-1.50317300	-0.12858800
P	-1.85277000	-0.19405400	-0.18577800
C	-2.74693600	-1.33519500	0.93022000
C	-2.89654900	1.30919400	-0.07190600
C	-2.35132000	-0.82948800	-1.82810100
H	-3.81552900	-1.38666900	0.68819800
H	-2.31061700	-2.33567700	0.84977500
H	-2.63050600	-1.00198600	1.96622800
H	-2.54088100	2.06316000	-0.78210200
H	-3.94794000	1.08596000	-0.28995900
H	-2.82809500	1.73893600	0.93282000
H	-1.99180200	-0.15509800	-2.61193700
H	-1.89833600	-1.81224000	-1.99403200
H	-3.44134600	-0.91766700	-1.90824500
C	0.28019500	1.69036900	0.57586700
O	0.20373200	2.80584700	0.82533200
C	0.99874500	0.14960700	-1.76952200

C	2.09607200	-0.13611500	-0.95988800
H	0.57417800	-0.63593500	-2.39299600
H	0.83872600	1.16494200	-2.13298400
C	2.70460600	-1.51109100	-0.94977800
C	3.06483500	0.94272700	-0.56285100
H	1.99531400	-2.28245200	-1.26288300
H	3.56418900	-1.54019500	-1.63739600
H	3.08634100	-1.78510500	0.04127200
H	2.63314200	1.94572500	-0.63630400
H	3.43315700	0.80468200	0.46131400
H	3.94642600	0.91401400	-1.22178800

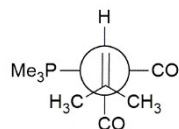
TS_{rotate}-ma in entry 10



Co	-0.32279000	0.53235800	-0.12407200
C	-1.27081100	2.00358500	-0.17551800
O	-1.84127300	2.99760600	-0.23839100
H	0.19360900	1.25721700	-1.34966100
P	1.78711200	-0.03667700	-0.13991900
C	2.82965900	1.08089800	0.86564400
C	2.29330600	-1.67428700	0.52056500
C	2.68140000	-0.03130400	-1.73639400
H	3.89040000	0.80608100	0.81195400
H	2.70306200	2.10854500	0.51193500
H	2.50273300	1.04442900	1.91000500
H	1.93202700	-2.47216300	-0.13734400
H	3.38459100	-1.75552100	0.59355600
H	1.85657800	-1.83051400	1.51284900
H	2.19937800	-0.71499800	-2.44232100
H	2.64682800	0.97342100	-2.16806300
H	3.72748100	-0.33450000	-1.60869000
C	-0.51819200	0.10824300	1.57121100
O	-0.59910900	-0.16990100	2.68447200
C	-1.09015200	-0.81912600	-1.68499400
C	-1.74309300	-1.25509800	-0.56692700
H	-1.57081500	-0.13697200	-2.38082100
H	-0.23836100	-1.37457600	-2.07538200
C	-3.13597500	-0.80374800	-0.24251400
C	-1.31382800	-2.50342500	0.14639000
H	-3.41897100	0.10040600	-0.78925100
H	-3.85070700	-1.59730100	-0.50813800

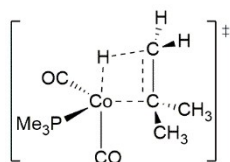
H	-3.26821300	-0.61122600	0.82892700
H	-0.27646600	-2.77116400	-0.07464700
H	-1.42611300	-2.42845900	1.23438400
H	-1.94923100	-3.34227900	-0.17398400

c in entry 10



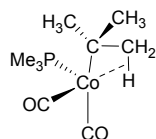
Co	-0.34280600	-0.54736900	0.12535500
C	-1.25352600	-2.04663600	0.21532100
O	-1.79836300	-3.05266900	0.30148700
H	0.24170800	-1.19573200	1.36684900
P	1.75881200	0.03229400	0.09706500
C	2.89470800	-1.39361800	-0.05974200
C	2.38708700	1.11748000	-1.24397200
C	2.45356400	0.87081900	1.57209100
H	3.94405900	-1.07547300	-0.09415300
H	2.74726600	-2.06854900	0.78860500
H	2.65771800	-1.94918900	-0.97219600
H	1.87036600	2.08255400	-1.22771500
H	3.46513900	1.29259500	-1.14536500
H	2.19342600	0.65302100	-2.21625900
H	1.99748400	1.85646500	1.71010000
H	2.24692300	0.27177300	2.46450000
H	3.53741000	1.00311100	1.47268500
C	-0.61427200	-0.14247600	-1.56371500
O	-0.75137900	0.13814000	-2.67015300
C	-1.66502400	1.30266200	0.57659000
C	-1.17385200	0.72340500	1.71248900
C	-1.05337900	2.54988400	0.00944200
C	-3.05851300	1.01646200	0.09981300
H	-1.65197200	3.42296700	0.30921300
H	-0.03191600	2.71260100	0.36903900
H	-1.03727000	2.54883200	-1.08711000
H	-3.12927300	0.98646600	-0.99382000
H	-3.44291000	0.07100700	0.49326600
H	-3.73188400	1.82039400	0.43352000
H	-0.32141500	1.15303700	2.23379500
H	-1.78409800	0.03700800	2.29390800

TS_{ma} in entry 10



Co	-0.37937600	-0.48058900	0.14148700
C	-0.65605000	-2.23528500	0.25460100
O	-0.80658400	-3.37150100	0.31718900
H	-0.08452900	-0.58679300	1.62436300
P	1.72214700	0.22752700	0.05960500
C	2.98944200	-1.08733200	0.22064000
C	2.29702500	1.08143100	-1.45891800
C	2.30692000	1.40154700	1.34713300
H	4.00898500	-0.68625200	0.15761400
H	2.86210200	-1.59664900	1.18141000
H	2.84716600	-1.83164400	-0.56917100
H	1.68900000	1.97549300	-1.63586300
H	3.35121800	1.37561700	-1.38779300
H	2.17318100	0.42136300	-2.32361400
H	1.73472700	2.33442600	1.30671400
H	2.16732200	0.96099000	2.34016900
H	3.36949100	1.64010100	1.21572800
C	-0.73484300	-0.20971100	-1.54641100
O	-0.95390300	0.01568900	-2.65216500
C	-1.26797200	0.55187700	1.74463800
C	-1.79326100	1.03465600	0.53306600
H	-1.89355600	-0.09129800	2.36296800
H	-0.60249700	1.19732200	2.32045700
C	-3.18705200	0.63086500	0.12967200
C	-1.38354600	2.39617900	0.03740800
H	-3.43387400	-0.38092600	0.46570100
H	-3.92315200	1.32309800	0.56836600
H	-3.33223200	0.66803700	-0.95625100
H	-0.36281800	2.65831400	0.33642400
H	-1.44313100	2.47460700	-1.05501100
H	-2.05654000	3.16831000	0.44239600

e in entry 10



Co	-0.40502100	0.56743800	-0.25207100
C	0.36555800	2.10356000	-0.69305000

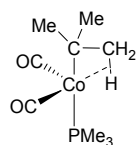
O	0.84003200	3.10821300	-0.97752300
P	1.53580500	-0.54040800	0.15299100
C	2.97361200	0.59045800	0.31728100
C	1.63744900	-1.39840300	1.77358000
C	2.28224100	-1.79941200	-0.96699700
H	3.88325600	0.04990800	0.60567500
H	3.15531500	1.10835600	-0.63004900
H	2.75980700	1.35087900	1.07566300
H	0.94370500	-2.24231100	1.81106100
H	2.65225200	-1.76579000	1.97038000
H	1.35434700	-0.69657100	2.56522800
H	1.62309000	-2.66394600	-1.09024800
H	2.44173800	-1.35671100	-1.95614200
H	3.24757700	-2.15145200	-0.58233000
C	-1.24342600	1.14276800	1.16017600
O	-1.73715100	1.47082900	2.14528600
C	-1.36696100	-0.68571700	-1.81035100
C	-1.68750200	-0.95983900	-0.37611000
H	-2.24620500	-0.43932600	-2.41679900
H	-0.79083400	-1.48003100	-2.29626000
C	-3.12782400	-0.64996100	-0.02002200
C	-1.32511900	-2.33394100	0.12770000
H	-0.71236200	0.25355800	-1.97123900
H	-3.80495700	-1.38605700	-0.48455800
H	-3.30095800	-0.70043300	1.06154800
H	-3.43844000	0.34390000	-0.36094800
H	-2.06041500	-3.08137700	-0.21552700
H	-0.34375300	-2.67829200	-0.21394000
H	-1.33587600	-2.36842000	1.22420400

TS_{iso}-ma in entry 10

Co	-0.35586600	0.39670700	-0.09538700
C	-0.46650700	2.20157700	-0.23382800
O	-0.51773000	3.34673900	-0.17927300
P	1.77575800	-0.26993200	-0.09237400
C	-0.68035800	0.07575000	1.55744800
O	-0.91024000	-0.16579900	2.66091400
C	-3.27249400	-0.16265000	-0.22562100
C	-1.92309100	-0.78630300	-0.47462200
C	-1.31851600	-0.53315200	-1.79534200
C	-1.84453500	-2.21135400	0.01700200
H	-1.96296900	0.01842900	-2.48736900
H	-0.37798700	0.19276200	-1.77314000
H	-0.89907700	-1.42066100	-2.28096200

H	-4.07159800	-0.73963900	-0.72128700
H	-3.51152600	-0.14541700	0.84447100
H	-3.32381000	0.86756100	-0.59290800
H	-0.84496200	-2.64161200	-0.11977100
H	-2.09567400	-2.28746300	1.08132700
H	-2.56124000	-2.85236900	-0.52272400
C	2.30805600	-1.43984800	-1.40688100
H	3.37242600	-1.68985100	-1.31536300
H	1.72584400	-2.36503900	-1.34387200
H	2.13599700	-0.99835400	-2.39441900
C	3.06775000	1.02241000	-0.25986800
H	4.08090100	0.60349900	-0.21197900
H	2.93969200	1.54166900	-1.21537700
H	2.94932700	1.76451400	0.53623500
C	2.36543100	-1.15632900	1.40022600
H	2.26244600	-0.51226200	2.27952200
H	1.74838300	-2.04586700	1.56854000
H	3.41517900	-1.46012400	1.30592600

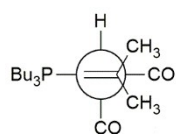
g in entry 10



Co	0.31628900	0.00000100	-0.03246000
C	0.37031600	1.55779100	-0.85082500
O	0.36439000	2.50281000	-1.50680800
P	-1.88736900	-0.00000300	0.22755300
C	-2.82585500	1.41387200	-0.46005300
C	-2.82585900	-1.41387500	-0.46005000
C	-2.46641500	0.00001000	1.96901700
H	-3.89993800	1.31400200	-0.26399300
H	-2.46721700	2.34872400	-0.01791900
H	-2.66644400	1.47548900	-1.54123100
H	-2.46723300	-2.34873000	-0.01791100
H	-3.89994300	-1.31399600	-0.26400200
H	-2.66643800	-1.47549700	-1.54122600
H	-2.08587600	-0.88618800	2.48681400
H	-2.08587800	0.88622100	2.48679200
H	-3.56165600	0.00001000	2.02612200
C	0.37031300	-1.55779000	-0.85082400
O	0.36438400	-2.50281300	-1.50680100
C	3.06452000	-1.23743800	0.13777600
C	2.25089600	-0.00000100	0.44525000

H	2.56030200	-2.16243200	0.43826000
H	4.03171000	-1.20553200	0.66766800
C	1.62635100	0.00001400	1.81339100
C	3.06453300	1.23742100	0.13775400
H	3.29183900	1.31461600	-0.93242400
H	2.56032700	2.16242700	0.43822200
H	4.03172400	1.20551400	0.66764400
H	1.86036500	0.89527000	2.39926400
H	0.47989900	0.00000100	1.78440100
H	1.86038000	-0.89522100	2.39928900
H	3.29182600	-1.31465400	-0.93239900

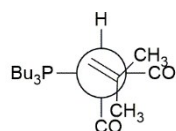
a in entry 11



Co	-1.52295300	-0.35552100	-0.28939000
C	-2.81490600	0.84250300	-0.40519900
O	-3.66140500	1.60204200	-0.55404900
H	-1.25176000	0.16227900	-1.67580100
P	0.55196100	0.37313200	-0.15848500
C	-1.63895600	-0.81259400	1.42445500
O	-1.65958500	-1.07171300	2.54133000
C	1.68053100	-0.29102300	-1.45730500
C	3.11487300	0.20876700	-1.48477200
H	1.18144900	-0.08819600	-2.41621000
H	1.66031700	-1.38507300	-1.34692400
C	3.96430800	-0.54242700	-2.49779600
H	3.13942100	1.28247700	-1.72308600
H	3.57983000	0.11307700	-0.49112300
C	5.38894100	-0.02767900	-2.55728800
H	3.96079500	-1.61403400	-2.24659400
H	3.49493800	-0.46936100	-3.49028400
H	5.99549300	-0.57848100	-3.28357900
H	5.41752200	1.03145500	-2.84156400
H	5.88426000	-0.11471600	-1.58220600
C	0.72892800	2.19641200	-0.36044400
C	-0.01579300	3.00434600	0.68879000
H	0.34685300	2.43236500	-1.36526200
H	1.79614400	2.46206700	-0.35068500
C	0.05684000	4.50072800	0.43388900
H	-1.06886700	2.68880100	0.72447000
H	0.39405300	2.78999900	1.68854400

C	-0.67887400	5.30272400	1.48932400
H	1.11116900	4.81382000	0.38955100
H	-0.36035700	4.71706400	-0.56091500
H	-0.62661000	6.37962500	1.29816000
H	-1.73937900	5.02613100	1.52885600
H	-0.26000800	5.12519700	2.48768900
C	1.49070700	0.06659100	1.40261800
C	1.81695600	-1.40007100	1.63425900
H	0.86044200	0.44032000	2.22223200
H	2.40644500	0.67670700	1.41652500
C	2.31471900	-1.67384000	3.04339500
H	0.92743600	-2.01948700	1.43889200
H	2.57484200	-1.73645300	0.90901700
C	2.68025600	-3.12947000	3.25624000
H	3.18317600	-1.03124400	3.25435600
H	1.53774200	-1.37193600	3.76152900
H	3.03011000	-3.32075700	4.27594200
H	1.81876100	-3.78420500	3.07632000
H	3.47669600	-3.44492400	2.57067900
C	-1.19786400	-2.26578400	-1.06154400
C	-2.55671200	-1.98636000	-1.18787400
H	-0.55347900	-2.20692200	-1.93749000
H	-0.85118600	-2.94002600	-0.27824300
C	-3.14215100	-1.62212700	-2.52468300
C	-3.56147500	-2.59605600	-0.24961200
H	-3.96529900	-0.90291600	-2.43312100
H	-2.39727000	-1.19673100	-3.20309800
H	-3.56185100	-2.52171200	-3.00123000
H	-4.37706800	-1.90058500	-0.01588300
H	-4.02371100	-3.47780300	-0.71992100
H	-3.11477000	-2.92419300	0.69428900

TS_{rotate}-ma in entry 11

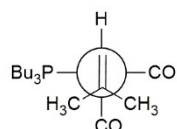


Co	-1.48714800	0.07586700	-0.55277700
C	-2.77261200	1.22728200	-0.87985700
O	-3.56091500	2.03123200	-1.10657800
H	-0.95106200	0.82143400	-1.75989800
P	0.63939900	0.37297700	-0.11898600
C	-1.89682600	-0.40491400	1.08710800
O	-2.11613500	-0.68485800	2.18148100

C	1.83638900	-0.30740000	-1.34957700
C	3.31180200	-0.00450800	-1.15045700
H	1.49261000	0.06103700	-2.32762300
H	1.67866000	-1.39509900	-1.37862000
C	4.18492200	-0.69934700	-2.18356100
H	3.48859900	1.08003600	-1.20331800
H	3.63771500	-0.31265100	-0.14456200
C	5.65680900	-0.38117800	-2.00883900
H	4.02441300	-1.78629700	-2.12021500
H	3.85377500	-0.40913600	-3.19193100
H	6.27842700	-0.88850200	-2.75384100
H	5.84437600	0.69554200	-2.10263600
H	6.01545800	-0.68748700	-1.01821900
C	1.11773100	2.15165000	-0.05675700
C	0.22937900	3.00031900	0.83591700
H	1.07086800	2.51877000	-1.09348600
H	2.16635800	2.23206700	0.26478000
C	0.64806400	4.46094600	0.85324500
H	-0.81397400	2.91604700	0.49982600
H	0.24123700	2.60912100	1.86590800
C	-0.24413800	5.30775400	1.73947500
H	1.69389600	4.53985200	1.18757100
H	0.63475000	4.85159600	-0.17547400
H	0.05856800	6.36013100	1.74265600
H	-1.28813300	5.26555000	1.40644000
H	-0.22154900	4.95566500	2.77828200
C	1.28956400	-0.25726600	1.49093100
C	1.28048400	-1.77409500	1.57541100
H	0.63846600	0.16215200	2.27112600
H	2.29620900	0.14266500	1.68125700
C	1.43181900	-2.29761300	2.99305600
H	0.33829800	-2.16014400	1.15495800
H	2.08072600	-2.19075100	0.94343100
C	1.42173000	-3.81231000	3.04841300
H	2.36250900	-1.90646000	3.43136900
H	0.61475200	-1.89290500	3.60826200
H	1.52250500	-4.18876300	4.07160400
H	0.48540400	-4.21512600	2.64117900
H	2.24268900	-4.23878700	2.45845000
C	-1.38191600	-1.58592600	-2.03612000
C	-2.41494000	-2.00046700	-1.25055500
H	-1.56926400	-1.06267200	-2.96937200
H	-0.39435000	-2.02834800	-1.92390800
C	-3.84449700	-1.72389900	-1.60482100

C	-2.23208000	-3.08161700	-0.22680200
H	-4.42712000	-1.40682900	-0.73155200
H	-3.94314000	-0.95680600	-2.37808200
H	-4.31585500	-2.64587800	-1.97766800
H	-2.81074400	-2.90200500	0.68648700
H	-2.59507600	-4.03321500	-0.64197700
H	-1.18269000	-3.22231400	0.05208200

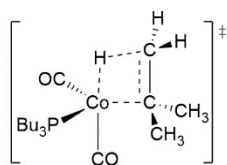
c in entry 11



Co	-1.55046500	-0.14994800	-0.54514200
C	-3.04570700	0.74583800	-0.78038100
O	-3.97706900	1.39885000	-0.93825100
H	-1.17451700	0.76446500	-1.69560900
P	0.50639400	0.47780800	-0.13151200
C	-1.84736900	-0.80925100	1.05604600
O	-2.01354300	-1.21822800	2.11876400
C	1.78430600	-0.04998700	-1.35741600
C	3.20894300	0.43960400	-1.16032700
H	1.40028700	0.27374000	-2.33645100
H	1.76370900	-1.14977900	-1.38428100
C	4.16037300	-0.12348500	-2.20433100
H	3.24193200	1.53841100	-1.20205200
H	3.57643600	0.16686700	-0.15890800
C	5.58038400	0.37644700	-2.02561600
H	4.13947200	-1.22283500	-2.15738700
H	3.79255600	0.13734000	-3.20800100
H	6.25950300	-0.03593500	-2.77896200
H	5.62962100	1.46963400	-2.10224300
H	5.97737300	0.10265400	-1.04021900
C	0.71271500	2.31105700	-0.12529900
C	-0.28718300	3.03679200	0.75787400
H	0.60156500	2.63949500	-1.16987900
H	1.73945800	2.55784900	0.18265500
C	-0.10490400	4.54497700	0.72766000
H	-1.30801400	2.77844900	0.44182400
H	-0.20086400	2.68303900	1.79795400
C	-1.11006700	5.26587200	1.60441800
H	0.91907100	4.79813500	1.04259300
H	-0.19215500	4.89737000	-0.31126100
H	-0.97728600	6.35247500	1.57505000

H	-2.13775900	5.05019900	1.28825400
H	-1.02121400	4.95162400	2.65177600
C	1.26535500	0.03120600	1.49404300
C	1.51396200	-1.45605500	1.67168100
H	0.56342100	0.38377000	2.26374100
H	2.19372100	0.60303100	1.63950800
C	1.86300100	-1.83170500	3.10147900
H	0.62193600	-2.02183400	1.36741200
H	2.32010200	-1.78924000	0.99798400
C	2.11782000	-3.31782400	3.25822700
H	2.74317500	-1.25820800	3.42978100
H	1.03837500	-1.52052400	3.76018900
H	2.35110200	-3.58972100	4.29284700
H	1.23974900	-3.90182300	2.95451000
H	2.95823800	-3.64667300	2.63413400
C	-1.38245700	-1.54999500	-2.25758200
C	-1.85574700	-2.37678400	-1.28205700
H	-2.05852300	-1.10164800	-2.98045200
H	-0.33025300	-1.56266500	-2.53340300
C	-0.95372200	-3.34237300	-0.57298100
C	-3.31874700	-2.67987100	-1.15092400
H	-3.94265700	-1.94867700	-1.67250600
H	-3.52798400	-3.67181800	-1.57896800
H	-3.64127100	-2.71915000	-0.10372100
H	-1.20061300	-3.44890000	0.49052700
H	-1.07423100	-4.34144000	-1.01732800
H	0.10236400	-3.06796700	-0.65878100

TS_{ma} in entry 11

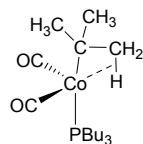


Co	-1.49888000	-0.47788400	-0.58911200
C	-2.87792400	0.64453300	-0.75960800
O	-3.71879800	1.42437100	-0.82958000
H	-1.13970200	-0.03908800	-1.99361400
P	0.44088400	0.51053100	-0.16214300
C	-1.75842800	-1.10182900	1.01956700
O	-1.89698300	-1.52933700	2.07912000
C	1.81104100	0.19342400	-1.36309900
C	3.17935300	0.78409800	-1.06976000
H	1.43495500	0.55997200	-2.33144700

H	1.88871600	-0.89790900	-1.47737200
C	4.18989400	0.47386300	-2.16281800
H	3.10896100	1.87529700	-0.94823800
H	3.56179400	0.40179800	-0.11057500
C	5.55541100	1.06732100	-1.87703800
H	4.27122900	-0.61703700	-2.28222300
H	3.81013500	0.84997500	-3.12466300
H	6.27723600	0.83925900	-2.66807600
H	5.50260500	2.15915200	-1.78504000
H	5.96710700	0.68270700	-0.93561900
C	0.31427100	2.35029400	-0.20384800
C	-0.58368000	2.91863200	0.88500500
H	-0.09894900	2.59105800	-1.19518600
H	1.31193900	2.80950200	-0.15172500
C	-1.04398700	4.33452900	0.58247300
H	-1.46750200	2.27625400	1.01903300
H	-0.05408500	2.90377000	1.85004200
C	-1.91231800	4.90864600	1.68400800
H	-0.16715300	4.97849500	0.41431500
H	-1.59990900	4.33026000	-0.36740100
H	-2.24651100	5.92619500	1.45601200
H	-2.80823000	4.29512400	1.83887800
H	-1.37367400	4.94522500	2.63920100
C	1.22451300	0.21506300	1.48171400
C	1.67538400	-1.22183400	1.68029600
H	0.45847300	0.46489100	2.23032300
H	2.05647900	0.91811000	1.64050300
C	2.05815600	-1.52772300	3.11798900
H	0.87077800	-1.90543500	1.37115700
H	2.52669700	-1.44881400	1.01826400
C	2.50839100	-2.96344600	3.30156100
H	2.85089200	-0.83676600	3.44307900
H	1.19425000	-1.31959100	3.76691200
H	2.77186200	-3.18296600	4.34144200
H	1.71767600	-3.66497400	3.00748100
H	3.38770300	-3.18833600	2.68491400
C	-1.58725000	-2.48530600	-1.24178000
C	-1.26739700	-1.64718700	-2.32413900
C	-0.52647200	-3.39335000	-0.67748500
C	-2.98310400	-3.03856100	-1.12492200
H	-0.69618500	-3.62621300	0.38130700
H	-0.53572200	-4.35676800	-1.21107300
H	0.48117300	-2.97365600	-0.77327200
H	-0.25504000	-1.68298200	-2.72940500

H	-2.03164900	-1.45267300	-3.07653500
H	-3.25317600	-3.25790500	-0.08497600
H	-3.73293900	-2.34988400	-1.52587500
H	-3.06260500	-3.98841700	-1.67740200

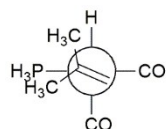
g in entry 11



Co	-1.43727600	-0.32583400	-0.42127500
C	-1.69867600	0.94627100	-1.60670000
O	-1.88000700	1.88213300	-2.25367100
P	0.65757200	0.29721500	-0.03703400
C	-1.91807200	-0.25750600	1.26820400
O	-2.22839400	-0.07317600	2.36189400
C	1.81453500	-0.17257300	-1.39749800
C	3.28944000	0.14583800	-1.22223300
H	1.41443800	0.32307500	-2.29537400
H	1.67508000	-1.24859700	-1.57759700
C	4.11519600	-0.26473100	-2.43129400
H	3.43013100	1.22227900	-1.04171100
H	3.68557100	-0.36284200	-0.32960600
C	5.58877900	0.04745600	-2.26014100
H	3.97689800	-1.34069800	-2.61580000
H	3.72393100	0.24213600	-3.32587000
H	6.17626400	-0.25149200	-3.13429200
H	5.75260200	1.12112400	-2.10596400
H	6.00727800	-0.47263800	-1.38957100
C	0.93852100	2.10993200	0.12133500
C	0.00490900	2.78843000	1.11061100
H	0.79783100	2.53790900	-0.88306500
H	1.98740000	2.29044500	0.39906400
C	0.23226900	4.28894000	1.18413200
H	-1.03938400	2.58619700	0.83093300
H	0.13254000	2.35401300	2.11478400
C	-0.69910500	4.96617100	2.17015300
H	1.27981200	4.48790100	1.45782400
H	0.09825900	4.72222700	0.18160600
H	-0.53289200	6.04749700	2.21591700
H	-1.74900500	4.80483000	1.89787800
H	-0.56318100	4.56844800	3.18341000
C	1.45436700	-0.36751300	1.48480400
C	1.47488000	-1.88568400	1.52997000

H	0.87720500	0.02217800	2.33571800
H	2.46993100	0.04436500	1.58112700
C	2.06151200	-2.42787100	2.82250800
H	0.44960800	-2.26851400	1.40306500
H	2.05013800	-2.28359500	0.67794100
C	2.07849600	-3.94327200	2.85955600
H	3.08191700	-2.03626900	2.95206200
H	1.48219400	-2.03664500	3.67183600
H	2.50025800	-4.32701400	3.79419900
H	1.06586100	-4.35351200	2.76307200
H	2.67530500	-4.35511000	2.03613900
C	-2.96920900	-1.45650500	-1.00062100
C	-1.82116800	-2.39389100	-1.26028300
C	-3.94388400	-1.94608600	0.04679400
C	-3.71955500	-1.04424000	-2.24784300
H	-0.79737300	-1.92093100	-1.04957300
H	-1.82865800	-3.28278300	-0.62033100
H	-1.73502300	-2.69699300	-2.30986200
H	-3.44494800	-2.35268200	0.93345300
H	-4.61193700	-1.14281200	0.38086800
H	-4.58587900	-2.74490100	-0.36253100
H	-3.05157000	-0.77058800	-3.07211900
H	-4.36067400	-1.86830400	-2.60543800
H	-4.37926600	-0.18904100	-2.05677100

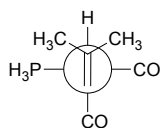
TS_{rotate}-(anti-ma) in entry 12



Co	0.41115400	0.09187400	-0.11249900
C	1.33138800	1.52532200	-0.56057200
O	1.91143000	2.44878000	-0.91210600
H	-0.28209900	0.54810800	-1.37093000
P	0.28030000	-1.75240600	-1.24573400
H	0.78502600	-2.98729500	-0.76900900
H	-0.96677300	-2.25239900	-1.69497200
H	0.92608600	-1.78922900	-2.50077000
C	1.45816600	-0.54910100	1.16637100
O	2.14886400	-0.97718400	1.97320900
C	-0.97745400	0.72714600	1.47359900
C	-1.84322700	0.38008400	0.47764100
H	-0.80281700	0.05176600	2.30815000
H	-0.70189000	1.76630200	1.63566900

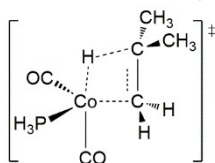
C	-2.47959600	1.42339800	-0.39323000
C	-2.56050600	-0.93478200	0.49633900
H	-3.47257800	1.67311900	0.01004100
H	-1.89039300	2.34401600	-0.43457800
H	-2.63331500	1.06910800	-1.41841100
H	-2.04726200	-1.68444100	1.10767200
H	-3.56956400	-0.79498700	0.91204800
H	-2.70507000	-1.34376000	-0.51112700

d in entry 12



Co	0.36943000	0.11947400	-0.14606900
C	0.40283700	1.72365300	-0.85590900
O	0.39172100	2.74996200	-1.36622500
H	-0.50920600	-0.04334300	-1.36468100
P	1.02031200	-1.82043500	-0.89923300
H	2.03036600	-2.59088100	-0.27186000
H	0.09720300	-2.88048800	-1.07629500
H	1.56562800	-1.87216500	-2.20051100
C	1.68353500	0.31950600	1.02520400
O	2.54792200	0.43543800	1.76727000
C	-1.83355200	-0.18026400	0.54668000
C	-0.96192100	-0.18774700	1.59641900
H	-0.64788800	-1.12483600	2.05199300
C	-2.59964800	1.05544900	0.17747700
H	-2.13877800	1.96450500	0.57485600
H	-2.69905300	1.16907600	-0.90765900
H	-3.61907000	0.98730900	0.58500500
H	-0.79775100	0.70963300	2.18830800
C	-2.41134400	-1.45612400	0.01178600
H	-1.84182200	-2.33664500	0.32400600
H	-3.43575300	-1.57665300	0.39275800
H	-2.47975300	-1.45482200	-1.08185700

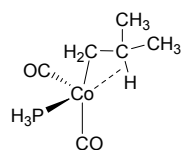
TS_{anti-ma} in entry 12



Co	0.32590300	-0.10166000	0.05512500
C	0.76914400	-1.48972200	1.04844100

O	1.02375400	-2.39786600	1.69981200
H	-0.81773000	-0.06197900	1.03876500
P	0.87066400	1.92759500	0.83914300
H	2.15223800	2.47533900	0.59360700
H	0.15232000	3.09538700	0.46493700
H	0.86018900	2.20240000	2.22674300
C	1.57580000	-0.26611900	-1.17661500
O	2.37460200	-0.36168500	-1.99143200
C	-1.00759600	0.25923800	-1.49577900
C	-1.80687000	-0.04005300	-0.38732300
H	-0.94077800	1.28932100	-1.84578300
H	-0.84940800	-0.49954600	-2.25974800
C	-2.41690900	-1.41172000	-0.26251000
C	-2.64605200	1.05970000	0.21635000
H	-3.40075600	-1.42106100	-0.75311800
H	-1.79484800	-2.17909300	-0.73155700
H	-2.57370300	-1.69564200	0.78414600
H	-2.14289300	2.03074400	0.17420900
H	-3.58331900	1.14890000	-0.34956600
H	-2.91258400	0.85459600	1.25941100

f in entry 12



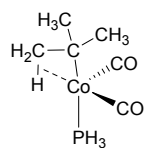
Co	-0.43193500	0.08319700	-0.00526800
C	-1.64381900	0.08403600	1.28665200
O	-2.42293000	0.08547800	2.12468400
P	-0.84010100	-1.92642700	-0.78901700
H	-1.25634900	-1.97240200	-2.13870900
H	0.18891700	-2.89316600	-0.91944600
H	-1.82681500	-2.80519600	-0.28216800
C	-0.87544200	1.60623200	-0.76549700
O	-1.16514300	2.56853000	-1.31504200
C	1.24579500	0.10227400	-1.04825900
C	1.83586100	0.06242400	0.33144000
C	2.54961800	1.34977700	0.71319400
C	2.70414400	-1.16021300	0.58902400
H	3.46496900	1.46123600	0.11800300
H	1.91916500	2.22581700	0.52756500
H	2.83642400	1.35791500	1.77152200
H	2.17932300	-2.09209500	0.35085400
H	3.60544400	-1.11882600	-0.03571300

H	3.02546800	-1.21498100	1.63610900
H	1.47178200	1.01180700	-1.61010300
H	1.48230500	-0.77052400	-1.66760200
H	0.98079400	-0.03875500	1.11073000

TS_{iso}-(anti-ma) in entry 12

Co	0.34923700	0.10624500	-0.00369800
C	0.71126200	1.70104000	-0.81587400
O	1.03804500	2.71531300	-1.23310200
P	1.12084000	-1.63100600	-1.15715500
H	2.16318300	-2.42071200	-0.61988200
H	0.26134200	-2.71302600	-1.47666300
H	1.67891400	-1.51261800	-2.45384400
C	1.47395100	0.00303000	1.29762800
O	2.20416200	-0.06479900	2.18169700
C	-1.04686900	0.12926700	1.39796100
C	-1.83644000	-0.08644200	0.18108000
H	-1.11149500	-0.07264500	-0.78600200
H	-1.01211300	-0.69853800	2.10762800
H	-1.15064600	1.09878600	1.88756600
C	-2.49860800	-1.45083000	0.07873700
H	-3.36957800	-1.49490200	0.74369100
H	-2.84982700	-1.65865500	-0.93941700
H	-1.81063000	-2.25070000	0.37229700
C	-2.78367100	1.05171500	-0.17246600
H	-3.19740400	0.93798600	-1.18158100
H	-3.62333500	1.07047300	0.53259500
H	-2.27582700	2.02024000	-0.12036400

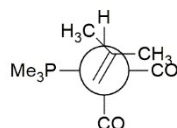
h in entry 12



Co	0.40816500	0.00746800	0.13360100
C	0.71046400	1.62792000	0.77237000
O	0.93179400	2.63260100	1.27859200
P	1.95818500	0.00793300	-1.42798300
H	3.05616300	-0.87538200	-1.33437400
H	1.59446700	-0.31599300	-2.75628100
H	2.69707200	1.17265600	-1.73325500
C	0.77215000	-1.59119500	0.79279000
O	1.03301200	-2.57858700	1.31432000
C	-1.32953700	-0.02042900	1.04981600

C	-1.87210000	-0.02507600	-0.35375900
H	-0.98931100	-0.01381000	-1.09481500
H	-1.55686000	-0.91927900	1.62869900
H	-1.58500700	0.86738300	1.63392800
C	-2.63918800	-1.29445100	-0.68895200
H	-3.56423100	-1.34058600	-0.10019800
H	-2.91658000	-1.33600800	-1.74930500
H	-2.05081700	-2.18932300	-0.45692600
C	-2.66789100	1.22749400	-0.68502600
H	-2.94561400	1.26653500	-1.74538300
H	-3.59406700	1.25063400	-0.09664700
H	-2.10028300	2.13484500	-0.44965800

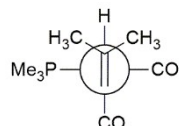
TS_{rotate}-(anti-ma) in entry 13



Co	-0.34990800	-0.42911600	0.07442400
C	-1.35205200	-1.41191300	1.12164600
O	-1.99122900	-2.01664700	1.85886400
H	-0.46822500	0.44180700	1.30846100
P	1.68216100	0.37403400	0.23612800
C	2.70039200	-0.62919300	1.37890400
C	2.74855500	0.40053700	-1.25832400
C	1.98697800	2.06246200	0.88117900
H	3.72284800	-0.24063100	1.46592700
H	2.23085700	-0.64010900	2.36716100
H	2.73760200	-1.66169000	1.01676100
H	2.31570500	1.06555200	-2.01359600
H	3.76186900	0.74977500	-1.02563900
H	2.81360800	-0.60219300	-1.69268900
H	1.61807100	2.81375600	0.17601100
H	1.45870100	2.19918500	1.82948600
H	3.05900300	2.23340500	1.03661900
C	0.14289300	-1.68236300	-1.06536800
O	0.51361600	-2.50243600	-1.77926700
C	-1.25814500	0.69814000	-1.61226300
C	-1.88756300	1.22589100	-0.52369800
H	-0.43631500	1.22703700	-2.09264100
H	-1.73203200	-0.08172200	-2.20317000
C	-1.49972700	2.56710600	0.02276700
C	-3.24365100	0.75244700	-0.09418800
H	-4.00752200	1.46820900	-0.43333100

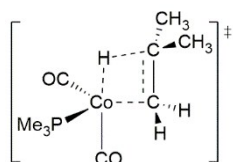
H	-3.49086600	-0.22944700	-0.50830200
H	-3.32953900	0.69406400	0.99696800
H	-0.49620500	2.86762500	-0.29129200
H	-2.20514200	3.32686900	-0.34574000
H	-1.54249500	2.59811100	1.11692000

d in entry 13



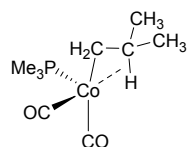
Co	0.39559400	-0.46678800	-0.07230000
C	1.45239100	-1.48434300	-1.03149600
O	2.12526200	-2.11342900	-1.71630300
H	0.58776400	0.34778200	-1.33268800
P	-1.63023100	0.35256700	-0.28970800
C	-2.51239800	0.92268100	1.21694800
C	-1.95996900	1.73575400	-1.44391900
C	-2.81206800	-0.89866900	-0.91759800
H	-3.55142100	1.19724400	0.99795400
H	-2.50869900	0.12280400	1.96561900
H	-2.00680100	1.79178400	1.65019000
H	-1.60868700	1.46088900	-2.44323600
H	-3.03193600	1.96268800	-1.49017500
H	-1.42225600	2.63620900	-1.13392800
H	-2.46196800	-1.27520200	-1.88345800
H	-2.85529200	-1.74505800	-0.22452300
H	-3.81971100	-0.48096900	-1.03571500
C	-0.18984700	-1.66724600	1.07864400
O	-0.63768900	-2.43748100	1.80455300
C	1.37732400	0.57156400	1.60964500
C	1.77981700	1.29274900	0.52282200
H	0.56830500	0.92416500	2.24717200
H	2.01861000	-0.19646000	2.03523700
C	1.15841300	2.61806500	0.19665700
C	3.12062500	1.06855500	-0.11177500
H	3.81822500	1.85402400	0.21520200
H	3.55291900	0.10148300	0.16093600
H	3.07096000	1.12340500	-1.20508000
H	0.18024300	2.74971800	0.67124700
H	1.80988300	3.42648400	0.56071500
H	1.04597500	2.76640500	-0.88331200

TS_{anti-ma} in entry 13



Co	0.42903300	0.47729100	-0.02621700
C	1.04435100	1.60915100	1.19477200
O	1.43458700	2.33120100	1.99740800
H	0.93162300	-0.58732800	0.92867200
P	-1.58929300	-0.42799900	0.26320600
C	-1.84645500	-1.68660000	1.57295600
C	-2.88332100	0.79435800	0.69873500
C	-2.39185100	-1.24455200	-1.17515600
H	-2.89994400	-1.98367500	1.64668400
H	-1.24260900	-2.57570300	1.36604600
H	-1.52292400	-1.27858700	2.53576000
H	-2.94879600	1.55185100	-0.08951800
H	-3.86670700	0.32386600	0.82289100
H	-2.60930800	1.30365600	1.62794100
H	-2.43336900	-0.53959200	-2.01323400
H	-1.80922500	-2.11335000	-1.49911400
H	-3.41148100	-1.57548000	-0.94156200
C	-0.14125900	1.60719200	-1.23223200
O	-0.55976100	2.30641800	-2.04222500
C	1.48323900	-0.47594100	-1.51975300
C	1.82860600	-1.14783300	-0.33453700
H	0.81224300	-0.95873700	-2.23037500
H	2.18650300	0.23162800	-1.95477100
C	1.34600100	-2.56781400	-0.15332200
C	3.18451100	-0.89175300	0.27720800
H	0.35120100	-2.71897700	-0.58559300
H	2.03509500	-3.25382900	-0.66407700
H	1.31349200	-2.86464800	0.90186900
H	3.51254200	0.13891200	0.11534200
H	3.18898100	-1.08229200	1.35670500
H	3.92663800	-1.56278600	-0.17739300

f in entry 13



Co	0.34551500	-0.57787500	-0.03383900
C	-0.35909800	-1.57878700	-1.29820500

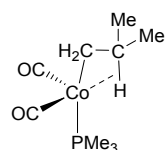
O	-0.84828300	-2.21375800	-2.12046600
H	1.33433700	0.53344700	-1.14297400
P	-1.58940200	0.48053800	0.25268700
C	-2.39608800	1.20781000	-1.22884400
C	-2.89065100	-0.68551900	0.80368400
C	-1.80229500	1.83444600	1.47072200
H	-3.39146300	1.60732100	-0.99952700
H	-1.77843500	2.01301800	-1.64024500
H	-2.49559700	0.43639600	-2.00022900
H	-2.59951400	-1.14061900	1.75505400
H	-3.85792000	-0.18274100	0.92566100
H	-2.99844700	-1.48890200	0.06779600
H	-1.48316900	1.49795900	2.46196400
H	-1.19793600	2.70579100	1.19918500
H	-2.85301200	2.14308500	1.52258300
C	1.16807700	-1.83669900	0.86691300
O	1.66605500	-2.63998100	1.51669000
C	1.36894700	0.73407600	1.02815800
C	1.86303400	1.15823900	-0.33169200
H	0.80663600	1.50199300	1.56561800
H	2.15792700	0.35092400	1.68109300
C	1.51355000	2.59827600	-0.67542700
C	3.34400500	0.88065900	-0.53764400
H	0.44276400	2.79910300	-0.55058100
H	2.05715000	3.28617100	-0.01493000
H	1.78012600	2.84767300	-1.71003300
H	3.59048300	-0.15905400	-0.29652000
H	3.65520500	1.07042200	-1.57234500
H	3.94392800	1.52747500	0.11597900

TS_{iso}-(anti-ma) in entry 13

Co	-0.36334400	-0.51337600	-0.07225200
C	-0.65182800	-1.72769800	1.24149900
O	-0.76238000	-2.57368900	2.00851500
P	1.56657300	0.56525300	0.24078300
C	0.22635900	-1.45359200	-1.38108000
O	0.63754400	-2.05502000	-2.27279700
C	-1.80078500	0.09417300	-1.29371600
C	-1.99411100	0.95069800	-0.11980400
H	-1.17173500	0.68595000	0.73522000
H	-1.45674400	0.58635100	-2.20552100
H	-2.56722400	-0.65812400	-1.48483700
C	-1.73060700	2.43025400	-0.35422700
H	-2.54674000	2.86862200	-0.94111900

H	-1.66607100	2.98749800	0.58879100
H	-0.79883400	2.58476900	-0.90975600
C	-3.28976700	0.70560500	0.63940300
H	-3.28976900	1.20307500	1.61669800
H	-4.13832600	1.09659200	0.06505800
H	-3.45309900	-0.36438500	0.80251700
C	2.94127600	-0.53348600	0.75148100
H	3.88126500	0.01750800	0.88037600
H	2.68402500	-1.03132400	1.69176400
H	3.08706900	-1.31015000	-0.00713900
C	2.33600200	1.40832700	-1.19770700
H	2.49168700	0.68230600	-2.00304700
H	1.67031900	2.18967000	-1.57903400
H	3.30125200	1.86159300	-0.93888900
C	1.67028900	1.88317900	1.51395100
H	0.99886500	2.70845500	1.25390900
H	1.35310200	1.48247400	2.48202500
H	2.69036200	2.27639500	1.60749400

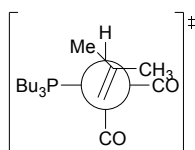
h in entry 13



Co	-0.24577200	0.02475300	-0.49263700
C	-0.06054300	-1.54368000	-1.26410700
O	0.08523900	-2.51765400	-1.85706100
P	1.70482400	-0.00144500	0.52623000
C	2.93364300	-1.22817100	-0.04877400
C	2.70056900	1.53368600	0.53641000
C	1.60897600	-0.39187400	2.31557300
H	3.86512400	-1.16251500	0.52577100
H	2.52186700	-2.23758700	0.05055500
H	3.15553700	-1.06267000	-1.10775700
H	2.11914900	2.34915100	0.97843500
H	3.62942300	1.40563900	1.10467200
H	2.94957600	1.82146200	-0.48999700
H	1.02515500	0.37657700	2.83220600
H	1.10209300	-1.35256100	2.45443800
H	2.60583800	-0.44518900	2.77005400
C	-0.11813800	1.65583400	-1.14984300
O	0.00292000	2.67649800	-1.66348700
C	-2.19136800	-0.01808100	-0.79830700
C	-2.22574700	-0.03926100	0.70452200

C	-2.89976200	1.18537400	1.30284600
C	-2.78164200	-1.33315900	1.27699500
H	-1.14201000	0.00988300	1.10445200
H	-2.59124300	-0.91627700	-1.27556400
H	-2.63262800	0.87281900	-1.25195300
H	-3.97205300	1.17643300	1.06874500
H	-2.79734500	1.21673500	2.39491300
H	-2.47704300	2.11062700	0.89527100
H	-2.28361300	-2.20725700	0.84253500
H	-2.66170200	-1.38169100	2.36685900
H	-3.85382600	-1.41501400	1.05659200

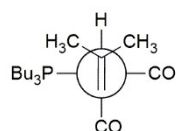
TS_{rotate}-(anti-ma) in entry 14



Co	-1.54630300	-0.63485800	-0.10979400
C	-3.10935500	-0.14783700	-0.74645100
O	-4.09365900	0.21072800	-1.21742200
H	-1.24275000	-0.56859500	-1.59514700
P	0.38717300	0.40713100	-0.16346400
C	-1.81005500	-0.27107400	1.59356200
O	-1.94727800	0.00481300	2.70071400
C	1.66021000	-0.13680900	-1.38960400
C	3.00525100	0.56892000	-1.40196300
H	1.16632400	-0.04538600	-2.36883300
H	1.80924800	-1.21446700	-1.24521200
C	3.90233700	0.07021300	-2.52441000
H	2.87468100	1.65630900	-1.50685700
H	3.52378800	0.42050300	-0.44187000
C	5.25214000	0.76023000	-2.53825800
H	4.03636100	-1.01750600	-2.42524300
H	3.39388900	0.21931900	-3.48865900
H	5.89230300	0.39625400	-3.34857000
H	5.14307200	1.84412400	-2.66758700
H	5.79065500	0.59911000	-1.59609900
C	0.15581800	2.17398000	-0.64394600
C	-0.83808400	2.93157900	0.21921100
H	-0.18709100	2.16342700	-1.68951300
H	1.13047700	2.68414200	-0.62996200
C	-1.01316300	4.37460800	-0.22395700
H	-1.80926700	2.41693300	0.19562500
H	-0.51629900	2.91662800	1.27287000

C	-2.01691900	5.12333500	0.63074600
H	-0.03945400	4.88721900	-0.19704900
H	-1.32984500	4.39223400	-1.27761400
H	-2.13895200	6.16229200	0.30687900
H	-3.00415600	4.64749000	0.59087500
H	-1.70861900	5.14069500	1.68344500
C	1.36712100	0.57312400	1.39178700
C	1.84265500	-0.76133400	1.94183900
H	0.72716400	1.07249700	2.13236300
H	2.21793200	1.24847200	1.21727300
C	2.74222100	-0.61059800	3.15669500
H	0.97089700	-1.38032000	2.20436400
H	2.38385500	-1.32627900	1.16446200
C	3.20278600	-1.94534200	3.70833100
H	3.61389600	0.00532100	2.88610600
H	2.20780100	-0.04445200	3.93393300
H	3.85748400	-1.82733600	4.57791900
H	2.35070100	-2.56182200	4.01973900
H	3.75821400	-2.51679900	2.95404100
C	-1.33915700	-2.78064800	0.50289200
C	-1.45557000	-2.88212300	-0.85002800
H	-0.36518000	-2.86334000	0.98195100
H	-2.20437000	-2.91387000	1.14766100
C	-0.25687000	-3.15478800	-1.70722900
C	-2.76912100	-3.17425900	-1.51055500
H	-0.26161000	-2.57074600	-2.63397500
H	0.68038900	-2.96101900	-1.17654500
H	-0.25664200	-4.21517600	-2.00009600
H	-2.90883400	-2.58381700	-2.42321600
H	-2.79987100	-4.23242600	-1.81051000
H	-3.61958700	-2.98680300	-0.84886200

d in entry 14

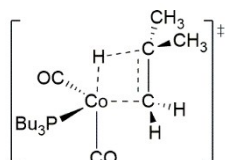


Co	-1.52999000	-0.68212200	-0.16008700
C	-3.08416600	-0.20843200	-0.83536700
O	-4.05785800	0.14896200	-1.32865100
H	-1.18721900	-0.59877400	-1.63538200
P	0.37582300	0.41376700	-0.15258200
C	-1.83032300	-0.34396100	1.54208400
O	-1.98483200	-0.09063200	2.65252200

C	1.67880700	-0.03304800	-1.38838700
C	2.98496600	0.74244500	-1.37627000
H	1.18354600	0.06180000	-2.36672800
H	1.88326600	-1.10502000	-1.27434000
C	3.92342200	0.29701300	-2.48723600
H	2.79889900	1.82179300	-1.47972600
H	3.49643100	0.61747000	-0.40933500
C	5.23458200	1.05804200	-2.47931400
H	4.11381900	-0.78246000	-2.38976400
H	3.42096700	0.42266200	-3.45793700
H	5.90414800	0.73234500	-3.28208600
H	5.06984400	2.13522200	-2.60577800
H	5.76832900	0.92130600	-1.53062300
C	0.09298100	2.19186900	-0.56610400
C	-0.94455300	2.88511200	0.29953700
H	-0.22407500	2.21145100	-1.61991800
H	1.05006400	2.73108500	-0.50862200
C	-1.14962700	4.33899900	-0.09243900
H	-1.90003700	2.34560400	0.23012100
H	-0.65046900	2.83743100	1.36036600
C	-2.19068600	5.02769400	0.76814500
H	-0.19113200	4.87618600	-0.02558700
H	-1.44511200	4.38829600	-1.15132800
H	-2.33695600	6.07371400	0.47900600
H	-3.16258900	4.52541500	0.69212400
H	-1.90241500	5.01577400	1.82658800
C	1.33212200	0.54831100	1.42219600
C	1.83880000	-0.79147100	1.92687600
H	0.66205200	0.99602000	2.16936500
H	2.16297000	1.25684200	1.28934200
C	2.62155800	-0.67584200	3.22382500
H	0.98573900	-1.47200600	2.07439600
H	2.47398500	-1.27262400	1.16468500
C	3.11167800	-2.01894000	3.72777100
H	3.47381500	0.00427100	3.07322100
H	1.98809600	-0.19575900	3.98437200
H	3.67689400	-1.92713800	4.66100300
H	2.27389500	-2.70121700	3.91704700
H	3.76634000	-2.50484900	2.99345700
C	-1.29298700	-2.89689500	-0.91565900
C	-1.46532400	-2.83245400	0.43434700
C	-2.43958400	-3.18076500	-1.83991100
C	0.06035900	-3.14816800	-1.50788200
H	-2.38547600	-2.58295700	-2.75651800

H	-2.40973000	-4.23712800	-2.14617400
H	-3.40937000	-2.99478200	-1.36948900
H	-2.44776800	-2.97474400	0.87801400
H	-0.61618400	-2.93079400	1.10751600
H	0.23362200	-2.55863800	-2.41482900
H	0.86541200	-2.94230600	-0.79491800
H	0.13815700	-4.20639900	-1.79870500

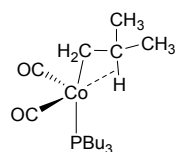
TS_{anti-ma} in entry 14



Co	-1.47105200	-0.88600700	-0.11685600
C	-2.86752800	-0.06644900	-0.89211100
O	-3.70235800	0.56170000	-1.36887000
H	-1.02180600	-1.25716200	-1.51830600
P	0.33546100	0.40168700	-0.15906000
C	-1.77764500	-0.60016400	1.57760200
O	-1.93500000	-0.42267800	2.70297200
C	1.65905800	0.02256600	-1.39600800
C	2.91442300	0.87823900	-1.39522700
H	1.15757800	0.07264200	-2.37517700
H	1.93010000	-1.03325700	-1.26420000
C	3.87047000	0.50377700	-2.51753200
H	2.66081800	1.94499700	-1.48587900
H	3.44095900	0.77745600	-0.43378500
C	5.13745400	1.33605100	-2.49978200
H	4.12085400	-0.56490700	-2.43901300
H	3.35835900	0.61822600	-3.48460200
H	5.82185400	1.06088900	-3.30892100
H	4.91337200	2.40449100	-2.60818900
H	5.67978000	1.21301500	-1.55412300
C	-0.09961500	2.13883200	-0.61231200
C	-1.03019000	2.82114900	0.37680000
H	-0.58118200	2.07563600	-1.60012500
H	0.81446000	2.73677200	-0.73931200
C	-1.58815700	4.12958300	-0.15757200
H	-1.86485000	2.15170800	0.63286500
H	-0.49742300	3.01163600	1.32152200
C	-2.47212700	4.83662300	0.85059000
H	-0.75819100	4.78711000	-0.45896200
H	-2.15689000	3.92427100	-1.07692600

H	-2.88043700	5.77233100	0.45439400
H	-3.32004700	4.20604100	1.14447100
H	-1.91725200	5.08098700	1.76505800
C	1.28013400	0.65025200	1.40576700
C	1.89454300	-0.63138000	1.94141600
H	0.57089200	1.05403600	2.14224700
H	2.04686500	1.42606600	1.25966700
C	2.59154300	-0.43608200	3.27722900
H	1.10911600	-1.39689600	2.04680300
H	2.61510500	-1.04335700	1.21558400
C	3.20145400	-1.71856900	3.80741000
H	3.36927100	0.33578600	3.17209700
H	1.86887800	-0.03433400	4.00299100
H	3.70241600	-1.56885200	4.76951400
H	2.43662500	-2.49140500	3.95249200
H	3.94458800	-2.12441000	3.10946600
C	-1.17219900	-2.84239600	-1.01093100
C	-1.58039700	-2.89654300	0.33114800
C	-2.17400200	-3.20408600	-2.08153300
C	0.24092700	-3.25106900	-1.34622900
H	-1.92080400	-2.75759900	-3.05012300
H	-2.18819900	-4.29462000	-2.21591400
H	-3.18479100	-2.88217500	-1.81502200
H	-2.61416300	-3.14498600	0.56495800
H	-0.85458800	-3.17055300	1.09558800
H	0.58912500	-2.80846100	-2.28700000
H	0.94220900	-2.97593900	-0.55147600
H	0.28387500	-4.34245200	-1.46681900

h in entry 14



Co	0.65367600	-1.39604500	-0.51727500
C	-0.22093000	-1.74951200	-1.99790100
O	-0.87385500	-2.04209700	-2.89993700
P	-0.61560900	0.32671900	0.00240500
C	0.60317300	-2.18179900	1.05897600
O	0.48434900	-2.73780600	2.05903300
C	-0.37878500	1.73271900	-1.17070700
C	-1.10245500	3.03529300	-0.87693200
H	-0.67838500	1.33584400	-2.15307800
H	0.70537700	1.90225600	-1.25050600

C	-0.86616800	4.08213600	-1.95413900
H	-2.18462000	2.85830700	-0.78054300
H	-0.77687400	3.44114900	0.09345900
C	-1.58066900	5.38677400	-1.66161900
H	0.21511600	4.25901700	-2.05578800
H	-1.19361800	3.68237500	-2.92530600
H	-1.40603300	6.13468800	-2.44183000
H	-2.66493400	5.23819300	-1.58607200
H	-1.24571100	5.81954800	-0.71081000
C	-2.43609300	0.06056200	-0.03822600
C	-2.88266700	-1.17676600	0.72363300
H	-2.71721600	-0.02895700	-1.09894400
H	-2.94314600	0.95643800	0.34979800
C	-4.38805900	-1.37614600	0.67478400
H	-2.37705300	-2.06239100	0.31142900
H	-2.56029600	-1.11497400	1.77543100
C	-4.83031800	-2.61799400	1.42353900
H	-4.88889100	-0.48794400	1.08948400
H	-4.70954300	-1.43600600	-0.37591700
H	-5.91562700	-2.75728000	1.38308600
H	-4.36616200	-3.51913200	1.00522200
H	-4.54346000	-2.56801300	2.48114000
C	-0.33979200	1.06433400	1.66717800
C	1.10941900	1.45734100	1.89568700
H	-0.63964500	0.30179300	2.40090800
H	-1.01307200	1.92197000	1.81216800
C	1.37151300	2.00120000	3.28928400
H	1.75218100	0.58051800	1.72199700
H	1.42226600	2.20731300	1.15029500
C	2.83037900	2.35855900	3.49637900
H	0.73668900	2.88272600	3.46574100
H	1.05746600	1.25338800	4.03246500
H	3.02308400	2.73893400	4.50474700
H	3.47633000	1.48461800	3.34452500
H	3.15587100	3.12907800	2.78629600
C	2.87842400	-1.04430700	-1.01190900
C	2.24518700	-2.40511700	-1.08705900
C	3.33235600	-0.51014700	-2.36107200
C	3.97175100	-0.94486400	0.04037700
H	3.65892100	0.53595400	-2.29633800
H	4.17750600	-1.09972800	-2.73926600
H	2.52619400	-0.56755700	-3.10134100
H	2.21083500	-2.83656500	-2.09028800
H	2.64561900	-3.13329200	-0.37760800

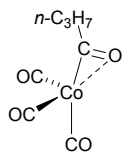
H	4.30096300	0.09177700	0.19208400
H	3.63145600	-1.33623300	1.00628600
H	4.84685500	-1.53195500	-0.26658100
H	2.08489600	-0.27778600	-0.66041100

4 Structures in Table 4

TS_{Co}-(off-cycle) (L = CO)

Co	0.77514200	-0.46888000	0.01415100
C	0.40906700	-1.17361500	-1.57859300
O	0.14142100	-1.72854000	-2.53931600
C	0.44418400	-0.89461800	1.71052100
O	0.19806000	-1.27875500	2.75666500
C	2.58020100	-0.74214100	0.01918300
O	3.70603900	-0.89064400	0.02091700
C	-0.95123500	0.36082600	-0.04079400
O	-0.71452600	1.53482000	-0.14872000
C	-2.31817700	-0.24683700	0.02936300
C	-3.46678200	0.74245600	-0.04836400
H	-2.35875500	-0.84194700	0.95592600
H	-2.37740800	-0.99928900	-0.77353600
C	-4.80949500	0.04263900	0.02944700
H	-3.36912100	1.47704600	0.76122400
H	-3.38756400	1.31868600	-0.97912500
H	-5.64053700	0.75272600	-0.02704900
H	-4.93565700	-0.67540900	-0.79025800
H	-4.91769900	-0.51445800	0.96827500
C	2.12523300	2.40531700	-0.10852200
O	1.91649800	3.51039900	-0.16091800

(n-C₃H₈CO)Co(CO)₄



Co	0.92259100	0.05955500	-0.01893100
C	0.49111800	1.33406900	1.19239100
O	0.25397000	2.14209800	1.95985500
C	0.39159200	0.06189000	-1.74215400
O	0.03491900	0.07393300	-2.82445900
C	2.57553900	0.76430000	-0.36166800
O	3.59676200	1.20377200	-0.59154400
C	-0.96470100	-0.71059800	0.20062200
O	-1.13352700	-1.88785800	0.27045800
C	-2.11282100	0.27772200	0.21659100

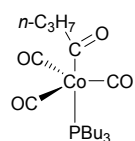
C	-3.46548500	-0.34635900	-0.07754200
H	-1.88955400	1.10239900	-0.47418700
H	-2.11298200	0.73973800	1.21732100
C	-4.57217800	0.68936100	-0.03652900
H	-3.43331700	-0.83359400	-1.06136900
H	-3.66056900	-1.14938600	0.64307300
H	-5.54918500	0.24544500	-0.25246100
H	-4.63930200	1.16538300	0.94956800
H	-4.40524500	1.48675000	-0.77114800
C	1.55240400	-1.51820300	0.70164200
O	1.92379900	-2.49167100	1.14821900

TS_{Co}-(off-cycle) (L = PBu₃)

Co	-1.08168300	-0.03999300	-0.32116900
C	-0.97962600	-1.77331900	-0.56995300
O	-0.89554000	-2.86850600	-0.91185600
C	-1.28018000	1.31970900	-1.41536600
O	-1.34907800	2.10408200	-2.25346600
C	-2.97150000	-0.11406900	-0.10708700
O	-3.24933200	0.29378000	0.99521800
C	-3.99257900	-0.58448000	-1.10587600
H	-3.82632600	-0.00753400	-2.02992100
H	-3.72295200	-1.61638400	-1.38228500
C	-5.43667200	-0.49526300	-0.64850000
H	-5.66790000	0.54226700	-0.37430700
H	-5.56190500	-1.07581300	0.27460400
C	-6.39343400	-0.98648400	-1.71741500
H	-6.30198600	-0.39709800	-2.63844900
H	-7.43692900	-0.92393000	-1.39125900
H	-6.19505600	-2.03259800	-1.98250400
C	-1.00498100	-0.45288400	2.55087500
O	-1.52986300	-1.28846600	3.09838700
P	1.13310400	0.32792200	-0.09119000
C	2.03833200	-0.16316500	-1.61881300
C	1.58773900	2.09889100	0.12862100
C	2.06395000	-0.47796000	1.27912500
C	3.54341400	0.03950600	-1.64575300
H	1.55820200	0.40016800	-2.43385700
H	1.78476300	-1.21626000	-1.81033200
C	0.82227000	2.76854400	1.25921900
H	1.36842700	2.60133000	-0.82620200
H	2.67171600	2.18775200	0.29180500
C	1.99862800	-1.99481300	1.27737100
H	1.64097300	-0.08536800	2.21414500

H	3.10753400	-0.13111900	1.24528500
C	4.15602500	-0.37163600	-2.97523200
H	3.79047100	1.09363800	-1.44754000
H	4.02058700	-0.53791400	-0.83884100
C	1.12616100	4.25296300	1.36964400
H	-0.25942900	2.62208700	1.11315200
H	1.05590400	2.27834700	2.21726100
C	2.69111700	-2.60530900	2.48451000
H	0.95020100	-2.32691600	1.25980600
H	2.44835200	-2.39572900	0.35486000
C	5.65860800	-0.17325900	-3.00673700
H	3.91026300	-1.42496500	-3.17661400
H	3.68280600	0.20330700	-3.78499300
C	0.36845200	4.91420900	2.50409100
H	2.20908300	4.39552300	1.50611500
H	0.87916900	4.74300100	0.41591600
C	2.63845300	-4.12020500	2.47714200
H	3.73657800	-2.26304100	2.51980000
H	2.21969600	-2.21673200	3.40048200
H	6.09197700	-0.47127000	-3.96689600
H	5.92492700	0.87753100	-2.83828100
H	6.15443600	-0.76279900	-2.22563500
H	0.58594000	5.98500700	2.57413300
H	-0.71490400	4.80522400	2.37362800
H	0.62491700	4.46228000	3.47021200
H	3.13189900	-4.55227700	3.35376100
H	1.60284800	-4.48077100	2.47020200
H	3.13002400	-4.53091700	1.58667200

(n-C₃H₇CO)Co(CO)₃(PBU₃)



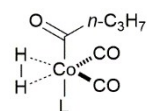
Co	-1.14023100	0.01075400	0.11003400
C	-1.08430000	0.70511100	1.77706900
O	-1.02411000	1.13089300	2.83505200
P	1.09525400	0.20788800	-0.13964200
C	-3.15197300	0.03341000	0.23615900
O	-3.72847500	0.86948100	0.86895800
C	1.76818500	-0.82707500	-1.50631700
C	3.26567000	-0.78196300	-1.75854700
H	1.21343600	-0.51098900	-2.40355700
H	1.44442900	-1.86001000	-1.31708300

C	3.67525100	-1.66005200	-2.93061700
H	3.59292700	0.25033900	-1.95330000
H	3.81249800	-1.10801400	-0.86020900
C	5.16892200	-1.62359300	-3.18661300
H	3.35019800	-2.69357800	-2.73977800
H	3.13045000	-1.33912000	-3.83083300
H	5.45569400	-2.25805300	-4.03134800
H	5.50981100	-0.60520800	-3.41029900
H	5.73158400	-1.96922900	-2.31061100
C	1.68588800	1.89617200	-0.57776000
C	1.14857400	3.00065600	0.31747500
H	1.38908800	2.07694900	-1.62215900
H	2.78576200	1.89499500	-0.56081000
C	1.67009400	4.37087900	-0.08239900
H	0.04947000	3.00270900	0.28734500
H	1.41523600	2.80504600	1.36813900
C	1.12771500	5.47461800	0.80404700
H	2.77030800	4.36796400	-0.05043900
H	1.40259500	4.56540900	-1.13186900
H	1.50462200	6.45937100	0.50936300
H	0.03274700	5.51444300	0.76260900
H	1.40610200	5.31551700	1.85302000
C	2.13498700	-0.20374700	1.32182100
C	1.94567300	-1.61960900	1.83770400
H	1.87894400	0.51931800	2.10934100
H	3.18854000	-0.01750900	1.06467700
C	2.82663700	-1.92110400	3.03872300
H	0.89088200	-1.77625000	2.10842800
H	2.15991600	-2.34945400	1.04033800
C	2.63137700	-3.33168100	3.55842300
H	3.88111300	-1.76221500	2.76610000
H	2.61186400	-1.19303200	3.83505600
H	3.26888700	-3.54174300	4.42329800
H	1.59250800	-3.50088800	3.86600100
H	2.86609200	-4.07602300	2.78761600
C	-3.90730700	-1.02137800	-0.55371100
C	-5.40276100	-0.78266500	-0.64934400
C	-6.08980100	-1.87467500	-1.44654200
H	-3.44836600	-1.10121900	-1.55010300
H	-3.70237100	-1.99133100	-0.07367500
H	-5.69719900	-1.93328600	-2.46953600
H	-5.94150500	-2.86005200	-0.98701800
H	-7.16959900	-1.70736700	-1.51996600
H	-5.58664000	0.19871900	-1.10610200

H	-5.82628200	-0.71848100	0.36052300
C	-1.40930700	1.02323800	-1.33085700
O	-1.53708700	1.66836600	-2.27127200
C	-1.07232300	-1.77631600	-0.00962200
O	-0.98451800	-2.91720700	-0.08824100

5 Structures in Table 5

[Co]-H₂-a



L = CO

Co	-1.07293500	0.00618500	0.29229800
C	-0.74527600	-1.65829900	-0.26468500
O	-0.53417200	-2.70476000	-0.66713900
C	-0.70722200	1.63553500	-0.34045200
O	-0.45784600	2.65351300	-0.79091000
C	-2.82500100	0.00864100	-0.23378500
O	-3.89656900	0.01241700	-0.61048600
C	0.88476600	0.02420400	0.79273700
O	1.16120100	0.11533600	1.95025600
C	1.92472100	-0.07554200	-0.30072500
C	3.35875000	0.04833800	0.17968900
H	1.69239800	0.68199900	-1.06439400
H	1.76662000	-1.03458500	-0.81840400
C	4.34009600	-0.06659900	-0.97066700
H	3.48742800	1.00601000	0.70038100
H	3.55896700	-0.72425600	0.93268800
H	5.37675100	0.02008800	-0.62966600
H	4.24385100	-1.03136500	-1.48415300
H	4.17550100	0.71729700	-1.72047800
H	-1.48040300	0.44196200	1.96492900
H	-1.41778200	-0.35386600	2.00060700

L = PH₃

Co	0.92759100	-0.00000200	0.31407400
C	0.64540700	1.61781900	-0.35188200
O	0.46855500	2.63838700	-0.84172500
C	0.64541100	-1.61781500	-0.35189900
O	0.46855800	-2.63838000	-0.84174900
C	-0.98988100	-0.00001300	0.81348900
O	-1.27767700	-0.00002600	1.97427300
C	-2.03503500	-0.00000900	-0.28385400

C	-3.46901300	0.00001700	0.21211100
H	-1.84156300	-0.86821300	-0.93207400
H	-1.84153800	0.86816800	-0.93210100
C	-4.45525800	0.00000900	-0.93981700
H	-3.63168100	-0.87317600	0.85679600
H	-3.63165900	0.87323500	0.85676700
H	-5.49214500	0.00005000	-0.58785900
H	-4.32622900	0.88278500	-1.57858100
H	-4.32628000	-0.88281400	-1.57852400
H	1.31996600	-0.40405500	1.96778700
H	1.31994700	0.40401200	1.96780500
P	3.11307000	0.00000900	-0.27101700
H	3.63400800	-1.05825400	-1.04729200
H	4.11687700	0.00001800	0.72455200
H	3.63401000	1.05825800	-1.04730900

L = PMe₃

Co	-0.21169300	0.00000000	0.42765200
C	-0.00895100	-1.60207700	-0.28016300
O	0.07514000	-2.61288300	-0.82031500
C	-0.00895000	1.60207600	-0.28016600
O	0.07514100	2.61288000	-0.82032100
C	1.72552000	0.00000100	0.85112500
O	2.07625800	0.00000500	1.99764900
C	2.72344300	-0.00000200	-0.29154200
C	4.17930000	0.00000200	0.13475900
H	2.49927400	0.86851300	-0.93015000
H	2.49927700	-0.86852300	-0.93014200
C	5.11111000	-0.00000200	-1.06176000
H	4.37243400	0.87292800	0.77151500
H	4.37243600	-0.87291900	0.77152300
H	6.16382200	0.00000000	-0.75961800
H	4.95195300	-0.88269200	-1.69403200
H	4.95195000	0.88268100	-1.69404000
H	-0.53779900	0.40573200	2.08790500
H	-0.53779900	-0.40572900	2.08790500
P	-2.40323000	0.00000000	-0.07031400
C	-3.37889600	1.42440000	0.53205500
H	-2.96808100	2.35223000	0.12074000
H	-4.43368900	1.34348900	0.24378000
H	-3.31237600	1.48290300	1.62327100
C	-3.37889500	-1.42440000	0.53205400
H	-4.43368900	-1.34348900	0.24378000
H	-2.96808000	-2.35223000	0.12074000

H	-3.31237600	-1.48290400	1.62327000
C	-2.77212300	0.00000000	-1.85873300
H	-2.32661300	-0.88500700	-2.32483600
H	-3.85153500	0.00000000	-2.05054600
H	-2.32661300	0.88500800	-2.32483600

L = P Bu₃

Co	-1.20981200	0.04378900	-0.28193500
C	-1.15441800	-1.70738000	-0.07192800
O	-1.11098900	-2.83496700	0.14554100
C	-1.54935500	1.32110700	0.88138000
O	-1.72444300	2.11612100	1.69339500
C	-3.16550600	-0.14753900	-0.55452100
O	-3.63356300	0.08318500	-1.63466100
C	-4.03103400	-0.58348600	0.61293900
C	-5.50124000	-0.76105600	0.28394300
H	-3.89585200	0.15636000	1.41750200
H	-3.60265600	-1.51012800	1.02447500
C	-6.29683500	-1.19598200	1.49961700
H	-5.90016700	0.17813600	-0.12011200
H	-5.60719000	-1.49437200	-0.52607900
H	-7.35926800	-1.32616100	1.26748000
H	-5.92959600	-2.14985500	1.89904200
H	-6.22647700	-0.45869900	2.30941400
H	-1.13081600	0.93329400	-1.77734100
H	-1.02954100	0.16371900	-2.01009800
P	1.02159500	0.27252000	0.02999200
C	1.63237800	-0.64425700	1.50566300
C	1.64143000	1.98172700	0.33370500
C	2.10406200	-0.28439600	-1.35387500
C	3.12114300	-0.60079300	1.80432600
H	1.29343000	-1.68421300	1.39782400
H	1.05401300	-0.24163200	2.35178700
C	1.19772900	2.99422600	-0.70930000
H	2.73928400	1.95839100	0.39544200
H	1.27699600	2.27984800	1.32867100
C	1.96114600	-1.75566400	-1.70382200
H	3.14880500	-0.04045000	-1.10783600
H	1.84078200	0.33304200	-2.22510100
C	3.48169500	-1.40439700	3.04386700
H	3.69369500	-0.98965500	0.94757900
H	3.45539200	0.43833700	1.94261900
C	1.70900800	4.39427900	-0.41300400
H	1.54475300	2.68768200	-1.70913400

H	0.09951000	3.01217900	-0.76814100
C	2.89278200	-2.17705900	-2.82814900
H	2.15824400	-2.38144700	-0.81862300
H	0.92091600	-1.96950800	-1.99059000
C	4.96592400	-1.36288900	3.34934800
H	2.90935200	-1.02203300	3.90207600
H	3.15310100	-2.44556400	2.90863000
C	1.26399700	5.40360200	-1.45287300
H	1.35806600	4.70099600	0.58362400
H	2.80766200	4.37680800	-0.35049300
C	2.74136000	-3.64240300	-3.18585700
H	2.69850100	-1.55130000	-3.71221800
H	3.93309000	-1.96561900	-2.53725500
H	5.21762900	-1.94456300	4.24197000
H	5.55512500	-1.76741900	2.51702500
H	5.30865600	-0.33484000	3.51993600
H	1.63301200	6.41036800	-1.23185800
H	1.62687400	5.13231100	-2.45199400
H	0.17020200	5.45903000	-1.50922900
H	3.41594200	-3.93878200	-3.99560900
H	2.95761900	-4.28638800	-2.32460400
H	1.71828700	-3.86853100	-3.50938500

L= a₅-PhobPC₅

O	-2.52897100	1.28995400	-2.09020800
O	-0.81433500	-0.97891700	2.47081700
P	0.97228800	0.76680800	-0.30944000
C	-1.87527600	0.60118200	-1.44485300
C	-0.86472800	-0.79908900	1.33687200
C	1.31601600	2.34467600	-1.23371700
C	0.13337500	3.31930400	-1.24344700
C	-0.68035000	3.47397900	0.04021300
C	0.10016900	3.66606700	1.33726800
C	0.54964400	2.37253000	2.01057400
C	1.58662100	1.52081800	1.27710200
C	2.81242600	2.32852700	0.84366300
C	2.59042300	2.91576400	-0.56831000
C	2.41670600	-0.26648900	-0.84289700
C	2.77346200	-1.38386400	0.12435200
C	3.77767600	-2.36023700	-0.46298700
C	4.18358700	-3.45489700	0.50717600
C	5.17488900	-4.43021200	-0.09674700
H	1.53577200	2.06973400	-2.27451700
H	-0.55725900	3.03653600	-2.04746500

H	0.52893300	4.30441000	-1.53536100
H	-1.34595400	2.60760200	0.16535600
H	-1.35327300	4.32877300	-0.10803800
H	-0.54327800	4.19056000	2.05588800
H	0.95571400	4.33994100	1.17840500
H	0.98345700	2.62631700	2.98950200
H	-0.33840900	1.76365100	2.23101300
H	1.87422800	0.69872700	1.94658100
H	3.69855200	1.68284100	0.84686400
H	3.02053800	3.12070700	1.57500600
H	3.46283700	2.70726000	-1.19804000
H	2.51528500	4.00908500	-0.52897300
H	2.13208300	-0.68731700	-1.81801800
H	3.29292800	0.36760300	-1.03052500
H	3.18440300	-0.95758900	1.05251700
H	1.86755300	-1.93145000	0.42686600
H	3.35402800	-2.81448800	-1.37335300
H	4.67438800	-1.81242400	-0.79653000
H	4.61107400	-2.99814000	1.41269000
H	3.28471900	-3.99312400	0.84321300
H	4.75707300	-4.92320400	-0.98310500
H	5.46264100	-5.21540200	0.60999800
H	6.09309600	-3.91963200	-0.41289900
Co	-0.94283700	-0.47352600	-0.39410800
C	-2.56957300	-1.61536000	-0.42230100
O	-2.54761100	-2.64986700	-1.02792200
C	-3.80354300	-1.15092100	0.32665500
C	-5.02235700	-2.03759800	0.15416100
H	-4.01817400	-0.11542600	0.02236600
H	-3.52706700	-1.06762200	1.38968900
C	-6.21083400	-1.51076700	0.93503900
H	-5.26872900	-2.11425400	-0.91292800
H	-4.77691600	-3.05936500	0.47038400
H	-7.09422800	-2.14641500	0.81240600
H	-5.99264700	-1.45690500	2.00916500
H	-6.48755400	-0.49960800	0.61071700
H	-0.25905700	-1.48110100	-1.65669200
H	-0.05714700	-1.86702900	-0.97806500

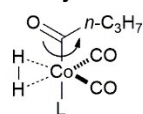
L = PBu₃ (*i*-C₃H₇ instead of *n*-C₃H₇)

Co	1.31238000	-0.09906200	0.19499400
C	1.09061700	-1.83179300	-0.04480200
O	0.92091300	-2.94217100	-0.29029300
C	1.68475100	1.16083600	-0.98232700

O	1.86475400	1.94339100	-1.80431000
C	3.28249700	-0.31399500	0.37257500
O	3.83139800	0.34794600	1.20928200
C	4.06840500	-1.28872200	-0.51004000
C	5.54888700	-1.27066100	-0.17331000
H	3.65767900	-2.28571300	-0.28056700
H	5.98786900	-0.29145700	-0.39682800
H	5.72984500	-1.47111800	0.88643200
P	-0.90700800	0.30646600	0.01386200
C	-1.67306200	-0.51848900	-1.44341900
C	-1.39603200	2.06817800	-0.22001700
C	-1.95565800	-0.19172400	1.44554800
C	-3.16439500	-0.33301100	-1.66484300
H	-1.42750200	-1.58726700	-1.37094800
H	-1.10279900	-0.15173300	-2.31115200
C	-0.81148500	3.01691700	0.81334500
H	-2.49377700	2.13553300	-0.21767900
H	-1.06582900	2.35844900	-1.22912200
C	-1.92003700	-1.67770300	1.75859400
H	-2.98772400	0.14468200	1.26334500
H	-1.59403400	0.38053800	2.31236100
C	-3.65782000	-1.07483500	-2.89712000
H	-3.72705200	-0.68602700	-0.78639600
H	-3.40796400	0.73484500	-1.76925700
C	-1.22065500	4.46033900	0.57127600
H	-1.12667000	2.71775200	1.82593300
H	0.28590200	2.94326600	0.80924900
C	-2.81926100	-2.04546400	2.92727900
H	-2.22021800	-2.26307900	0.87476100
H	-0.88753600	-1.98610000	1.97996800
C	-5.14498500	-0.89158000	-3.12673100
H	-3.09510100	-0.72899200	-3.77689700
H	-3.42063700	-2.14425600	-2.79515100
C	-0.63720200	5.40646400	1.60207000
H	-0.90044100	4.75937200	-0.43794800
H	-2.31878400	4.53427800	0.57043900
C	-2.77657400	-3.52695600	3.24586500
H	-2.52098500	-1.46115500	3.81073800
H	-3.85195500	-1.73797700	2.70261500
H	-5.49242100	-1.42962700	-4.01458300
H	-5.72779100	-1.25736400	-2.27226800
H	-5.39922500	0.16672800	-3.26369700
H	-0.93210200	6.44482700	1.41917000
H	-0.96724800	5.14438200	2.61495600

H	0.45876400	5.36982300	1.59856200
H	-3.42698600	-3.78438800	4.08806400
H	-3.09743900	-4.12787600	2.38613800
H	-1.76038500	-3.84873900	3.50354900
H	6.08471400	-2.02276500	-0.76389900
C	3.83827300	-1.01228100	-1.98844800
H	4.39895900	-1.72899500	-2.59869700
H	2.78306500	-1.08429000	-2.26909800
H	4.18934100	-0.00755800	-2.25701600
H	1.24735100	-0.02614900	1.93667600
H	1.34588500	0.74939200	1.72508200

TS_{acyl-rotate}



L = CO

Co	-0.93670500	-0.05348400	-0.26264600
C	-2.61180200	-0.71693000	-0.63445300
O	-3.65050100	-1.12224700	-0.84917800
C	-0.47297400	-1.44542200	0.76264900
O	-0.23884300	-2.30991200	1.46946900
C	-1.53506000	1.50251500	0.45541300
O	-1.90302000	2.44823900	0.96479700
C	0.92421900	0.70927300	-0.04377900
O	1.10984200	1.89010200	-0.03355700
C	2.08273500	-0.27294100	-0.04891300
H	2.06036800	-0.79258800	0.92244900
H	1.87595700	-1.05993400	-0.78900900
C	3.43963000	0.36512600	-0.28058000
H	3.60950400	1.13893000	0.47794100
H	3.43381000	0.89492300	-1.24232400
C	4.55150500	-0.66544300	-0.25096500
H	4.59532400	-1.18105800	0.71641200
H	5.53163200	-0.20841900	-0.42184200
H	4.41016000	-1.43405800	-1.02120000
H	-0.64714600	0.38060600	-1.88641400
H	-0.38791700	-0.40086000	-1.83304900

L = PH₃

Co	-0.81011400	-0.00331300	-0.22225100
C	-0.40470100	-1.40677000	0.78472900
O	-0.21769500	-2.29423400	1.48537900
C	-1.43219000	1.54550300	0.45099900

O	-1.83709000	2.49235600	0.94015100
C	1.02752300	0.72268300	-0.02873600
O	1.23736600	1.90126700	-0.00266900
C	2.17463900	-0.27657000	-0.05028000
H	2.14533400	-0.81353400	0.91119500
H	1.95723800	-1.04739400	-0.80389400
C	3.54104800	0.34483100	-0.27093500
H	3.72732300	1.09631700	0.50605600
H	3.54127500	0.89945500	-1.21862900
C	4.63594300	-0.70450900	-0.27148100
H	4.66979500	-1.24892600	0.68050000
H	5.62447200	-0.26064800	-0.42935900
H	4.48080600	-1.44826200	-1.06324400
H	-0.57929900	0.39179400	-1.85537600
H	-0.32794200	-0.39698300	-1.79604500
P	-2.89625100	-0.80476300	-0.64404000
H	-3.29605900	-2.06021200	-0.13455300
H	-3.30791800	-1.01909800	-1.97893700
H	-4.03241600	-0.07773800	-0.22499300

L = PMe₃

Co	-0.14066200	0.19835600	-0.11022800
C	0.13903900	-1.19764800	0.93411800
O	0.21317600	-2.08047300	1.66651100
C	-0.59069100	1.82084300	0.48586900
O	-0.92491500	2.81943000	0.93127000
C	1.77471400	0.73749100	-0.05437300
O	2.12270200	1.88586700	-0.09009900
C	2.80749700	-0.38263100	-0.08987400
H	2.75403600	-0.89170600	0.88601000
H	2.47642300	-1.14163700	-0.81423900
C	4.22599800	0.07113400	-0.37664600
H	4.52474800	0.81994100	0.36719300
H	4.25440000	0.59349100	-1.34218100
C	5.19536400	-1.09544300	-0.37780200
H	5.20416600	-1.60936100	0.59171100
H	6.22138400	-0.77379600	-0.58631200
H	4.92581800	-1.84188600	-1.13579200
H	0.02011100	0.47435500	-1.77517200
H	0.17339800	-0.33730900	-1.68327100
P	-2.31250300	-0.37677200	-0.31340100
C	-3.28277200	-0.22731300	1.22612400
H	-4.33278300	-0.50133800	1.07059500
H	-2.85477500	-0.87886600	1.99508900

H	-3.23286400	0.80284500	1.59353300
C	-2.67692100	-2.09120700	-0.83341900
H	-3.75616400	-2.27634100	-0.89196400
H	-2.22989900	-2.28410200	-1.81397100
H	-2.23366600	-2.79243000	-0.11876500
C	-3.29838000	0.60952300	-1.49594900
H	-2.86828800	0.52313000	-2.49909400
H	-4.34320200	0.27831000	-1.52754900
H	-3.26820500	1.66557600	-1.20839700

L = PBu₃

Co	1.09738000	-0.55754700	-0.20680700
C	1.52218800	0.70204100	-1.36368000
O	1.69208100	1.51133000	-2.16338500
C	0.42236600	-2.14235800	-0.68527600
O	-0.02056800	-3.12535800	-1.06579100
C	2.91925700	-1.35353200	-0.28574300
O	3.11627000	-2.53488700	-0.19668900
C	4.09127500	-0.38053600	-0.34035800
H	4.06318900	0.09381700	-1.33443400
H	3.89369300	0.44298600	0.36237500
C	5.44872500	-1.00864000	-0.08933400
H	5.60682900	-1.82350900	-0.80667500
H	5.45329400	-1.48720700	0.89899200
C	6.56514400	0.01316800	-0.18740800
H	6.59610100	0.47906100	-1.18046700
H	7.54745500	-0.43670000	-0.00706900
H	6.43601300	0.82130500	0.54393200
H	1.28003100	-0.77425600	1.46410300
H	1.53930800	0.00313900	1.32731400
P	-0.95947100	0.37620600	0.03678300
C	-2.07749500	0.01018800	-1.37843300
C	-1.02445200	2.21622000	0.12925200
C	-1.91107300	-0.12849600	1.53169600
C	-3.50626500	0.51994700	-1.30772300
H	-2.06675800	-1.07958000	-1.51930000
H	-1.56258400	0.41711700	-2.26285300
C	-0.06397800	2.82204100	1.13895400
H	-2.05524700	2.52982800	0.35034200
H	-0.79164800	2.58856000	-0.88000800
C	-2.21514200	-1.61571700	1.59846400
H	-2.83868500	0.46210700	1.58230900
H	-1.30953800	0.16710400	2.40375900
C	-4.30654700	0.15889100	-2.54927700

H	-4.01393600	0.10471700	-0.42312300
H	-3.51984900	1.61246000	-1.17785000
C	-0.15318300	4.33821100	1.18970900
H	-0.26025800	2.41661700	2.14464700
H	0.96627800	2.52414500	0.89357200
C	-3.02766900	-1.98692200	2.82805200
H	-2.76120700	-1.93514300	0.69652500
H	-1.27554800	-2.18740900	1.59299000
C	-5.73949000	0.64793100	-2.47722500
H	-3.80876300	0.57879700	-3.43584300
H	-4.28724500	-0.93227200	-2.68761100
C	0.81621700	4.94035900	2.18755400
H	0.04029600	4.74371800	0.18542900
H	-1.18306200	4.63601100	1.43811000
C	-3.33060400	-3.47088300	2.89292100
H	-2.48178100	-1.67345400	3.73068500
H	-3.96523300	-1.41020400	2.83229100
H	-6.30889400	0.38379100	-3.37423000
H	-6.26421300	0.21550800	-1.61625300
H	-5.78381800	1.73882700	-2.36978200
H	0.74998400	6.03273700	2.21668800
H	0.62270500	4.57238800	3.20285100
H	1.85259900	4.68010300	1.94022900
H	-3.91029200	-3.73306600	3.78397000
H	-3.90578100	-3.79750300	2.01791100
H	-2.40851700	-4.06403000	2.91256000

L= a₅-PhobPC₅

Co	1.10192900	-0.39185100	0.27894900
C	1.45012700	-0.94652000	-1.35873500
O	1.64421100	-1.35880200	-2.41406300
C	0.96953300	-1.42541700	1.73607300
O	0.93108600	-2.13636600	2.62949800
C	3.05251500	-0.25144500	0.67409000
O	3.51165400	-0.48554500	1.75798600
C	3.94457800	0.29880400	-0.43249500
H	4.03097700	-0.49459900	-1.19204600
H	3.41372500	1.11424800	-0.94536600
C	5.32029100	0.74085300	0.02938600
H	5.82540000	-0.10022700	0.51985000
H	5.21558100	1.50972300	0.80658500
C	6.15447600	1.26471200	-1.12382200
H	6.29497800	0.49852800	-1.89666100
H	7.14935300	1.58429400	-0.79565800

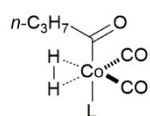
H	5.67683500	2.12628200	-1.60763500
H	1.03852300	1.14807100	0.99434800
H	1.18765500	1.29939200	0.19399500
P	-1.13889900	-0.28593100	-0.24284300
C	-1.88152300	-1.30506000	-1.61048100
C	-2.58929400	-0.65393100	0.86716500
C	-1.53325100	1.42549500	-0.84801000
C	-1.46178700	-2.77863900	-1.57019700
C	-3.40703700	-1.08846400	-1.47962300
H	-1.52643900	-0.87920900	-2.55953600
C	-2.50859200	-1.99624500	1.59344300
C	-3.79191000	-0.56843400	-0.07710000
H	-2.63253900	0.13489500	1.63028400
C	-1.71551200	2.46561800	0.24605700
H	-0.68875500	1.70070700	-1.49642200
H	-2.41895400	1.40432400	-1.49625400
C	-1.37555200	-3.46168700	-0.20683900
H	-0.48744300	-2.88705300	-2.06203400
H	-2.17031600	-3.33318400	-2.20472300
H	-3.75007800	-0.38230700	-2.24436000
H	-3.92355000	-2.02999000	-1.70085700
C	-2.55313700	-3.26468500	0.74482800
H	-3.35729500	-2.02653100	2.29367000
H	-1.61091300	-2.02143400	2.22419200
H	-4.13629700	0.47033500	-0.14389100
H	-4.63612400	-1.13472200	0.33859200
C	-1.71714400	3.88363100	-0.29836200
H	-2.66082400	2.28400300	0.77942300
H	-0.92672600	2.37168500	1.00812200
H	-0.45064500	-3.15167800	0.29944200
H	-1.24482300	-4.53570100	-0.39387800
H	-2.57710600	-4.10989200	1.44515300
H	-3.50417500	-3.32713500	0.19402700
C	-1.96145300	4.93412200	0.76979600
H	-0.75533000	4.08344500	-0.79805300
H	-2.48239700	3.97492600	-1.08654900
C	-1.94632500	6.34468400	0.21414600
H	-2.92593000	4.73530800	1.26122100
H	-1.20099500	4.83352700	1.55889300
H	-0.98111500	6.57783800	-0.25202400
H	-2.12513100	7.09531000	0.99086900
H	-2.71734900	6.47710500	-0.55497300

L = PBu₃ (*i*-C₃H₇ instead of *n*-C₃H₇)

Co	1.29590200	0.12019700	-0.24412700
C	1.18857300	-1.58806000	-0.69841900
O	1.05090900	-2.67048300	-1.05940600
C	1.27293900	1.45090400	-1.42868200
O	1.21151800	2.26044200	-2.23503600
C	3.28212800	0.14836800	-0.32695000
O	3.88645200	1.16006700	-0.55917700
C	4.06543900	-1.12719900	0.02440900
C	5.24522100	-0.80434500	0.92466400
H	3.39481400	-1.82683400	0.53973800
H	5.93179900	-0.10930400	0.43097900
H	4.92465100	-0.33968100	1.86454400
P	-0.95650100	0.27147100	0.02519200
C	-1.90909100	-0.49019900	-1.35499200
C	-1.64564400	1.98078700	0.08695400
C	-1.66079200	-0.47720600	1.55510100
C	-3.42560200	-0.46285500	-1.27182500
H	-1.55147900	-1.52381500	-1.46100000
H	-1.56077400	0.02752700	-2.26244800
C	-0.94558500	2.89640700	1.07727200
H	-2.71957000	1.92314000	0.31769700
H	-1.56422900	2.39317200	-0.93036300
C	-1.41500000	-1.97040500	1.68627900
H	-2.73734900	-0.25244900	1.59958900
H	-1.20050600	0.05236900	2.40227700
C	-4.07796900	-1.12569600	-2.47489200
H	-3.76626900	-0.97090600	-0.35597000
H	-3.78822700	0.57300900	-1.19429900
C	-1.55267000	4.28915800	1.10904500
H	-0.98391000	2.46323800	2.09006900
H	0.12223000	2.96870000	0.82407900
C	-2.02084600	-2.54939900	2.95404700
H	-1.82552800	-2.50379100	0.81408900
H	-0.33319000	-2.17044300	1.67148200
C	-5.59177400	-1.10203300	-2.39883200
H	-3.73864100	-0.62328600	-3.39283600
H	-3.72022400	-2.16293200	-2.55519400
C	-0.84756900	5.20401000	2.09087900
H	-1.51344500	4.72089700	0.09787500
H	-2.62145400	4.21697600	1.36159200
C	-1.76750700	-4.03798700	3.08850600
H	-1.61195800	-2.01715700	3.82614600
H	-3.10303600	-2.34896700	2.96478100
H	-6.05381100	-1.58130900	-3.26792200

H	-5.95365000	-1.62473000	-1.50473400
H	-5.97195200	-0.07416800	-2.35000700
H	-1.28772500	6.20632700	2.10646900
H	-0.89848300	4.80669300	3.11226600
H	0.21373700	5.31449200	1.83803500
H	-2.20670200	-4.44811400	4.00367400
H	-2.19252100	-4.59162800	2.24236000
H	-0.69329500	-4.25767300	3.11107100
H	5.79982200	-1.71718300	1.17230200
C	4.52650800	-1.74959800	-1.28810800
H	5.05520200	-2.69166700	-1.10336800
H	3.69358900	-1.96180400	-1.96744400
H	5.21441100	-1.06954300	-1.80452900
H	1.53887400	0.08275400	1.43148500
H	1.55137600	0.89257600	1.24328000

[Co]-H₂-b



L = CO

Co	0.93001200	0.01228400	-0.26927600
C	1.03404200	-1.64302600	0.41627500
O	1.11011000	-2.66815300	0.90494200
C	0.93227300	1.59689300	0.56799700
O	0.94880500	2.57956500	1.14315300
C	2.67217100	0.09309300	-0.81965900
O	3.76988200	0.14248900	-1.10765500
H	0.31028400	0.47111800	-1.82295500
H	0.35697200	-0.33856700	-1.87153800
C	-0.93615800	-0.07267200	0.49163200
O	-1.15293200	-0.17891800	1.66032500
C	-2.05312100	0.02159800	-0.53535900
C	-3.44750800	-0.03841600	0.05985600
H	-1.90343000	-0.78204100	-1.27231300
H	-1.90566300	0.95421800	-1.10163200
C	-4.51285300	0.08216000	-1.01258200
H	-3.56565400	-0.97682700	0.61613100
H	-3.55961300	0.75895900	0.80528200
H	-5.52108000	0.03614400	-0.58849900
H	-4.42983400	1.03151300	-1.55635600
H	-4.43230400	-0.72383100	-1.75276100

L = PH₃

Co	0.79796800	0.00000500	-0.21495300
C	0.92089300	-1.59871000	0.55849300
O	1.02388400	-2.59814000	1.10355200
C	0.92079500	1.59863100	0.55868400
O	1.02373100	2.59800400	1.10385900
H	0.25602400	0.41082700	-1.78544000
H	0.25603500	-0.41068800	-1.78547700
C	-1.04755500	-0.00008500	0.50452000
O	-1.29344000	-0.00021200	1.67448600
C	-2.15446900	0.00002400	-0.54301300
C	-3.55515400	-0.00000600	0.04000100
H	-2.00048500	-0.87282500	-1.19524600
H	-2.00045900	0.87297900	-1.19509800
C	-4.61040500	0.00009800	-1.04921300
H	-3.67678600	-0.87277700	0.69382400
H	-3.67676300	0.87265800	0.69397000
H	-5.62347400	0.00007400	-0.63358000
H	-4.52200100	0.88313200	-1.69466800
H	-4.52202000	-0.88283000	-1.69481600
P	2.94767900	0.00012800	-0.91334300
H	3.80466900	-1.05803500	-0.53977500
H	3.80460400	1.05830400	-0.53966300
H	3.26231600	0.00020700	-2.29215300

L = PMe₃

Co	-0.12502200	0.01864900	0.02326200
C	-0.19140300	-1.50638600	-0.87137300
O	-0.30467900	-2.46284700	-1.49367300
C	-0.25541300	1.66925300	-0.60464000
O	-0.40366800	2.70942200	-1.06275600
H	0.23613900	0.29995600	1.67305300
H	0.26866900	-0.51909600	1.59801300
C	1.78199100	0.09634000	-0.52055400
O	2.13914200	0.24336000	-1.65486100
C	2.79491800	-0.05334100	0.61064600
C	4.24306700	-0.01530600	0.16113900
H	2.57086300	-0.99376500	1.13732300
H	2.59267900	0.73874200	1.34791600
C	5.19580600	-0.17409900	1.33029300
H	4.41371000	-0.80370500	-0.58299800
H	4.43445400	0.92767000	-0.36664300
H	6.24281300	-0.14536600	1.01027600
H	5.05889700	0.62293400	2.07238700
H	5.03885800	-1.12848500	1.84909300

P	-2.32498300	-0.06425200	0.45820900
C	-2.93175000	-1.50209700	1.41078800
H	-4.01899400	-1.46679800	1.54825100
H	-2.66995400	-2.42686300	0.88585000
H	-2.45064300	-1.52633400	2.39391300
C	-3.05099000	1.34547800	1.36861000
H	-2.86051700	2.27180100	0.81658300
H	-4.13275000	1.22715100	1.50327000
H	-2.57846000	1.43805400	2.35184200
C	-3.36112300	-0.12250100	-1.04396200
H	-3.10063000	-1.00519900	-1.63692400
H	-4.42940800	-0.15610000	-0.79975200
H	-3.16234200	0.76214100	-1.65802800

L = PBu₃

Co	1.15353600	-0.17940100	-0.39672300
C	0.80458800	-1.86475600	-0.81829400
O	0.55471700	-2.93127600	-1.15612400
C	1.29910500	1.20064900	-1.49055400
O	1.33372800	2.07093900	-2.23715900
H	1.63216200	0.47179400	1.11233500
H	1.50447100	-0.32478500	1.27237300
C	3.02386900	-0.59743200	-0.91064600
O	3.35193200	-0.91279200	-2.01966600
C	4.05479700	-0.49001400	0.20967900
C	5.47652100	-0.79948200	-0.21887500
H	3.73628300	-1.16013700	1.02290300
H	3.98481300	0.52318100	0.63417100
C	6.44915300	-0.67237600	0.93787800
H	5.51579100	-1.80983100	-0.64528200
H	5.76315300	-0.12798200	-1.03815100
H	7.47738100	-0.89440200	0.63281400
H	6.44448600	0.34187100	1.35723300
H	6.19474000	-1.36037300	1.75427000
P	-1.01062900	0.30792800	0.04155500
C	-2.14144600	-0.28277900	-1.28594500
C	-1.44379700	2.09553900	0.16961800
C	-1.72301300	-0.36957300	1.60139500
C	-3.63069700	-0.03911400	-1.11325500
H	-1.94172400	-1.35494600	-1.42159500
H	-1.77321600	0.19371600	-2.20771300
C	-0.56611800	2.87711100	1.13287400
H	-2.50071700	2.18814100	0.45948600
H	-1.35773500	2.51570600	-0.84414900

C	-1.69074300	-1.88576800	1.68934500
H	-2.75075100	0.00681200	1.71789800
H	-1.14069600	0.06443700	2.42758400
C	-4.43976200	-0.58354000	-2.28004700
H	-3.98886800	-0.50571100	-0.18205100
H	-3.83476100	1.03703500	-1.00853000
C	-0.95394400	4.34423800	1.21288700
H	-0.61857300	2.43501400	2.14101800
H	0.48687000	2.79404300	0.82536700
C	-2.30551600	-2.40678300	2.97778800
H	-2.22021200	-2.33035200	0.83157000
H	-0.65214700	-2.23965400	1.60897300
C	-5.92709000	-0.34049600	-2.11666300
H	-4.08270800	-0.12384000	-3.21344800
H	-4.24258200	-1.66059500	-2.38613400
C	-0.07235100	5.12387500	2.16843300
H	-0.90021600	4.78522800	0.20642800
H	-2.00761600	4.42756700	1.51935100
C	-2.26286700	-3.91946200	3.06834700
H	-1.77829400	-1.96272700	3.83569200
H	-3.34532600	-2.05394000	3.05355900
H	-6.50243800	-0.73574100	-2.96000900
H	-6.31069900	-0.81658100	-1.20572300
H	-6.14944300	0.73111200	-2.04107500
H	-0.35613300	6.17998900	2.21989100
H	-0.13123300	4.71778400	3.18593500
H	0.97985000	5.08096500	1.86199300
H	-2.70754900	-4.28769100	3.99855400
H	-2.80754500	-4.38301700	2.23679300
H	-1.23200900	-4.29116700	3.02566700

L= a₅-PhobPC₅

O	1.35617300	-2.98904800	-1.61015100
O	0.83249100	-0.05009500	2.79718100
P	-1.21511100	-0.21524700	-0.35406500
C	1.20288200	-2.01318900	-1.02984000
C	0.91667500	-0.22318900	1.66671200
C	-2.34923900	-1.20082300	-1.45158800
C	-2.09250400	-2.71071500	-1.39986000
C	-1.79387500	-3.34558100	-0.04220700
C	-2.69965100	-2.95784100	1.12273800
C	-2.29551600	-1.67692600	1.84642700
C	-2.40553700	-0.36463600	1.06833900
C	-3.77736600	-0.18357800	0.41399900

C	-3.77370300	-0.79492300	-1.00506500
C	-1.55375300	1.50234400	-0.97065500
C	-1.25362200	2.59807400	0.03923600
C	-1.32342100	3.98697100	-0.57144800
C	-1.07532000	5.09507800	0.43607900
C	-1.13513600	6.47527900	-0.18842200
H	-2.17707900	-0.86434900	-2.48334100
H	-1.26317500	-2.95589000	-2.07500400
H	-2.97550000	-3.20220200	-1.83688500
H	-0.75498600	-3.13490600	0.24876300
H	-1.83063800	-4.43371000	-0.18320800
H	-2.67007800	-3.76439200	1.86701100
H	-3.75072800	-2.90852900	0.79987500
H	-2.93147200	-1.56943300	2.73797000
H	-1.27207900	-1.79706500	2.22785500
H	-2.19189400	0.45438200	1.76862800
H	-4.02410400	0.88356000	0.36296300
H	-4.55659400	-0.63788700	1.04005200
H	-4.19657000	-0.07871400	-1.71884700
H	-4.42818700	-1.67342900	-1.05303300
H	-0.92143300	1.62550900	-1.86191800
H	-2.59044900	1.58522600	-1.32190500
H	-1.96396800	2.53779000	0.87799300
H	-0.25882900	2.44410900	0.48527100
H	-0.59008700	4.06353800	-1.39073300
H	-2.30854400	4.13334200	-1.04402200
H	-1.81359000	5.01895700	1.24862800
H	-0.09539000	4.94045000	0.91220900
H	-0.38414100	6.58622100	-0.98034200
H	-0.95681800	7.26763100	0.54583300
H	-2.11537800	6.66362800	-0.64365700
Co	1.02691900	-0.52784400	-0.07244000
C	2.95917600	-0.80766500	0.30203400
O	3.38002300	-1.72629000	0.94572600
C	3.90106800	0.23873900	-0.28436200
C	5.36659800	0.00256800	0.02764500
H	3.57680500	1.22511800	0.08145200
H	3.73223200	0.27081000	-1.37171100
C	6.24692800	1.07776900	-0.57992200
H	5.50433800	-0.03829500	1.11557100
H	5.66113600	-0.98871900	-0.33943900
H	7.30633900	0.91122400	-0.35767900
H	6.14361200	1.11213600	-1.67200000
H	5.98582400	2.07346500	-0.19923700

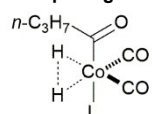
H	1.34481900	0.60481100	-1.32949700
H	1.32885300	1.06301800	-0.65184700

L = PBu₃ (*i*-C₃H₇ instead of *n*-C₃H₇)

Co	1.27019300	0.00273100	-0.35489500
C	1.05809100	-1.67400700	-0.87523800
O	0.91074200	-2.74398900	-1.26188300
C	1.36835700	1.45833300	-1.36072100
O	1.37979900	2.37093700	-2.05409200
C	3.17704700	-0.30200100	-0.81989400
O	3.55946500	-0.41330500	-1.95085900
C	4.16780700	-0.46756700	0.34769500
C	5.59075900	-0.18628400	-0.10171800
H	3.88954500	0.23527100	1.14436800
H	5.90200600	-0.89522800	-0.87570700
H	5.69476600	0.81931300	-0.52186100
P	-0.93552400	0.31106000	0.02814700
C	-1.98262900	-0.31970200	-1.34903900
C	-1.51350200	2.05278800	0.20342900
C	-1.62795900	-0.47514600	1.54502000
C	-3.49059900	-0.20250500	-1.20879300
H	-1.69413700	-1.36685200	-1.51627200
H	-1.63162000	0.21817000	-2.24337800
C	-0.73645300	2.86247900	1.22790300
H	-2.58428900	2.05136700	0.45433300
H	-1.42372000	2.51691900	-0.79067800
C	-1.45805800	-1.98401100	1.59312200
H	-2.68888300	-0.19783500	1.63969400
H	-1.11226900	-0.01470800	2.40065100
C	-4.22371600	-0.75722800	-2.42009500
H	-3.83263500	-0.73715000	-0.30864800
H	-3.78389300	0.84820600	-1.06450700
C	-1.23105000	4.29556700	1.33252200
H	-0.80153000	2.38572800	2.21926600
H	0.33224900	2.86354700	0.96710100
C	-2.06266200	-2.59778200	2.84494300
H	-1.91619400	-2.44956900	0.70585400
H	-0.38857100	-2.23840000	1.53907400
C	-5.72953300	-0.64386800	-2.28751100
H	-3.88361600	-0.22767900	-3.32230400
H	-3.93576800	-1.80864300	-2.56765900
C	-0.45208400	5.10277900	2.35217800
H	-1.16243800	4.77203600	0.34331200
H	-2.30097800	4.29513100	1.59012000

C	-1.88291400	-4.10218900	2.89610600
H	-1.60692500	-2.13302600	3.73235100
H	-3.13263100	-2.34442000	2.89390400
H	-6.24976200	-1.04515700	-3.16316900
H	-6.09430600	-1.19135800	-1.40955100
H	-6.04146900	0.40140600	-2.17084900
H	-0.81172600	6.13454400	2.42044800
H	-0.52958300	4.66081200	3.35334800
H	0.61364600	5.14251600	2.09628300
H	-2.32062900	-4.53731400	3.80037700
H	-2.35595400	-4.58854000	2.03427100
H	-0.82123600	-4.37645000	2.87859700
H	6.28293900	-0.27711200	0.74380300
C	4.03937000	-1.89329400	0.87392700
H	4.76481600	-2.07391400	1.67539600
H	3.04089400	-2.11134900	1.26839500
H	4.24381100	-2.61387100	0.07138100
H	1.55777400	-0.18457900	1.32156600
H	1.65829200	0.62125000	1.19232700

TS_{splitting}



L = CO

Co	-0.92133700	-0.12488500	-0.23641400
C	-2.52053200	-0.88228600	-0.74768500
O	-3.46680900	-1.38315400	-1.12115700
C	-0.66412800	-1.00601100	1.32558500
O	-0.45386800	-1.58987800	2.27818300
C	-1.54870300	1.57507500	0.05692500
O	-1.91555100	2.63819000	0.18912100
C	0.94396700	0.57146500	0.06396600
O	1.13154700	1.59110600	0.65565400
C	2.08084800	-0.27927900	-0.46516900
H	1.92725100	-1.30738700	-0.10338600
H	1.95216000	-0.35039500	-1.55571300
C	3.46403700	0.23097200	-0.10801100
H	3.58689700	1.25182100	-0.49126900
H	3.55313200	0.31489600	0.98268700
C	4.54646000	-0.67724700	-0.65905300
H	4.49031200	-0.75219900	-1.75220000
H	5.54785200	-0.31333400	-0.40748900
H	4.45823800	-1.69525400	-0.25951500

H	-0.53761500	0.07989500	-1.67562000
H	-0.27638100	-1.10239700	-1.16807000

L = PH₃

Co	-0.79486600	-0.07038000	-0.20151200
C	-0.73014600	-1.04051900	1.31169200
O	-0.65791300	-1.69085700	2.24575200
C	-1.32678400	1.64192800	0.06745500
O	-1.64719800	2.72585500	0.19250400
C	1.06401100	0.47577000	0.22660500
O	1.28407700	1.32482700	1.03872100
C	2.18327100	-0.25879900	-0.48921400
H	2.01950700	-1.33649500	-0.33928500
H	2.03910900	-0.10467500	-1.56865800
C	3.57812600	0.15241800	-0.05726900
H	3.70563400	1.23148700	-0.21100100
H	3.68821300	-0.00373200	1.02349500
C	4.64240100	-0.61954200	-0.81338100
H	4.56824000	-0.45154800	-1.89520500
H	5.65199100	-0.32749900	-0.50591800
H	4.54951800	-1.70017700	-0.64705600
H	-0.38165200	0.07731300	-1.64604500
H	-0.20746500	-1.07811200	-1.15460700
P	-2.81159100	-0.81467900	-0.89980600
H	-3.43568700	-1.90948700	-0.26145700
H	-2.91655500	-1.29506800	-2.22129200
H	-3.94260000	0.03230600	-0.92621100

L = PMe₃

Co	-0.13937800	-0.12957100	-0.01913000
C	-0.50891900	-1.89218200	-0.03483000
O	-0.77085900	-2.99995100	-0.09975600
C	-0.08609900	0.60531000	1.60995800
O	-0.08502400	1.13197200	2.62516700
C	1.79845700	-0.53526300	0.16596900
O	2.18653700	-1.49546400	0.76821100
C	2.77160600	0.44832200	-0.46392600
H	2.53180800	0.50679000	-1.53585300
H	2.52810800	1.44747800	-0.07156900
C	4.23509100	0.11361000	-0.24827900
H	4.44301100	0.05526400	0.82780300
H	4.44025100	-0.89116000	-0.63927900
C	5.14251900	1.13434300	-0.90795300
H	4.97297700	2.14143700	-0.50621800

H	6.20112500	0.89687500	-0.75771300
H	4.96906000	1.18538600	-1.99043500
H	0.24120400	1.08948600	-0.81950600
H	0.13827400	0.00986200	-1.49742000
P	-2.27721600	0.44707200	-0.37818300
C	-3.49769300	-0.16410300	0.83766100
H	-3.24222900	0.20714600	1.83586300
H	-4.51580300	0.15817800	0.58905600
H	-3.47118300	-1.25830000	0.87111400
C	-2.99372400	-0.11522500	-1.96089200
H	-4.03490600	0.20983600	-2.07325800
H	-2.40268000	0.28025200	-2.79269100
H	-2.95512000	-1.20851300	-2.01352500
C	-2.61815600	2.24147900	-0.39689900
H	-2.02225700	2.72087400	-1.17963800
H	-3.67972500	2.45145400	-0.57414100
H	-2.32420500	2.67979800	0.56282700

L = PBu₃

Co	1.14901800	0.15692700	-0.52077500
C	0.96976100	1.53734300	-1.66484200
O	0.82783300	2.44897800	-2.33520000
C	1.05919000	-1.45573300	-1.28509800
O	1.00015100	-2.51436600	-1.71536900
C	3.10854900	0.11400300	-0.84841600
O	3.59437300	0.53472400	-1.86015200
C	3.97090000	-0.51282900	0.23598600
H	3.80878500	0.06565900	1.15778300
H	3.55468500	-1.50735000	0.45810300
C	5.44671500	-0.59876700	-0.10295800
H	5.57571100	-1.16844500	-1.03228900
H	5.82938000	0.40604900	-0.32287400
C	6.24039400	-1.23438600	1.02246300
H	5.89037300	-2.25252600	1.23528400
H	7.30746400	-1.29909200	0.78413800
H	6.14715700	-0.66018500	1.95311400
H	1.43757400	-0.30084800	0.88326300
H	1.51121800	0.96611700	0.70089700
P	-1.03454800	0.24750800	0.05304200
C	-2.16955800	-0.41063800	-1.24132900
C	-1.72481300	1.92797800	0.36395100
C	-1.49801900	-0.65937200	1.58549000
C	-3.66075400	-0.41326700	-0.95151100
H	-1.82416400	-1.42721900	-1.47832100

H	-1.95204500	0.18207500	-2.14374200
C	-0.91698300	2.76854700	1.33829000
H	-2.75917500	1.82154700	0.72307300
H	-1.78317300	2.43239300	-0.61301600
C	-1.25097400	-2.15647800	1.51169400
H	-2.55114300	-0.44761600	1.82519800
H	-0.89842100	-0.22161000	2.39657700
C	-4.46704500	-1.00735400	-2.09576400
H	-3.87057900	-0.98315900	-0.03279300
H	-4.01547700	0.61008700	-0.75797100
C	-1.54695200	4.12835600	1.58971300
H	-0.80640700	2.23783700	2.29762500
H	0.10486000	2.90049800	0.95499800
C	-1.62036000	-2.87108900	2.80114800
H	-1.82295100	-2.59770300	0.67974600
H	-0.19242600	-2.34445800	1.27827000
C	-5.95696000	-1.00640400	-1.81628800
H	-4.25595400	-0.44493500	-3.01736300
H	-4.11999800	-2.03336600	-2.28874500
C	-0.73418000	4.97178900	2.55215300
H	-1.65983200	4.65582300	0.63065300
H	-2.56811100	3.99326800	1.97744300
C	-1.37157800	-4.36459800	2.72578400
H	-1.04663300	-2.43497600	3.63262500
H	-2.67802200	-2.67668500	3.03568700
H	-6.52990000	-1.43684800	-2.64388700
H	-6.19358100	-1.58721100	-0.91615200
H	-6.33071100	0.01195500	-1.65291100
H	-1.19182200	5.95080300	2.72757300
H	-0.63206500	4.47713000	3.52604300
H	0.27861100	5.14563200	2.16912500
H	-1.63777000	-4.87277100	3.65829200
H	-1.95750500	-4.82535800	1.92101200
H	-0.31607600	-4.58146200	2.52181200

L = a₅-PhobPC₅

P	-1.12581300	-0.35375700	-0.37128500
C	-1.90033900	-1.46184600	-1.64663800
C	-1.44016600	-2.91959700	-1.55167200
C	-1.32834400	-3.55895700	-0.16691300
C	-2.46653300	-3.31576600	0.81867400
C	-2.35926400	-2.01240300	1.60517900
C	-2.50988600	-0.70649000	0.82412200
C	-3.75901100	-0.69775800	-0.06149700

C	-3.42390500	-1.27335400	-1.45607000
C	-1.60016200	1.31321000	-1.02781600
C	-1.65214400	2.40764000	0.02579500
C	-1.79466400	3.79145800	-0.58388200
C	-1.90049000	4.89315600	0.45504800
C	-2.02731200	6.27023900	-0.16645800
H	-1.60078900	-1.07910900	-2.63205700
H	-0.46481900	-3.01769500	-2.04642200
H	-2.13460600	-3.51576000	-2.16362000
H	-0.39515300	-3.24085900	0.31679200
H	-1.20824100	-4.63912200	-0.32248000
H	-2.46462800	-4.13128600	1.55383700
H	-3.44274500	-3.38918000	0.31672100
H	-3.14280600	-2.01154500	2.37772600
H	-1.40653800	-2.01042200	2.15407100
H	-2.53689600	0.11516400	1.55296000
H	-4.13557800	0.32714100	-0.15877100
H	-4.56672200	-1.26549000	0.41927100
H	-3.81549800	-0.60937900	-2.23507000
H	-3.92737000	-2.23473900	-1.61381200
H	-0.83813100	1.55348200	-1.78236100
H	-2.55667900	1.25700200	-1.56328800
H	-2.49471200	2.22918000	0.71161700
H	-0.74589200	2.37534400	0.64962400
H	-0.93424600	3.98935300	-1.24339200
H	-2.68084400	3.81763800	-1.23935000
H	-2.76441300	4.69555300	1.10768000
H	-1.01899100	4.85754900	1.11258100
H	-1.15963900	6.50326100	-0.79594400
H	-2.10478500	7.05819000	0.58986700
H	-2.91730000	6.33815500	-0.80446000
Co	1.08750500	-0.32392600	0.20463600
C	1.63398600	-1.93946200	-0.33664200
C	0.70951200	-0.14247600	1.95890100
C	3.01313000	-0.00684500	0.58873200
H	1.10509300	1.14669900	-0.13939500
H	1.28944800	0.37651600	-1.11650700
O	2.07517000	-2.91518100	-0.73931900
O	0.44487400	0.04362400	3.05201100
O	3.48885400	-0.22099800	1.66641600
C	3.86419600	0.49782300	-0.56562800
H	3.69354500	-0.16682500	-1.42594600
H	3.44748000	1.46686600	-0.87860700
C	5.34296700	0.61686100	-0.24971100

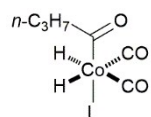
H	5.47975400	1.28260600	0.61185500
H	5.72728900	-0.35940400	0.07281000
C	6.12699700	1.12600200	-1.44406800
H	5.77627700	2.11623700	-1.76167200
H	7.19606400	1.21361200	-1.22301700
H	6.02504000	0.45545900	-2.30672400

L = P Bu₃ (*i*-C₃H₇ instead of *n*-C₃H₇)

Co	1.15556000	-0.51232400	-0.39666500
C	0.52762700	-2.02912500	-1.15084200
O	0.10825400	-3.00251500	-1.56902600
C	1.60800300	0.75706200	-1.56874500
O	1.91172900	1.61572900	-2.26271500
C	3.01619100	-1.17933700	-0.48045900
O	3.30714600	-2.23125500	-0.97567900
C	4.11060500	-0.30119300	0.14431500
C	5.26364400	-0.15044300	-0.83455900
H	3.68815300	0.68636800	0.36723300
H	5.69812900	-1.12649700	-1.07425700
H	4.93827700	0.31000800	-1.77522700
P	-0.89644100	0.34053900	0.00247300
C	-2.15403400	-0.02299300	-1.29529800
C	-0.98405600	2.17714200	0.13071500
C	-1.67868500	-0.20897100	1.57490700
C	-3.55827300	0.52398400	-1.10311100
H	-2.18307900	-1.11616800	-1.40869300
H	-1.71811200	0.35014800	-2.23513000
C	0.01651200	2.79370500	1.09367900
H	-2.00716200	2.45994100	0.41945100
H	-0.82567300	2.57293700	-0.88463000
C	-1.97333400	-1.69884800	1.62223700
H	-2.59328500	0.37712900	1.75178900
H	-0.97551800	0.05748500	2.37705600
C	-4.49866000	0.09742800	-2.21939200
H	-3.97145400	0.18727000	-0.13936000
H	-3.53780600	1.62284300	-1.05349200
C	-0.12050700	4.30464100	1.18105800
H	-0.10726200	2.36029600	2.09914700
H	1.03932400	2.53366600	0.78470600
C	-2.55622100	-2.13433200	2.95654300
H	-2.67333900	-1.97463500	0.81742000
H	-1.05101900	-2.26471900	1.42299400
C	-5.89905500	0.64922600	-2.03939900
H	-4.08579600	0.42428400	-3.18532400

H	-4.52924600	-1.00129100	-2.26688800
C	0.88606900	4.92138800	2.13219300
H	-0.00125500	4.73594000	0.17581400
H	-1.14299100	4.56224700	1.49631100
C	-2.85522300	-3.61991000	2.99908500
H	-1.85403700	-1.86831300	3.76074600
H	-3.47259400	-1.55931300	3.15935500
H	-6.57034300	0.33580600	-2.84536700
H	-6.34134200	0.31171300	-1.09387700
H	-5.89573600	1.74610600	-2.02273400
H	0.78317100	6.00984300	2.18996400
H	0.76771800	4.52537900	3.14839800
H	1.91395000	4.70426400	1.81737900
H	-3.27199700	-3.92718500	3.96372500
H	-3.57759000	-3.90270600	2.22347800
H	-1.94847300	-4.21237100	2.82782800
H	6.05131400	0.48072200	-0.40663600
C	4.55632900	-0.95774600	1.44241800
H	5.32950900	-0.35603700	1.93395400
H	3.72518500	-1.07762400	2.14752700
H	4.97429200	-1.95117200	1.24279400
H	1.25650600	-1.06033700	1.00847400
H	1.55743900	0.18289500	0.87622600

[Co]-2H



L = CO

Co	-0.91594600	-0.15486800	-0.18313800
C	-2.41771900	-1.02479400	-0.79363600
O	-3.26205400	-1.61773200	-1.26332200
C	-0.74048200	-0.76832400	1.51320700
O	-0.55933100	-1.19723100	2.54896000
C	-1.61112600	1.53566000	-0.00670500
O	-2.02446000	2.58715800	0.03999000
C	0.94659300	0.58608300	-0.06190600
O	1.12053300	1.72385900	0.25713000
C	2.08911300	-0.35868500	-0.36169300
H	1.96635800	-1.24148900	0.28490000
H	1.92997500	-0.74261300	-1.38017900
C	3.46931900	0.25058800	-0.20467900
H	3.56094900	1.12186900	-0.86550000
H	3.58418400	0.64231300	0.81412700

C	4.55688500	-0.76208600	-0.50821400
H	4.47360600	-1.14597800	-1.53262900
H	5.55647800	-0.32840300	-0.40161900
H	4.50105200	-1.62568000	0.16626100
H	-0.55493800	0.15919200	-1.59429900
H	-0.24013300	-1.37686300	-0.66664000

L = PH₃

Co	-0.79931000	-0.08924100	-0.15157400
C	-0.69846300	-0.78389700	1.50273200
O	-0.56883100	-1.27690200	2.52148700
C	-1.49616900	1.57727300	0.05032900
O	-1.93053500	2.62377600	0.10813800
C	1.05340900	0.60125800	-0.01280100
O	1.25476600	1.72497700	0.34318500
C	2.18172800	-0.35249500	-0.34841400
H	2.05238000	-1.24875700	0.27763600
H	2.00640700	-0.70806900	-1.37413300
C	3.57203200	0.23319600	-0.19094800
H	3.66800900	1.12220600	-0.82723900
H	3.70494600	0.59380800	0.83713500
C	4.64293300	-0.78352100	-0.53749400
H	4.54224100	-1.13572000	-1.57187300
H	5.64986000	-0.36660400	-0.43054700
H	4.58348600	-1.66644900	0.11135500
H	-0.46770400	0.25378500	-1.56786400
H	-0.17297000	-1.33564700	-0.66153300
P	-2.66067700	-1.08958200	-0.91392800
H	-3.89601100	-0.41727900	-1.06584400
H	-3.17078000	-2.24088300	-0.27400300
H	-2.58436200	-1.62284200	-2.21457500

L = PMe₃

Co	-0.15261000	0.17568400	0.01183400
C	-0.05076900	-0.26976700	1.74122100
O	0.01580800	-0.63436500	2.82143400
C	-0.61425100	1.91933500	-0.07751300
O	-0.93662800	3.00178100	-0.21326300
C	1.78532200	0.60486900	-0.05808600
O	2.17896900	1.72354100	0.11471600
C	2.74371000	-0.54021300	-0.32684600
H	2.54612400	-1.31894600	0.42616400
H	2.43744000	-0.99729500	-1.27931200
C	4.20921100	-0.15003600	-0.34417800

H	4.36842000	0.63480000	-1.09489000
H	4.47901500	0.30715700	0.61657600
C	5.09932300	-1.34458200	-0.62923000
H	4.86544300	-1.79650600	-1.60156800
H	6.15949100	-1.07001600	-0.64307300
H	4.97407300	-2.12801700	0.12910800
H	0.07128900	0.19310700	-1.46583700
H	0.23850800	-1.21451000	-0.33238800
P	-2.23433800	-0.56390400	-0.35163700
C	-3.54881100	0.06193700	0.75772900
H	-3.60784200	1.15319900	0.68570300
H	-4.52874000	-0.36162700	0.50725800
H	-3.30848900	-0.19301900	1.79550100
C	-2.45796400	-2.37019900	-0.22093900
H	-3.49921400	-2.66237700	-0.40118900
H	-1.81091500	-2.87147100	-0.94678300
H	-2.15992600	-2.70352400	0.77871100
C	-2.91790200	-0.18996200	-2.00210400
H	-2.26702500	-0.61604200	-2.77134100
H	-3.93156500	-0.59080300	-2.12154800
H	-2.94297300	0.89503600	-2.14948600

L = PBu₃

Co	1.07426600	-0.42820800	-0.60824300
C	1.50030200	0.89617200	-1.73104700
O	1.79101600	1.79679500	-2.37132500
C	0.50219600	-1.82318200	-1.60209000
O	0.11851900	-2.73826600	-2.15801000
C	2.94291500	-1.10227300	-0.61421300
O	3.28122100	-1.99621500	-1.33792200
C	3.92719100	-0.43081900	0.32534600
H	3.89190700	0.65110300	0.12353600
H	3.51883100	-0.53225500	1.34180500
C	5.34629000	-0.95940800	0.24211100
H	5.34613800	-2.03817400	0.44436400
H	5.71582500	-0.85684100	-0.78642300
C	6.26608400	-0.23887600	1.20929300
H	5.92826900	-0.35644500	2.24682600
H	7.29295400	-0.61605300	1.15517000
H	6.30171000	0.83827500	1.00208100
H	1.07242900	-1.33110900	0.58236100
H	1.48843000	0.43898500	0.52439000
P	-0.97241600	0.31595400	-0.04118700
C	-2.35143200	-0.21042300	-1.14685300

C	-1.18357100	2.14542900	0.00560200
C	-1.51975900	-0.20469900	1.63691500
C	-3.75091100	0.29251400	-0.83302300
H	-2.33480400	-1.31016100	-1.15462500
H	-2.05282700	0.08706800	-2.16358900
C	-0.19581300	2.88177100	0.89460200
H	-2.21187100	2.36609400	0.32797600
H	-1.09971600	2.50058600	-1.03346300
C	-1.84139800	-1.68651000	1.73938600
H	-2.38107200	0.40460000	1.95007100
H	-0.69130400	0.04474400	2.31434200
C	-4.80839900	-0.38274300	-1.69182800
H	-3.99351100	0.12542500	0.22829500
H	-3.80581500	1.38068000	-0.98406200
C	-0.43143900	4.38321300	0.89793500
H	-0.26137800	2.50207000	1.92660500
H	0.83267300	2.67189900	0.56869300
C	-2.08876700	-2.13076400	3.17149300
H	-2.72870700	-1.92465500	1.13154100
H	-1.01574600	-2.27646700	1.31148700
C	-6.20302500	0.14269500	-1.41500400
H	-4.55633500	-0.24421900	-2.75377500
H	-4.77285000	-1.46894000	-1.51838200
C	0.55579100	5.12019400	1.78135400
H	-0.36686000	4.76036000	-0.13378300
H	-1.46046900	4.59215600	1.22770000
C	-2.44211200	-3.60183500	3.26684200
H	-1.19292200	-1.91869200	3.77356300
H	-2.89344200	-1.52025700	3.60901700
H	-6.95883200	-0.35423000	-2.03167400
H	-6.48417700	-0.00860900	-0.36538500
H	-6.27028100	1.21881600	-1.61688600
H	0.38244900	6.20122800	1.77808200
H	0.48980200	4.77948800	2.82204600
H	1.58745600	4.95118900	1.44988200
H	-2.61156500	-3.91735900	4.30144000
H	-3.35335700	-3.82993700	2.70015300
H	-1.64089000	-4.22930400	2.85810100

L= a₅-PhobPC₅

O	1.73572700	-3.30967300	-0.20167100
O	0.38455300	-0.08821200	3.14920800
P	-1.13714400	-0.22711900	-0.36170000
C	1.38799700	-2.24917500	0.04128500

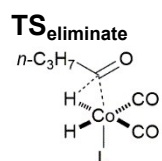
C	0.64885100	-0.30814500	2.06492300
C	-1.94343000	-1.21864000	-1.70701500
C	-1.69190700	-2.72453400	-1.59241100
C	-1.80644200	-3.38241100	-0.21596100
C	-2.97255800	-2.97372900	0.67794600
C	-2.74051300	-1.70002700	1.48651300
C	-2.65014100	-0.38488800	0.71262000
C	-3.80709100	-0.20584300	-0.27467800
C	-3.43817400	-0.82631000	-1.64168800
C	-1.31307900	1.48916900	-1.03096100
C	-1.32223900	2.57407200	0.03365900
C	-1.15611300	3.96381200	-0.55591900
C	-1.21973900	5.06560800	0.48625700
C	-1.03569100	6.44616300	-0.11284300
H	-1.51035600	-0.87891300	-2.65816700
H	-0.69199900	-2.94743400	-1.98937200
H	-2.39236700	-3.21941600	-2.28276300
H	-0.88244300	-3.21753500	0.35273600
H	-1.84177500	-4.46714500	-0.38187700
H	-3.14774400	-3.78157100	1.40070300
H	-3.90602800	-2.90345100	0.10035300
H	-3.56902500	-1.59264200	2.20259900
H	-1.83688300	-1.83155100	2.10035400
H	-2.62616000	0.43333800	1.44559800
H	-4.02785700	0.86112200	-0.39460400
H	-4.72388600	-0.65418000	0.13111800
H	-3.67052200	-0.11761400	-2.44464900
H	-4.05236800	-1.71121900	-1.84781100
H	-0.44749900	1.62128600	-1.69434200
H	-2.20813300	1.56714300	-1.66171100
H	-2.26319700	2.53488200	0.60388700
H	-0.51847300	2.39237700	0.76389600
H	-0.19410400	4.01792800	-1.09046400
H	-1.93020900	4.13628700	-1.32193000
H	-2.18411500	5.01172600	1.01405200
H	-0.45199200	4.88373600	1.25311200
H	-0.06486200	6.53428500	-0.61589300
H	-1.08475000	7.23447300	0.64552200
H	-1.80856600	6.66125400	-0.86129200
Co	1.01042200	-0.52064500	0.30776600
C	2.95242100	-0.19350500	0.56559600
O	3.42901100	-0.14355900	1.66305800
C	3.79864200	-0.02403100	-0.68102300
C	5.27935300	0.17298400	-0.41806100

H	3.37309200	0.82038500	-1.24307900
H	3.62147700	-0.89828400	-1.32627000
C	6.05585700	0.33836400	-1.71045600
H	5.42196200	1.04726300	0.22993900
H	5.66627100	-0.67980300	0.15461000
H	7.12632100	0.48135900	-1.52842600
H	5.94849000	-0.54090000	-2.35823800
H	5.70218000	1.20552200	-2.28256600
H	1.24237800	-0.32321900	-1.15073000
H	1.15856500	0.96265700	0.20006400

L = P Bu₃ (*i*-C₃H₇ instead of *n*-C₃H₇)

Co	1.18462100	-0.40137700	-0.57358700
C	0.64825800	-1.77400100	-1.61825500
O	0.28286700	-2.67619400	-2.20641300
C	1.65372500	0.94605400	-1.65237200
O	1.97078300	1.85923400	-2.26158700
C	3.04950900	-1.08018000	-0.50862700
O	3.37558100	-2.05609000	-1.12372900
C	4.06585000	-0.34190800	0.37071300
C	5.47509700	-0.50247400	-0.17329000
H	3.78923800	0.72096300	0.38889800
H	5.77587700	-1.55512600	-0.17500800
H	5.56048100	-0.13627600	-1.20210500
P	-0.88054300	0.32999700	-0.06104300
C	-2.22295400	-0.16497500	-1.22501400
C	-1.09329000	2.15808200	0.02767700
C	-1.48341700	-0.23446700	1.58385800
C	-3.63132200	0.33179200	-0.94271200
H	-2.20700500	-1.26412900	-1.26202600
H	-1.89140500	0.15957100	-2.22309000
C	-0.12900300	2.87138100	0.96013300
H	-2.12965200	2.36949600	0.32998600
H	-0.98442900	2.54090000	-0.99920800
C	-1.81123300	-1.71763200	1.63472600
H	-2.35324000	0.36836300	1.88569000
H	-0.67696200	-0.00631100	2.29460700
C	-4.66145200	-0.31670600	-1.85375000
H	-3.90809000	0.13550000	0.10514900
H	-3.67983400	1.42391400	-1.06461500
C	-0.37380900	4.37063200	1.00579500
H	-0.21348600	2.45885200	1.97807500
H	0.90731600	2.67765300	0.64933300
C	-2.10487400	-2.20080800	3.04534100

H	-2.67945700	-1.93581000	0.99271400
H	-0.97373400	-2.29810000	1.21692900
C	-6.06355300	0.20392800	-1.60716400
H	-4.37518300	-0.14891100	-2.90272600
H	-4.63297600	-1.40742300	-1.70992700
C	0.59193800	5.08500400	1.93058800
H	-0.29202100	4.78038100	-0.01218200
H	-1.41015900	4.56339700	1.32216800
C	-2.46525700	-3.67264400	3.08818700
H	-1.22784800	-2.00905500	3.68103400
H	-2.92121400	-1.59972600	3.47426200
H	-6.79982400	-0.27371100	-2.26155500
H	-6.37856800	0.02379800	-0.57181500
H	-6.12276700	1.28545500	-1.78069100
H	0.41169600	6.16455600	1.95815100
H	0.50856800	4.71114100	2.95857400
H	1.63070600	4.93266400	1.61356700
H	-2.66856600	-4.01613800	4.10765700
H	-3.35862700	-3.88133300	2.48661400
H	-1.65320200	-4.29152300	2.68782200
H	6.18802200	0.05494100	0.44559400
C	3.96121300	-0.90089100	1.78391400
H	4.67527500	-0.39900300	2.44677400
H	2.95869100	-0.77501500	2.20456300
H	4.19859800	-1.97232500	1.78631500
H	1.14052400	-1.33120300	0.59487800
H	1.55022600	0.44005700	0.59345000



L = CO

Co	-0.92531100	-0.19282100	-0.10817900
C	-2.30156800	-1.08203700	-0.90895600
O	-3.08600800	-1.69960000	-1.44979500
C	-0.77090000	-0.65164900	1.62594900
O	-0.61771200	-0.99186100	2.70031900
C	-1.69411300	1.46462400	0.02952300
O	-2.16273800	2.49231200	0.09440900
H	-0.14897300	0.18666900	-1.36087400
H	-0.26892400	-1.50199000	-0.33281900
C	0.94802100	0.61594200	-0.29234000
O	1.09645800	1.79717500	-0.18589100

C	2.09785500	-0.36395500	-0.33086900
H	1.94668800	-1.10070200	0.47240800
H	1.99399700	-0.94719500	-1.25867100
C	3.46782800	0.27913400	-0.23118800
H	3.54133100	0.84102500	0.70860200
H	3.58098800	1.02526700	-1.02812300
C	4.57131800	-0.75785100	-0.31517000
H	4.48738200	-1.50031700	0.48825800
H	5.56323600	-0.30159000	-0.23613700
H	4.53703100	-1.30445600	-1.26585700

L = PH₃

Co	-0.81458500	-0.13313800	-0.05227900
C	-0.75851200	-0.68468600	1.63750800
O	-0.66627400	-1.08502800	2.70248100
C	-1.58108600	1.49916200	0.13329300
O	-2.07478700	2.51650500	0.23633500
H	-0.01078500	0.26513200	-1.30169700
H	-0.20820600	-1.47543500	-0.29196900
C	1.04535600	0.63915100	-0.28589900
O	1.22180000	1.81979700	-0.17257100
C	2.18511300	-0.35756400	-0.31313000
H	2.02786100	-1.07749700	0.50366600
H	2.07394500	-0.95570200	-1.23041900
C	3.56267800	0.27112600	-0.22632200
H	3.64447600	0.84581400	0.70493000
H	3.68218800	1.00558700	-1.03338800
C	4.65626600	-0.77716300	-0.29785800
H	4.56655300	-1.50782200	0.51589600
H	5.65317800	-0.32992700	-0.22689200
H	4.61496600	-1.33711800	-1.24069200
P	-2.50016000	-1.13061000	-1.10994000
H	-3.07847700	-2.28482500	-0.53866100
H	-3.71161100	-0.47185200	-1.42598900
H	-2.26270200	-1.67284100	-2.38964800

L = PMe₃

Co	-0.20293000	0.25106300	0.14685600
C	0.02418700	0.36403400	1.90327600
O	0.17397900	0.36355300	3.03722700
C	-0.71741800	1.92357800	-0.27145800
O	-1.08872400	2.96342900	-0.54832600
H	0.49699500	-0.00920100	-1.20693300
H	0.10861200	-1.19323000	0.39268800

C	1.70125500	0.50751300	-0.53097100
O	2.06855900	1.57686900	-0.93729600
C	2.67098700	-0.60860000	-0.19728700
H	2.53086100	-0.87163000	0.86172300
H	2.34723000	-1.50515800	-0.74747700
C	4.12313900	-0.27798200	-0.48408300
H	4.40722000	0.62572700	0.06977000
H	4.23759100	-0.01683000	-1.54433200
C	5.03790100	-1.43164200	-0.12035300
H	4.96045400	-1.68389400	0.94479300
H	6.08826800	-1.19952600	-0.32555900
H	4.78620800	-2.33794900	-0.68575600
P	-2.15591500	-0.70598100	-0.28176100
C	-2.86177100	-1.64937200	1.11589400
H	-3.04169900	-0.97849600	1.96203800
H	-3.80491700	-2.13669600	0.84077900
H	-2.14479600	-2.41061600	1.43884100
C	-2.13828700	-1.95852800	-1.61154300
H	-3.12468300	-2.41821000	-1.74731000
H	-1.82731200	-1.49246700	-2.55159900
H	-1.40866100	-2.73613400	-1.36569900
C	-3.57685400	0.33879700	-0.77750600
H	-3.34369000	0.87020200	-1.70593900
H	-4.48191800	-0.26074600	-0.93249000
H	-3.77728100	1.08825900	-0.00488600

L = PBu₃

Co	-1.07836500	-0.66060900	-0.11677100
C	-0.92879900	-2.28357400	0.58509900
O	-0.81852700	-3.29861400	1.10220000
C	-0.84227000	-0.97759800	-1.87143400
O	-0.63863600	-1.15349100	-2.97875700
H	-2.02499600	0.54363300	-0.32679500
H	-1.17369000	-0.24577000	1.31761300
C	-3.10039100	-0.44908600	-0.26207800
O	-3.66544200	-0.63035400	-1.30767900
C	-3.84732200	-0.36609300	1.05465500
H	-3.47926700	-1.17515900	1.70315700
H	-3.52863500	0.55762200	1.56071600
C	-5.35671400	-0.42823300	0.91877100
H	-5.63990000	-1.36052600	0.41425200
H	-5.69823600	0.37663100	0.25464700
C	-6.04093700	-0.32764200	2.26857100
H	-5.73277500	-1.14258900	2.93566800

H	-7.13130400	-0.37413500	2.17791400
H	-5.79428400	0.61429200	2.77492200
P	0.86193300	0.39748300	0.16448700
C	1.72205000	-0.08988800	1.72007300
C	0.74783400	2.22862700	0.30382700
C	2.14586300	0.16826300	-1.13877500
C	3.08584200	0.51594000	2.00216200
H	1.78239300	-1.18845500	1.70702600
H	1.01709700	0.14782500	2.53025000
C	0.17626300	2.90016200	-0.93352400
H	1.74179200	2.64015300	0.53249800
H	0.10763600	2.42898100	1.17632500
C	2.63710300	-1.26663100	-1.24973900
H	2.98454700	0.85923400	-0.96497000
H	1.68446400	0.47717600	-2.08771800
C	3.69442600	-0.01501000	3.29082100
H	3.77853500	0.31226600	1.17103100
H	3.01204000	1.61192600	2.06757000
C	-0.02937800	4.39403000	-0.74481100
H	0.84466400	2.73610300	-1.79326800
H	-0.78056100	2.42797100	-1.20334000
C	3.44581500	-1.51112500	-2.51259000
H	3.24604200	-1.52583700	-0.36963200
H	1.78225100	-1.96140100	-1.22865800
C	5.05107800	0.59399400	3.58500700
H	3.00433800	0.18031300	4.12511400
H	3.77845700	-1.11015900	3.22625000
C	-0.58281000	5.06225200	-1.98799100
H	-0.70764200	4.56010100	0.10553100
H	0.92534000	4.86141000	-0.45933600
C	3.97254900	-2.92992500	-2.59707900
H	2.81541500	-1.29050000	-3.38712800
H	4.28012000	-0.79450300	-2.55622900
H	5.48375700	0.20441600	4.51214600
H	5.76397600	0.38646600	2.77738300
H	4.98446300	1.68428800	3.68639900
H	-0.73485300	6.13687300	-1.84370100
H	0.09491800	4.93769800	-2.84151700
H	-1.54807600	4.62835900	-2.27554000
H	4.54505400	-3.10127100	-3.51435800
H	4.63055200	-3.16191800	-1.75042700
H	3.15286600	-3.65844500	-2.58018800

L = a₅-PhobPC₅

Co	0.67867700	-0.95454000	0.37668100
C	0.57109400	-2.72467000	0.30151200
O	0.55301200	-3.86216700	0.17922700
C	0.38221300	-0.59510900	2.11660900
O	0.16229100	-0.32043500	3.19968000
H	1.61798200	0.24651900	0.18429900
H	0.82071400	-1.08605300	-1.10848700
C	2.69279100	-0.79096000	0.51374100
O	3.22550800	-0.62020900	1.57588400
C	3.47315500	-1.16203600	-0.73197500
H	3.09583100	-2.13179200	-1.08996300
H	3.19281900	-0.45023100	-1.52289600
C	4.97659000	-1.20685000	-0.53625500
H	5.22069300	-1.92386800	0.25757700
H	5.32721700	-0.23402900	-0.16729200
C	5.69271400	-1.57573700	-1.82134700
H	5.37642400	-2.56060400	-2.18754300
H	6.77907400	-1.61021600	-1.68769900
H	5.48374100	-0.85243700	-2.61983300
P	-1.14103400	0.11954900	-0.36069900
C	-2.18399800	-0.51645100	-1.75355700
C	-2.65537000	0.51767300	0.64533300
C	-0.64605300	1.77697300	-1.01850700
C	-2.47779000	-2.01519400	-1.65473400
C	-3.44622300	0.37682300	-1.74409200
H	-1.61485900	-0.34882400	-2.67880600
C	-3.23778400	-0.68237000	1.39286700
C	-3.62693800	1.09538800	-0.38686300
H	-2.37518500	1.27369000	1.39201500
C	-0.25188800	2.77530400	0.05681100
H	0.21115100	1.57198100	-1.67583700
H	-1.43654900	2.19456900	-1.65610700
C	-2.88159000	-2.59148400	-0.29603800
H	-1.59551400	-2.56950100	-2.00346400
H	-3.26933000	-2.23642000	-2.38734200
H	-3.38209300	1.11750300	-2.54935100
H	-4.32395700	-0.23614900	-1.98171800
C	-3.86485900	-1.79525100	0.55622100
H	-4.00832300	-0.29091500	2.07390800
H	-2.46646700	-1.12192200	2.04275300
H	-3.44259600	2.16987700	-0.50347500
H	-4.66057400	1.00910900	-0.02576600
C	0.40016500	4.02048700	-0.51857100
H	-1.13885500	3.06930800	0.63953000

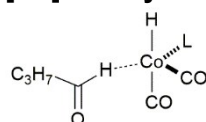
H	0.43669800	2.30264200	0.77461500
H	-1.98337600	-2.76910000	0.30957300
H	-3.29623100	-3.59095300	-0.48212600
H	-4.34321200	-2.48868900	1.26067400
H	-4.68962700	-1.40249300	-0.05675200
C	0.76159400	5.04884400	0.53780100
H	1.30618900	3.73168500	-1.07543700
H	-0.27077500	4.47855900	-1.26397700
C	1.42460600	6.27913900	-0.05005000
H	-0.14620200	5.33926000	1.08824200
H	1.42438100	4.58500800	1.28347800
H	2.35090900	6.01757000	-0.57630100
H	1.68107400	7.01596600	0.71818600
H	0.76902800	6.77565900	-0.77635100

L = PBu₃ (*i*-C₃)

Co	1.06387000	-0.85618400	-0.26071400
C	0.83771900	-1.83395000	1.23269400
O	0.66100800	-2.41538200	2.19606800
C	0.75740600	-2.04253800	-1.54663500
O	0.55071100	-2.75020700	-2.42130500
C	3.08664600	-0.86870400	-0.14910900
O	3.64600400	-1.53755800	0.67722500
C	3.85669200	-0.17154100	-1.27232400
C	5.23579700	-0.78106900	-1.44343200
H	3.27557700	-0.29049600	-2.19712100
H	5.84072500	-0.64247100	-0.54083400
H	5.18492100	-1.85714000	-1.63667300
P	-0.76266100	0.39935500	-0.03088600
C	-1.85878000	0.33944000	-1.51035400
C	-0.43067100	2.19902000	0.16674800
C	-1.90106400	0.03588500	1.37458400
C	-3.10298700	1.21144300	-1.51111600
H	-2.12857000	-0.71862700	-1.64569000
H	-1.21412200	0.58175000	-2.36781900
C	0.41427000	2.54354500	1.38115500
H	-1.38702700	2.74067200	0.20426000
H	0.08021800	2.51621700	-0.75560100
C	-2.63891900	-1.28559500	1.22373000
H	-2.61036900	0.86621800	1.50959000
H	-1.27586800	0.01439000	2.27921300
C	-4.00083600	0.92697100	-2.70465700
H	-3.68228600	1.06330800	-0.58618600
H	-2.82067700	2.27475100	-1.51886700

C	0.81455500	4.00887400	1.41776000
H	-0.13276300	2.29247800	2.30362700
H	1.31948700	1.91796700	1.39261700
C	-3.30254200	-1.73642900	2.51401900
H	-3.40072500	-1.20126900	0.43282700
H	-1.94673000	-2.07133500	0.88057900
C	-5.22643700	1.81850400	-2.73528600
H	-3.42131900	1.04937800	-3.63183500
H	-4.30404200	-0.13074700	-2.68269200
C	1.67038200	4.34235700	2.62373700
H	1.35815800	4.25541200	0.49283800
H	-0.08843800	4.63807600	1.40848000
C	-4.07323800	-3.03078500	2.34622000
H	-2.53195400	-1.85521800	3.29030300
H	-3.97192000	-0.94130700	2.87630800
H	-5.87032200	1.60234600	-3.59392900
H	-5.83303000	1.69230900	-1.82986400
H	-4.94680700	2.87768900	-2.79302100
H	1.95906500	5.39827400	2.64401900
H	1.14040900	4.12804600	3.55998000
H	2.59245300	3.74811800	2.63062500
H	-4.54194800	-3.35354400	3.28143000
H	-4.86906700	-2.92700500	1.59816700
H	-3.41584000	-3.84218400	2.01100100
H	5.76069300	-0.30767100	-2.28114800
C	3.95250500	1.31545200	-0.94999300
H	4.54136500	1.83392100	-1.71482900
H	2.96897600	1.79558500	-0.90149600
H	4.45443900	1.46983800	0.01470700
H	2.05524600	0.09782400	0.42036600
H	1.17276700	0.09098800	-1.41311700

[Co]-aldehyde



L = CO

Co	-1.36106200	0.15264400	-0.34475800
C	-1.04308300	1.90043700	-0.33282800
O	-0.83671900	3.01625500	-0.41691700
C	-1.71853000	-1.36762400	-1.19495600
O	-1.94388000	-2.29210500	-1.81754200
C	-2.43107500	-0.00877500	1.09096300
O	-3.12908800	-0.10142000	1.98307700

H	0.33080800	-0.45605300	0.66183000
H	-0.56055400	0.32522000	-1.61875300
C	1.42468100	-0.62004700	0.93408200
O	1.70787700	-1.20437200	1.93727100
C	2.38229600	-0.04885700	-0.06059800
H	2.11699300	-0.47592000	-1.04261100
H	2.13587900	1.02177100	-0.16680900
C	3.84542400	-0.25605600	0.26950300
H	4.05825400	0.17371600	1.25688000
H	4.04460100	-1.33066900	0.37168100
C	4.75158600	0.35441500	-0.78171700
H	4.58699300	1.43504700	-0.87475400
H	5.80897500	0.20423700	-0.54250800
H	4.57340800	-0.08655900	-1.77029800

L = PH₃

Co	-1.41604000	-0.32911100	-0.00086900
C	-1.33736000	-1.97799200	-0.55971400
O	-1.31991500	-3.04423100	-0.97146100
H	0.37516600	0.49070400	-1.94990100
H	-2.23172600	-0.22848800	-1.28628200
C	1.10399600	0.86016100	-1.18683200
O	0.93412600	1.92934900	-0.65522100
C	2.25432800	-0.05579700	-0.91876400
H	1.82661400	-1.03318900	-0.63733600
H	2.74957900	-0.25149400	-1.88519200
C	3.23889600	0.44111400	0.11849200
H	3.64728700	1.40805400	-0.20322200
H	2.70690300	0.65004400	1.05565400
C	4.35727300	-0.55458400	0.35649100
H	4.91682000	-0.75776400	-0.56529400
H	5.07322000	-0.19129800	1.10052200
H	3.96835300	-1.51445900	0.71817300
P	-2.01254000	1.78267000	0.04518500
H	-1.50475700	2.72398900	0.96532200
H	-3.38974800	2.01218400	0.24728700
H	-1.84287800	2.52630100	-1.13482700
C	-0.51032000	-0.44576900	1.51716900
O	0.07147400	-0.54654700	2.49665100

L = PMe₃

Co	0.64638100	1.06686500	0.01104500
C	0.09123400	2.65721500	-0.46601100
O	-0.22509000	3.70023200	-0.81321500

H	-0.90111300	0.18284600	-2.26404500
H	1.59448000	1.30220400	-1.16497100
C	-1.34822900	-0.61563500	-1.62460200
O	-0.83005800	-1.70409100	-1.56494500
C	-2.60949100	-0.23670700	-0.91581900
H	-2.43816500	0.73780700	-0.43094600
H	-3.36285600	-0.02057100	-1.69330200
C	-3.11897300	-1.27017700	0.06754000
H	-3.35082900	-2.19989200	-0.46800600
H	-2.31444700	-1.53284400	0.76817600
C	-4.33091700	-0.77398600	0.83083300
H	-5.15237100	-0.50847200	0.15343000
H	-4.71091400	-1.52917300	1.52627600
H	-4.08981700	0.12022500	1.41869700
C	-0.35355100	0.74629100	1.42263900
O	-0.99568600	0.54024600	2.35130900
P	1.89197500	-0.74109800	0.10623200
C	3.46817500	-0.38238600	0.95888800
C	2.43617900	-1.47478500	-1.47014100
C	1.25762700	-2.19784900	1.00949100
H	4.10667700	-1.27337400	0.99191100
H	3.99502400	0.41777000	0.43075400
H	3.27432300	-0.04539200	1.98156700
H	2.99809600	-0.73179800	-2.04317100
H	3.06719000	-2.35406000	-1.29372300
H	1.55407400	-1.77271200	-2.04467700
H	2.00283600	-3.00136800	1.04121800
H	0.99165900	-1.91749200	2.03387800
H	0.35859700	-2.56557300	0.50311900

L = PBu₃

Co	-0.47826900	-1.35952100	0.45168800
C	-1.50991500	-2.45746200	1.34464700
O	-2.15930700	-3.15054900	1.98358600
C	-0.03232600	-2.34241600	-0.93920000
O	0.28953800	-2.96490700	-1.84721000
H	-2.31472400	-0.37329600	-0.41668100
H	-0.77295500	-0.44972300	1.64862200
C	-3.22368100	0.28486200	-0.30011100
O	-3.34869600	1.27271900	-0.97373600
C	-4.18350500	-0.18211600	0.74450300
H	-4.42897300	-1.23354100	0.51735200
H	-3.61480600	-0.24651700	1.68780100
C	-5.42919300	0.66481200	0.89729000

H	-5.95415900	0.71551300	-0.06574400
H	-5.13816400	1.69906300	1.12269000
C	-6.34963100	0.12587400	1.97495900
H	-6.67478100	-0.89732200	1.74946400
H	-7.24996500	0.73883800	2.08540400
H	-5.84980400	0.09719100	2.95110600
P	0.95091400	0.27668600	0.07882000
C	1.73363400	0.92174400	1.61529500
C	0.22438600	1.77269400	-0.70344300
C	2.37554700	-0.12901600	-1.01518000
C	2.85221600	1.93775600	1.46284500
H	2.07584200	0.04522200	2.18396400
H	0.90347900	1.33804800	2.20412200
C	-0.35574800	1.52303300	-2.08651700
H	0.99307400	2.55821700	-0.74906400
H	-0.56198900	2.13342000	-0.02417700
C	3.26987000	-1.21848500	-0.44327800
H	2.95152600	0.78156400	-1.23736900
H	1.94702000	-0.46542900	-1.96981700
C	3.37804700	2.41588200	2.80733000
H	3.68622500	1.50997900	0.88597200
H	2.50593700	2.80840900	0.88519100
C	-0.98840000	2.77109800	-2.67735200
H	0.42810300	1.15613200	-2.76750800
H	-1.11497400	0.72936100	-2.03591800
C	4.24520000	-1.77145000	-1.46854300
H	3.82925600	-0.83338300	0.42354000
H	2.65284900	-2.04256500	-0.05009500
C	4.49659500	3.42910600	2.66477900
H	2.54941000	2.84826400	3.38750800
H	3.72605100	1.54892800	3.38858600
C	-1.64473200	2.49860500	-4.01556100
H	-1.73728600	3.15600400	-1.97192000
H	-0.22284800	3.55611700	-2.77902800
C	5.16428300	-2.82530600	-0.88356100
H	3.67497400	-2.19372800	-2.30950900
H	4.83719000	-0.94587000	-1.89228700
H	4.86955600	3.76846400	3.63655400
H	5.34759300	3.00798900	2.11526600
H	4.16183900	4.31644900	2.11342100
H	-2.07877500	3.40452500	-4.45147400
H	-0.92709800	2.09483300	-4.74135700
H	-2.45257800	1.76565800	-3.90525400
H	5.85604600	-3.22736900	-1.63082900

H	5.76740500	-2.41755700	-0.06278400
H	4.59191400	-3.66851200	-0.47814600

L= a₅-PhobPC₅

Co	-0.65357900	-1.51866200	0.43957800
C	-0.19945000	-3.21007200	0.43640000
O	0.09592400	-4.31343800	0.37141700
C	-0.89797100	-1.21557800	2.16132200
O	-1.03422000	-1.00194600	3.27880100
H	1.76166400	-1.24017800	0.93264000
H	-0.41768500	-1.68053900	-1.06658500
C	2.81083800	-0.99989100	0.60821000
O	3.55140900	-0.38561500	1.32869600
C	3.15246500	-1.49130300	-0.76251200
H	3.00323300	-2.58488300	-0.76200000
H	2.36088900	-1.12765600	-1.44130800
C	4.53532700	-1.11632700	-1.25144700
H	5.28442500	-1.49335700	-0.54330800
H	4.64379300	-0.02261500	-1.22936300
C	4.80722300	-1.64614900	-2.64564400
H	4.73554300	-2.74033000	-2.67875400
H	5.80717800	-1.37286600	-2.99754800
H	4.08476000	-1.25356500	-3.37212500
P	-1.21875200	0.44977100	-0.34716800
C	-2.24514000	0.54812200	-1.88293100
C	-2.33336700	1.63548100	0.54627200
C	0.25676200	1.46112300	-0.79080500
C	-3.31992400	-0.54261200	-1.91826900
C	-2.79285200	1.99257600	-1.90869800
H	-1.56629200	0.38648700	-2.73146700
C	-3.56126800	0.95958100	1.15754700
C	-2.68663100	2.67120000	-0.52294700
H	-1.76007000	2.09177700	1.36534400
C	1.05435400	1.94784800	0.40956200
H	0.87438000	0.80069500	-1.41745100
H	-0.03787600	2.30300900	-1.43168900
C	-4.01804500	-0.87333900	-0.60111000
H	-2.86617900	-1.46755000	-2.29705700
H	-4.07282300	-0.24784800	-2.66548300
H	-2.24434200	2.58311300	-2.65155200
H	-3.83265100	1.97968400	-2.25630100
C	-4.55950300	0.30748800	0.20353900
H	-4.09309800	1.72567600	1.74162400
H	-3.23441700	0.20741400	1.88946500

H	-1.91407900	3.44947700	-0.54557500
H	-3.62029100	3.18662300	-0.26078100
C	2.44302600	2.42529900	0.02431400
H	0.51140400	2.76110400	0.91558600
H	1.14699700	1.14472400	1.15775700
H	-3.32830900	-1.45598500	0.03431800
H	-4.84113100	-1.56260500	-0.83096700
H	-5.39946000	-0.04287800	0.81756900
H	-4.99685000	1.05959700	-0.47080500
C	3.26283800	2.90731600	1.20648300
H	2.98162500	1.59958900	-0.46950300
H	2.36755000	3.22292000	-0.73322400
C	4.69563200	3.21509300	0.81948600
H	2.78484900	3.79614500	1.64624900
H	3.25229000	2.13367500	1.98673000
H	5.19672800	2.31149600	0.45006100
H	5.27984200	3.58978800	1.66639000
H	4.74551800	3.97001300	0.02407100

L = PBu₃ (*i*-C₃H₇ instead of *n*-C₃H₇)

Co	0.41623500	-1.32268700	-0.91952000
C	1.27839000	-2.23739300	-2.13846900
O	1.82265600	-2.79228100	-2.97825700
C	0.16592200	-2.53583000	0.33385700
O	-0.03645800	-3.31108400	1.15397000
H	2.33753400	-0.46774000	-0.14322800
H	0.53452400	-0.24035000	-1.99276900
C	3.37178600	-0.04864400	0.03368900
O	3.85369100	-0.05883000	1.13345100
C	4.00668200	0.53430200	-1.19730600
H	3.91345300	-0.23453200	-1.98363500
C	3.15980200	1.73446800	-1.62078200
H	3.19650700	2.52071800	-0.85456400
H	2.11190800	1.45551800	-1.78543500
P	-0.83452100	0.24697700	-0.00418300
C	-1.70871100	1.31410200	-1.22374200
C	0.10086400	1.44970900	1.02745600
C	-2.16432000	-0.33718800	1.12626700
C	-2.73126300	2.30544400	-0.69725800
H	-2.16396300	0.63624100	-1.95971300
H	-0.90716300	1.83138300	-1.77245000
C	0.78391500	0.82793900	2.23673700
H	-0.57696100	2.25537900	1.34546900
H	0.84567300	1.91319400	0.36298500

C	-3.17837000	-1.23151200	0.43042800
H	-2.65492900	0.52336500	1.60500100
H	-1.66549900	-0.89724600	1.92983200
C	-3.32493600	3.15864700	-1.80735800
H	-3.54614600	1.77761100	-0.17879900
H	-2.27737300	2.96654200	0.05688900
C	1.71611300	1.80302400	2.93584500
H	0.02651500	0.47368000	2.95271800
H	1.35829500	-0.06273900	1.94153000
C	-4.11989100	-1.91599800	1.40675800
H	-3.76571400	-0.64666400	-0.29485700
H	-2.65375500	-1.99563400	-0.16540800
C	-4.35238500	4.14732000	-1.29268500
H	-2.51500400	3.69253200	-2.32627600
H	-3.77920800	2.50195400	-2.56423200
C	2.39722500	1.18275900	4.13895900
H	2.47687800	2.14659600	2.21847300
H	1.15156400	2.70047500	3.23342600
C	-5.15245000	-2.77776000	0.70758800
H	-3.52755600	-2.52818100	2.10326700
H	-4.61912800	-1.15583300	2.02684300
H	-4.77381100	4.75789900	-2.09776900
H	-5.18667600	3.63389000	-0.79894100
H	-3.91230700	4.83209500	-0.55721600
H	3.06098700	1.89239800	4.64372300
H	1.66370600	0.83554900	4.87773600
H	3.00156700	0.31982400	3.83769500
H	-5.82112500	-3.27485700	1.41776400
H	-5.77648800	-2.18160800	0.03021400
H	-4.67364300	-3.55887500	0.10471900
H	3.54205600	2.16321300	-2.55303100
C	5.45745300	0.90786200	-0.98033000
H	6.05680700	0.04933700	-0.66213900
H	5.89588400	1.31096900	-1.89958100
H	5.54799900	1.67183300	-0.19970500

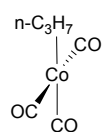
6 Structures in Figure 6

TS_{alkyl-rotate-alkane}

C	3.22368800	0.50520400	1.01313400
C	1.70784700	0.61240600	0.91760000
C	1.21582700	0.70520000	-0.51912100
H	1.35736200	1.48107400	1.49083000
H	1.85403000	0.13216900	-1.20117500
H	1.20310000	1.73487500	-0.88998000

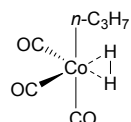
O	-2.91583000	-1.47352300	0.97871200
O	0.37735400	-2.26989600	-1.89622600
C	0.02311000	-1.47690900	-1.15977700
C	-2.00384700	-0.95447500	0.53565900
Co	-0.55838700	-0.14115100	-0.13325800
C	-1.14222600	1.53837700	-0.02267700
O	-1.49467900	2.62086300	-0.04970200
H	3.70320500	1.36565600	0.53192600
H	3.56636600	0.46588100	2.05307300
H	3.58710600	-0.39663600	0.50696100
H	1.26897900	-0.26769000	1.43222900

o



Co	0.56981600	0.00000300	-0.13257000
C	0.36549000	-1.76747800	-0.28516400
O	0.17724000	-2.88151300	-0.40954100
C	0.36532900	1.76746500	-0.28519300
O	0.17697100	2.88148000	-0.40958600
C	2.26917000	0.00008700	0.40490600
O	3.35300400	0.00013300	0.75695100
C	-1.41153100	-0.00008500	-0.60619600
H	-1.69665900	0.87181900	-1.20989600
H	-1.69663000	-0.87208700	-1.20976600
C	-2.17646700	-0.00000600	0.70962900
C	-3.68242000	-0.00006100	0.49160400
H	-1.89850200	0.87452500	1.31684900
H	-1.89845600	-0.87443300	1.31697700
H	-4.23361900	-0.00001100	1.43897600
H	-3.99817400	0.88300000	-0.07698100
H	-3.99812800	-0.88321500	-0.07686200

[Co]-H2-alkane



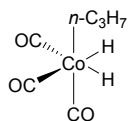
Co	0.63741500	0.00001300	0.36903900
C	0.29349000	1.63448700	-0.26100200
O	0.00697400	2.65061500	-0.69107300
C	0.29363900	-1.63448200	-0.26098400

O	0.00723000	-2.65063100	-0.69107700
C	2.40353400	0.00004900	-0.01566100
O	3.50577300	0.00008300	-0.29534800
C	-1.38671900	-0.00006700	0.72927100
H	-1.56695800	-0.87994200	1.36239400
H	-1.56702500	0.87973000	1.36248300
C	-2.33351100	-0.00004100	-0.45229100
C	-3.78650400	-0.00005500	-0.00255500
H	-2.15179500	-0.87412100	-1.09321900
H	-2.15179800	0.87406500	-1.09318300
H	-4.47687700	-0.00005500	-0.85358200
H	-4.01360300	-0.88327700	0.60704800
H	-4.01361700	0.88315600	0.60705900
H	0.83395000	0.40310200	2.06807800
H	0.83414600	-0.40288900	2.06819600

TS_{splitting}-alkane

Co	0.62516800	-0.00002700	0.35643800
C	0.27126500	1.51182200	-0.58875800
O	0.02245400	2.49762500	-1.09578600
C	0.27112000	-1.51179800	-0.58882400
O	0.02208500	-2.49752300	-1.09589200
C	2.43623200	-0.00006900	0.24039700
O	3.57099600	-0.00011400	0.23644500
C	-1.36000800	-0.00006000	0.88362600
H	-1.50099200	-0.87991900	1.52128900
H	-1.50096600	0.87956700	1.52161300
C	-2.37646500	0.00018200	-0.24040700
C	-3.79609600	0.00003300	0.30677500
H	-2.24277000	-0.87457700	-0.89247600
H	-2.24278300	0.87526500	-0.89204600
H	-4.54153000	0.00022900	-0.49651500
H	-3.98115500	-0.88322500	0.92998600
H	-3.98117000	0.88297500	0.93043000
H	0.75563200	0.70414000	1.65948100
H	0.75562600	-0.70428800	1.65942900

[Co]-2H-alkane



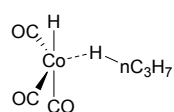
Co	-0.62179100	0.00085100	-0.33501700
C	-0.27137000	1.47967200	0.66583300

O	-0.03972900	2.45122600	1.20529600
C	-0.26787700	-1.47000000	0.67533800
O	-0.01529200	-2.43491300	1.21730100
C	-2.43477000	0.00601500	-0.31919400
O	-3.56566900	0.00690800	-0.40953200
C	1.34391800	-0.02847300	-0.92938200
H	1.47727700	-0.94630500	-1.51208800
H	1.47147300	0.80633000	-1.62596200
C	2.38406200	0.04482400	0.17140100
C	3.79193500	-0.02545400	-0.40086900
H	2.25049600	-0.77049800	0.89712100
H	2.27920200	0.97366100	0.75011500
H	4.55421900	0.03233200	0.38443500
H	3.95100600	-0.96199300	-0.94883400
H	3.97606800	0.79717400	-1.10241400
H	-0.73156700	0.86257500	-1.52806200
H	-0.74166800	-0.86080700	-1.52737900

TS_{eliminate-alkane}

Co	-0.59847400	0.03992300	-0.18255300
C	-0.29480100	1.26150600	1.12983000
O	-0.11358700	2.08257200	1.89492500
C	-0.42354400	-1.52644400	0.71153200
O	-0.25377600	-2.52259900	1.23095700
C	-2.36469800	0.04108900	-0.56517900
O	-3.45577000	0.06969100	-0.88293300
C	1.31307100	-0.24815300	-1.02071100
H	1.52798400	-1.29877500	-1.25716100
H	1.44622100	0.30927000	-1.95345600
C	2.33627800	0.23647000	0.00081100
C	3.75094300	-0.00065900	-0.50351600
H	2.19827900	-0.27615500	0.96293000
H	2.19357700	1.30646900	0.20027500
H	4.50001900	0.35710800	0.21174800
H	3.94027500	-1.06734100	-0.67460000
H	3.92676600	0.51906300	-1.45323800
H	-0.59745400	1.24693500	-1.04249500
H	-0.24138900	-0.56684400	-1.47905900

[Co]-alkane



Co	-0.87134300	0.23769200	0.13508400
----	-------------	------------	------------

C	-0.18081000	1.39886900	1.29165700
O	0.19908500	2.19553400	2.00866700
C	-0.38906900	-1.32584400	0.87354400
O	-0.07934100	-2.31588700	1.34099800
C	-2.08488600	-0.29318200	-1.04991700
O	-2.90446500	-0.55476400	-1.79355600
C	1.83140200	-0.03661200	-1.49627900
H	1.73123800	-1.11402600	-1.67934300
H	2.12755700	0.43099600	-2.44354000
C	2.83585700	0.24875300	-0.39682000
C	4.22567000	-0.24279400	-0.75411900
H	2.50693900	-0.22411100	0.54033300
H	2.86399700	1.32848600	-0.19129400
H	4.95124600	-0.04122100	0.04086500
H	4.22831800	-1.32449800	-0.93718700
H	4.59423500	0.24038100	-1.66747100
H	-1.33628800	1.55763500	-0.44289100
H	0.82585300	0.35312600	-1.25194600

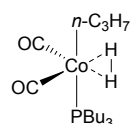
7 Structures in Figure 7

TS_{H2}-alkane

Co	-1.44794200	-0.00994300	-0.59124300
C	-1.32851500	1.16928900	-1.89238000
O	-1.29264500	2.04794800	-2.63008500
P	0.70106400	0.21916700	-0.05382600
C	-1.96839500	-0.26094700	1.06432600
O	-2.28800900	-0.26347100	2.16805300
C	1.85327100	-0.30826700	-1.39507700
C	3.34499500	-0.22798000	-1.11909500
H	1.58838200	0.31324200	-2.26434800
H	1.56867000	-1.33222500	-1.67553600
C	4.17579100	-0.64944000	-2.32098200
H	3.62653900	0.79615900	-0.83055300
H	3.60935700	-0.86538600	-0.26126100
C	5.66554300	-0.57474500	-2.05047500
H	3.89639500	-1.67281100	-2.61310800
H	3.91652900	-0.01435400	-3.18103000
H	6.25643500	-0.87961900	-2.92021100
H	5.97142400	0.44523800	-1.78692800
H	5.95150500	-1.22529600	-1.21472200
C	1.21349800	1.95829100	0.27130800
C	0.28730200	2.68494800	1.23375800
H	1.22389400	2.47257300	-0.70207100
H	2.24708800	1.97113600	0.64752500

C	0.72102700	4.11868700	1.48738600
H	-0.73829200	2.67153300	0.83519400
H	0.23698300	2.14736200	2.19420000
C	-0.20968000	4.84366000	2.43953500
H	1.74717100	4.12529800	1.88560800
H	0.77048300	4.65520900	0.52793200
H	0.10715800	5.87663200	2.61662400
H	-1.23288900	4.87543000	2.04634000
H	-0.25301100	4.34068500	3.41340500
C	1.30785700	-0.66500900	1.44307500
C	1.11426100	-2.17006000	1.36757900
H	0.74705400	-0.25943300	2.29754700
H	2.36395400	-0.41160700	1.61735400
C	1.52528100	-2.87787500	2.64766300
H	0.05919700	-2.39644100	1.14713300
H	1.68837800	-2.58503200	0.52326100
C	1.33832900	-4.37987300	2.56396400
H	2.57589900	-2.64046700	2.87425600
H	0.94008700	-2.47157700	3.48596300
H	1.63263600	-4.88261000	3.49093900
H	0.29078700	-4.63857000	2.36771800
H	1.93674900	-4.81104600	1.75177300
C	-3.32446600	-0.35887300	-1.22498600
C	-4.03263400	-1.54960000	-0.59984600
H	-3.23480700	-0.52643700	-2.31092100
H	-3.93825400	0.54646300	-1.10968700
C	-5.32297000	-1.89424400	-1.32782300
H	-3.37442600	-2.43245600	-0.59645400
H	-4.25873100	-1.34847600	0.45735000
H	-5.84375500	-2.74370800	-0.86901500
H	-6.01370600	-1.04165400	-1.32751500
H	-5.12925000	-2.15142700	-2.37684100
H	-1.07657900	-1.97091900	-1.31333500
H	-0.79832200	-2.37801800	-1.88695000

[Co]-H₂-alkane



Co	-1.43552500	-0.15790600	-0.63299000
C	-1.49210000	1.24475400	-1.69738900
O	-1.57383000	2.20440400	-2.32314900
P	0.70073900	0.20526300	-0.09233600

C	-1.97159000	-0.26746100	1.04018400
O	-2.33374100	-0.25095900	2.13057400
C	1.87701600	-0.27360600	-1.43008100
C	3.36335700	-0.10174800	-1.16795600
H	1.56799400	0.31356100	-2.30860600
H	1.65104500	-1.31829700	-1.68887300
C	4.20991900	-0.51763100	-2.36075600
H	3.58904100	0.94568900	-0.91676100
H	3.66713100	-0.69356600	-0.29048900
C	5.69438000	-0.34572700	-2.10602500
H	3.98957700	-1.56570000	-2.61324000
H	3.90811500	0.06913200	-3.24104500
H	6.29669200	-0.64844700	-2.96865200
H	5.94139600	0.69971200	-1.88374300
H	6.02336300	-0.94603700	-1.24876000
C	1.13950000	1.96355600	0.23197700
C	0.22368600	2.64686300	1.23493400
H	1.09472300	2.48548800	-0.73628400
H	2.18423900	2.01685300	0.57184200
C	0.60208000	4.09990100	1.46787500
H	-0.81728900	2.58773900	0.88509900
H	0.24319200	2.10981400	2.19669400
C	-0.31455300	4.78223500	2.46411700
H	1.64485100	4.15569500	1.81590200
H	0.57914900	4.63595800	0.50720700
H	-0.03821000	5.82925300	2.62602400
H	-1.35580300	4.76537200	2.12059200
H	-0.28736600	4.27968100	3.43881200
C	1.35120600	-0.64138300	1.40880400
C	1.25981300	-2.15592300	1.34011800
H	0.76215300	-0.27118300	2.26015900
H	2.38787200	-0.31819300	1.58583000
C	1.75552900	-2.82951400	2.60888100
H	0.21694700	-2.45302300	1.15044100
H	1.83887000	-2.53379600	0.48181700
C	1.66324800	-4.34084700	2.53528100
H	2.79541600	-2.52428900	2.80106400
H	1.17279400	-2.45779400	3.46465900
H	2.02056100	-4.81934200	3.45288000
H	0.62860300	-4.66759400	2.37534700
H	2.26058300	-4.73627700	1.70426700
C	-3.38532000	-0.45061700	-1.14690000
C	-3.96499500	-1.78286900	-0.71090200
H	-3.43821700	-0.37327000	-2.24262300

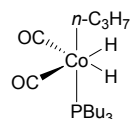
H	-3.99304500	0.37339200	-0.74889000
C	-5.38989500	-1.97199500	-1.21039500
H	-3.34057300	-2.61066800	-1.07952500
H	-3.95114000	-1.87199800	0.38505600
H	-5.81239300	-2.93439500	-0.89697600
H	-6.04913000	-1.18158500	-0.83083800
H	-5.43453600	-1.93161600	-2.30595000
H	-1.05404200	-1.39997600	-1.76346800
H	-1.11159200	-1.80127700	-1.05320500

TS_{splitting}-alkane

Co	-1.48615800	-0.05855300	-0.61646500
C	-1.75479700	1.52786300	-1.39136100
O	-1.93241400	2.51616700	-1.93893800
P	0.65149500	0.28025800	-0.10052500
C	-2.07458700	-0.14597400	1.06890000
O	-2.45796400	-0.26952100	2.13976600
C	1.80036500	-0.25400300	-1.43578300
C	3.29307900	-0.13233000	-1.18421300
H	1.50544900	0.32887900	-2.32145900
H	1.52864300	-1.29184000	-1.67495700
C	4.11557700	-0.62060600	-2.36646800
H	3.56275400	0.91273600	-0.96947700
H	3.57943100	-0.70638500	-0.28919200
C	5.60712700	-0.49847700	-2.12488000
H	3.85280400	-1.66695400	-2.58237900
H	3.83121800	-0.05238200	-3.26457100
H	6.19196500	-0.85308500	-2.97975800
H	5.89619500	0.54327600	-1.93880600
H	5.91771600	-1.08243200	-1.24962100
C	1.16140600	2.02193300	0.21736700
C	0.32998200	2.72116600	1.28073400
H	1.07559700	2.55565100	-0.74194900
H	2.22537300	2.04300100	0.49543100
C	0.73786700	4.17194700	1.47627700
H	-0.73599500	2.67464300	1.01340500
H	0.41815900	2.18923200	2.24139600
C	-0.08982500	4.86595700	2.53995700
H	1.80561900	4.21964100	1.73881700
H	0.64203900	4.70429600	0.51806100
H	0.20699300	5.91124700	2.67395700
H	-1.15560700	4.85685200	2.28169800
H	0.01225300	4.36759000	3.51186900
C	1.27032000	-0.57918900	1.40722400

C	1.16869800	-2.09353500	1.34867300
H	0.67828900	-0.20028200	2.25270700
H	2.30844900	-0.26440400	1.59333300
C	1.66137600	-2.75753800	2.62378300
H	0.12561400	-2.38654900	1.15861200
H	1.74553000	-2.48163200	0.49386800
C	1.56015500	-4.26895600	2.56410900
H	2.70321000	-2.45698500	2.81345900
H	1.08109400	-2.37508100	3.47672300
H	1.91437400	-4.74114400	3.48622700
H	0.52375000	-4.59086000	2.40621000
H	2.15523900	-4.67528800	1.73681900
C	-3.36058000	-0.59437700	-1.21989500
C	-3.76321200	-2.01811700	-0.89720300
H	-3.39855000	-0.43336700	-2.30474200
H	-4.07506600	0.11043900	-0.77116900
C	-5.18245100	-2.32098400	-1.35420200
H	-3.06478500	-2.72055700	-1.37383800
H	-3.67984200	-2.20921100	0.18294000
H	-5.47493700	-3.35428500	-1.13153400
H	-5.90725100	-1.65941800	-0.86343100
H	-5.29030900	-2.17266000	-2.43606300
H	-1.05903000	-0.75626500	-1.87159200
H	-1.14195100	-1.51174000	-0.75822000

[Co]-2H-alkane



Co	-1.50328200	-0.00619900	-0.51252500
C	-1.87533300	1.66347200	-1.03037900
O	-2.10856500	2.70428400	-1.43879400
P	0.68100700	0.23376700	-0.20207700
C	-1.98914000	-0.20748900	1.19862000
O	-2.30391300	-0.43788900	2.27234400
C	1.68639500	-0.59829000	-1.49803400
C	3.19647600	-0.59932000	-1.33670400
H	1.39482300	-0.11914900	-2.44454900
H	1.29841200	-1.62407400	-1.56808500
C	3.89267100	-1.33564300	-2.47070900
H	3.58149900	0.43061800	-1.29231300
H	3.48104000	-1.06602300	-0.38094300
C	5.40096200	-1.34052000	-2.31890800

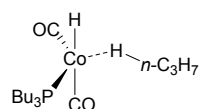
H	3.51481400	-2.36785700	-2.51724100
H	3.61140600	-0.87386100	-3.42879700
H	5.89450900	-1.87286000	-3.13843300
H	5.80265600	-0.31979200	-2.30153100
H	5.70519500	-1.82462400	-1.38260400
C	1.31605200	1.96231400	-0.21247500
C	0.76365100	2.81949100	0.91657000
H	1.03135600	2.38641100	-1.18769600
H	2.41484400	1.95792400	-0.17981100
C	1.01445700	4.30214000	0.69828000
H	-0.31863000	2.65021900	1.03103900
H	1.21412700	2.51053200	1.87223700
C	0.51233500	5.14943500	1.85042500
H	2.09102800	4.47211400	0.54464000
H	0.52586200	4.61200700	-0.23780300
H	0.68689900	6.21693800	1.68148400
H	-0.56524300	5.01259700	2.00230700
H	1.00975500	4.87943300	2.79023600
C	1.34332100	-0.41950400	1.38751700
C	1.19477500	-1.92297900	1.55166900
H	0.79414400	0.09854500	2.18730600
H	2.39642200	-0.11564400	1.49169600
C	1.56921700	-2.39322000	2.94733900
H	0.15988500	-2.22370300	1.33032500
H	1.81820100	-2.44773200	0.81066100
C	1.45311100	-3.89684900	3.10069800
H	2.59437200	-2.06777800	3.18159200
H	0.92090200	-1.88938300	3.68007900
H	1.71613600	-4.22832600	4.11047200
H	0.43061400	-4.23768700	2.89805600
H	2.11459800	-4.42082400	2.39963400
C	-3.38256600	-0.57235300	-1.07927700
C	-3.71192400	-2.03943500	-0.89832600
H	-3.49681000	-0.29165200	-2.13327900
H	-4.09570500	0.04407200	-0.51220000
C	-5.14298700	-2.35113600	-1.30966200
H	-3.01463500	-2.65146600	-1.48700100
H	-3.55860100	-2.34279200	0.14815800
H	-5.38460000	-3.41405800	-1.18806700
H	-5.86236200	-1.77839200	-0.71079100
H	-5.31828500	-2.09067100	-2.36114800
H	-1.17961200	-0.33754200	-1.92317600
H	-1.18452400	-1.45650800	-0.56336900

TS_{eliminate}-alkane

Co	-1.49654900	-0.29155500	-0.27948900
C	-2.45432300	1.21807600	-0.31683500
O	-2.99543300	2.22255400	-0.41213100
P	0.60986400	0.33483700	-0.06834400
C	-1.72059900	-0.88372100	1.38569700
O	-1.81723900	-1.28799700	2.45219900
C	1.68097500	-0.11247600	-1.50011500
C	3.16625800	0.19035600	-1.40828000
H	1.23238400	0.39748900	-2.36568400
H	1.51392300	-1.18383400	-1.68245200
C	3.91575600	-0.22839900	-2.66359000
H	3.33241100	1.26466300	-1.23661400
H	3.61047300	-0.32176100	-0.54081300
C	5.39965000	0.07042500	-2.58071600
H	3.75671200	-1.30309800	-2.83797200
H	3.47673500	0.28090700	-3.53437300
H	5.93179600	-0.23517100	-3.48747200
H	5.58226100	1.14279600	-2.43858000
H	5.86435300	-0.45214100	-1.73539500
C	0.83778700	2.15819100	0.06581100
C	0.25944100	2.74828200	1.34305000
H	0.33312600	2.58690000	-0.81370400
H	1.90285000	2.41657300	-0.02146200
C	0.12194900	4.26001300	1.27783200
H	-0.72701100	2.30599500	1.55374100
H	0.89559200	2.47688900	2.19949900
C	-0.41532600	4.84784500	2.56753800
H	1.09878100	4.70617000	1.03607900
H	-0.54229400	4.52148300	0.44054400
H	-0.52065700	5.93615900	2.51054500
H	-1.40205300	4.43419600	2.80902000
H	0.24660700	4.62513500	3.41370600
C	1.53898000	-0.29592000	1.39340000
C	1.72202600	-1.80499100	1.38645600
H	0.96000600	0.00354700	2.27910000
H	2.50886300	0.21881300	1.47055000
C	2.20436400	-2.34050500	2.72401800
H	0.77290400	-2.29634200	1.12074400
H	2.43342100	-2.09593400	0.59758800
C	2.42979100	-3.83927100	2.70093000
H	3.13198500	-1.82304000	3.01278900
H	1.46438600	-2.08290400	3.49668300
H	2.76608000	-4.21942900	3.67106500

H	1.50849100	-4.37408400	2.43962400
H	3.18803000	-4.11688900	1.95811800
C	-2.66320000	-1.82419300	-1.13157500
C	-4.07578500	-1.25623100	-1.24385200
H	-2.69543400	-2.72612100	-0.50555100
H	-2.35101100	-2.15990000	-2.12845100
C	-5.03689200	-2.29668800	-1.79879800
H	-4.42870100	-0.91367600	-0.26200100
H	-4.07518700	-0.37169500	-1.89405500
H	-6.05595800	-1.90257200	-1.88973800
H	-4.72427100	-2.63588200	-2.79442200
H	-5.08186100	-3.18228500	-1.15253500
H	-1.22515200	0.10655500	-1.69666000
H	-1.10666300	-1.62213000	-0.81493100

[Co]-alkane

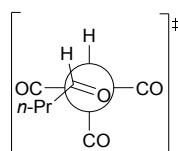


Co	-1.55713200	0.97748600	-0.36796600
C	-3.13182600	1.45502800	-0.96864000
O	-4.13504600	1.79526800	-1.39958100
P	0.62604900	0.82069900	-0.19797200
C	-1.97115200	0.21630400	1.16295200
O	-2.20209600	-0.25734000	2.18293400
C	1.49078100	0.32171400	-1.74381500
C	2.99881600	0.15638000	-1.67266600
H	1.21477300	1.08713500	-2.48301900
H	1.01247600	-0.60379100	-2.09517300
C	3.60127500	-0.20210300	-3.02202800
H	3.46788400	1.08244500	-1.30547600
H	3.26659800	-0.62409500	-0.94409700
C	5.10645100	-0.37075100	-2.95830900
H	3.13339900	-1.12640000	-3.39256800
H	3.33955400	0.57629200	-3.75398600
H	5.53240400	-0.62909600	-3.93320100
H	5.59620900	0.55071800	-2.61986700
H	5.38871700	-1.16471600	-2.25582900
C	1.37826700	2.44167700	0.23091700
C	0.64842700	3.14035800	1.36751200
H	1.33785400	3.05708000	-0.67979900
H	2.44019600	2.29927300	0.47945200
C	1.27609700	4.47421500	1.73343600
H	-0.40489800	3.28771100	1.08281100

H	0.62535100	2.49332700	2.25935800
C	0.53660800	5.17176400	2.85816500
H	2.32865700	4.31768100	2.01488200
H	1.29923500	5.11840400	0.84156500
H	0.99241400	6.13346500	3.11535300
H	-0.50818200	5.36427300	2.58617200
H	0.52642800	4.55850300	3.76764000
C	1.29289600	-0.32526300	1.08247800
C	0.88742600	-1.76375800	0.80317800
H	0.87027300	0.00416900	2.04302500
H	2.38419900	-0.22219800	1.16690800
C	1.08058500	-2.70057700	1.98128500
H	-0.17103100	-1.79325500	0.50351100
H	1.44450200	-2.14977800	-0.06557200
C	0.62916000	-4.11051000	1.65205800
H	2.13656000	-2.69828800	2.29124000
H	0.51239700	-2.31598800	2.84162000
H	0.76238200	-4.79623300	2.49504400
H	-0.43369600	-4.12826400	1.37763000
H	1.18995100	-4.52010000	0.80208200
C	-1.69800800	-2.24589100	-1.75477800
C	-2.62370000	-2.83180100	-0.70648400
H	-0.71698800	-2.74223400	-1.73824200
H	-2.10912200	-2.37299600	-2.76410800
C	-2.85493200	-4.31640500	-0.91338000
H	-2.20796800	-2.66166500	0.29844800
H	-3.58218400	-2.29363800	-0.71823200
H	-3.51525500	-4.74333700	-0.15075800
H	-3.30899500	-4.51545500	-1.89223000
H	-1.90825800	-4.87199400	-0.87974100
H	-1.09165300	1.71199700	-1.62869200
H	-1.53482000	-1.16676200	-1.59920400

7 Structures in Figure S5

TS_{rotate}

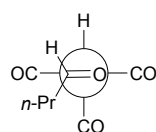


O	-3.40111000	-1.69463400	-0.79241200
O	-0.10981000	2.61425100	-1.25717400
C	-0.49548600	1.63831300	-0.80702300
C	-2.52631200	-1.02009500	-0.51995900
H	-1.02996500	-0.15419000	-1.70817400

Co	-1.18822300	0.12414100	-0.22965900
C	-1.52937900	0.58000000	1.48174700
O	-1.75591600	0.88194700	2.55361300
H	1.14634900	-1.51019200	-1.32951700
C	1.18020000	-1.05542700	-0.31185400
C	2.28426800	-0.07767200	-0.07694500
H	2.07818200	0.49089200	0.83947300
H	2.33851800	0.62800200	-0.91898600
O	0.40926600	-1.44013400	0.54406600
C	3.61243200	-0.82833100	0.03734200
H	3.76384200	-1.44611200	-0.85999200
H	3.55634700	-1.52800200	0.88227900
C	4.77987200	0.12187200	0.21651700
H	5.72832400	-0.41678300	0.30718000
H	4.86842600	0.80833000	-0.63379700
H	4.65900400	0.73284200	1.11862600

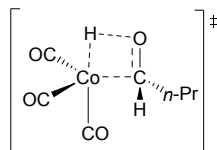
pathway B to alcohol

p



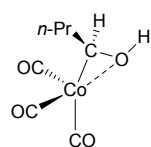
O	-3.58347500	-1.48091400	-0.55411700
O	-0.46182100	2.88539100	-0.76746500
C	-0.69778600	1.79920000	-0.50467500
C	-2.62807300	-0.89331900	-0.36715200
H	-1.44613400	0.25474200	-1.65018400
Co	-1.18087000	0.13961200	-0.17134600
C	-1.02336100	0.12895100	1.62797300
O	-0.93904200	0.14167000	2.76160100
H	1.06629200	-0.37520500	-1.91494000
C	1.10061200	-0.65776500	-0.83742500
C	2.19268900	-0.03040300	-0.03262900
H	1.97418500	-0.14941400	1.03679200
H	2.25480200	1.04420500	-0.25712600
O	0.36325400	-1.53667400	-0.42327000
C	3.52373100	-0.69890000	-0.38267700
H	3.69406400	-0.63303500	-1.46729000
H	3.45649500	-1.77030600	-0.14980300
C	4.68181900	-0.06752000	0.36429400
H	5.63215200	-0.55241200	0.12001800
H	4.78059600	0.99671900	0.11958100
H	4.54191800	-0.14205600	1.44905000

TS_{add-alcohol-a}



Co	-0.94880400	0.02542700	-0.10393100
H	-0.86189800	0.82509000	-1.44504800
C	-1.61716500	1.53086300	0.61010500
O	-2.10353800	2.44050000	1.09738600
C	-2.24540900	-0.94887800	-0.88103500
O	-3.07601600	-1.54630200	-1.38017200
C	-0.52894900	-1.08759300	1.25323100
O	-0.27951500	-1.75480300	2.14277000
C	0.95264100	0.77134100	-0.36249800
O	0.47355400	0.46314400	-1.53692800
H	0.95753200	1.83885000	-0.09421100
C	2.08836500	-0.05565200	0.15224800
H	2.15839100	0.03683900	1.24498500
H	1.90171100	-1.11430700	-0.07771800
C	3.40457800	0.38566900	-0.48577800
H	3.56415800	1.45668500	-0.29247500
H	3.32252700	0.28210900	-1.57635700
C	4.57901700	-0.41803500	0.03607700
H	5.52191700	-0.10416400	-0.42289700
H	4.68755700	-0.30685800	1.12179800
H	4.45146500	-1.48737300	-0.17048800

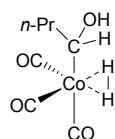
r



Co	-0.94061500	-0.00460900	0.07037200
H	0.20921100	-1.46162700	1.84770400
C	-1.51533100	-1.44350300	-0.80430500
O	-1.87344200	-2.30116200	-1.47098900
C	-2.51430400	0.55813400	0.74787200
O	-3.49915200	0.90865400	1.19987600
C	-0.45420600	1.52002600	-0.72442500
O	-0.19155000	2.44220200	-1.34532100
C	0.87369500	-0.70924900	0.14298400
O	0.54566700	-0.61934500	1.52069300
H	0.99159100	-1.75537800	-0.16724600

C	2.08623700	0.11655500	-0.16184000
H	2.13071000	0.29322400	-1.24635200
H	1.97347500	1.10581400	0.30641800
C	3.38162700	-0.52982100	0.31304700
H	3.49185100	-1.51653300	-0.16174300
H	3.31451100	-0.71707800	1.39388400
C	4.59272100	0.32952900	0.00696200
H	5.52333200	-0.13811600	0.34454400
H	4.68810800	0.51349100	-1.07022400
H	4.51898300	1.30781000	0.49712400

[Co]-H₂-alcohol-B



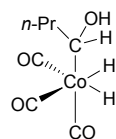
Co	1.10491500	0.00716400	0.29591100
H	-0.69511600	-1.43952600	2.25382500
C	0.74431600	1.71859700	-0.04961300
O	0.46879400	2.79528900	-0.30828600
C	2.86380500	0.09260700	-0.18196100
O	3.94688300	0.14465200	-0.52407800
C	0.72280400	-1.46131300	-0.66256600
O	0.45076300	-2.35586900	-1.31212500
C	-0.88805400	-0.11578500	0.82450400
O	-1.15597400	-1.36287900	1.41304300
H	-0.99335400	0.68240100	1.57973300
C	-1.89411500	0.08760500	-0.28107000
H	-1.64810300	0.99685500	-0.84617300
H	-1.82149500	-0.74288500	-0.99902600
C	-3.32658800	0.18270100	0.22906500
H	-3.39829900	1.00484500	0.95775500
H	-3.57478400	-0.73338500	0.77898900
C	-4.31440200	0.40446600	-0.89987400
H	-5.34489600	0.47386800	-0.53574900
H	-4.09606800	1.32986600	-1.44768300
H	-4.27770800	-0.41746900	-1.62550000
H	1.47849000	-0.68194300	1.86202900
H	1.40832100	0.11115800	2.01283800

TS_{splitting}-alcohol-B

Co	1.09610100	-0.00786700	0.28690800
H	-0.55313600	-1.92663900	1.84719300
C	0.70655800	1.68244500	-0.22822500

O	0.48614400	2.77093700	-0.47169200
C	2.91504900	0.08042300	0.08063200
O	4.04845500	0.09622000	0.03550200
C	0.71115200	-1.21552300	-1.02100900
O	0.45117400	-2.01118500	-1.78688400
C	-0.88191200	-0.27739200	0.87193800
O	-1.14142400	-1.62284400	1.14908200
H	-0.95738900	0.33127300	1.78447400
C	-1.91864400	0.17126600	-0.13111600
H	-1.74684700	1.22064300	-0.40499400
H	-1.82136800	-0.40960500	-1.06104100
C	-3.34237300	0.03140100	0.39622900
H	-3.43102100	0.57887600	1.34706100
H	-3.53774700	-1.02069900	0.63373000
C	-4.36294600	0.54922400	-0.59873600
H	-5.38717600	0.44669200	-0.22497400
H	-4.20086200	1.61047300	-0.82618100
H	-4.30465100	0.00208200	-1.54789100
H	1.35549900	-1.00645500	1.36831900
H	1.27388900	0.38968100	1.71145000

[Co]-2H-alcohol-B



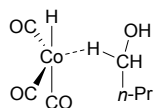
Co	-1.08210600	-0.00280000	-0.28438400
H	0.53218500	-2.21766100	-1.47557200
C	-0.67122000	1.65925500	0.30657500
O	-0.44973500	2.73389000	0.60075200
C	-2.90860900	0.12051500	-0.23551400
O	-4.03916900	0.14469700	-0.32320500
C	-0.77196200	-1.13232900	1.11603200
O	-0.55055200	-1.86844000	1.94868700
C	0.87497800	-0.40718400	-0.85648000
O	1.12315500	-1.78617900	-0.85059400
H	0.94625300	-0.00693500	-1.87623900
C	1.92631400	0.23143200	0.01998600
H	1.79165800	1.32155100	0.01913900
H	1.80327300	-0.09681600	1.06443000
C	3.34673900	-0.07997300	-0.43817600
H	3.45267100	0.19838000	-1.49787200
H	3.51303400	-1.16216300	-0.39281800
C	4.37873900	0.65177400	0.39804600

H	5.40085100	0.42603100	0.07615200
H	4.24816800	1.73972400	0.33790200
H	4.30062000	0.37459200	1.45678500
H	-1.32678200	-1.10755400	-1.24856300
H	-1.16453200	0.55377900	-1.65292300

TS_{eliminate}-alcohol-B

Co	1.06973400	0.04047200	-0.19232900
H	-0.50948800	2.37153200	-1.23289600
C	0.66640400	-1.53864000	0.58674300
O	0.43619600	-2.54911400	1.05400800
C	2.78492200	-0.33314900	-0.60799400
O	3.85659500	-0.50780900	-0.94761000
C	0.93808300	1.18306500	1.23171300
O	0.83756200	1.94188600	2.06947000
C	-0.90500400	0.48508200	-0.94402500
O	-1.08971900	1.84751700	-0.67143500
H	-1.11315100	0.31452200	-2.01262600
C	-1.92677600	-0.29400500	-0.15097000
H	-1.77213300	-1.36858900	-0.32052500
H	-1.77917300	-0.11782800	0.92499400
C	-3.35732300	0.06659200	-0.53109000
H	-3.49327400	-0.08049500	-1.61355900
H	-3.52152800	1.13496100	-0.34750200
C	-4.36760800	-0.76397500	0.23646400
H	-5.39729100	-0.50602000	-0.03209700
H	-4.23621800	-1.83624900	0.04403400
H	-4.26436400	-0.61423000	1.31825700
H	1.42181000	1.23853800	-1.00447400
H	0.46072200	-0.31854600	-1.49123000

[Co]-alcohol-B

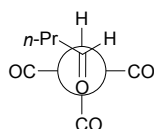


Co	-1.51544300	-0.13526200	0.14371800
H	0.91066400	-2.44564800	-1.26208800
C	-1.16471000	1.49028200	0.81522600
O	-0.94450200	2.52233700	1.24066000
C	-2.70021500	0.27004900	-1.11162200
O	-3.49915200	0.45486400	-1.90037200
C	-0.82429100	-1.18127100	1.41900400
O	-0.45435800	-1.89804900	2.21771100
C	1.28185400	-0.52621600	-1.18604400

O	1.48558300	-1.85421800	-0.76622600
H	1.49883900	-0.41070300	-2.26252100
C	2.17108000	0.37630700	-0.37068500
H	1.92985900	1.42236600	-0.61595000
H	1.92492900	0.24428100	0.69500300
C	3.65208300	0.12020000	-0.58921600
H	3.88508900	0.23834500	-1.65871700
H	3.87379000	-0.92649700	-0.34666200
C	4.52064400	1.04835900	0.23695900
H	5.58777700	0.86066200	0.07906700
H	4.33147200	2.10074100	-0.01002800
H	4.32204100	0.92706500	1.30905100
H	-1.87966100	-1.51243600	-0.37766600
H	0.21292400	-0.23183300	-1.04576700

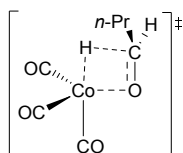
pathway to formate

q



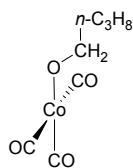
O	-2.65682300	-2.26005200	-1.14632900
O	-0.18189000	2.62249600	-1.25940600
C	-0.54649000	1.64104600	-0.80751800
C	-2.06580300	-1.37599300	-0.73830600
H	-0.44770100	-0.31367300	-1.54460100
Co	-1.15204500	0.07003100	-0.25716200
C	-2.15728200	0.60736600	1.13969200
O	-2.80309600	0.95459300	2.00732400
H	1.18070800	-1.91752900	-0.18270700
C	1.23376000	-0.95651500	0.38263400
C	2.35309800	-0.04838600	-0.00739500
H	2.23042100	0.91786300	0.49877900
H	2.31118600	0.12447600	-1.09339600
O	0.46510900	-0.75522500	1.29939200
C	3.69504500	-0.68801800	0.34841000
C	4.86153400	0.17531000	-0.08996000
H	3.76419900	-1.68051200	-0.12044700
H	3.73710300	-0.86095900	1.43247800
H	5.82187200	-0.27963600	0.17208800
H	4.85405200	0.33231600	-1.17510600
H	4.82380800	1.16347300	0.38309300

TS_{add}-formate



O	-2.73399300	-1.80331200	-1.54603900
O	-0.68961800	2.70531300	-1.21022400
C	-0.70406500	1.67573900	-0.73144500
C	-2.04012800	-1.13330900	-0.93897900
H	0.20626600	-0.57647200	-0.94929500
Co	-0.95775400	-0.03979400	-0.03748300
C	-2.12545100	0.29721900	1.27079700
O	-2.83376500	0.50491400	2.13274500
H	1.03880200	-1.94094700	0.00874200
C	1.04965100	-0.83679100	0.12924900
C	2.29250700	-0.16910600	-0.42400700
H	2.12867700	0.91784600	-0.44313000
H	2.47658000	-0.49420700	-1.45867100
O	0.54835400	-0.37136400	1.22174700
C	3.49092000	-0.49865700	0.45423500
C	4.76478100	0.14314800	-0.05879600
H	3.61474900	-1.59069700	0.51026900
H	3.27639700	-0.16483100	1.47777700
H	5.62285900	-0.09019900	0.57955900
H	5.00549100	-0.19919900	-1.07274900
H	4.67037800	1.23505700	-0.09737400

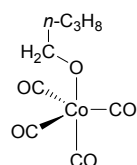
S



O	-4.04369000	0.38160600	0.39108400
O	-0.62608000	2.98937700	-0.26315900
C	-0.88549100	1.89611800	-0.16815000
C	-2.92170200	0.26423300	0.22397400
H	1.14212400	-1.73288100	-1.22975900
Co	-1.19036100	0.07192300	-0.03205800
C	-1.33402900	-1.71454100	0.05286300
O	-1.42247000	-2.84271700	0.10273300
H	1.37133000	-1.70682700	0.53054000
C	1.44078300	-1.08521900	-0.38453800
C	2.88089300	-0.65743800	-0.57097100
H	2.95433100	-0.05382900	-1.48848800

H	3.49473700	-1.55664700	-0.74217200
O	0.62188300	0.04411200	-0.29504400
C	3.43419600	0.12509000	0.60619700
C	4.88325200	0.52363600	0.40504100
H	3.33436200	-0.48057500	1.52071700
H	2.81355400	1.01563500	0.76739000
H	5.27837300	1.08964200	1.25562800
H	5.52515000	-0.35622400	0.26885600
H	5.00123500	1.14948100	-0.48854800

t



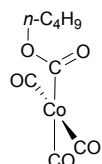
O	-4.05831100	0.87784500	0.33355500
O	-0.07356800	2.94303200	-0.01332000
C	-0.62233900	1.95226700	-0.04032900
C	-2.97213500	0.60773600	0.14421500
H	1.48309700	-1.16087100	0.96918100
Co	-1.25022100	0.20713000	-0.14365800
C	-1.16913400	-0.99417700	1.25795600
O	-1.08929500	-1.74463700	2.10399100
H	1.40253600	0.59052800	1.22400800
C	1.54085600	-0.18710000	0.44319800
C	2.92120700	-0.02403300	-0.16236500
H	3.06115400	-0.79517300	-0.93477100
H	3.67144000	-0.22818200	0.61849000
O	0.59019000	-0.08966000	-0.56840800
C	3.15655900	1.35261400	-0.75761300
C	4.54928400	1.50036400	-1.33851700
H	2.99101000	2.11578300	0.01925100
H	2.40132100	1.54206700	-1.53135900
H	4.71469500	2.49469300	-1.76727400
H	5.32075100	1.33917500	-0.57462400
H	4.72580000	0.76612800	-2.13456100
C	-1.50241200	-0.52483700	-1.85817800
O	-1.52229200	-0.99113300	-2.88772200

TS_{inesrt}-formate

O	-3.18921900	-0.22717500	-2.17016400
O	0.30392700	-2.32239000	-0.85724200
C	-0.25907700	-1.40141000	-0.45957200

C	-2.44162500	-0.10994100	-1.31998600
H	1.60544900	1.49789000	0.10432100
Co	-1.26137800	0.01780900	-0.00977300
C	-1.31306500	1.84144800	0.04853100
O	-1.25732600	2.97454400	0.08405000
H	1.52686000	0.30163600	-1.19404100
C	1.64825000	0.41401600	-0.10181900
C	2.97661300	-0.15903200	0.33376200
H	2.98389400	-1.23731200	0.11519000
H	3.06178500	-0.06751700	1.42640300
O	0.60519800	-0.23444700	0.59578500
C	4.15118100	0.52466300	-0.34424700
C	5.48362300	-0.05444000	0.09013800
H	4.12423700	1.60315700	-0.12637400
H	4.04587700	0.43894500	-1.43638200
H	6.32733400	0.44148000	-0.40106900
H	5.62610900	0.04728100	1.17291600
H	5.54653700	-1.12371900	-0.14549100
C	-2.10996100	-0.52733200	1.62058800
O	-2.66339400	-0.88434700	2.54057700

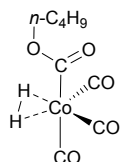
u



O	-2.30692800	-2.67386600	-0.46526100
O	0.43672300	-0.64650900	1.58415800
C	0.09134600	-0.52678800	0.44021700
C	-2.08738300	-1.59146000	-0.20019700
H	2.52136800	-1.73291600	-1.26206000
Co	-1.69886900	0.13122000	0.09934300
C	-3.38207300	0.77042700	0.06152100
O	-4.44385700	1.17570300	0.05399400
H	2.27276400	-1.80522700	0.49886400
C	2.22562100	-1.15395200	-0.38121900
C	3.08991500	0.07088200	-0.20969100
H	2.74266900	0.64160800	0.66373600
H	2.96097100	0.72699400	-1.08340100
O	0.85195600	-0.78647400	-0.62700400
C	4.55530600	-0.29146300	-0.03986100
C	5.43339400	0.93279000	0.13141700
H	4.89279300	-0.87485200	-0.90994000

H	4.66896900	-0.95699700	0.82866200
H	6.48825600	0.66686600	0.25432400
H	5.36004500	1.59879900	-0.73692000
H	5.13501500	1.51396400	1.01220400
C	-0.83629800	1.66991800	-0.21132600
O	-0.25193800	2.60573400	-0.48249700

[Co]-H₂-formate



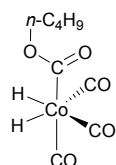
O	2.62965200	2.42622900	0.90992900
O	-0.52280400	1.28872900	1.02486200
C	-0.14485100	0.70628400	0.04925500
C	2.26642500	1.46225600	0.43284300
H	-2.62331100	0.99532200	-1.96994800
Co	1.64160600	-0.09340000	-0.23893600
C	3.27553100	-0.88695900	-0.35331000
O	4.29246300	-1.39004000	-0.39042600
H	-2.35343900	1.84332100	-0.42844000
C	-2.29975900	0.87102600	-0.93103100
C	-3.13145300	-0.16495800	-0.21555300
H	-2.75504000	-0.28882800	0.80983900
H	-3.00517300	-1.13684400	-0.71569600
O	-0.92154200	0.45971600	-1.02339300
C	-4.60134500	0.21741300	-0.18291700
C	-5.44908900	-0.81988600	0.52735000
H	-4.96770300	0.35909400	-1.21116200
H	-4.71365200	1.19360400	0.31164700
H	-6.50713800	-0.53936300	0.54981400
H	-5.37717200	-1.79695700	0.03415600
H	-5.12158200	-0.95559500	1.56504900
C	0.81017300	-1.49109400	0.51156500
O	0.26010600	-2.34751800	1.02074500
H	1.25707700	-0.37421300	-1.92622400
H	1.58698200	0.36084100	-1.93069600

TS_{splitting}-formate

O	2.32343000	2.43371400	1.25826900
O	-0.53366700	1.71794500	-0.16121100
C	-0.15130900	0.63284500	-0.49641200
C	2.07731300	1.46571800	0.72768000

H	-2.65073300	-0.52595300	-2.13366300
Co	1.66734800	-0.06557400	-0.22230700
C	3.35869200	-0.74739400	-0.31643500
O	4.39552300	-1.18599900	-0.44852300
H	-2.39186100	1.13555400	-1.55042200
C	-2.31946900	0.07595600	-1.28076000
C	-3.12609600	-0.23454000	-0.04385900
H	-2.74508800	0.36100100	0.79800100
H	-2.97904900	-1.29106900	0.22626400
O	-0.93411500	-0.27639900	-1.10311800
C	-4.60428000	0.04946800	-0.24871900
C	-5.42647600	-0.26509000	0.98586600
H	-4.97580400	-0.53512900	-1.10408400
H	-4.73812900	1.10519300	-0.52751400
H	-6.49074100	-0.05796800	0.83385400
H	-5.33280300	-1.32117200	1.26692700
H	-5.09422600	0.32994000	1.84505200
C	0.89880200	-1.30664500	0.86883900
O	0.36268300	-2.09008000	1.48992000
H	1.41065300	-0.75549800	-1.51636400
H	1.81550200	0.51025400	-1.59566700

[Co]-2H-formate



O	2.25722800	2.46175400	1.24744700
O	-0.52763100	1.68792200	-0.33985800
C	-0.14485800	0.57577500	-0.57240500
C	2.03625000	1.47599500	0.74149600
H	-2.64205900	-0.72608000	-2.09999400
Co	1.66624500	-0.07990800	-0.18599800
C	3.35944200	-0.72438200	-0.38515900
O	4.38575400	-1.14449000	-0.61852800
H	-2.38034900	0.98288700	-1.67748100
C	-2.31133800	-0.04618100	-1.30760800
C	-3.12227900	-0.23573100	-0.04904900
H	-2.74737200	0.44236600	0.73076900
H	-2.97099800	-1.25951100	0.32533300
O	-0.92790100	-0.38417800	-1.09337100
C	-4.60088400	0.01895600	-0.28613800
C	-5.42603500	-0.17215500	0.97156500

H	-4.96692100	-0.65130800	-1.07867700
H	-4.73835600	1.04020700	-0.67134700
H	-6.49085100	0.01222100	0.79589800
H	-5.32770100	-1.19337400	1.35958400
H	-5.10015000	0.50963900	1.76632800
C	0.93979700	-1.21781300	1.03920000
O	0.41427500	-1.94875700	1.72772500
H	1.34463600	-1.04453500	-1.24776200
H	1.83712300	0.62019600	-1.47944500

TS_{eliminate-formate}

O	2.42260400	2.17241400	1.57146500
O	-0.49370700	1.74975800	-0.05672700
C	-0.13339200	0.71579300	-0.54526800
C	2.11596800	1.28995500	0.93462600
H	-2.66212700	-0.20253000	-2.27601300
Co	1.61492400	-0.13289100	-0.12530800
C	3.25561800	-0.65655500	-0.69678200
O	4.23939300	-1.01634600	-1.13396200
H	-2.39008100	1.35918700	-1.46597100
C	-2.30927600	0.27185400	-1.35429600
C	-3.08237900	-0.21778700	-0.15414700
H	-2.68279400	0.25486300	0.75445000
H	-2.92346000	-1.30058700	-0.04109400
O	-0.91983300	-0.09408700	-1.26802400
C	-4.56636000	0.08094900	-0.28026900
C	-5.35511800	-0.41155100	0.91739300
H	-4.95723100	-0.37971100	-1.20023600
H	-4.71181600	1.16442700	-0.40335900
H	-6.42384900	-0.19399800	0.82227000
H	-5.24918400	-1.49587700	1.04401700
H	-5.00397500	0.05907600	1.84357900
C	0.94663400	-1.29221400	1.09236700
O	0.46367100	-2.04802000	1.78867600
H	1.21485600	-1.19425200	-1.06802500
H	1.25952200	0.72505100	-1.31948200

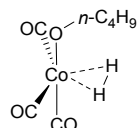
HCOOC₄H₉

O	-2.19020900	1.21199800	0.37140300
C	-2.39154000	0.22775700	-0.27612500
H	-0.15999400	-1.86870600	0.61170300
H	-0.59494300	-0.32541200	1.38374000
C	-0.39730500	-0.81658200	0.42383600
C	0.71731500	-0.12702000	-0.32383000

H	0.43511300	0.91725300	-0.51754100
H	0.84372600	-0.60664900	-1.30553500
O	-1.61057400	-0.84745200	-0.34641400
C	2.02305200	-0.17401800	0.45122000
C	3.15431800	0.51281900	-0.28875700
H	2.29220400	-1.22141400	0.65576500
H	1.88126700	0.29613800	1.43560000
H	4.09326200	0.47631400	0.27296600
H	3.33461800	0.04279500	-1.26323500
H	2.92240100	1.56825900	-0.47523900
H	-3.27642800	0.06732300	-0.91620100

pathway A to alcohol

[Co]-H₂-alcohol-A



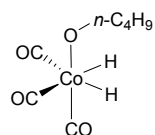
C	1.31568300	0.94135600	-0.69729300
O	-3.96184900	-1.03006800	-0.14864300
O	0.26234500	-2.60043300	-0.35455800
C	-0.38645300	-1.69498200	-0.16188300
C	-2.89060500	-0.65814100	-0.04176400
H	1.22806700	0.31915000	-1.61239800
Co	-1.22594700	-0.08870300	0.09671000
C	-1.61722400	1.68488500	0.01998200
O	-1.76617500	2.80424000	-0.04539400
H	0.97628200	1.95579000	-0.99066500
O	0.55665800	0.42713000	0.35288300
H	-0.68960900	-0.05022000	2.58514600
H	-1.25889800	-0.28299500	3.01563200
C	2.77290600	0.99030400	-0.28546800
H	3.34781900	1.49896800	-1.07588800
H	2.86495400	1.61450400	0.61628000
C	3.36050900	-0.38472000	-0.02268100
H	3.24345400	-1.00514900	-0.92566100
H	2.77218400	-0.88041900	0.76069300
C	4.82172400	-0.32460800	0.37725700
H	5.24014300	-1.31922500	0.56602900
H	5.43160600	0.14576400	-0.40470200
H	4.95750100	0.26729200	1.29114200

TS_{splitting}-alcohol-A

C	-1.33225500	1.07295600	0.08879800
---	-------------	------------	------------

O	3.99709200	-0.99978000	-0.45884700
O	-0.15635000	-2.07766000	1.43151000
C	0.46208200	-1.34136100	0.83890300
C	2.92507000	-0.64074900	-0.37713900
H	-1.19545600	0.83136500	1.16799300
Co	1.22439300	-0.10453600	-0.36326000
C	1.50049000	1.51302200	0.53009400
O	1.70284300	2.52897000	0.98259200
H	-1.02185300	2.13240100	-0.02650900
O	-0.61213600	0.22723700	-0.74157000
H	1.48444200	0.48941100	-1.68613700
H	1.09788000	-1.00347800	-1.52781500
C	-2.80753700	0.94891200	-0.24059600
H	-3.36155400	1.70712700	0.33622200
H	-2.95187200	1.19894200	-1.30224800
C	-3.37058900	-0.43153100	0.04563300
H	-2.80563400	-1.17422700	-0.53220400
H	-3.20091400	-0.67810200	1.10609600
C	-4.84900000	-0.53076200	-0.27612400
H	-5.25125800	-1.52831400	-0.06854300
H	-5.43553600	0.18893500	0.30938600
H	-5.03800400	-0.31464300	-1.33512800

[Co]-2H-alcohol-A



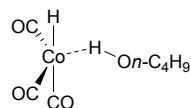
C	-1.39368300	-0.44742600	-1.24160200
O	3.99235800	0.68771600	-0.87600300
O	1.44995100	-2.39948500	1.54668200
C	1.43498400	-1.45374700	0.93185400
C	2.93275700	0.42625300	-0.56899800
H	-1.32800700	0.50973900	-1.79848300
Co	1.23388100	0.01111700	-0.22731000
C	0.66171700	1.44164300	0.85548900
O	0.14716000	2.28014600	1.40882600
H	-1.06138100	-1.23353600	-1.94661000
O	-0.60838800	-0.42635000	-0.09295100
H	0.95538500	0.80860700	-1.43284400
H	1.34702600	-0.88270700	-1.39218900
C	-2.83655500	-0.68360900	-0.84277200
H	-3.43877900	-0.79569300	-1.75897900
H	-2.90774800	-1.64233200	-0.30662800

C	-3.40934500	0.43014900	0.01605900
H	-2.80993500	0.52160800	0.93128400
H	-3.29586600	1.38880400	-0.51488800
C	-4.86686800	0.20125600	0.36584700
H	-5.27467200	1.00514800	0.98846600
H	-5.48918700	0.13569300	-0.53593000
H	-4.99831700	-0.73882900	0.91646700

TS_{eliminate}-alcohol-A

C	1.48337900	-0.84596000	-0.78603500
O	-3.84279200	0.00457100	-1.35706900
O	-1.20523800	2.59434200	1.25666300
C	-1.22396500	1.59030200	0.73667000
C	-2.82341200	0.01232800	-0.85285800
H	1.40294800	-1.62247400	0.00132400
Co	-1.19470200	-0.01828300	-0.17610000
C	-1.21299200	-1.32604300	1.19415600
O	-1.19366900	-2.18514900	1.93064300
H	1.11178000	-1.31412400	-1.71439100
O	0.72363600	0.28085200	-0.44431100
H	-1.11909400	-1.13262300	-1.15881300
H	-0.47019700	0.55103300	-1.35645100
C	2.93082100	-0.43520900	-0.94853700
H	3.50125100	-1.31008300	-1.30034600
H	2.99994800	0.31922600	-1.74700200
C	3.55412700	0.10459000	0.32657000
H	2.98329300	0.97942600	0.66286500
H	3.45128300	-0.64779700	1.12429900
C	5.01442100	0.46947200	0.14444600
H	5.46047600	0.86005700	1.06542100
H	5.60845800	-0.39971100	-0.16588300
H	5.13702800	1.23689700	-0.63022000

[Co]-alcohol-A

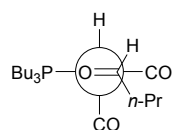


C	1.81619500	1.53951000	0.13970400
O	-3.58085700	2.05319300	-0.06452000
O	-2.57098600	-2.04018900	1.64682300
C	-2.22191900	-1.29826900	0.85948800
C	-2.85134000	1.18476000	-0.14739400
H	1.55816800	1.40419300	-0.92640000
Co	-1.66961800	-0.11537800	-0.37204500

C	-0.28099700	-0.99971700	-1.08666500
O	0.60173700	-1.49877100	-1.59471700
H	1.67224500	2.60523700	0.37782700
O	0.98643200	0.73242500	0.95642100
H	-1.18994500	0.89725900	-1.39564500
H	0.06764700	1.02025200	0.86333600
C	3.25013100	1.13984600	0.37847200
H	3.90053600	1.83368100	-0.17579800
H	3.48339800	1.28381400	1.44413700
C	3.55994500	-0.29000700	-0.02925900
H	2.89788200	-0.97314300	0.51819700
H	3.31737200	-0.42369300	-1.09451100
C	5.01021200	-0.65410600	0.22091700
H	5.23241600	-1.68468300	-0.07525000
H	5.68972400	0.00235400	-0.33751700
H	5.26627000	-0.55543700	1.28319100

8 Structures in Figure S6 **pathway to formate**

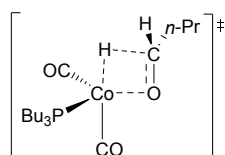
q



Co	-0.94523300	0.88006600	-0.45676100
C	-1.47998000	2.44923200	-0.98559500
O	-1.76378100	3.49649700	-1.35871400
H	-0.33532800	0.95419300	-1.83938200
P	1.08456500	0.04216500	-0.17258300
C	-1.34447200	0.97807000	1.27930500
O	-1.52119200	1.07851900	2.40578400
C	1.50758300	-1.27342800	-1.38400800
C	2.85087300	-1.96359700	-1.22520300
H	1.43028300	-0.79385400	-2.37073000
H	0.67981300	-1.99453400	-1.35084400
C	3.08211400	-3.02001500	-2.29427500
H	3.66947200	-1.22826900	-1.26654700
H	2.92525300	-2.43853200	-0.23481000
C	4.42153000	-3.71398100	-2.14414400
H	2.26738400	-3.75815200	-2.25386200
H	3.00901900	-2.55236900	-3.28744400
H	4.57986800	-4.47370400	-2.91655000
H	5.25041700	-2.99846700	-2.21242200
H	4.50398400	-4.21330000	-1.17072300

C	2.43939000	1.27033300	-0.36551800
C	2.24195700	2.52435200	0.46972300
H	2.47541300	1.52898100	-1.43449200
H	3.39895500	0.79241300	-0.11823100
C	3.37526700	3.52231800	0.30262400
H	1.28737400	2.99793200	0.19656300
H	2.14742600	2.25990400	1.53542600
C	3.16710500	4.77694300	1.12789100
H	4.32760400	3.04416300	0.57795400
H	3.47074500	3.78395800	-0.76199700
H	3.98575000	5.49297000	1.00125900
H	2.23730100	5.28634700	0.84725700
H	3.09762000	4.54225600	2.19727700
C	1.44790300	-0.71874300	1.46555000
C	0.56869200	-1.92268900	1.76792700
H	1.27957600	0.06514500	2.21832400
H	2.51429900	-0.98200700	1.52811900
C	0.64799300	-2.34794800	3.22419700
H	-0.47721300	-1.70338100	1.50371600
H	0.85597600	-2.76761200	1.12264800
C	-0.18765000	-3.57906700	3.51399200
H	1.69865700	-2.53202700	3.49676300
H	0.31724100	-1.51116200	3.85811000
H	-0.13770400	-3.87149800	4.56806000
H	-1.24268400	-3.40734800	3.26856400
H	0.14755200	-4.43692200	2.91791700
C	-2.60717700	-0.28271300	-1.25210200
H	-2.59825400	0.04276100	-2.31312400
C	-3.90383600	-0.08871100	-0.52322200
H	-4.27924600	0.93250300	-0.67930700
H	-3.74128500	-0.22598700	0.55463300
O	-1.72825600	-1.07456600	-0.85830000
C	-4.93448500	-1.09870400	-1.02466700
H	-5.05081900	-0.99341400	-2.11365300
H	-4.54675700	-2.11356900	-0.85848200
C	-6.27639700	-0.92694500	-0.34054200
H	-7.01261300	-1.65496700	-0.69696000
H	-6.18659800	-1.05243100	0.74525900
H	-6.68827600	0.07388200	-0.51875700

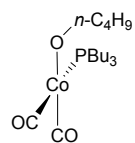
TS_{add}-formate



Co	-1.16888300	0.83666700	0.22861900
C	-1.80531200	2.40010100	-0.25850400
O	-2.16215900	3.43119700	-0.61335500
H	-1.56068900	0.34467200	-1.19625600
P	0.90338000	0.02588500	-0.25593800
C	-0.76094500	1.31791100	1.87041600
O	-0.45957800	1.59607900	2.93794900
C	0.92774900	-1.47874800	-1.32348100
C	2.27248100	-2.12701700	-1.60445300
H	0.44445400	-1.18264300	-2.26720800
H	0.24298500	-2.19876800	-0.85175300
C	2.14554400	-3.35700100	-2.48943100
H	2.95155100	-1.40715300	-2.08653500
H	2.76167600	-2.41529900	-0.66167400
C	3.48495500	-4.00791100	-2.77333100
H	1.46950200	-4.07965000	-2.00840900
H	1.65584700	-3.07569100	-3.43384600
H	3.38517200	-4.89372300	-3.40902000
H	4.16509000	-3.31342400	-3.28191700
H	3.97822400	-4.32335600	-1.84562400
C	2.03104000	1.18301400	-1.14151500
C	2.12602000	2.54933300	-0.48290400
H	1.63978800	1.28453600	-2.16529000
H	3.02997700	0.72963600	-1.22529700
C	3.04807600	3.49731600	-1.23114300
H	1.12155600	2.99231000	-0.41085700
H	2.48059000	2.44650000	0.55540200
C	3.12935900	4.86199700	-0.57581700
H	4.05226000	3.05227000	-1.30043800
H	2.69536300	3.59882000	-2.26861500
H	3.79306300	5.54098200	-1.12110000
H	2.14205500	5.33671300	-0.52460600
H	3.50662800	4.78773000	0.45159400
C	1.90751300	-0.46703900	1.20870700
C	1.27772800	-1.60192800	2.00287800
H	1.99061900	0.42748500	1.84302700
H	2.93299500	-0.71931900	0.89993400
C	1.92140700	-1.78168300	3.36722600
H	0.19792000	-1.42650000	2.12292100
H	1.35449000	-2.54307000	1.43581600

C	1.32992900	-2.94627100	4.13652800
H	3.00697300	-1.92059000	3.24647700
H	1.80144800	-0.85125300	3.94295300
H	1.78763700	-3.06138200	5.12460700
H	0.25144100	-2.81456700	4.28503900
H	1.46922200	-3.89133400	3.59691800
C	-2.39945200	-0.74427300	-0.57933400
H	-2.01075700	-1.41394500	-1.38079900
C	-3.82214300	-0.29941300	-0.83098100
H	-3.89568600	0.20919600	-1.80394000
H	-4.10833400	0.42683000	-0.05876500
O	-2.00941500	-0.99204500	0.61301200
C	-4.75651000	-1.50095600	-0.79555600
H	-4.43036900	-2.24240200	-1.54131900
H	-4.66246800	-1.99347500	0.18189700
C	-6.19841200	-1.10906600	-1.05226400
H	-6.86925400	-1.97408500	-1.02234100
H	-6.55245800	-0.39107100	-0.30272000
H	-6.31429500	-0.63529900	-2.03499000

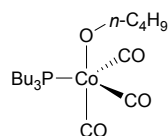
S



Co	0.09682100	-1.68336400	-0.68241300
C	-1.38080300	-2.54180800	-0.41739700
O	-2.37196000	-3.11255700	-0.30343700
H	2.69579500	-1.93611900	-2.16592400
P	-0.95016800	0.29265000	-0.27736200
C	0.99580700	-3.20831300	-0.77807000
O	1.54427100	-4.20730700	-0.79532100
C	-0.50397200	1.57292000	-1.51248100
C	-0.80349100	3.01701600	-1.14719800
H	-1.03347500	1.28802000	-2.43446100
H	0.56124500	1.41170300	-1.71717900
C	-0.48292700	3.96982300	-2.28809700
H	-1.86045200	3.14498200	-0.86297300
H	-0.22001200	3.31344400	-0.26183200
C	-0.75223500	5.41738200	-1.92731300
H	0.56997800	3.84163600	-2.57889800
H	-1.07154700	3.68603300	-3.17323300
H	-0.52106600	6.09664000	-2.75431000

H	-1.80500800	5.57216000	-1.65988900
H	-0.14949300	5.73156400	-1.06624400
C	-2.79392700	0.32578100	-0.27258300
C	-3.44746200	-0.23072800	0.98539300
H	-3.11444200	-0.24960600	-1.15356200
H	-3.13135500	1.35800500	-0.44330800
C	-4.91795600	-0.55093800	0.77781200
H	-2.93303500	-1.14130200	1.32669700
H	-3.34344600	0.49299200	1.80733200
C	-5.58438400	-1.04917900	2.04461900
H	-5.43730500	0.34392100	0.40202300
H	-5.00851400	-1.30697900	-0.01623100
H	-6.64178100	-1.28488300	1.88675400
H	-5.09672800	-1.95908200	2.41517200
H	-5.53009700	-0.30110900	2.84532800
C	-0.53204700	1.00415600	1.36587100
C	0.95013300	1.23134600	1.60149000
H	-0.92654100	0.30806000	2.11879700
H	-1.09830800	1.94153800	1.48494000
C	1.21461000	1.91905500	2.92962800
H	1.48014400	0.26856100	1.55416200
H	1.38074700	1.83217000	0.78638200
C	2.69302900	2.12961200	3.19020600
H	0.68827200	2.88639300	2.94793900
H	0.77087700	1.32522100	3.74337400
H	2.87324700	2.64031200	4.14196700
H	3.23067800	1.17435600	3.22013500
H	3.15502900	2.73321600	2.39850000
C	2.75616400	-1.01146800	-1.56308300
H	3.17809000	-0.24818400	-2.24541000
C	3.73171400	-1.21846500	-0.41551300
H	4.58962700	-1.81590000	-0.76485700
H	3.23534800	-1.82463700	0.36143300
O	1.50065400	-0.57468900	-1.14780000
C	4.23826600	0.07769200	0.19270800
H	4.83296400	0.61750100	-0.56010000
H	3.38446700	0.72975000	0.42054100
C	5.06809200	-0.15175300	1.44022900
H	5.44400600	0.78386900	1.86984100
H	4.47954300	-0.65869700	2.21711900
H	5.93550700	-0.79084100	1.23068900

t



O	-3.08897400	-2.46246100	-1.02718900
O	0.71919100	-2.35235300	-3.28985400
C	0.23100700	-2.11848900	-2.28862700
C	-2.00277100	-2.15207300	-0.85195200
H	2.66890000	-2.37865300	-0.74973200
Co	-0.34004000	-1.62962600	-0.62369800
H	2.42181300	-1.75919800	0.88599300
C	2.50115100	-1.44020300	-0.17896900
C	3.71831000	-0.54503300	-0.31148500
H	3.51912200	0.39446000	0.22883200
H	3.84490700	-0.26510800	-1.36820300
O	1.37710700	-0.75763100	-0.60591600
C	4.98770500	-1.18315400	0.22262200
C	6.17811100	-0.24619800	0.15359400
H	5.20190500	-2.10550500	-0.33807000
H	4.82649400	-1.50067100	1.26461200
H	7.09453900	-0.71091700	0.53327200
H	6.37327700	0.07330700	-0.87767900
H	5.99910000	0.66118500	0.74484800
C	-0.05613900	-2.58267200	0.92765900
O	0.08390300	-3.15574800	1.90227600
P	-0.99358500	0.50124700	-0.16260200
C	-0.24493100	1.65691200	-1.37627200
C	-2.78462000	0.93499400	-0.20054000
C	-0.49302900	1.11299500	1.50387300
C	-0.28253100	3.13979700	-1.04641700
H	-0.76641300	1.45842600	-2.32558200
H	0.78410500	1.30008200	-1.51384700
C	-3.59549500	0.32518600	0.93479600
H	-3.16661600	0.58513300	-1.17152400
H	-2.89972200	2.02844200	-0.19976300
C	0.99727200	1.07757500	1.78986700
H	-1.02511200	0.48384300	2.23257900
H	-0.89536600	2.13185000	1.62635200
C	0.30293700	3.98695500	-2.16523400
H	-1.31325800	3.47425000	-0.84848800
H	0.27813200	3.33658900	-0.11995700
C	-5.09008700	0.35168800	0.66339700
H	-3.28474200	-0.71555700	1.12062400
H	-3.38544100	0.86384900	1.87078300

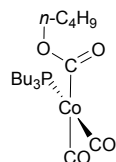
C	1.35093900	1.57889400	3.17806100
H	1.36602700	0.05270600	1.66349500
H	1.54424200	1.66656500	1.03856900
C	0.28967500	5.46735200	-1.83895100
H	1.33102200	3.65351100	-2.36895100
H	-0.25861400	3.80031200	-3.09280000
C	-5.89850300	-0.19996000	1.82073700
H	-5.40125300	1.38384100	0.44149300
H	-5.29655900	-0.22669700	-0.24942700
C	2.84590100	1.50799900	3.42708300
H	0.99400100	2.61260400	3.30630200
H	0.81487000	0.98188800	3.93155300
H	0.71110000	6.07059800	-2.64969200
H	-0.73132800	5.82657000	-1.65900800
H	0.87246400	5.68038900	-0.93427000
H	-6.97347000	-0.18651900	1.61386200
H	-5.61909900	-1.23791700	2.03935200
H	-5.73247500	0.38114500	2.73628900
H	3.11579200	1.83431800	4.43684100
H	3.21740400	0.48272700	3.29850600
H	3.39586900	2.13949800	2.71771300

TS_{inesrt}-formate

O	-3.08897400	-2.46246100	-1.02718900
O	0.71919100	-2.35235300	-3.28985400
C	0.23100700	-2.11848900	-2.28862700
C	-2.00277100	-2.15207300	-0.85195200
H	2.66890000	-2.37865300	-0.74973200
Co	-0.34004000	-1.62962600	-0.62369800
H	2.42181300	-1.75919800	0.88599300
C	2.50115100	-1.44020300	-0.17896900
C	3.71831000	-0.54503300	-0.31148500
H	3.51912200	0.39446000	0.22883200
H	3.84490700	-0.26510800	-1.36820300
O	1.37710700	-0.75763100	-0.60591600
C	4.98770500	-1.18315400	0.22262200
C	6.17811100	-0.24619800	0.15359400
H	5.20190500	-2.10550500	-0.33807000
H	4.82649400	-1.50067100	1.26461200
H	7.09453900	-0.71091700	0.53327200
H	6.37327700	0.07330700	-0.87767900
H	5.99910000	0.66118500	0.74484800
C	-0.05613900	-2.58267200	0.92765900
O	0.08390300	-3.15574800	1.90227600

P	-0.99358500	0.50124700	-0.16260200
C	-0.24493100	1.65691200	-1.37627200
C	-2.78462000	0.93499400	-0.20054000
C	-0.49302900	1.11299500	1.50387300
C	-0.28253100	3.13979700	-1.04641700
H	-0.76641300	1.45842600	-2.32558200
H	0.78410500	1.30008200	-1.51384700
C	-3.59549500	0.32518600	0.93479600
H	-3.16661600	0.58513300	-1.17152400
H	-2.89972200	2.02844200	-0.19976300
C	0.99727200	1.07757500	1.78986700
H	-1.02511200	0.48384300	2.23257900
H	-0.89536600	2.13185000	1.62635200
C	0.30293700	3.98695500	-2.16523400
H	-1.31325800	3.47425000	-0.84848800
H	0.27813200	3.33658900	-0.11995700
C	-5.09008700	0.35168800	0.66339700
H	-3.28474200	-0.71555700	1.12062400
H	-3.38544100	0.86384900	1.87078300
C	1.35093900	1.57889400	3.17806100
H	1.36602700	0.05270600	1.66349500
H	1.54424200	1.66656500	1.03856900
C	0.28967500	5.46735200	-1.83895100
H	1.33102200	3.65351100	-2.36895100
H	-0.25861400	3.80031200	-3.09280000
C	-5.89850300	-0.19996000	1.82073700
H	-5.40125300	1.38384100	0.44149300
H	-5.29655900	-0.22669700	-0.24942700
C	2.84590100	1.50799900	3.42708300
H	0.99400100	2.61260400	3.30630200
H	0.81487000	0.98188800	3.93155300
H	0.71110000	6.07059800	-2.64969200
H	-0.73132800	5.82657000	-1.65900800
H	0.87246400	5.68038900	-0.93427000
H	-6.97347000	-0.18651900	1.61386200
H	-5.61909900	-1.23791700	2.03935200
H	-5.73247500	0.38114500	2.73628900
H	3.11579200	1.83431800	4.43684100
H	3.21740400	0.48272700	3.29850600
H	3.39586900	2.13949800	2.71771300

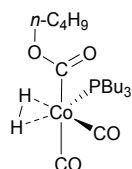
u



O	-0.15518300	-3.72544900	2.54301500
O	0.86190200	-2.30365300	-1.12825300
C	0.82934000	-1.78327500	-0.03797700
C	-0.40760800	-2.80351100	1.91903700
H	3.08339900	-1.24271600	-1.15064700
Co	-0.77177900	-1.36508900	0.97243000
H	3.46304800	-2.62291700	-0.12296500
C	3.20273500	-1.55546000	-0.10346100
C	4.24962900	-0.73356300	0.60102100
H	4.31618400	-1.04895800	1.65240700
H	3.92419600	0.31881800	0.62090200
O	1.96459700	-1.38259600	0.59433700
C	5.60992600	-0.84229100	-0.06482000
C	6.66242400	-0.00499800	0.63541000
H	5.52883100	-0.53586100	-1.11892100
H	5.92455600	-1.89637200	-0.08637200
H	7.64179700	-0.08627900	0.15257800
H	6.38509500	1.05645200	0.64210000
H	6.78383100	-0.31393000	1.68081600
C	-2.31272600	-0.97701700	1.74075800
O	-3.32715900	-0.72367400	2.21004000
P	-0.81762600	0.43775900	-0.35329700
C	0.78111500	1.32218100	-0.57234300
C	-1.33108800	-0.02261400	-2.05499600
C	-1.99980100	1.76560200	0.12028800
C	0.76550400	2.58907500	-1.40937400
H	1.46831000	0.58848100	-1.01461000
H	1.17854700	1.51725400	0.43404300
C	-2.51715000	-0.97481300	-2.06484200
H	-0.46365500	-0.50536000	-2.52499700
H	-1.55437400	0.89086500	-2.62550400
C	-1.66285600	2.41708200	1.45252400
H	-2.99446800	1.29994200	0.16834400
H	-2.04918000	2.51563900	-0.68207500
C	2.16019500	3.17533200	-1.56588400
H	0.34750400	2.38342700	-2.40695900
H	0.10752000	3.34655200	-0.95722500
C	-2.95372300	-1.34063500	-3.47269700
H	-2.24560800	-1.88792900	-1.51338800

H	-3.37023200	-0.53545700	-1.52190100
C	-2.78246800	3.30605300	1.96669700
H	-1.43813100	1.64479700	2.20548200
H	-0.73940600	3.00947700	1.35732700
C	2.16911500	4.44059800	-2.40051700
H	2.58031100	3.37727000	-0.56893800
H	2.82064800	2.41978100	-2.01796500
C	-4.12458200	-2.30355200	-3.48201400
H	-3.21461100	-0.42452200	-4.02461600
H	-2.09955300	-1.78064300	-4.00797200
C	-2.42599500	3.98883000	3.27217600
H	-3.03158600	4.05790400	1.20235400
H	-3.69048300	2.69806000	2.09522800
H	3.17678600	4.85495400	-2.50729700
H	1.78209500	4.25394700	-3.40981900
H	1.54006900	5.21863000	-1.95060500
H	-4.43289500	-2.56526300	-4.49950600
H	-3.87310900	-3.23665200	-2.96377700
H	-4.99712000	-1.87474700	-2.97358500
H	-3.24095200	4.61997200	3.64098100
H	-2.19931500	3.25418200	4.05431900
H	-1.54080800	4.62705800	3.15959000

[Co]-H₂-formate



O	-1.38262600	-3.99940400	1.31477900
O	0.84992600	-2.35630800	-0.80378700
C	0.83679500	-1.76214400	0.24687300
C	-1.11830800	-2.88806400	1.33089200
H	3.09642900	-1.48408200	-0.91013000
Co	-0.72538200	-1.16393400	1.26685100
H	3.42637700	-2.75949600	0.26005800
C	3.21614600	-1.68506700	0.16341000
C	4.30846400	-0.84015100	0.76426500
H	4.37795600	-1.04138600	1.84325300
H	4.02883900	0.22151800	0.67081300
O	1.99771100	-1.37851000	0.84830500
C	5.65231600	-1.08280800	0.10024200
C	6.75208100	-0.22491200	0.69486300
H	5.56882900	-0.88814400	-0.97979600

H	5.91869300	-2.14660800	0.18949900
H	7.71922900	-0.40350700	0.21362400
H	6.52333400	0.84283100	0.58917000
H	6.87542400	-0.42471100	1.76629800
C	-2.28509600	-0.61912600	1.93554800
O	-3.31136300	-0.27309600	2.30476900
P	-0.74437500	0.42788000	-0.30487300
C	0.87471400	1.24670300	-0.63975300
C	-1.26778000	-0.18998000	-1.95549700
C	-1.88575100	1.84780400	-0.02107800
C	0.89658700	2.38825900	-1.64090400
H	1.55178600	0.44842400	-0.97235800
H	1.27091600	1.57219100	0.33367500
C	-2.51878200	-1.05092500	-1.90390600
H	-0.42907800	-0.77701700	-2.35293800
H	-1.41696200	0.67204100	-2.62249600
C	-1.53559800	2.67903300	1.20236600
H	-2.89580800	1.42776200	0.08515500
H	-1.91038500	2.47577900	-0.92332000
C	2.30395000	2.92572600	-1.85062100
H	0.49132100	2.05580900	-2.60874500
H	0.24573300	3.21131400	-1.30845000
C	-2.96557100	-1.50550300	-3.28274200
H	-2.32318100	-1.92875100	-1.27149600
H	-3.34458900	-0.50634000	-1.41648900
C	-2.62613700	3.67385100	1.56266400
H	-1.34683200	2.02255500	2.06639800
H	-0.59033000	3.21814800	1.03271200
C	2.34844100	4.06674500	-2.84754100
H	2.71300300	3.25361500	-0.88287500
H	2.95725700	2.10575000	-2.18572700
C	-4.19919800	-2.38500100	-3.22796300
H	-3.15843000	-0.62537000	-3.91526100
H	-2.13850400	-2.04619600	-3.76600300
C	-2.25863000	4.52851900	2.75937200
H	-2.83843700	4.31325300	0.69233900
H	-3.55779700	3.12401100	1.76401600
H	3.36507700	4.44625100	-2.99276500
H	1.97190100	3.75223100	-3.82865200
H	1.72776100	4.90863400	-2.51663400
H	-4.51588400	-2.71148600	-4.22404400
H	-4.01679300	-3.28502100	-2.62860500
H	-5.04486100	-1.85647500	-2.77038300
H	-3.05265100	5.23660400	3.01760400

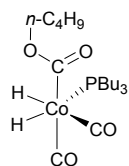
H	-2.06953500	3.90981300	3.64513900
H	-1.34822200	5.11044400	2.56928500
H	0.23097500	-0.91888700	2.70383800
H	0.28732500	-0.19668200	2.34692200

TS_{splitting}-formate

O	2.23604900	-3.51637300	-0.49698700
O	-0.77495100	-2.59097200	0.53928700
C	-0.81321600	-1.87562400	-0.43433800
C	1.67059700	-2.58781900	-0.83312200
H	-3.02384200	-1.78403700	0.84078400
Co	0.73042600	-1.13309600	-1.36998900
H	-3.36777200	-2.93364400	-0.44976200
C	-3.18116000	-1.87040800	-0.24312200
C	-4.31879000	-0.99787700	-0.70449500
H	-4.42441300	-1.07745300	-1.79618900
H	-4.06623500	0.05474000	-0.49951900
O	-2.00146100	-1.45379700	-0.93707400
C	-5.62795400	-1.35733700	-0.02437400
C	-6.77358200	-0.47237600	-0.47539600
H	-5.50674600	-1.28471000	1.06721800
H	-5.86865500	-2.41189200	-0.22586300
H	-7.71560400	-0.73517000	0.01701700
H	-6.56985400	0.58301400	-0.25568100
H	-6.93403200	-0.55211700	-1.55752200
C	2.02464200	-0.33932200	-2.32317000
O	2.81606600	0.20115900	-2.94235100
P	0.73694100	0.35931200	0.30222800
C	-0.92802400	0.94493600	0.82946600
C	1.47178600	-0.31905200	1.84342100
C	1.67602800	1.91532600	0.00668100
C	-1.00031000	2.06887700	1.84803700
H	-1.44322200	0.05670500	1.22086900
H	-1.46830600	1.21331400	-0.08930200
C	2.97127600	-0.55784200	1.74074200
H	0.94113300	-1.26643900	2.02030800
H	1.24646100	0.34090700	2.69313600
C	1.07637400	2.78161600	-1.08996200
H	2.69996300	1.62096600	-0.26476000
H	1.75746500	2.47565900	0.95037600
C	-2.43985600	2.39607300	2.21526400
H	-0.44898300	1.80116000	2.76235100
H	-0.51503300	2.97777800	1.46146300
C	3.48557000	-1.49636800	2.81905500

H	3.22494100	-0.97848900	0.75437700
H	3.51014900	0.40028900	1.80017300
C	2.00117100	3.91068500	-1.51256100
H	0.83140400	2.16467500	-1.96842300
H	0.11602300	3.20264500	-0.75453600
C	-2.54177600	3.51490500	3.23281800
H	-2.99205600	2.66456700	1.30179100
H	-2.92940600	1.48872000	2.60070700
C	4.98289000	-1.71324400	2.72927900
H	3.21762100	-1.09708500	3.80906100
H	2.95945500	-2.45852900	2.73202800
C	1.38180900	4.79807600	-2.57394700
H	2.27328800	4.50988300	-0.63026500
H	2.94352900	3.48090400	-1.88430500
H	-3.58123900	3.74310200	3.48987400
H	-2.02293100	3.25439600	4.16358600
H	-2.08637400	4.43881700	2.85531800
H	5.34641000	-2.39469200	3.50520600
H	5.26181500	-2.14237800	1.75891600
H	5.53107300	-0.76890100	2.83730900
H	2.05666000	5.60371900	-2.88066700
H	1.12720000	4.22237200	-3.47208600
H	0.45614500	5.26368300	-2.21352500
H	0.04585600	-1.62573600	-2.60840200
H	-0.26796200	-0.42630300	-2.23942100

[Co]-2H-formate



O	2.27618100	-3.41116000	-0.22505500
O	-0.84708500	-2.64420000	0.56583700
C	-0.89038500	-1.89913700	-0.38559200
C	1.67595600	-2.53766900	-0.63441300
H	-3.08340300	-1.75113300	0.94055100
Co	0.66548200	-1.18683000	-1.31215500
H	-3.43594400	-2.91254100	-0.33746800
C	-3.24847100	-1.84751200	-0.14162500
C	-4.38954400	-0.97979500	-0.60312700
H	-4.50074500	-1.06966300	-1.69343000
H	-4.13545100	0.07470400	-0.41027800
O	-2.07552400	-1.43413800	-0.84836300

C	-5.69479600	-1.33365400	0.08716900
C	-6.84378500	-0.45438100	-0.36651900
H	-5.56846300	-1.25093600	1.17742000
H	-5.93535000	-2.39027700	-0.10342100
H	-7.78310000	-0.71361600	0.13296700
H	-6.64039100	0.60332900	-0.15796200
H	-7.00934500	-0.54458500	-1.44705100
C	1.80623700	-0.45609600	-2.48412000
O	2.45057800	0.05725100	-3.27252200
P	0.79268200	0.34480200	0.30955100
C	-0.83931400	0.90375800	0.94854100
C	1.67570600	-0.24116300	1.81054600
C	1.66540800	1.90135800	-0.13926500
C	-0.85443300	2.05308500	1.94133900
H	-1.30115200	0.01260500	1.39759500
H	-1.45357700	1.13794900	0.06779600
C	3.16900700	-0.43957700	1.59284500
H	1.19208900	-1.19251100	2.07945700
H	1.50125700	0.45164000	2.64570800
C	0.94403700	2.72356800	-1.19619800
H	2.65852900	1.60534900	-0.50725600
H	1.83887000	2.49663600	0.77024200
C	-2.26924500	2.38852700	2.38816600
H	-0.24784400	1.81002600	2.82686300
H	-0.39629000	2.95252800	1.50259700
C	3.80272700	-1.31318500	2.66208700
H	3.35768900	-0.89224000	0.60606600
H	3.67600000	0.53707700	1.56826200
C	1.81687400	3.83026900	-1.76363600
H	0.60375200	2.07410100	-2.01681700
H	0.02713200	3.16090000	-0.77174500
C	-2.30908500	3.52784800	3.38716200
H	-2.87556000	2.63940700	1.50477300
H	-2.73416000	1.48985000	2.82098900
C	5.29319900	-1.49083000	2.45265000
H	3.60652900	-0.87714900	3.65334600
H	3.30362300	-2.29336500	2.66141900
C	1.08234000	4.68270400	-2.77923500
H	2.19148300	4.45933100	-0.94169200
H	2.70799000	3.37901100	-2.22564700
H	-3.33122800	3.76359200	3.70051800
H	-1.73649200	3.28496400	4.29077300
H	-1.87583400	4.44298000	2.96480200
H	5.74341600	-2.12402300	3.22388100

H	5.50198800	-1.95754800	1.48198900
H	5.81751200	-0.52720200	2.47033900
H	1.72044200	5.47095800	-3.19158600
H	0.72371000	4.07629100	-3.61976300
H	0.20623200	5.16877100	-2.33233800
H	0.12880900	-2.06902300	-2.37860500
H	-0.30878200	-0.30452400	-1.98818900

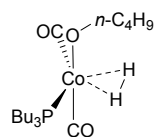
TS_{eliminate-formate}

O	2.83103100	-2.98404200	0.19182200
O	-0.56210200	-3.06987700	0.34742100
C	-0.64213300	-2.23512300	-0.52024600
C	2.09573300	-2.31816700	-0.36596900
H	-2.74189800	-2.02582800	0.93949500
Co	0.92182800	-1.24841800	-1.23260600
H	-3.19202800	-3.16757500	-0.32493300
C	-2.97237900	-2.10825300	-0.13242600
C	-4.12142300	-1.21125600	-0.51132200
H	-4.34529800	-1.32654600	-1.58162900
H	-3.81296200	-0.16254000	-0.37842700
O	-1.83462100	-1.70965300	-0.90003300
C	-5.36136400	-1.48650300	0.32041300
C	-6.50295200	-0.55042400	-0.02498800
H	-5.11284100	-1.39141000	1.38871400
H	-5.67627300	-2.53141200	0.18110600
H	-7.39735000	-0.75298100	0.57313800
H	-6.22116400	0.49623500	0.14706500
H	-6.78537300	-0.63998700	-1.08104100
C	1.93257500	-0.69179100	-2.59550600
O	2.50570900	-0.27144200	-3.49005600
P	0.76328900	0.36466200	0.26869400
C	-0.95034800	0.64272200	0.87745000
C	1.70602900	0.08682400	1.82525100
C	1.33054400	2.02914200	-0.27387800
C	-1.22962800	1.84878100	1.75605300
H	-1.21512100	-0.27996800	1.41594200
H	-1.59452200	0.65257200	-0.01134200
C	3.21518100	0.17522900	1.65417300
H	1.41332600	-0.91727500	2.17044900
H	1.37071500	0.79479400	2.59662200
C	0.52637600	2.61835400	-1.42041400
H	2.38348200	1.92383600	-0.57222800
H	1.32000900	2.70316300	0.59726800
C	-2.69585600	1.90925800	2.15931500

H	-0.60740500	1.82576300	2.66374800
H	-0.96396000	2.78126000	1.23443700
C	3.97162600	-0.42786800	2.82563800
H	3.52860700	-0.32954600	0.72664600
H	3.51306600	1.22748900	1.53003200
C	0.99068800	4.01700500	-1.79146000
H	0.59636000	1.96158000	-2.29942900
H	-0.54429200	2.65024800	-1.16380700
C	-3.00442300	3.08216600	3.06831000
H	-3.31599800	1.96269200	1.25108700
H	-2.97463600	0.96441600	2.65137900
C	5.47405300	-0.30723500	2.66627100
H	3.64821400	0.05942500	3.75804300
H	3.68829400	-1.48587400	2.92665000
C	0.20644600	4.59739800	-2.95170000
H	0.90469200	4.67380200	-0.91208200
H	2.06257700	3.98879400	-2.03815500
H	-4.06259800	3.11914300	3.34666900
H	-2.42210800	3.02987300	3.99645000
H	-2.75840400	4.03549000	2.58442700
H	6.01298000	-0.74820300	3.51102800
H	5.81657000	-0.81599800	1.75682600
H	5.78500800	0.74210600	2.58912500
H	0.54335500	5.60621800	-3.21145800
H	0.30729900	3.97509000	-3.84899200
H	-0.86373000	4.65781500	-2.71792400
H	0.08721200	-2.40277400	-1.79978500
H	-0.04510300	-0.35795500	-1.92817300

pathway A to alcohol

[Co]-H₂-alcohol-A



Co	-0.81547900	-1.73175200	-0.45766100
C	-2.52868200	-1.69054900	-0.70009300
O	-3.66133700	-1.64902000	-0.88803800
H	1.72702800	-3.36935600	0.34465900
P	-0.72506400	0.52835200	-0.23829900
C	-0.75572900	-3.48910000	-0.68011600
O	-0.73073600	-4.61726400	-0.83602800
C	0.41347400	1.19151800	-1.51643200
C	0.97608500	2.58571700	-1.29929800

H	-0.14632500	1.14282400	-2.46311200
H	1.21450200	0.44803100	-1.59811400
C	1.91140900	2.99590500	-2.42571700
H	0.16815600	3.32924800	-1.20866100
H	1.52908100	2.62623400	-0.34844000
C	2.49976200	4.37737900	-2.21817000
H	2.71666800	2.25017300	-2.50860300
H	1.36946500	2.95565300	-3.38242500
H	3.17482100	4.66259000	-3.03159400
H	1.71396200	5.14090700	-2.16071200
H	3.07155600	4.42932800	-1.28338700
C	-2.26464500	1.50564100	-0.49268100
C	-3.28775800	1.36795500	0.62677700
H	-2.69484900	1.16222100	-1.44528000
H	-2.00103500	2.56339800	-0.63842200
C	-4.66984400	1.84318000	0.21196400
H	-3.35522800	0.32154800	0.96476300
H	-2.95539200	1.94021400	1.50552300
C	-5.67458000	1.75524500	1.34334000
H	-4.60327600	2.87830500	-0.15661300
H	-5.01288400	1.24159100	-0.64270200
H	-6.66970500	2.09236600	1.03563800
H	-5.77382500	0.72410000	1.70378000
H	-5.36835000	2.37096200	2.19818300
C	-0.15315300	1.16422100	1.39406000
C	1.19888300	0.68704900	1.89146300
H	-0.93090000	0.86694500	2.11168400
H	-0.19143100	2.26463400	1.34550200
C	1.49480700	1.17547400	3.29819700
H	1.23491500	-0.40797700	1.85121800
H	1.99898300	1.02030500	1.21188700
C	2.85791300	0.71839900	3.78016400
H	1.43050500	2.27422700	3.33612000
H	0.71227400	0.80752400	3.98033600
H	3.07239200	1.05681500	4.79931500
H	2.93280600	-0.37617800	3.77241100
H	3.65571900	1.10107300	3.13098100
C	1.98904800	-2.48760600	-0.27108800
H	2.13471100	-2.86760800	-1.30375300
C	3.30675500	-1.92666100	0.23345100
H	4.06056900	-2.73051400	0.22543700
H	3.18961400	-1.62978500	1.28851900
O	1.00331800	-1.50776400	-0.23189800
C	3.81681900	-0.74267200	-0.56814900

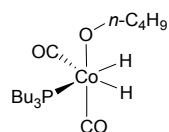
H	3.94502900	-1.04215200	-1.62045100
H	3.04963400	0.04347500	-0.57256200
C	5.11392700	-0.18348900	-0.01711100
H	5.48017500	0.66904800	-0.60035800
H	4.98486700	0.15763600	1.01911500
H	5.90761800	-0.94124500	-0.00818300
H	-1.06740200	-1.67849600	2.22405500
H	-1.16745800	-1.55928000	2.95990700

TS_{splitting}-alcohol-A

Co	-0.40877800	-1.87297300	0.04180900
C	-2.06409400	-2.42601700	-0.15185200
O	-3.13975800	-2.79092900	-0.26148400
H	1.99832100	-1.97029800	2.07357700
P	-0.85660400	0.33558200	-0.16697800
C	0.33661400	-2.42103300	-1.55786800
O	0.97134800	-2.71992500	-2.45082800
C	0.27427100	1.09084100	-1.40157100
C	0.36681700	2.60681700	-1.43607000
H	-0.05467200	0.70245500	-2.37851800
H	1.25421500	0.63522500	-1.20565600
C	1.29385300	3.09506200	-2.53809700
H	-0.62756200	3.05925500	-1.57806200
H	0.73202100	2.98620600	-0.46953000
C	1.40909000	4.60622000	-2.57208000
H	2.28694300	2.64277700	-2.39869900
H	0.93211100	2.72252000	-3.50814000
H	2.07826900	4.94933700	-3.36782900
H	0.43203400	5.07664300	-2.73909500
H	1.79914100	4.99673500	-1.62402700
C	-2.53120400	0.85108300	-0.73817900
C	-3.62860300	0.64805400	0.29762200
H	-2.74289800	0.25382900	-1.63837600
H	-2.50765100	1.90143800	-1.06262300
C	-5.01951800	0.67220200	-0.31292400
H	-3.48873600	-0.30533200	0.83117900
H	-3.55648500	1.42800800	1.07005800
C	-6.11046000	0.51792700	0.72787800
H	-5.15642400	1.61135800	-0.87038100
H	-5.09701100	-0.13235600	-1.05972500
H	-7.10960900	0.52945500	0.28051500
H	-6.00517900	-0.42807500	1.27306700
H	-6.07227400	1.32631300	1.46850800

C	-0.64822000	1.31537200	1.37600700
C	0.71972300	1.22607100	2.02940200
H	-1.41406700	0.94831100	2.07413100
H	-0.91129200	2.36192000	1.15112500
C	0.80980000	2.05554200	3.29805500
H	0.94905400	0.17511100	2.24645200
H	1.50392200	1.54419300	1.32587400
C	2.17598900	1.94783000	3.94741400
H	0.58241400	3.10895000	3.07096400
H	0.03113100	1.72900600	4.00437500
H	2.24102800	2.52676500	4.87468800
H	2.41591100	0.90479900	4.18967100
H	2.96381200	2.31092900	3.27564200
C	2.28588300	-1.90003900	1.00219900
H	2.37235600	-2.94954400	0.64767800
C	3.64089200	-1.22847500	0.88008900
H	4.35942200	-1.74585300	1.53621500
H	3.56222800	-0.19666100	1.26148100
O	1.35803000	-1.18302600	0.26772000
C	4.16649100	-1.20838200	-0.54434100
H	4.22040200	-2.24180800	-0.92171600
H	3.43815700	-0.69720600	-1.18893700
C	5.52436700	-0.54309500	-0.65591100
H	5.89731100	-0.53128400	-1.68608500
H	5.48557300	0.49748000	-0.30840300
H	6.27368600	-1.05842000	-0.04132300
H	-0.12714400	-3.07120900	0.89647900
H	-0.57950900	-1.94925400	1.52936700

[Co]-2H-alcohol-A



Co	-0.49015000	-1.84667500	-0.09376600
C	-2.15138400	-2.39840100	-0.12970000
O	-3.22494500	-2.78279800	-0.10168200
H	1.85864300	-2.13062500	1.93981800
P	-0.82985600	0.38652000	-0.15668200
C	0.10235000	-2.16270500	-1.81649600
O	0.62604800	-2.36312400	-2.80210400
C	0.29993000	1.18153700	-1.36611000
C	0.43655400	2.69352200	-1.30508500
H	-0.06128900	0.86960200	-2.35898100

H	1.26940900	0.68489400	-1.22260000
C	1.34200200	3.22875100	-2.40315200
H	-0.54848600	3.18046700	-1.38422300
H	0.84230900	2.99812500	-0.32850500
C	1.50280100	4.73475300	-2.33865800
H	2.32457300	2.73984500	-2.32912700
H	0.93730200	2.93425700	-3.38296900
H	2.15527600	5.11237600	-3.13259800
H	0.53582000	5.24347600	-2.43851500
H	1.93644600	5.04762900	-1.38083400
C	-2.50258100	0.97038100	-0.65894600
C	-3.57547700	0.73115500	0.39544500
H	-2.74759000	0.42318100	-1.58218700
H	-2.46494700	2.03531800	-0.92977200
C	-4.98053500	0.76103500	-0.18107300
H	-3.41837200	-0.23594400	0.89813200
H	-3.48883000	1.48825100	1.18880000
C	-6.04343900	0.55179000	0.87883000
H	-5.14240200	1.71800300	-0.70012600
H	-5.06560800	-0.01702800	-0.95490500
H	-7.05352600	0.57039400	0.45711700
H	-5.91418800	-0.41510200	1.38065200
H	-5.99502400	1.32891700	1.65160600
C	-0.55379500	1.25799700	1.43696000
C	0.83400000	1.08840000	2.02944100
H	-1.30614000	0.86618100	2.13592900
H	-0.79403700	2.32310400	1.28689600
C	1.00524500	1.83512200	3.33983700
H	1.03582100	0.02007100	2.17474100
H	1.60015000	1.42389100	1.31411800
C	2.39089100	1.63239000	3.92194600
H	0.81302000	2.90852500	3.18555400
H	0.24236700	1.49589100	4.05720300
H	2.52072600	2.15334200	4.87634200
H	2.59318100	0.56760600	4.09391100
H	3.16563400	1.99900800	3.23684600
C	2.19611000	-2.04240800	0.88509500
H	2.26534000	-3.08492700	0.50909600
C	3.57534400	-1.41024600	0.84277100
H	4.25154000	-1.98276700	1.49839300
H	3.51816400	-0.39528900	1.27096400
O	1.32358100	-1.28044300	0.12758900
C	4.15602700	-1.34053600	-0.55855500
H	4.18119900	-2.35469400	-0.98774500

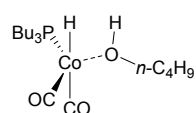
H	3.47498700	-0.76561400	-1.20103500
C	5.54396200	-0.73065000	-0.58525000
H	5.95632900	-0.68087000	-1.59921700
H	5.53584400	0.29091600	-0.18336100
H	6.24704000	-1.31001700	0.02696100
H	-0.16442700	-3.24227000	0.30480000
H	-0.67987800	-1.82609200	1.37649900

TS_{eliminate}-alcohol-A

C	2.30806800	-1.82074700	0.90005600
O	-2.89192200	-2.39216300	2.00144200
O	-1.46037700	-2.61682500	-2.28124900
C	-1.10439900	-2.30446000	-1.24577600
C	-1.99117200	-2.15944700	1.33472100
H	2.26271400	-0.74917000	1.18501600
Co	-0.57848300	-1.76469300	0.40360200
H	2.16805000	-2.38254200	1.84116500
O	1.32117000	-2.14173700	-0.03661200
H	-0.18027500	-1.43211900	1.80527600
H	0.28420400	-2.98051100	0.60900200
C	3.67184300	-2.11909100	0.31262900
H	4.43321500	-1.96258200	1.09412400
H	3.71773700	-3.18562000	0.04491800
C	4.00875400	-1.27235900	-0.90272400
H	3.24355200	-1.43047600	-1.67417700
H	3.94673300	-0.20598300	-0.62863900
C	5.38575100	-1.57911400	-1.45796200
H	5.62555200	-0.96676700	-2.33421100
H	6.16761200	-1.40212100	-0.70825400
H	5.46327600	-2.63066200	-1.76130800
P	-0.64269800	0.47128900	-0.06694100
C	0.87128600	0.95135600	-0.99067900
C	-2.00537800	1.06685000	-1.15673400
C	-0.73589200	1.64914300	1.34777700
C	1.00032200	2.39291400	-1.44977000
H	0.92547200	0.26052900	-1.84566300
H	1.72283800	0.66649200	-0.35784700
C	-3.38654500	0.65020800	-0.67809300
H	-1.81326300	0.65762600	-2.16094400
H	-1.94643300	2.16175500	-1.24797500
C	0.47516700	1.61204400	2.26347200
H	-1.63876200	1.37759900	1.91472300
H	-0.90261800	2.66741300	0.96472900
C	2.36782600	2.67416300	-2.05258400

H	0.22226700	2.62769800	-2.19194200
H	0.83121200	3.08619200	-0.61041000
C	-4.49923500	1.18282600	-1.56516800
H	-3.44833200	-0.44770900	-0.63503000
H	-3.55137800	0.99437900	0.35579200
C	0.31717300	2.51276800	3.47728500
H	0.65767800	0.57794100	2.59456500
H	1.37899400	1.91094900	1.70855300
C	2.49187600	4.08950200	-2.58056800
H	3.14013100	2.48547100	-1.29161400
H	2.56497800	1.94980200	-2.85738800
C	-5.87303100	0.74827600	-1.09394600
H	-4.44275700	2.28124200	-1.60073500
H	-4.33012800	0.84273900	-2.59798800
C	1.53536100	2.48431300	4.37915300
H	0.11886000	3.54302000	3.14450500
H	-0.57607000	2.20515000	4.04119100
H	3.48343700	4.28607100	-3.00114800
H	1.75560700	4.28584000	-3.36973100
H	2.31993700	4.82681800	-1.78641600
H	-6.66939500	1.13471100	-1.73827700
H	-5.96099700	-0.34482900	-1.08105100
H	-6.07389000	1.10074300	-0.07476300
H	1.41441300	3.13181000	5.25371200
H	1.73413800	1.46977100	4.74519100
H	2.43356800	2.81762700	3.84473100

[Co]-alcohol-A



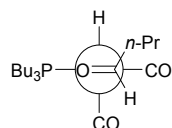
C	2.23958500	-2.41089000	0.09551300
O	-1.75378500	-4.10130500	1.41967800
O	-2.66300000	-1.76870100	-2.29796600
C	-1.94400400	-1.76583700	-1.39934100
C	-1.41717600	-3.17334100	0.83288700
H	2.10719900	-1.72141300	0.93904500
Co	-0.94783700	-1.69514900	0.04453200
H	2.02839500	-3.41992400	0.47897400
O	1.25005700	-2.03127200	-0.85402000
H	-0.33947500	-1.51022600	1.43252900
H	1.10736500	-2.74808700	-1.48080900
C	3.64130800	-2.30526800	-0.46168100
H	4.34626000	-2.67509700	0.29924500

H	3.75129200	-2.98397500	-1.32359700
C	4.01711000	-0.89076600	-0.86849800
H	3.30286300	-0.52779500	-1.62040300
H	3.89856900	-0.22552900	0.00291100
C	5.43088000	-0.79029800	-1.40505000
H	5.68619700	0.23472700	-1.69515700
H	6.16718000	-1.11518600	-0.65942700
H	5.56548800	-1.42439600	-2.29014700
P	-0.71962400	0.49899800	0.00713100
C	0.72640700	1.05108500	-0.99098200
C	-2.12100200	1.43668700	-0.73444100
C	-0.49069400	1.36873500	1.61783200
C	0.97881400	2.54259200	-1.12950600
H	0.61263500	0.57919200	-1.97785300
H	1.59776300	0.55176500	-0.54854800
C	-3.44737400	1.18226400	-0.03563900
H	-2.18045100	1.12413400	-1.78830000
H	-1.88921200	2.51175400	-0.73549100
C	0.85171200	1.11220200	2.27899700
H	-1.29979700	1.01456100	2.27192300
H	-0.65169000	2.44775100	1.47227300
C	2.35245700	2.82947800	-1.71578000
H	0.20754700	3.00157500	-1.76601800
H	0.89877300	3.04781600	-0.15408600
C	-4.62810800	1.75695100	-0.79947000
H	-3.59292600	0.10021600	0.10625700
H	-3.42317000	1.61292200	0.97784900
C	0.95825000	1.74871600	3.65478700
H	1.01230100	0.02623700	2.36595000
H	1.67053800	1.49009300	1.64397700
C	2.59968000	4.30944900	-1.92973600
H	3.11982200	2.41130000	-1.04496900
H	2.46317000	2.28478900	-2.66602400
C	-5.94443000	1.54002700	-0.07952700
H	-4.46535500	2.83188000	-0.97293200
H	-4.66481500	1.29496100	-1.79764800
C	2.30557200	1.49987500	4.30375700
H	0.77426600	2.83075900	3.57220800
H	0.15392100	1.35817300	4.29553500
H	3.59588100	4.50634700	-2.33938500
H	1.86773000	4.73803100	-2.62533300
H	2.51542900	4.86623800	-0.98808500
H	-6.79239100	1.94542600	-0.64140000
H	-6.13593600	0.47215300	0.08100900

H	-5.94284500	2.02090600	0.90663600
H	2.37643200	1.95899400	5.29528300
H	2.49491500	0.42616500	4.42439000
H	3.12196400	1.90707000	3.69400800

pathway B to alcohol

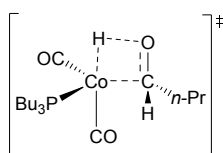
q



C	2.87038500	0.32153600	0.56199500
H	3.27174300	-0.08462100	1.51472700
O	2.32170800	-3.36944600	-0.43380000
C	1.84354800	-2.38368100	-0.09244700
H	1.14649300	-0.77448300	-1.18179100
Co	1.05453700	-0.88970500	0.32315800
C	0.61891600	-1.21815900	2.02369300
O	0.26582700	-1.46702200	3.08316900
C	3.80296400	0.27123000	-0.61154300
H	4.26399800	-0.72314800	-0.69401400
H	3.23097200	0.45317900	-1.53116900
O	1.88184200	1.07780600	0.59621000
C	4.89078400	1.33085600	-0.44720600
H	5.41721000	1.17295700	0.50605900
H	4.41563200	2.31885400	-0.37015600
C	5.88085200	1.30885900	-1.59512200
H	6.65719600	2.07250700	-1.47973000
H	6.38232400	0.33620600	-1.66912300
H	5.37959100	1.48926300	-2.55377000
P	-0.89301700	-0.02542300	-0.26765000
C	-0.73176300	1.48940200	-1.29650100
C	-1.92707300	-1.14672600	-1.29473700
C	-2.04337600	0.46773600	1.08463500
C	-2.01348900	2.17468400	-1.73634300
H	-0.13226000	1.18561400	-2.16730100
H	-0.08571800	2.17394300	-0.73089300
C	-2.10019600	-2.53042400	-0.69106500
H	-1.42984200	-1.21967500	-2.27372500
H	-2.90765200	-0.67852300	-1.46624200
C	-1.49269500	1.58706100	1.95513300
H	-2.21044800	-0.43217800	1.69439600
H	-3.02258600	0.74014500	0.66345500
C	-1.74191500	3.41490900	-2.57327700

H	-2.64080200	1.48171900	-2.31803700
H	-2.61685800	2.46153300	-0.86111300
C	-2.96118200	-3.44019800	-1.55088000
H	-1.11165400	-2.98872100	-0.54022200
H	-2.54731500	-2.45280300	0.31322400
C	-2.27592400	1.75872500	3.24556200
H	-0.43415200	1.39854600	2.19069400
H	-1.49816700	2.53448900	1.39394500
C	-3.01610200	4.10469400	-3.01915200
H	-1.11789700	4.11157300	-1.99399300
H	-1.13825600	3.13510600	-3.44953100
C	-3.12029600	-4.82282100	-0.94959600
H	-3.94901700	-2.97773400	-1.69822400
H	-2.51536600	-3.51545200	-2.55415700
C	-1.76078100	2.91010300	4.08628400
H	-3.34121500	1.90865500	3.01156500
H	-2.22502000	0.82138900	3.82025400
H	-2.81220100	4.99628700	-3.62112300
H	-3.64014700	3.43544800	-3.62442600
H	-3.61947800	4.42030500	-2.15894000
H	-3.73948300	-5.47442900	-1.57487500
H	-2.14811400	-5.31428800	-0.82289000
H	-3.58987900	-4.77393500	0.04065400
H	-2.32032500	3.01926000	5.02118300
H	-0.70539900	2.76709900	4.34799000
H	-1.83411300	3.86188700	3.54555500

TS_{add}-alcohol-B

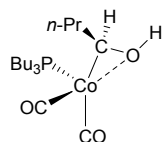


C	2.13806300	-0.25607200	-0.90972900
H	1.94367000	0.82455200	-0.80239500
O	-1.23664400	-3.56452300	-1.55400400
C	-0.52312800	-2.74701300	-1.18663900
H	0.46223000	-0.79882100	-2.07018800
Co	0.52032100	-1.42063500	-0.63087300
C	1.00581200	-2.03008900	0.96437100
O	1.26547900	-2.33048100	2.04093100
C	3.42320100	-0.72391400	-0.28946200
H	3.43895900	-0.46784300	0.78087900
H	3.48001700	-1.81996600	-0.35693700
O	1.83904700	-0.78304600	-2.08486000

C	4.63174300	-0.10053600	-0.98058100
H	4.54806600	0.99634800	-0.94362400
H	4.60867400	-0.37018200	-2.04528800
C	5.93783500	-0.54282300	-0.35088100
H	6.80508900	-0.09546800	-0.84788800
H	5.98441600	-0.26271100	0.70896400
H	6.05370700	-1.63222500	-0.40296000
P	-0.84453400	0.26432600	-0.22188000
C	-0.81203000	1.73216600	-1.34871100
C	-2.62223600	-0.22201900	-0.30493100
C	-0.72633000	0.99178900	1.46996000
C	-1.56696900	2.98119300	-0.92611600
H	-1.20219200	1.35541600	-2.30746400
H	0.24088200	1.97797900	-1.54810800
C	-3.03398100	-1.24193700	0.74552200
H	-2.77154100	-0.63710200	-1.31324800
H	-3.25999600	0.67111100	-0.23373900
C	0.61774700	1.62655700	1.78051700
H	-0.90860200	0.16391900	2.17042000
H	-1.54645300	1.71139200	1.61819200
C	-1.54300200	4.05925700	-1.99828000
H	-2.61391400	2.73941200	-0.68655600
H	-1.13725800	3.39016400	0.00122500
C	-4.38066600	-1.87756400	0.44354400
H	-2.27150600	-2.03225400	0.82852000
H	-3.07347800	-0.76239300	1.73544400
C	0.69412900	2.17212300	3.19642900
H	1.41493800	0.88214500	1.63385200
H	0.83466900	2.44003600	1.06919700
C	-2.28003600	5.31470700	-1.57536100
H	-0.49842700	4.30073500	-2.24574600
H	-1.98146900	3.65873600	-2.92439300
C	-4.80834200	-2.86123600	1.51456500
H	-5.13990500	-1.08869700	0.32909600
H	-4.32628700	-2.38427300	-0.53156400
C	2.04510600	2.78613900	3.50634000
H	-0.10215300	2.91775900	3.34308100
H	0.47741500	1.36035900	3.90664300
H	-2.25901300	6.08509800	-2.35297500
H	-3.33290300	5.10204000	-1.35225300
H	-1.83846100	5.74966300	-0.67018000
H	-5.77476100	-3.32244600	1.28636400
H	-4.07548600	-3.66993500	1.62341200
H	-4.89984600	-2.37173000	2.49215800

H	2.09560800	3.17571600	4.52827400
H	2.84974400	2.04873000	3.39552500
H	2.27036600	3.61702400	2.82613200

r



C	2.03530800	-0.39496800	-0.78326100
H	1.95026400	0.70107000	-0.73122100
O	-1.67037900	-3.26262900	-1.56992100
C	-0.84633200	-2.57096800	-1.16998900
H	1.35535200	-0.18032300	-2.63555200
Co	0.43814300	-1.48311300	-0.60978700
C	1.05866700	-2.43045600	0.73159400
O	1.40475900	-2.95863900	1.69288800
C	3.37815700	-0.85218700	-0.29069000
H	3.40358600	-0.75309100	0.80575900
H	3.48526300	-1.92780700	-0.49699400
O	1.84143200	-0.84105800	-2.12953900
C	4.54484000	-0.08805700	-0.90171900
H	4.43209300	0.98473900	-0.67916200
H	4.49966700	-0.17790000	-1.99610300
C	5.88510000	-0.58203900	-0.39292100
H	6.72259300	-0.02655400	-0.82841400
H	5.95673500	-0.48519000	0.69772100
H	6.03288900	-1.64208300	-0.63260600
P	-0.85591100	0.27752900	-0.23721200
C	-0.68664300	1.78653100	-1.30774600
C	-2.67882100	-0.00886900	-0.32323600
C	-0.67680000	0.93867400	1.47861700
C	-1.32595500	3.08411200	-0.83974400
H	-1.10397500	1.49116500	-2.28404800
H	0.38652800	1.95640900	-1.48351400
C	-3.19507800	-0.99764500	0.71234600
H	-2.87835400	-0.38793500	-1.33702400
H	-3.21945800	0.94426000	-0.23299900
C	0.71378600	1.43983100	1.82491800
H	-0.93643000	0.10512100	2.14668100
H	-1.43257900	1.72161300	1.64814600
C	-1.18698600	4.20078300	-1.86231700
H	-2.39347100	2.93192600	-0.61997300
H	-0.87063200	3.40819900	0.10848700

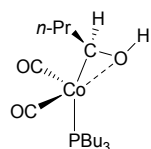
C	-4.57883200	-1.52558900	0.37359200
H	-2.50026400	-1.84601300	0.81303800
H	-3.22076000	-0.51811300	1.70256300
C	0.80847500	1.96852200	3.24601000
H	1.43589600	0.62099300	1.68998700
H	1.02620300	2.23439500	1.12743200
C	-1.80706700	5.50088600	-1.38920900
H	-0.12114500	4.35349200	-2.09010100
H	-1.65066900	3.88533100	-2.80903000
C	-5.11574900	-2.46391200	1.43610400
H	-5.26877800	-0.67944400	0.23178300
H	-4.53414600	-2.04292200	-0.59630200
C	2.20753300	2.43854900	3.59291000
H	0.08986500	2.79196400	3.37816900
H	0.49124000	1.18116700	3.94580100
H	-1.70504100	6.29910400	-2.13157100
H	-2.87757600	5.37893800	-1.18305400
H	-1.33657600	5.85189300	-0.46252500
H	-6.10794600	-2.84978000	1.18015000
H	-4.45250600	-3.32671300	1.57246300
H	-5.19869000	-1.96100500	2.40769500
H	2.27342800	2.81610800	4.61852800
H	2.93437200	1.62264200	3.49525000
H	2.53370300	3.24488300	2.92400300

TS_{iso}-alcohol-B

Co	-1.16320100	0.75830600	-0.18511000
C	-1.38777200	2.45429700	-0.80970200
O	-1.55063700	3.55895600	-1.07373300
P	0.99307400	0.07025400	-0.18750100
C	-1.35790100	0.89883200	1.50948500
O	-1.46897500	0.94280000	2.65768400
C	1.35833800	-1.30147700	-1.38397100
C	2.77296900	-1.85257700	-1.45129600
H	1.05750800	-0.92783900	-2.37575700
H	0.65776600	-2.11815800	-1.14008500
C	2.88725700	-3.04671800	-2.38528700
H	3.46520000	-1.06606700	-1.78591800
H	3.11709500	-2.14696700	-0.44795000
C	4.30329400	-3.58069000	-2.47516100
H	2.20705600	-3.84099400	-2.04135900
H	2.52878700	-2.76084500	-3.38578500
H	4.37579800	-4.44327800	-3.14549400
H	4.99361200	-2.81477400	-2.84929900

H	4.67210500	-3.89666600	-1.49153300
C	2.31830400	1.29321500	-0.58799100
C	2.25244600	2.53682800	0.28312500
H	2.18327900	1.56739500	-1.64565200
H	3.30843600	0.82129800	-0.50070300
C	3.28486100	3.58162000	-0.10624500
H	1.24504900	2.97543900	0.22530300
H	2.39804800	2.26423100	1.34056300
C	3.21520100	4.81701700	0.76984400
H	4.29141800	3.13907800	-0.05436400
H	3.13546800	3.85980800	-1.16032300
H	3.95816500	5.56811900	0.48171000
H	2.22754400	5.28975100	0.70957800
H	3.39100100	4.56750300	1.82361100
C	1.60616600	-0.61533300	1.41569200
C	0.87993200	-1.87848100	1.84696800
H	1.43980800	0.17423900	2.16301300
H	2.69358700	-0.77886200	1.37665200
C	1.15409100	-2.24998600	3.29447300
H	-0.20525300	-1.74530000	1.70886100
H	1.16478200	-2.72099800	1.19594100
C	0.46153900	-3.53451600	3.70439200
H	2.24006700	-2.33994900	3.44970700
H	0.82568400	-1.42245100	3.94047200
H	0.65433200	-3.79001100	4.75147200
H	-0.62551600	-3.45409100	3.58117100
H	0.79673300	-4.38150900	3.09247400
C	-2.52688800	-0.57900200	-0.33908900
H	-2.29612000	-1.57577000	0.06212400
C	-3.97466900	-0.21025800	-0.28847900
H	-4.25253300	-0.06725100	0.76635000
H	-4.10457300	0.77121300	-0.76802800
C	-4.89618800	-1.23761100	-0.93577200
H	-4.59890500	-1.37533100	-1.98522100
H	-4.75270400	-2.21408600	-0.44808700
C	-6.35423800	-0.82908700	-0.85708500
H	-6.52423700	0.12962500	-1.36203500
H	-7.01556400	-1.56788700	-1.32210100
H	-6.67682400	-0.70713700	0.18438400
O	-1.98880100	-0.42137800	-1.64662600
H	-1.37892600	-1.13902600	-1.85520800

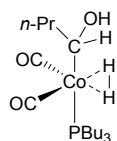
v



Co	-1.18911800	0.34854900	0.27848800
C	-1.53778300	1.29577100	-1.15790800
O	-1.71828400	2.05018000	-2.01017800
P	0.97339900	0.15499000	-0.15663400
C	-1.03168800	0.95803900	1.91648700
O	-0.88709200	1.49641100	2.92587700
C	1.25143500	-1.08568800	-1.49265500
C	2.68371300	-1.46686600	-1.82487000
H	0.74637700	-0.66639100	-2.37611500
H	0.66123400	-1.97416400	-1.22479400
C	2.76620800	-2.43855200	-2.99148600
H	3.27353000	-0.56843500	-2.06411900
H	3.17159100	-1.92034700	-0.94801400
C	4.19323800	-2.83048500	-3.32033700
H	2.17278200	-3.33516800	-2.75788800
H	2.28647300	-1.98746700	-3.87270500
H	4.24395900	-3.52949700	-4.16148900
H	4.79561100	-1.95293500	-3.58596100
H	4.68153900	-3.31150800	-2.46368700
C	1.84485400	1.65335200	-0.77424600
C	1.60164800	2.88040500	0.09051200
H	1.47776000	1.83420600	-1.79603400
H	2.92215200	1.44523700	-0.85512600
C	2.32663800	4.11041200	-0.42846000
H	0.52167500	3.08178000	0.14483900
H	1.91626900	2.68493100	1.12821200
C	2.07159000	5.33511900	0.42796800
H	3.40682800	3.90460800	-0.47942700
H	2.01072300	4.30368200	-1.46463200
H	2.59517300	6.21855000	0.04797400
H	1.00246100	5.57597300	0.46589300
H	2.40346200	5.17410100	1.46108800
C	2.06568200	-0.40208300	1.21855100
C	1.60438600	-1.70308400	1.85171200
H	2.06082100	0.39990500	1.97105800
H	3.10129700	-0.48577600	0.85700200
C	2.50710500	-2.16142000	2.98458100
H	0.57762400	-1.57468100	2.23050200
H	1.54586100	-2.49903800	1.09132000
C	2.02506200	-3.44753200	3.62612100

H	3.53077000	-2.29201700	2.60213200
H	2.57079400	-1.36404400	3.73970500
H	2.68356400	-3.77476300	4.43721400
H	1.01984600	-3.32752900	4.04872900
H	1.97493900	-4.26341000	2.89424500
C	-2.95299400	-0.40552100	0.50878000
H	-3.37120500	-0.37582300	1.52403500
H	-1.93312300	-1.96711200	1.16660400
C	-4.01806000	-0.29770200	-0.54126500
H	-4.38168800	0.74028400	-0.56476200
H	-3.56403000	-0.48201400	-1.52723400
O	-2.20754200	-1.61457900	0.31300100
C	-5.18648200	-1.25158200	-0.32832900
H	-5.64142400	-1.05495900	0.65462700
H	-4.80625500	-2.28189100	-0.28663700
C	-6.23484200	-1.12612500	-1.41678100
H	-7.07773200	-1.80767900	-1.25925700
H	-6.63914500	-0.10719000	-1.46359700
H	-5.81024200	-1.34994300	-2.40322700

[Co]-H₂-alcohol-B



Co	-0.96777900	-0.55188600	-0.47395200
H	-2.35126000	-1.86608600	-2.70251100
C	-1.31523600	-0.83955400	1.22713700
O	-1.54289700	-0.96147200	2.34725300
C	-1.37005800	0.85838900	-1.46300100
O	-1.64636000	1.82015500	-2.02388000
C	-2.83447200	-1.23318200	-0.91460500
O	-3.03201200	-1.30993100	-2.31310000
H	-2.84655900	-2.25365400	-0.48893200
C	-3.99057900	-0.44122100	-0.35474600
H	-3.84749100	-0.29822900	0.72568000
H	-3.99020700	0.56729300	-0.79676200
C	-5.34636300	-1.09207800	-0.59881500
H	-5.34060800	-2.10869300	-0.17575400
H	-5.49865900	-1.21498400	-1.67807200
C	-6.47980200	-0.28601100	0.00581300
H	-7.45631600	-0.75145500	-0.16786500
H	-6.35726400	-0.17377200	1.09085400
H	-6.51804200	0.72438600	-0.42058200

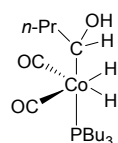
H	-0.34885300	-1.66862100	-1.63845500
H	-0.38439800	-2.10249700	-0.94314900
P	1.10384500	0.22701600	-0.04459800
C	2.25373900	0.05176100	-1.47686100
C	1.18818800	2.02713800	0.33334700
C	2.02803800	-0.50889200	1.36953600
C	3.68705000	0.52437200	-1.30524900
H	1.76490500	0.58857400	-2.30454500
H	2.23256800	-1.00830800	-1.76978900
C	0.21887600	2.46697600	1.41908500
H	0.96991800	2.55953000	-0.60507500
H	2.21900600	2.28995700	0.61310200
C	2.24904700	-2.00556100	1.23566000
H	1.43973500	-0.29894900	2.27431000
H	2.98501300	0.01958200	1.49362700
C	4.51181500	0.33165500	-2.56821300
H	3.70769700	1.58782000	-1.02306200
H	4.17068100	-0.01612100	-0.47667900
C	0.28996700	3.96062900	1.68841500
H	-0.80680100	2.19197600	1.13222100
H	0.42111300	1.92097900	2.35445000
C	2.96178600	-2.60191600	2.43796500
H	1.27997900	-2.50963000	1.09767000
H	2.83186800	-2.22429200	0.32611500
C	5.94311500	0.80309700	-2.40341200
H	4.49538900	-0.73122500	-2.85261300
H	4.03151700	0.86852300	-3.39969000
C	-0.67960900	4.39880500	2.76831500
H	1.31802800	4.23353400	1.97173800
H	0.08350100	4.50433600	0.75437200
C	3.18065200	-4.09550300	2.29901100
H	3.92640300	-2.09121900	2.57954700
H	2.37615900	-2.38959400	3.34460600
H	6.53033200	0.65978800	-3.31620300
H	5.98390000	1.86982900	-2.15096000
H	6.45103600	0.25938800	-1.59723900
H	-0.62641900	5.47633500	2.95517900
H	-1.71406200	4.16288100	2.49126800
H	-0.47457400	3.88915600	3.71783000
H	3.69352000	-4.51818300	3.16900000
H	2.22786900	-4.62751200	2.18874400
H	3.78698000	-4.32860700	1.41482600

TS_{splitting}-alcohol-B

Co	-1.01680400	-0.43487400	-0.43963000
H	-2.32282600	-1.58086500	-2.74607400
C	-1.39377600	-0.49669700	1.29994700
O	-1.57011400	-0.59633000	2.42683900
C	-1.53264700	1.07228000	-1.25973200
O	-1.84539700	2.01888300	-1.81714200
C	-2.85182200	-1.22144600	-0.91296800
O	-3.07879900	-1.18634500	-2.30154200
H	-2.78261300	-2.26502800	-0.56632100
C	-4.03824900	-0.54977100	-0.26298500
H	-3.90597900	-0.54000700	0.82806000
H	-4.08790900	0.50524100	-0.57557700
C	-5.36312100	-1.22857400	-0.59061900
H	-5.30167700	-2.29224100	-0.31321900
H	-5.52045800	-1.20885400	-1.67548200
C	-6.52742200	-0.57144800	0.12541400
H	-7.48199600	-1.05465400	-0.11033500
H	-6.40092100	-0.60785300	1.21518000
H	-6.61820200	0.48596800	-0.15365400
H	-0.53368600	-1.15129000	-1.67364600
H	-0.52107200	-1.85159100	-0.50001900
P	1.10832900	0.22240900	-0.09904200
C	2.21057700	-0.21780900	-1.50675700
C	1.38793900	2.03253900	0.09879900
C	1.96720800	-0.45967900	1.38176500
C	3.68618100	0.12247200	-1.39225200
H	1.76498400	0.27125100	-2.38627600
H	2.07146700	-1.29464600	-1.67869600
C	0.55166600	2.66596400	1.19908200
H	1.15076500	2.49623800	-0.87127600
H	2.45661300	2.21628500	0.28290000
C	2.07204400	-1.97495500	1.39514300
H	1.40369500	-0.11842200	2.26187300
H	2.96357200	0.00155600	1.45818200
C	4.47081800	-0.30833400	-2.62166100
H	3.82073100	1.20465400	-1.24407600
H	4.12313400	-0.35893400	-0.50348500
C	0.74797800	4.17048300	1.28421800
H	-0.51365200	2.44640100	1.03451300
H	0.80071200	2.21397100	2.17221300
C	2.75081400	-2.49873300	2.64986200
H	1.06800600	-2.41597900	1.30757200
H	2.62767500	-2.32621100	0.51087700
C	5.94448000	0.03143300	-2.51746100

H	4.34298700	-1.39087100	-2.77126800
H	4.03637800	0.16738000	-3.51346300
C	-0.08017600	4.79934400	2.38727900
H	1.81465300	4.39192400	1.44064900
H	0.48836700	4.62169200	0.31482600
C	2.85628200	-4.01096800	2.66144900
H	3.75237900	-2.05058300	2.73735100
H	2.19185600	-2.15366300	3.53240700
H	6.50215700	-0.28320100	-3.40547400
H	6.09656900	1.11145800	-2.39991700
H	6.40533100	-0.45726100	-1.65008300
H	0.06341800	5.88338900	2.44097200
H	-1.15039500	4.61628500	2.23313500
H	0.18175400	4.38354800	3.36803400
H	3.34502300	-4.38172000	3.56827600
H	1.86545100	-4.47794100	2.60711300
H	3.43430000	-4.37623200	1.80347800

[Co]-2H-alcohol-B



Co	-1.04071100	-0.26219800	-0.48795700
H	-2.45007600	-0.57799900	-3.00575600
C	-1.37470400	-0.62844800	1.22462000
O	-1.50581800	-0.93298600	2.31890900
C	-1.63205300	1.39830000	-0.82700900
O	-1.99401800	2.44601900	-1.09398600
C	-2.85162700	-0.97703300	-1.15150200
O	-3.18878800	-0.43314500	-2.40712900
H	-2.70052500	-2.06283000	-1.23933000
C	-4.01923400	-0.70022700	-0.23392400
H	-3.81918800	-1.13822800	0.75430900
H	-4.12498400	0.38537400	-0.07544600
C	-5.33827400	-1.25898700	-0.75503500
H	-5.21846500	-2.33451000	-0.95748500
H	-5.57095200	-0.79568500	-1.72081600
C	-6.47279700	-1.03750400	0.22677800
H	-7.42367100	-1.43390400	-0.14606500
H	-6.27041900	-1.52160700	1.19095500
H	-6.62019200	0.03133100	0.42740100
H	-0.64454700	-0.45067600	-1.91680600
H	-0.57289900	-1.66743500	-0.64577200

P	1.12265200	0.23787400	-0.15402700
C	2.19410700	-0.32040000	-1.54127100
C	1.51969900	2.02892200	0.00393700
C	1.91478700	-0.47352800	1.34935200
C	3.69432100	-0.12764600	-1.40536200
H	1.81305000	0.20130000	-2.43170400
H	1.94747300	-1.37906300	-1.70449100
C	0.87989200	2.68557200	1.21821900
H	1.16086800	2.50605600	-0.92098300
H	2.60963800	2.17029500	0.02899900
C	1.97078100	-1.99243000	1.35963500
H	1.32855700	-0.11739000	2.20869700
H	2.92113200	-0.04283200	1.46627000
C	4.45144000	-0.65988100	-2.61218700
H	3.93622900	0.93793400	-1.27517000
H	4.06718600	-0.63141500	-0.50033400
C	0.93418600	4.20280000	1.15577700
H	-0.16969400	2.36661700	1.31740700
H	1.38177100	2.34052800	2.13512900
C	2.41841600	-2.54552000	2.70232500
H	0.98351700	-2.40654500	1.10554600
H	2.65166400	-2.35104700	0.57172400
C	5.94984300	-0.46674600	-2.48765800
H	4.21824800	-1.72709800	-2.74319400
H	4.08113800	-0.16200200	-3.52065800
C	0.34273400	4.85390800	2.39014900
H	1.97772100	4.52569800	1.02070900
H	0.39708900	4.54216600	0.25730800
C	2.51367300	-4.05836200	2.70198400
H	3.39035300	-2.10599600	2.97409700
H	1.71238700	-2.21305100	3.47820500
H	6.48765700	-0.85366900	-3.35921100
H	6.20744800	0.59491500	-2.38770400
H	6.34523800	-0.98099000	-1.60293300
H	0.37668700	5.94669700	2.33374100
H	-0.70628900	4.56431100	2.52641700
H	0.88302300	4.55424700	3.29670000
H	2.82752700	-4.45033700	3.67486700
H	1.54703400	-4.51599900	2.45908100
H	3.23654400	-4.41178000	1.95622000

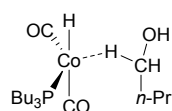
TS_{eliminate}-alcohol-B

Co	-1.09770000	0.11412500	-0.41865200
H	-2.29266100	-0.19611000	-2.90916400

C	-1.38365000	-0.18431000	1.30685900
O	-1.49720300	-0.38612000	2.42859900
C	-1.69606500	1.79714200	-0.65087400
O	-2.02213300	2.87264200	-0.85739200
C	-2.75557100	-0.98850400	-1.19573600
O	-3.09720500	-0.35971700	-2.40911300
H	-2.68142300	-2.07486700	-1.38695300
C	-3.91081400	-0.81431000	-0.23165500
H	-3.66248800	-1.29633000	0.72478100
H	-4.06576700	0.25303300	-0.01859200
C	-5.20366300	-1.41919700	-0.76523100
H	-5.03670300	-2.48122300	-1.00286500
H	-5.46374000	-0.93498500	-1.71425700
C	-6.34166200	-1.28191200	0.22783400
H	-7.27389500	-1.71311700	-0.15283500
H	-6.10987100	-1.78387000	1.17602200
H	-6.53962200	-0.22815700	0.46058000
H	-0.62984600	0.23100600	-1.84494800
H	-1.19641900	-1.30638000	-0.85411300
P	1.09989400	0.19403300	-0.18333800
C	2.03376300	-0.66752100	-1.51867300
C	1.76532500	1.91009900	-0.24850600
C	1.83926700	-0.47192700	1.36775400
C	3.54543200	-0.74832400	-1.39764900
H	1.74647800	-0.15293900	-2.44769500
H	1.59497800	-1.67233700	-1.60045500
C	1.33999300	2.76846600	0.93331500
H	1.38470800	2.34004900	-1.18767900
H	2.86170700	1.89078700	-0.32822000
C	1.63910600	-1.96985300	1.53495200
H	1.35774800	0.06258300	2.19895900
H	2.90722200	-0.20945100	1.41027200
C	4.17837800	-1.45478500	-2.58649400
H	3.98086900	0.25855500	-1.30874800
H	3.83054200	-1.27814400	-0.47594200
C	1.56663300	4.25085500	0.68932000
H	0.27553100	2.60086500	1.16164700
H	1.88983500	2.45866700	1.83525000
C	1.98858900	-2.45242500	2.93261500
H	0.59477200	-2.23706900	1.30966500
H	2.24650100	-2.51717700	0.79716800
C	5.68749700	-1.54264500	-2.47288900
H	3.74787300	-2.46310800	-2.67902400
H	3.90016900	-0.92792900	-3.51139600

C	1.18720500	5.09839800	1.88728000
H	2.62100700	4.42123100	0.42308800
H	0.98156900	4.55971400	-0.18991000
C	1.83009000	-3.95231600	3.08363400
H	3.02035100	-2.15516600	3.17490300
H	1.34821300	-1.93081300	3.65969500
H	6.13514900	-2.05303200	-3.33181400
H	6.14063700	-0.54550100	-2.41082000
H	5.98756300	-2.09164200	-1.57173000
H	1.34317200	6.16593300	1.70105900
H	0.13107500	4.96133500	2.14955800
H	1.77931600	4.82836200	2.77052900
H	2.07453900	-4.29153700	4.09548300
H	0.80029300	-4.26496500	2.87194400
H	2.48330700	-4.49416000	2.38835200

[Co]-alcohol-B



Co	0.34555100	-1.49925100	-0.17413600
H	2.00916500	0.13012700	-1.83116700
C	0.15097400	-1.90888100	1.52658900
O	-0.01734900	-2.16885600	2.63074700
C	1.40231000	-2.79466200	-0.69956700
O	2.07003300	-3.63592700	-1.09144600
C	2.87785800	0.64801100	-0.17077900
O	2.49502400	0.90214700	-1.50680200
H	3.04655400	1.63073700	0.29341800
C	4.12424100	-0.20391800	-0.06435500
H	4.30296100	-0.44122200	0.99672700
H	3.94122700	-1.17107600	-0.56091400
C	5.35390700	0.45399200	-0.66373000
H	5.54466600	1.40414300	-0.14099600
H	5.14247400	0.72427000	-1.70646100
C	6.58022500	-0.43437000	-0.58705500
H	7.46587800	0.04751800	-1.01491800
H	6.81864600	-0.69882000	0.45111300
H	6.42311300	-1.37428700	-1.13069700
H	0.37817400	-1.11898600	-1.66342500
H	2.04498500	0.16442600	0.37662700
P	-1.12235100	0.14973700	-0.20872600
C	-0.70806900	1.60511300	-1.25208400

C	-2.70111700	-0.46937600	-0.92080500
C	-1.63874500	0.87371500	1.40346700
C	-1.67845000	2.77310200	-1.22435700
H	-0.61331200	1.20180200	-2.27144600
H	0.30982300	1.92444900	-0.98929100
C	-3.14511800	-1.79647000	-0.32608400
H	-2.53269000	-0.57705100	-2.00222100
H	-3.48131500	0.29506400	-0.79080700
C	-0.49562300	1.55222800	2.14077900
H	-2.03816300	0.04836100	2.01053600
H	-2.47193900	1.57342100	1.24318100
C	-1.28103700	3.86571900	-2.20463100
H	-2.70053400	2.43589700	-1.45873200
H	-1.73009300	3.20475400	-0.21294200
C	-4.46113400	-2.28384300	-0.90723400
H	-2.35991100	-2.54959300	-0.49553400
H	-3.24160700	-1.71150100	0.76836900
C	-0.89862600	2.03925400	3.52219500
H	0.35216200	0.85604900	2.23599900
H	-0.11348800	2.40062100	1.55058400
C	-2.23035500	5.04702000	-2.17036600
H	-0.25613600	4.19576500	-1.98100100
H	-1.23983500	3.44379000	-3.21960000
C	-4.89498600	-3.61334500	-0.32190700
H	-5.23925600	-1.52465800	-0.73508000
H	-4.36380300	-2.36728500	-2.00012000
C	0.23991700	2.72899300	4.24731000
H	-1.75759400	2.72149700	3.43214400
H	-1.25743100	1.18275300	4.11254300
H	-1.93905100	5.82808600	-2.88009800
H	-3.25475000	4.74290400	-2.41927600
H	-2.26114200	5.50451900	-1.17365700
H	-5.84300900	-3.95922200	-0.74648100
H	-4.14634700	-4.39252800	-0.50917400
H	-5.02645200	-3.54531800	0.76501700
H	-0.05657900	3.07396600	5.24312600
H	1.09527200	2.05435000	4.37421400
H	0.59604600	3.60340100	3.68868200

9 Structures in Table S1

HCo(CO)₃

Co	0.00012700	-0.25339200	0.00000000
H	0.00054400	-1.76842700	0.00000000
C	0.00014000	-0.61153900	1.74216300
O	0.00014000	-0.91829200	2.83627400
C	0.00014000	-0.61153900	-1.74216300
O	0.00014000	-0.91829200	-2.83627400
C	-0.00038000	1.53858000	0.00000000
O	-0.00070300	2.67621100	0.00000000

Propene

C	-1.27243700	-0.21973300	0.00003500
C	-0.13130000	0.45546300	0.00006900
H	-1.28902800	-1.30929100	-0.00009400
H	-2.23781800	0.27972700	-0.00015900
H	-0.16708300	1.54720100	-0.00015000
C	1.22341300	-0.16153200	-0.00001300
H	1.80460300	0.14612900	-0.87837600
H	1.80490600	0.14638400	0.87808500
H	1.16636500	-1.25533600	0.00014700

4,6-dimethyl-1-heptene

C	3.77941200	-0.75949600	0.60031000
C	2.97751600	0.00934500	-0.12447100
H	4.72953700	-0.40009600	0.98761100
H	3.51762200	-1.79121900	0.83509000
H	3.28961600	1.03366900	-0.34024000
C	1.65680900	-0.42293000	-0.66819100
H	1.61374800	-0.21291500	-1.75048600
H	1.56396100	-1.51392100	-0.56226000
C	0.44787000	0.24646900	-0.00351300
H	0.51812400	0.03679400	1.07690400
C	-0.82931700	-0.38486300	-0.54960500
H	-0.78555400	-1.47448300	-0.37837600
H	-0.83514700	-0.25849500	-1.64620000
C	0.46445900	1.75227900	-0.20913500
H	1.38408300	2.20980700	0.17066400
H	0.38782300	1.99742400	-1.27855400
H	-0.36885100	2.24831600	0.29995300
C	-2.15457700	0.12602000	0.00702600
H	-2.25841800	1.19276700	-0.25018800
C	-2.23097000	-0.01562200	1.51862000
H	-2.06976600	-1.06145400	1.81727000
H	-1.48342700	0.59255500	2.03985400
H	-3.21577500	0.28289700	1.89720600

C	-3.30571700	-0.62017100	-0.64855700
H	-4.27783500	-0.24572900	-0.30668300
H	-3.27917700	-0.53112900	-1.74121000
H	-3.26347200	-1.69097300	-0.40526300

Isobutene

C	0.00049200	1.45451100	0.00000600
C	-0.00001900	0.12508300	0.00012700
H	-0.92502300	2.02702400	-0.00011500
H	0.92648900	2.02622900	-0.00009300
C	-1.26232900	-0.67533900	-0.00002800
H	-1.31139100	-1.33352000	-0.87821300
H	-1.31135800	-1.33357200	0.87812000
H	-2.15501800	-0.04261500	0.00003700
C	1.26189600	-0.67609800	0.00002800
H	1.31026600	-1.33519400	0.87750800
H	1.31083500	-1.33341000	-0.87885300
H	2.15496100	-0.04389100	0.00080900

2,4,4-trimethyl-1-pentene

C	2.04868400	1.31210700	0.04000400
C	1.51516900	0.12732200	-0.24730100
H	1.53789100	2.24345500	-0.19916800
H	3.02299500	1.40182200	0.51691500
C	2.24795400	-1.14810900	0.02943500
H	2.46014300	-1.67964100	-0.90853400
H	3.20115100	-0.97138200	0.53780600
H	1.65742300	-1.83930000	0.64307900
C	0.16813600	0.00556900	-0.90881500
H	0.15046400	-0.91280700	-1.51782900
H	0.03372800	0.83882600	-1.61479100
C	-1.06839900	-0.01908500	0.01594200
C	-2.29112300	-0.26443300	-0.86178900
H	-2.23039700	-1.23481500	-1.37163600
H	-3.21277000	-0.26101900	-0.26589500
H	-2.39351600	0.51043600	-1.63264000
C	-1.23281000	1.31651800	0.72999700
H	-0.37833000	1.54004300	1.37854100
H	-1.33510600	2.14266900	0.01355500
H	-2.13381300	1.31074400	1.35686100
C	-0.97245500	-1.13302400	1.05081000
H	-0.82433800	-2.11290800	0.57759200
H	-0.14966700	-0.96711000	1.75652500
H	-1.89679900	-1.19020600	1.63991500

10 Structures in Table S2**PH₃**

P	0.00000000	0.00000000	0.12889500
H	0.00000000	1.19192800	-0.64447300
H	-1.03224000	-0.59596400	-0.64447300
H	1.03224000	-0.59596400	-0.64447300

HCo(CO)₃(PH₃)

Co	-0.00005100	-0.12760700	-0.18421900
H	-0.00038100	-0.04852800	-1.67742000
C	1.59534400	-0.83990500	-0.54363900
O	2.59437300	-1.31112400	-0.83002400
C	-1.59536000	-0.84050000	-0.54285000
O	-2.59429200	-1.31201100	-0.82906700
C	0.00040600	-0.31265100	1.59780600
O	0.00094700	-0.43935400	2.73058800
P	-0.00046900	2.10038400	-0.27048600
H	1.05185200	2.85333300	0.29980800
H	0.00145200	2.74028300	-1.52736300
H	-1.05507700	2.85279000	0.29629800

PMe₃

P	0.00005600	0.00001900	-0.62425600
C	-0.51774300	1.52597400	0.28650400
H	0.12884800	2.36646700	0.01370300
H	-1.54217200	1.79967700	0.01350400
H	-0.47241100	1.39189900	1.37513600
C	1.58049600	-0.31469700	0.28651500
H	1.98511000	-1.29490900	0.01375200
H	2.32973800	0.43565400	0.01353600
H	1.44176100	-0.28691900	1.37515600
C	-1.06282200	-1.21131600	0.28644900
H	-2.11396000	-1.07150000	0.01350500
H	-0.78773400	-2.23542300	0.01362600
H	-0.96961400	-1.10500600	1.37511000

HCo(CO)₃(PMe₃)

Co	-0.77441400	-0.00010000	-0.16424300
H	-0.58601500	-0.00028600	-1.64863600
C	-1.52052800	-1.57913800	-0.53654300
O	-1.98864300	-2.58009700	-0.82873300
C	-1.52075900	1.57865500	-0.53715100
O	-1.98865300	2.57947500	-0.83016800

C	-0.88019400	0.00039700	1.61307300
O	-0.88649200	0.00108800	2.75647700
P	1.44112600	-0.00007200	-0.15824500
C	2.29161100	-0.00315100	-1.77562800
H	1.99257800	0.87977900	-2.34871100
H	3.38170900	-0.00295700	-1.65696500
H	1.99252900	-0.88819800	-2.34541300
C	2.23769100	1.41725500	0.68419900
H	1.91143700	1.45420300	1.72909400
H	3.33173900	1.34415600	0.65694700
H	1.93017900	2.35193200	0.20491000
C	2.23789300	-1.41403700	0.68965100
H	1.93006100	-2.35063700	0.21434500
H	3.33193300	-1.34117000	0.66159200
H	1.91216400	-1.44667000	1.73485300

PBu₃

P	0.37070700	-0.18350700	1.21572300
C	-0.83241200	1.24016900	1.22365700
C	-1.23284300	1.89032700	-0.08906200
H	-0.38778700	1.99271200	1.89296600
H	-1.72796900	0.88679100	1.75617500
C	-2.22589500	3.02613400	0.10248700
H	-0.34416800	2.27760200	-0.61021800
H	-1.67445400	1.14434500	-0.76810300
C	-2.62536300	3.67794300	-1.20691500
H	-3.11872200	2.64331900	0.61981300
H	-1.79178100	3.77748200	0.77936200
H	-3.34147700	4.49354000	-1.06053300
H	-1.75312700	4.09545400	-1.72519500
H	-3.08844300	2.95211900	-1.88705900
C	1.76547600	0.57487100	0.24443400
C	2.97388400	-0.34177400	0.14547100
H	2.04719400	1.50717300	0.75785700
H	1.42901700	0.86240100	-0.76298900
C	4.13879900	0.28887400	-0.59909200
H	3.29896400	-0.63634100	1.15542500
H	2.69408600	-1.28101800	-0.35839000
C	5.33737800	-0.63472900	-0.69608100
H	3.80915300	0.58408400	-1.60677000
H	4.42480200	1.22466800	-0.09517900
H	6.17332800	-0.17154600	-1.23091800
H	5.70066300	-0.91954900	0.29911300
H	5.08246400	-1.56203200	-1.22421200

C	-0.35796500	-1.26100000	-0.11527700
C	-1.69478300	-1.86836400	0.27430200
H	0.36870600	-2.06606400	-0.29830600
H	-0.44573200	-0.70748100	-1.06269300
C	-2.22764000	-2.84627100	-0.75987300
H	-1.60183800	-2.37770600	1.24682400
H	-2.44070700	-1.07243400	0.43033500
C	-3.56838500	-3.43615800	-0.36826400
H	-2.31015600	-2.33640100	-1.73185900
H	-1.49174200	-3.65074900	-0.90907000
H	-3.94354800	-4.14169000	-1.11714000
H	-3.50205400	-3.97343300	0.58594000
H	-4.32677000	-2.65279000	-0.24573700

HCo(CO)₃(PBU₃)

Co	-1.26833000	-1.35225700	-0.71140200
H	-0.02827000	-2.14543500	-0.42941400
C	-1.87099400	-2.27082600	0.70121100
O	-2.18274800	-2.87249700	1.62261700
C	-0.98274900	-2.03077800	-2.33558000
O	-0.74365400	-2.48261000	-3.35865800
C	-2.66474600	-0.30900900	-1.06697700
O	-3.53993300	0.38948400	-1.29955100
P	0.13981900	0.26360000	-0.14043600
C	1.53443400	0.45275100	-1.33306100
C	2.68341000	1.37283000	-0.95651200
H	1.06607400	0.78157800	-2.27373100
H	1.90477200	-0.56142000	-1.53912900
C	3.72681400	1.46944900	-2.05851000
H	2.31318400	2.38355300	-0.72682500
H	3.16953400	1.01693900	-0.03467500
C	4.88338100	2.37505200	-1.68377700
H	4.09845900	0.46119700	-2.29451900
H	3.24764400	1.83159300	-2.98020100
H	5.62912200	2.44064100	-2.48261900
H	4.53817800	3.39470600	-1.47238300
H	5.39678500	2.01352200	-0.78422900
C	-0.53505800	1.97605500	-0.02969200
C	-1.54278700	2.16561900	1.09429100
H	-1.00625000	2.18421900	-1.00218400
H	0.28902900	2.69546700	0.08009400
C	-2.32827100	3.45951200	0.96102800
H	-2.24527200	1.31798100	1.12804000
H	-1.02286500	2.15611300	2.06422200

C	-3.29711100	3.66796500	2.10797400
H	-1.62787600	4.30637200	0.89878000
H	-2.87330600	3.45149800	0.00537400
H	-3.86504000	4.59791000	2.00165800
H	-4.02077500	2.84605800	2.16894400
H	-2.77240800	3.71119600	3.07047400
C	0.96527700	0.07838000	1.49602100
C	1.82135900	-1.16817900	1.63785500
H	0.16545600	0.06467100	2.25001500
H	1.56043500	0.98433900	1.69146000
C	2.58042300	-1.19981100	2.95411900
H	1.18677500	-2.06264900	1.55651100
H	2.54112300	-1.24132800	0.80689200
C	3.40515900	-2.46134200	3.11635100
H	3.23048400	-0.31353200	3.01914500
H	1.86643300	-1.10665100	3.78614400
H	3.95401200	-2.47447600	4.06360200
H	2.77106700	-3.35573200	3.09073700
H	4.14054500	-2.56241100	2.30850600

a₅-PhobPC₅

P	0.54206500	-0.33736700	-0.84063800
C	1.66904300	-1.36856700	0.24750500
C	3.08290400	-1.43937000	-0.33937100
C	3.65250900	-0.15991500	-0.95065600
C	3.53698700	1.11272400	-0.11381800
C	2.21896800	1.86915500	-0.26311600
C	0.94563400	1.16523500	0.20832300
C	1.04089700	0.66527300	1.64963900
C	1.60809200	-0.76712000	1.66959200
C	-1.09566700	-0.84338800	-0.10320300
C	-2.22208600	0.12088000	-0.43316100
C	-3.58465800	-0.38507100	0.00756700
C	-4.71379800	0.58201600	-0.29977600
C	-6.06718400	0.05987400	0.14160900
H	1.26364700	-2.38973900	0.26618300
H	3.10359200	-2.21536900	-1.11719500
H	3.76471500	-1.79411700	0.45007700
H	3.17946000	0.01930100	-1.92834000
H	4.71118700	-0.34847100	-1.17543400
H	4.33695300	1.80264600	-0.41521100
H	3.73754500	0.89229400	0.94590800
H	2.30284100	2.81378500	0.29689100
H	2.09980600	2.15667400	-1.31905100

H	0.12028900	1.88311700	0.10229500
H	0.04372400	0.68156700	2.10696800
H	1.65416200	1.34816000	2.25565500
H	0.99018800	-1.40329800	2.31464400
H	2.60975000	-0.78577300	2.11921200
H	-1.31920400	-1.83157300	-0.53281900
H	-1.02947800	-0.99254000	0.98329000
H	-2.03120000	1.09559000	0.04365800
H	-2.23749900	0.32019300	-1.51670200
H	-3.78937500	-1.35379800	-0.47665400
H	-3.56584100	-0.59569100	1.08951900
H	-4.50788800	1.54758100	0.18684800
H	-4.72733600	0.79251000	-1.37995900
H	-6.30848300	-0.88782900	-0.35570200
H	-6.87547900	0.76368300	-0.08357900
H	-6.08689100	-0.12875600	1.22226600

HCo(CO)₃(a₅-PhobPC₅)

O	-1.61108700	2.46477500	-1.69881700
O	-0.67531600	2.48073900	2.69873000
P	0.37412500	-0.49186600	-0.22596200
C	-0.76503900	2.18491800	-0.98314000
C	-0.23184700	2.19323500	1.68461000
C	1.45657900	-1.44324800	-1.40024000
C	2.92208900	-1.00164200	-1.37342600
C	3.59130700	-0.75968800	-0.01817700
C	3.30349800	-1.74982200	1.10776200
C	2.00301300	-1.51708400	1.87520500
C	0.69035800	-1.73387800	1.12317100
C	0.65074700	-3.07939800	0.39432500
C	1.23932300	-2.92832100	-1.02663300
C	-1.30023800	-0.98787500	-0.84504600
C	-2.42446600	-0.73603500	0.14583300
C	-3.79801700	-0.86430200	-0.48927400
C	-4.93360000	-0.66090200	0.49720600
C	-6.29819600	-0.77465100	-0.15367500
H	1.07309900	-1.25846900	-2.41330000
H	3.02291000	-0.08047300	-1.96342500
H	3.49479300	-1.76388800	-1.92428700
H	3.34032900	0.24727400	0.34012700
H	4.67433100	-0.73346200	-0.19739300
H	4.11818400	-1.67457400	1.84043800
H	3.35347800	-2.78503500	0.73787500
H	1.99194900	-2.20093400	2.73741000

H	2.01661800	-0.50377700	2.30203100
H	-0.12995500	-1.65391000	1.84970500
H	-0.38383400	-3.43789600	0.33837400
H	1.19570300	-3.83842400	0.97128700
H	0.57219600	-3.40032900	-1.75697600
H	2.19212300	-3.46465700	-1.11297600
H	-1.46260500	-0.39432700	-1.75686000
H	-1.30334800	-2.03733700	-1.16581700
H	-2.34410100	-1.44060100	0.98859000
H	-2.32252900	0.26690700	0.58861600
H	-3.88670900	-0.13187000	-1.30827900
H	-3.89591400	-1.85401500	-0.96498100
H	-4.84418700	-1.39586000	1.31164200
H	-4.82661700	0.32462800	0.97468000
H	-6.42242700	-0.02813100	-0.94773900
H	-7.11110800	-0.62768900	0.56501900
H	-6.43899000	-1.76137900	-0.61227200
Co	0.53000900	1.71382900	0.14695600
H	1.60058000	1.31353600	1.10781900
C	1.92656900	2.51150100	-0.62582500
O	2.86283200	2.99228900	-1.07288000

11 Structures in Table S4

entry 1

axial



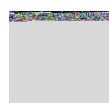
Co	0.01713800	-0.33366000	-0.00002700
C	-1.70284700	-0.72973400	0.00001900
C	1.75057700	-0.66085300	0.00002600
H	0.04783300	-1.83503100	-0.00008200
O	-2.78848500	-1.08451000	0.00003100
O	2.85178200	-0.96311900	0.00002500
P	-0.06234900	1.85845000	0.00000300
H	-0.73187500	2.51208700	-1.05892200
H	-0.73179100	2.51212500	1.05896000
H	1.09557000	2.66743600	0.00001000

equatorial



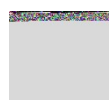
Co	0.08437200	-0.23519100	0.00358500
C	1.78124500	-0.65499300	0.00019300
O	2.87359600	-0.98600300	-0.00557000
H	-0.01434000	-1.75774300	0.01427900
P	-2.06313600	-0.56247800	-0.00322800
H	-3.04829700	0.45222400	-0.04916200
H	-2.57015800	-1.36760400	-1.04167900
H	-2.58599500	-1.28821900	1.08510700
C	0.18686500	1.53137300	-0.00132100
O	0.26129300	2.67230000	-0.00069800

entry 2 axial



Co	-1.02408300	0.14081300	-0.00005300
C	-1.02483900	1.90045100	0.00000300
O	-1.09607200	3.04291400	0.00006200
C	-1.62893400	-1.51190500	0.00000300
O	-2.08213100	-2.56237800	0.00006000
H	-2.51201600	0.40251000	-0.00008500
P	1.14634300	-0.19206000	-0.00000400
C	2.04393800	0.54430800	1.41732900
C	2.04401800	0.54430900	-1.41728700
C	1.78857800	-1.90670100	0.00001500
H	3.12307800	0.36273200	1.34582100
H	1.86582900	1.62429300	1.44176400
H	1.67452700	0.12250700	2.35666800
H	1.67466600	0.12250300	-2.35664700
H	1.86590300	1.62429300	-1.44173600
H	3.12315400	0.36274000	-1.34571500
H	1.42211400	-2.43896100	0.88372100
H	1.42215700	-2.43896700	-0.88370400
H	2.88473700	-1.93176600	0.00004300

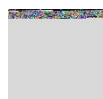
equatorial



Co	-0.80588900	-0.19159000	0.00001000
C	-2.45465000	-0.78893800	0.00007700
O	-3.50882100	-1.22996800	0.00012100
H	-0.48887200	-1.68972800	0.00024900

P	1.37457200	-0.19315900	0.00003400
C	2.12669000	-1.05379200	-1.42507000
C	2.28691600	1.39542900	-0.00038100
C	2.12657400	-1.05297300	1.42569700
H	3.22121300	-1.03320200	-1.36260900
H	1.78277200	-2.09156900	-1.44625500
H	1.81656000	-0.57629800	-2.35912600
H	2.01343000	1.98194200	0.88282000
H	3.37193800	1.23829800	-0.00022400
H	2.01361300	1.98138300	-0.88400700
H	1.81644900	-0.57487300	2.35944500
H	1.78258200	-2.09071100	1.44751200
H	3.22109900	-1.03249700	1.36325900
C	-1.05884200	1.54880700	-0.00024900
O	-1.18749200	2.68826500	-0.00041000

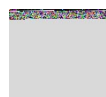
entry 3
axial



Co	-1.35010400	0.79319800	-1.47032000
C	-1.56926300	-0.51589900	-2.62396300
C	-1.62220800	2.31227900	-0.62685300
H	-2.33173400	1.44022700	-2.41957400
O	-1.77661200	-1.33410600	-3.39797700
O	-1.85175400	3.30689900	-0.10766700
P	0.04656200	-0.19747400	-0.07722000
C	1.42274600	-1.13551400	-0.86516000
C	2.38810800	-1.86874400	0.05013500
H	1.96059700	-0.42505300	-1.50955200
H	0.93853400	-1.84084200	-1.55740800
C	3.47893500	-2.59350400	-0.72300100
H	2.85917000	-1.16761600	0.75643300
H	1.84237900	-2.59603700	0.67057200
C	4.43347100	-3.34216300	0.18595600
H	3.01586600	-3.28891800	-1.43855200
H	4.03301100	-1.86532800	-1.33398300
H	5.22097300	-3.85382100	-0.37673300
H	4.92389000	-2.66240100	0.89375700
H	3.90638000	-4.10095600	0.77744300
C	-0.80332300	-1.47681500	0.94072300
C	-2.11617300	-0.98539900	1.53057300
H	-0.13031700	-1.83404900	1.73434100

H	-0.98985400	-2.33277600	0.27370900
C	-2.83130200	-2.05618300	2.33649000
H	-1.94115100	-0.10670600	2.17183100
H	-2.76885300	-0.63087100	0.71749300
C	-4.14388800	-1.56496900	2.91464300
H	-3.00738400	-2.93285900	1.69522700
H	-2.17142600	-2.40670400	3.14478500
H	-4.65570000	-2.34250200	3.49108900
H	-3.98832400	-0.70863300	3.58229700
H	-4.82811200	-1.23758700	2.12255600
C	0.88651100	0.84632400	1.18587500
C	1.83348200	1.86993700	0.58156600
H	1.41161800	0.20997700	1.91353700
H	0.08781100	1.35995600	1.74098100
C	2.36325700	2.85811000	1.60748100
H	2.68278800	1.35944700	0.09996800
H	1.32467200	2.42068900	-0.22567000
C	3.32569600	3.86010500	1.00146600
H	1.51544800	3.38376600	2.07143900
H	2.85550700	2.30727000	2.42340100
H	3.70099600	4.57104800	1.74469100
H	4.19485200	3.35921100	0.55710500
H	2.84338600	4.44008600	0.20533900

equatorial

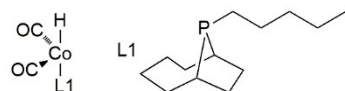


Co	1.51144400	-0.72569600	1.09080900
C	2.80607500	-1.06786400	2.21999100
O	3.63809000	-1.24761400	2.98344000
H	1.35252500	0.51662700	1.97388400
P	-0.16102800	0.31666400	0.12988400
C	1.64285800	-2.08594500	-0.01377200
O	1.72017800	-2.95151200	-0.76366400
C	-1.55069500	0.71206400	1.26557100
C	-2.70935700	1.50831000	0.68963200
H	-1.09122900	1.24604500	2.10898600
H	-1.90076200	-0.24246700	1.68419300
C	-3.80430700	1.75002700	1.71649900
H	-2.34982600	2.47825300	0.31292000
H	-3.14290100	0.99150800	-0.18075000
C	-4.95312800	2.56731800	1.15979200
H	-4.17393900	0.78156100	2.08555800

H	-3.37255500	2.25545900	2.59315200
H	-5.73672300	2.73463900	1.90591800
H	-4.61138300	3.55153100	0.81619600
H	-5.41879700	2.06798600	0.30093000
C	0.36978700	1.94847400	-0.52495400
C	1.67472900	1.86623800	-1.30181100
H	0.49248500	2.60698200	0.34748400
H	-0.42925000	2.37713800	-1.14718200
C	2.14839600	3.22197400	-1.79643300
H	2.44659000	1.41174900	-0.66089200
H	1.56435400	1.18565400	-2.16092200
C	3.45509200	3.13411800	-2.56023100
H	1.36993600	3.67177000	-2.43148500
H	2.25979400	3.89967600	-0.93690500
H	3.79213100	4.11428300	-2.91312600
H	4.25278500	2.71728300	-1.93363900
H	3.35966300	2.48325800	-3.43800700
C	-0.96943800	-0.48398500	-1.31985700
C	-1.72033600	-1.75488900	-0.95442900
H	-0.15960600	-0.72047700	-2.02583800
H	-1.63126200	0.22964700	-1.83182100
C	-2.07746400	-2.59722000	-2.16779300
H	-1.11936800	-2.36252600	-0.25916000
H	-2.64053200	-1.50237900	-0.40441200
C	-2.86898400	-3.83543300	-1.79729500
H	-2.64595000	-1.98347800	-2.88312900
H	-1.15170200	-2.88465200	-2.68819800
H	-3.11859800	-4.44133000	-2.67436000
H	-2.30374200	-4.47325700	-1.10701700
H	-3.81119800	-3.57277400	-1.30014900

entry 4

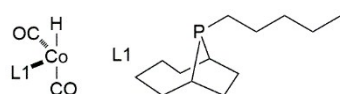
axial



O	-0.95786400	-2.87766000	-2.51774800
O	0.46038400	-1.99398000	2.86641500
P	-0.35729500	0.31747900	-0.25335500
C	-0.83959200	-2.42207000	-1.47350800
C	0.01840900	-1.88741500	1.81506400
C	-1.51400500	1.16327300	-1.43032100
C	-2.92701400	0.57394600	-1.33080000
C	-3.41867600	0.16587800	0.05640800

C	-3.28435900	1.21353200	1.16052500
C	-1.94434200	1.22468300	1.89225000
C	-0.70345000	1.57341300	1.07062900
C	-0.83403100	2.90099600	0.31941200
C	-1.41840200	2.66648100	-1.09262000
C	1.30211400	0.79671600	-0.89822300
C	2.43984500	0.32062000	-0.00956400
C	3.80368600	0.71975100	-0.54385000
C	4.95056600	0.23518800	0.32475800
C	6.30597900	0.63838000	-0.22201400
H	-1.14221400	0.98639700	-2.44883200
H	-2.98691100	-0.30975400	-1.98013700
H	-3.62896300	1.30451100	-1.76159000
H	-2.89913600	-0.75903000	0.37004700
H	-4.47310500	-0.12342600	-0.04257200
H	-4.05839700	1.02928300	1.91681000
H	-3.51122000	2.21394900	0.75972900
H	-2.00662600	1.95125800	2.71629000
H	-1.79764900	0.24493800	2.37027800
H	0.15797700	1.59067900	1.75356400
H	0.15056200	3.37672000	0.24188400
H	-1.45473100	3.60100900	0.89457000
H	-0.79156400	3.16967000	-1.83799900
H	-2.41058300	3.12524300	-1.18577600
H	1.38459100	0.33456100	-1.89328800
H	1.35356500	1.88376800	-1.05211000
H	2.31775200	0.71893200	1.01089600
H	2.38605400	-0.77391800	0.09240100
H	3.92515400	0.32528300	-1.56580800
H	3.85596000	1.81645800	-0.64322900
H	4.82527500	0.62834400	1.34499500
H	4.89499900	-0.85933400	0.42109500
H	6.46603000	0.22996800	-1.22755300
H	7.12711200	0.28458500	0.41002400
H	6.39594300	1.72921900	-0.29795100
Co	-0.57781200	-1.83350400	0.16183500
H	-0.76005100	-3.30402600	0.44681500

equatorial



O	-1.19172700	2.38537700	2.56784000
O	-0.39454600	4.25967700	-1.49887200

P	-0.30706800	-0.46193800	0.15897400
C	-0.94143600	2.12102700	1.47972100
C	-0.45534100	3.25891900	-0.94883900
C	-1.41201600	-1.39556100	1.31740400
C	-2.85637400	-0.88193700	1.24088200
C	-3.37534600	-0.45825700	-0.13142500
C	-3.19108300	-1.46301100	-1.26790800
C	-1.85861000	-1.36974000	-2.00697400
C	-0.59822500	-1.68133200	-1.20211200
C	-0.65315200	-3.03715500	-0.49243900
C	-1.23797800	-2.87978400	0.93089700
C	1.37799000	-0.86691100	0.78201200
C	2.48707700	-0.36948700	-0.13094400
C	3.87068300	-0.69395500	0.40241600
C	4.98716900	-0.19649600	-0.49822600
C	6.36451500	-0.52683100	0.04215900
H	-1.04362500	-1.23027800	2.33921500
H	-2.96190600	-0.02450400	1.91858300
H	-3.51433200	-1.66370900	1.65051300
H	-2.90327400	0.49829200	-0.41723600
H	-4.44259100	-0.22644200	-0.01975500
H	-3.98105300	-1.30124800	-2.01289400
H	-3.35477400	-2.48713600	-0.89780000
H	-1.88436900	-2.06648100	-2.85833000
H	-1.76237700	-0.36414300	-2.44196800
H	0.26068700	-1.62360700	-1.88478100
H	0.35617500	-3.46173200	-0.43518300
H	-1.24107100	-3.74975100	-1.08589900
H	-0.57901000	-3.37215100	1.65536700
H	-2.20314500	-3.39436100	1.01533600
H	1.45684200	-0.38683900	1.76873400
H	1.46580400	-1.94926200	0.95196500
H	2.37215800	-0.80556900	-1.13616100
H	2.38286000	0.71691600	-0.27015900
H	3.98819400	-0.25737100	1.40762300
H	3.96886500	-1.78332400	0.54084800
H	4.86433800	-0.63059300	-1.50215000
H	4.88710000	0.89084100	-0.63230500
H	6.52153200	-0.07854200	1.03113400
H	7.16228700	-0.16232100	-0.61338900
H	6.49932900	-1.61002200	0.15298000
Co	-0.51808400	1.69196000	-0.17364900
H	-0.07743000	1.25213000	-1.57186100

11 Structures in Table S4**H₂**

H	0.00000000	0.00000000	0.37308200
H	0.00000000	0.00000000	-0.37308200

CO

C	0.00000000	0.00000000	-0.64360600
O	0.00000000	0.00000000	0.48270400

TS_{co-ma}

Co	-1.53798700	-0.29647100	-0.36756300
C	-2.07172600	1.09780500	-1.29582300
O	-2.49845800	2.06362800	-1.74848600
P	0.49580400	0.56755600	-0.02579500
C	-1.69439700	-1.02066600	1.21789500
O	-1.84086400	-1.34451500	2.31123900
C	1.61502400	0.21434900	-1.44936200
C	3.05153800	0.70085300	-1.35687900
H	1.11246800	0.65741700	-2.32310700
H	1.58076000	-0.87098400	-1.61788200
C	3.85242000	0.36874100	-2.60602000
H	3.07861300	1.78879100	-1.19295300
H	3.55058800	0.25366100	-0.48330900
C	5.28738900	0.84995900	-2.51925200
H	3.82841000	-0.71854200	-2.77262500
H	3.35784200	0.81376500	-3.48218300
H	5.85738200	0.60675000	-3.42177800
H	5.33489400	1.93756400	-2.38402900
H	5.80923000	0.39434200	-1.66857400
C	0.52618900	2.40594300	0.08085600
C	-0.36812700	2.95663700	1.18190900
H	0.19294700	2.77967200	-0.89906300
H	1.55928900	2.75651900	0.21694200
C	-0.55621200	4.46046900	1.07637800
H	-1.35199300	2.46346900	1.14940000
H	0.05529000	2.70915900	2.16778000
C	-1.40888000	5.01754600	2.19896800
H	0.42791400	4.95369300	1.06847500
H	-1.01588600	4.69208500	0.10366000
H	-1.55087600	6.09941000	2.10866300
H	-2.40306200	4.55462500	2.20761800
H	-0.95315100	4.82592100	3.17833300
C	1.46681200	0.10019000	1.47073600

C	1.81395600	-1.37456200	1.56219800
H	0.85579800	0.39056600	2.33800900
H	2.37575300	0.71950100	1.51209400
C	2.58689200	-1.72170400	2.82313200
H	0.89128300	-1.97189700	1.53570600
H	2.39946600	-1.68610300	0.68200100
C	2.91292000	-3.20013700	2.90424400
H	3.51210100	-1.12675000	2.86089500
H	1.99844100	-1.41642900	3.70098000
H	3.46177400	-3.45148500	3.81754800
H	1.99972100	-3.80785000	2.89102600
H	3.52743700	-3.51931900	2.05313800
C	-2.72684000	-1.63883900	-2.44230200
C	-3.19860800	-1.21510900	-1.05851500
H	-3.44726400	-2.33009100	-2.91101600
H	-2.59732500	-0.79476200	-3.12933500
H	-1.76775500	-2.17718600	-2.41534000
C	-3.71691300	-2.40715400	-0.27621300
H	-4.02434500	-0.49833000	-1.16821500
H	-4.10983500	-2.12736500	0.70733100
H	-4.53719300	-2.90472000	-0.81947700
H	-2.94315800	-3.16986000	-0.11348500
C	0.05978200	-3.08077600	-0.79735600
O	-0.23121300	-4.02100300	-0.24696000

I

Co	-1.44916500	-0.34678800	-0.37815100
C	-1.72624700	0.92305600	-1.60514200
O	-1.89926500	1.75975500	-2.37059400
P	0.64432800	0.35472900	-0.03877800
C	-1.93459000	-0.00403000	1.30788300
O	-2.24100300	0.22014600	2.39007700
C	1.80366000	-0.16679900	-1.37170400
C	3.26720200	0.21478700	-1.22919600
H	1.38026400	0.25205800	-2.29779900
H	1.70150500	-1.25563600	-1.47807200
C	4.09992200	-0.26141700	-2.40920700
H	3.37447300	1.30577100	-1.13338000
H	3.68344300	-0.21205900	-0.30335500
C	5.56272800	0.11238300	-2.27349000
H	3.99671600	-1.35216100	-2.50839800
H	3.68722800	0.16107900	-3.33730200
H	6.15540100	-0.23426400	-3.12614700
H	5.69117200	1.19967900	-2.20467100

H	6.00286700	-0.32436900	-1.36848800
C	0.88547800	2.18017600	0.01022100
C	-0.05743000	2.91555800	0.94775900
H	0.75441500	2.54484500	-1.02014000
H	1.93052700	2.38592300	0.28504200
C	0.18901300	4.41508300	0.95392200
H	-1.09926000	2.71596400	0.65812500
H	0.04394300	2.52830200	1.97382000
C	-0.75758700	5.15113800	1.88150100
H	1.23172400	4.61359100	1.24499500
H	0.08705000	4.80100000	-0.07147900
H	-0.57592500	6.23080200	1.88051200
H	-1.80250900	4.99242600	1.58917400
H	-0.65416500	4.80045800	2.91568900
C	1.44611300	-0.19027800	1.52497800
C	1.51873200	-1.69842100	1.68995300
H	0.86507700	0.24830400	2.34898700
H	2.44885900	0.25931400	1.58093000
C	2.20246700	-2.10731600	2.98403900
H	0.50348300	-2.12113000	1.66073700
H	2.05405100	-2.15154000	0.83991500
C	2.26418300	-3.61246100	3.15375100
H	3.21787600	-1.68311900	3.00994100
H	1.66881500	-1.65394300	3.83268700
H	2.75692300	-3.90005600	4.08818100
H	1.25966100	-4.05221300	3.16168400
H	2.81672300	-4.08333900	2.33140400
C	-0.93963300	-1.98954000	-0.85230000
O	-0.62656100	-3.04969500	-1.15935800
C	-3.66233100	-1.36944100	-2.16302500
C	-3.40881000	-0.98910200	-0.71824500
H	-3.44346700	-0.56464600	-2.87197100
H	-3.07340100	-2.24353200	-2.46961200
H	-4.72113500	-1.64217600	-2.30242900
C	-3.83107100	-2.11973300	0.19818400
H	-3.99787800	-0.09436400	-0.47573200
H	-3.73529700	-1.87989700	1.26188400
H	-4.88813800	-2.37621200	0.02030900
H	-3.25463800	-3.03601800	0.01642500

TS_{insert}-ma

Co	-1.43219900	0.43788000	-0.39986000
C	-1.32703700	1.68716200	-1.71459000
O	-1.13917300	2.44641600	-2.55272700

P	0.70093200	0.17184900	-0.04930800
C	-1.75967300	1.13730700	1.23310200
O	-1.91988200	1.48791000	2.31404300
C	1.54132500	-0.89219600	-1.29207200
C	3.01939600	-1.18145400	-1.09218300
H	1.36944700	-0.39155000	-2.25772900
H	0.97236500	-1.82914100	-1.34890800
C	3.58815500	-2.03721800	-2.21330000
H	3.59651100	-0.24644700	-1.02977700
H	3.17866800	-1.69934300	-0.13355500
C	5.06033100	-2.34222400	-2.01927800
H	3.01377400	-2.97282200	-2.28101200
H	3.43290000	-1.52422000	-3.17403200
H	5.46235700	-2.95749200	-2.83076200
H	5.65594500	-1.42175800	-1.97905500
H	5.23448700	-2.88260200	-1.08055500
C	1.70883500	1.71364400	-0.10333100
C	1.18637600	2.85159600	0.75665900
H	1.74593000	2.02415100	-1.15902200
H	2.74050200	1.46343100	0.18568500
C	2.06600400	4.08805700	0.67256100
H	0.16252900	3.10979700	0.44988700
H	1.11018500	2.53335300	1.80834200
C	1.54034800	5.22916400	1.52096300
H	3.09048900	3.83003900	0.98118600
H	2.14240400	4.40481100	-0.37847400
H	2.17710600	6.11734800	1.45431100
H	0.53103500	5.52309400	1.20863200
H	1.48160200	4.94442400	2.57866200
C	1.15100100	-0.55492700	1.57938700
C	0.50805900	-1.90673100	1.83740800
H	0.83388900	0.16410500	2.34843200
H	2.24723200	-0.61968200	1.64922000
C	0.88030200	-2.47946300	3.19451000
H	-0.58643700	-1.81070000	1.76266700
H	0.79267700	-2.62162400	1.04913200
C	0.22561900	-3.82228200	3.45241600
H	1.97474100	-2.57498900	3.26364500
H	0.59397400	-1.76373200	3.97977800
H	0.49612800	-4.23000700	4.43193100
H	-0.86770200	-3.74294000	3.41833500
H	0.51941700	-4.55969300	2.69538600
C	-1.62276500	-1.20240600	-0.91301400
O	-1.47558800	-2.31472900	-1.25087000

C	-3.90112000	-0.87036200	-2.13173000
C	-3.37489100	-0.57520900	-0.74276700
H	-3.48631200	-0.19027300	-2.88274300
H	-3.67260200	-1.89661800	-2.44125300
H	-4.99402900	-0.75831700	-2.14656000
C	-3.92730800	-1.50597600	0.31508700
H	-3.64411300	0.45597600	-0.48942400
H	-3.57045600	-1.24996100	1.31826300
H	-5.02496400	-1.45345500	0.32740500
H	-3.65486900	-2.54932800	0.11526800

k

Co	-1.42177100	-0.58185900	0.69225300
C	-3.01767700	0.17305700	0.71960300
O	-4.00198700	0.76018000	0.71851900
P	0.40760000	0.29414400	-0.16472000
C	-0.94881100	-0.44574600	2.41772000
O	-0.62804500	-0.33255400	3.51196600
C	1.51954100	-0.73161700	-1.22343400
C	2.70480700	-0.03769600	-1.87668000
H	0.88380900	-1.19476400	-1.99012000
H	1.86893400	-1.55636600	-0.58450300
C	3.68341100	-1.03182600	-2.48134600
H	2.35339100	0.64547300	-2.66325400
H	3.24300800	0.59241300	-1.15160500
C	4.84224800	-0.35203800	-3.18333300
H	4.06022300	-1.69326700	-1.68577400
H	3.14772000	-1.68733700	-3.18395600
H	5.54743000	-1.07463800	-3.60670200
H	4.49103200	0.28410500	-4.00496600
H	5.40396800	0.29005200	-2.49344400
C	-0.03641900	1.69803700	-1.26593000
C	-0.75186800	2.83573500	-0.55605600
H	-0.67405500	1.27152800	-2.05409100
H	0.87657300	2.07178900	-1.75145900
C	-1.20879400	3.92047800	-1.51720200
H	-1.62141900	2.44635300	-0.00669900
H	-0.09284200	3.28383400	0.20449800
C	-1.91716600	5.05787500	-0.80808700
H	-0.34035800	4.30526400	-2.07351200
H	-1.87298100	3.47489000	-2.27199400
H	-2.24700500	5.83498500	-1.50541600
H	-2.80389600	4.69857900	-0.27192900
H	-1.26227600	5.53580800	-0.06873200

C	1.57724800	1.05030400	1.04575800
C	2.42231100	0.03068500	1.79388000
H	0.96196200	1.62173400	1.75488600
H	2.21598500	1.78506600	0.53335200
C	3.10912900	0.62358200	3.01253500
H	1.80023800	-0.82099000	2.11260700
H	3.18128000	-0.39620500	1.11914900
C	3.98833500	-0.38280100	3.72775900
H	3.70459200	1.49717300	2.70644100
H	2.34196800	1.00863200	3.70037200
H	4.47370100	0.04906700	4.60896500
H	3.40463900	-1.24794800	4.06542800
H	4.77978600	-0.76111100	3.06873600
C	-1.73199700	-1.26422500	-0.99318500
O	-1.83398500	-1.00655400	-2.15919300
C	-3.24561700	-3.20429400	-0.66447300
C	-1.83091900	-2.70212800	-0.41814600
H	-3.99763000	-2.55747100	-0.20061800
H	-3.44657600	-3.23492700	-1.74190500
H	-3.37505100	-4.21638600	-0.26372900
C	-0.78931300	-3.59570400	-1.07006300
H	-1.65008500	-2.68516200	0.68198900
H	0.23176400	-3.28511000	-0.82663400
H	-0.91026300	-4.63456200	-0.74096100
H	-0.90229600	-3.57112600	-2.16069300

TS_{acyl-iso}-ma

Co	-0.81707600	-1.24999300	-0.04781700
C	-1.75486000	-1.33304700	1.52757600
O	-2.41806600	-1.26194600	2.45924200
P	0.68244200	0.37469300	0.10227300
C	-0.60645800	-2.49965800	-1.31040800
O	-0.40287300	-3.26379700	-2.14319900
C	1.78917800	0.53604500	-1.36191100
C	2.96715700	1.48976200	-1.25978100
H	1.12243400	0.82186300	-2.18779600
H	2.13531800	-0.47940300	-1.60353900
C	3.76912800	1.55427800	-2.55004300
H	2.61984300	2.50227600	-1.00312100
H	3.63633100	1.18424600	-0.43975000
C	4.95106500	2.49864400	-2.45260000
H	4.11493600	0.54311400	-2.81206800
H	3.10625800	1.86258400	-3.37191900
H	5.52274600	2.53961700	-3.38555300

H	4.62561400	3.52062500	-2.22186700
H	5.64183000	2.19132100	-1.65748500
C	0.18300600	2.11441700	0.44979100
C	-0.97843800	2.21756900	1.42218700
H	-0.09171000	2.56496400	-0.51360000
H	1.05651400	2.66674900	0.82722900
C	-1.39022600	3.65184400	1.70403400
H	-1.83915700	1.66765600	1.01348500
H	-0.73450400	1.71435300	2.37197300
C	-2.59843200	3.73036200	2.61669600
H	-0.54380800	4.19797500	2.14733800
H	-1.60535000	4.15786400	0.75093000
H	-2.89788900	4.76420000	2.81780300
H	-3.46111000	3.21721900	2.17289000
H	-2.39972500	3.25038000	3.58289800
C	1.82019700	-0.00888400	1.50247000
C	2.37927900	-1.42011300	1.41795900
H	1.22970900	0.10631900	2.42367100
H	2.62951300	0.73420700	1.55560800
C	3.25698500	-1.78336000	2.60315300
H	1.54891400	-2.14392300	1.34354000
H	2.95773300	-1.54147500	0.48792000
C	3.81081100	-3.19118800	2.50607300
H	4.08114300	-1.05758800	2.67726200
H	2.67630700	-1.66907900	3.53069700
H	4.44108900	-3.44500100	3.36455700
H	3.00404800	-3.93277800	2.45931800
H	4.41944400	-3.31771300	1.60223600
C	-1.84053800	-0.21408700	-1.19476800
O	-1.52885400	0.74559700	-1.84029700
C	-4.19788800	0.31562200	-0.60243900
C	-3.29174800	-0.74863800	-1.20378300
H	-3.95632000	0.52074800	0.44708300
H	-4.11366000	1.25446800	-1.16209300
H	-5.24335200	-0.01092700	-0.64292400
C	-3.66770100	-1.06341400	-2.64400500
H	-3.35306100	-1.66512800	-0.60635200
H	-3.00690600	-1.81740900	-3.08600500
H	-4.69293100	-1.44808900	-2.69063300
H	-3.61059400	-0.16058400	-3.26194600
m			
Co	1.21201700	-0.35086300	-0.31200500
C	0.87466100	-2.06393900	-0.43698200

O	0.64232100	-3.16397000	-0.68695700
C	1.56709100	0.79020400	-1.60710600
O	1.70155700	1.43041800	-2.55368600
C	2.97589600	-0.59639300	0.21084200
O	2.92984200	-0.00802500	1.26670300
C	4.17114900	-1.34534200	-0.32279300
C	5.45053000	-0.96321700	0.40106000
H	3.92355000	-2.39977200	-0.10179400
H	5.70643500	0.08538400	0.20743600
H	5.35664500	-1.08328000	1.48392200
P	-0.88309000	0.36527500	0.00462900
C	-2.00636300	-0.06193800	-1.39087000
C	-1.02897600	2.19571300	0.13271300
C	-1.77392600	-0.20336900	1.51331000
C	-3.47016800	0.32302800	-1.26291600
H	-1.90256500	-1.14343900	-1.56108800
H	-1.55638600	0.41216800	-2.27697600
C	-0.08675200	2.78554900	1.17055100
H	-2.06928400	2.47802300	0.35102400
H	-0.79133600	2.59680800	-0.86479500
C	-1.95501400	-1.70897300	1.60131200
H	-2.74587700	0.31159800	1.55976000
H	-1.19376100	0.15316100	2.37586000
C	-4.27175300	-0.04209100	-2.50225700
H	-3.91952000	-0.17227800	-0.38787100
H	-3.56728200	1.40388200	-1.07831800
C	-0.09959300	4.30489700	1.17504400
H	-0.35424600	2.41978800	2.17425200
H	0.93787400	2.42421000	0.98955100
C	-2.79849100	-2.12107000	2.79634300
H	-2.42107000	-2.09770600	0.68152100
H	-0.97085600	-2.19536800	1.66024900
C	-5.73489100	0.33457600	-2.37815500
H	-3.82806300	0.45276200	-3.37890300
H	-4.17485400	-1.12170900	-2.69062300
C	0.82752400	4.88682100	2.22391700
H	0.18511800	4.66985400	0.17684100
H	-1.12762200	4.66193800	1.34074300
C	-2.95552200	-3.62509600	2.90290600
H	-2.34246600	-1.72332600	3.71544600
H	-3.78766700	-1.64306200	2.72463500
H	-6.30461200	0.06899000	-3.27453900
H	-6.20588400	-0.17323600	-1.52736900
H	-5.85607300	1.41332300	-2.21962300

H	0.82194200	5.98174400	2.21501700
H	0.53976300	4.56414100	3.23210500
H	1.86185600	4.55996900	2.06326500
H	-3.56723300	-3.91425200	3.76372400
H	-3.43192000	-4.03957800	2.00590800
H	-1.98225100	-4.11914500	3.00874600
H	6.28813200	-1.57904800	0.05561500
C	4.28763700	-1.19820000	-1.82988100
H	5.09916500	-1.82504400	-2.21450900
H	3.36219700	-1.48718600	-2.33825900
H	4.51206500	-0.16049000	-2.10696100

TS_{H2}-ma

Co	1.29046600	-0.19298100	0.04335700
C	1.02675300	-1.92738000	0.03132000
O	0.84913700	-3.04818100	-0.15996700
C	1.66131700	1.01052700	-1.18256300
O	1.81718000	1.69874900	-2.09062200
C	3.19470200	-0.41307300	0.30730500
O	3.59532700	0.27707800	1.20934200
C	4.09882600	-1.37194800	-0.45669500
C	5.55923800	-1.18413900	-0.08759200
H	3.76657000	-2.37388300	-0.13215000
H	5.91182800	-0.19131200	-0.39162900
H	5.72116600	-1.26889700	0.99050500
P	-0.90389900	0.34265700	0.02447700
C	-1.74102500	-0.37691700	-1.45083900
C	-1.27881700	2.14107500	-0.12342100
C	-1.96971100	-0.14740400	1.44726700
C	-3.23286600	-0.13848600	-1.60820100
H	-1.52098200	-1.45406900	-1.44906400
H	-1.19118700	0.02604600	-2.31563600
C	-0.56251900	2.99144800	0.91336500
H	-2.36572300	2.29694900	-0.06103300
H	-0.97367200	2.44573000	-1.13623100
C	-1.99914000	-1.64052700	1.72374900
H	-2.98548900	0.23536100	1.26603600
H	-1.59466400	0.39029800	2.32958500
C	-3.78033600	-0.74862700	-2.88884000
H	-3.77839400	-0.56097300	-0.74987900
H	-3.45236900	0.94002500	-1.60301200
C	-0.82800200	4.47662100	0.73299000
H	-0.86827100	2.69115900	1.92835100
H	0.52107800	2.80363600	0.86238000

C	-2.95344300	-2.00221600	2.84988900
H	-2.28751300	-2.19441300	0.81592600
H	-0.98782400	-1.99394300	1.97359300
C	-5.27037900	-0.52001500	-3.04851900
H	-3.23999700	-0.32790400	-3.74978600
H	-3.56073400	-1.82662500	-2.89891800
C	-0.11564700	5.32092000	1.77121800
H	-0.51330100	4.77755600	-0.27740600
H	-1.91212500	4.66189900	0.77545700
C	-2.96883600	-3.49013000	3.13958100
H	-2.67212900	-1.44431900	3.75573000
H	-3.96661100	-1.65797500	2.59166000
H	-5.65671500	-0.96174100	-3.97271400
H	-5.83210600	-0.95931300	-2.21485300
H	-5.50851800	0.55060500	-3.07178900
H	-0.30662100	6.38996400	1.63210200
H	-0.43767500	5.05862000	2.78660200
H	0.96980300	5.17143300	1.72696700
H	-3.66006600	-3.74328400	3.94998100
H	-3.27293400	-4.06410100	2.25568400
H	-1.97405300	-3.84837300	3.43050100
H	6.18403600	-1.93019200	-0.59173900
C	3.87824000	-1.26961500	-1.95714400
H	4.48690300	-2.01221500	-2.48454900
H	2.83132200	-1.43292100	-2.23313900
H	4.17140300	-0.27967100	-2.32962200
H	0.94463700	-0.08818200	2.36700700
H	1.32354900	0.56381100	2.34004300

TS_{co}-(anti-ma)

Co	-1.26801700	0.75617500	-0.21234800
C	-1.12115300	1.09516700	-1.92213200
O	-0.98646100	1.44810300	-3.00798800
P	0.83563700	0.09106300	-0.00756600
C	-1.39415700	1.49598000	1.38055500
O	-1.44446200	2.10365900	2.35341000
C	1.25355100	-1.35427500	-1.07270400
C	2.64374500	-1.95093800	-0.93736100
H	1.07892100	-1.01318500	-2.10521600
H	0.48122900	-2.11545200	-0.89212600
C	2.87177000	-3.10258900	-1.90374800
H	3.41058000	-1.18031100	-1.11067600
H	2.80694800	-2.31013500	0.09049200
C	4.25560600	-3.70675000	-1.76919900

H	2.10519700	-3.87346700	-1.73472700
H	2.71359800	-2.74808800	-2.93310700
H	4.41218600	-4.53463200	-2.46827300
H	5.03611500	-2.96079800	-1.96365800
H	4.42353600	-4.09536800	-0.75709100
C	2.10710400	1.33767300	-0.47442900
C	1.86808600	2.70043700	0.15593100
H	2.07586900	1.41987200	-1.57206600
H	3.10645700	0.95981400	-0.21249200
C	2.92439700	3.71813100	-0.23964700
H	0.87169300	3.06660900	-0.13401100
H	1.84305300	2.61392700	1.25416400
C	2.67559900	5.07943600	0.37950900
H	3.91802500	3.34663900	0.05400600
H	2.95049500	3.80256400	-1.33650200
H	3.43878300	5.80861400	0.08852400
H	1.70198200	5.48158300	0.07469100
H	2.67377100	5.02371200	1.47503600
C	1.34658200	-0.42666900	1.68324400
C	0.48716600	-1.55617900	2.22687400
H	1.24883300	0.46050700	2.32584500
H	2.41164900	-0.70095900	1.68909100
C	0.79221300	-1.88289800	3.67894200
H	-0.57807600	-1.28945400	2.12759800
H	0.62216900	-2.46220800	1.61466800
C	-0.06135500	-3.01856700	4.20772300
H	1.85910500	-2.13399800	3.77956900
H	0.63940800	-0.98068300	4.28964900
H	0.15919200	-3.24459300	5.25601700
H	-1.12892000	-2.77617400	4.14076400
H	0.09895800	-3.93859400	3.63204500
C	-3.25276400	0.85113100	-0.33637600
C	-3.61861700	-0.42674200	0.40498300
C	-5.00995300	-0.93620900	0.05456200
H	-3.60998400	0.81236600	-1.37410700
H	-3.72439500	1.72622500	0.12634500
H	-3.54916500	-0.26311600	1.49043700
H	-5.27431000	-1.83917600	0.61809200
H	-5.76650700	-0.17216700	0.27070400
H	-5.08895600	-1.17333400	-1.01355400
H	-2.88571600	-1.23003000	0.19308600
C	-2.08898800	-1.93752100	-2.23424400
O	-2.92567800	-1.69437400	-2.94932700

j

Co	-1.42026700	-0.29694000	-0.05314400
C	-1.83986400	0.84054400	-1.36358700
O	-2.12074400	1.58992000	-2.18534200
P	0.72015300	0.31406700	-0.08729500
C	-1.66286700	0.19374100	1.64875700
O	-1.84420700	0.48880200	2.74112400
C	1.65570700	-0.41555000	-1.49608200
C	3.14085300	-0.11182200	-1.59605300
H	1.12626000	-0.07281900	-2.39859700
H	1.48878600	-1.50120800	-1.46240700
C	3.77618700	-0.75875400	-2.81690300
H	3.31104200	0.97454100	-1.63823100
H	3.66322400	-0.46423500	-0.69291600
C	5.25935600	-0.46377400	-2.92232900
H	3.60919700	-1.84544300	-2.77883000
H	3.25711600	-0.41058800	-3.72217300
H	5.70920100	-0.93289900	-3.80325100
H	5.44677000	0.61479700	-2.99301000
H	5.80179600	-0.83047400	-2.04212400
C	1.03422500	2.11765800	-0.28518200
C	0.28207800	2.99834800	0.69856700
H	0.75031300	2.37561200	-1.31704600
H	2.11647800	2.29623500	-0.20330100
C	0.56240500	4.47610100	0.48127600
H	-0.79835600	2.81260600	0.61245200
H	0.54896300	2.72941100	1.73292600
C	-0.18993800	5.35566000	1.46033700
H	1.64441400	4.65975500	0.56451000
H	0.29264500	4.74564900	-0.55085400
H	0.01424100	6.41884900	1.29721300
H	-1.27332100	5.21073800	1.37200400
H	0.08425900	5.12271300	2.49659000
C	1.71462400	-0.10074600	1.40393100
C	1.75658200	-1.58484300	1.72501500
H	1.27055700	0.45085000	2.24506300
H	2.73049900	0.30117700	1.27220100
C	2.61120400	-1.89018400	2.94388600
H	0.73389800	-1.95456100	1.89105700
H	2.14134700	-2.15311700	0.86276600
C	2.64079000	-3.36982900	3.27227500
H	3.63422600	-1.52135000	2.77338700
H	2.22901900	-1.32075300	3.80425100
H	3.25830400	-3.58274300	4.15089700

H	1.63317000	-3.75089700	3.47720100
H	3.04397200	-3.95493900	2.43656000
C	-3.41081000	-0.83512500	-0.03140200
C	-3.96900000	-1.41027400	-1.31732900
C	-5.43851600	-1.77652600	-1.17100000
H	-3.97370200	0.06361000	0.25306100
H	-3.53201900	-1.55777700	0.78649000
H	-3.40183500	-2.30117700	-1.62195400
H	-5.85125100	-2.19154700	-2.09813500
H	-5.58447900	-2.52321200	-0.38064700
H	-6.04124800	-0.89959300	-0.90407400
H	-3.85473600	-0.69360200	-2.14292800
C	-1.07269300	-2.02188900	-0.37677200
O	-0.88326900	-3.13667900	-0.56556500

TS_{insert}-(anti-ma)

Co	-1.27777200	-0.64081100	0.23690700
C	-1.92544200	0.19951000	-1.12413800
O	-2.09592700	0.85368200	-2.08228500
P	0.62664800	0.36385100	-0.06271400
C	-1.35676200	-0.29561200	2.01022200
O	-1.33199000	-0.00791300	3.12055500
C	1.48765500	-0.21576600	-1.58243700
C	2.85951500	0.36475200	-1.88155700
H	0.78835800	-0.00467100	-2.40529200
H	1.53943400	-1.31185400	-1.51955600
C	3.43602600	-0.17106600	-3.18264900
H	2.80907600	1.46270200	-1.93821100
H	3.55823600	0.13632800	-1.06160500
C	4.80779100	0.39842500	-3.48590700
H	3.48620200	-1.26889000	-3.13112600
H	2.74268500	0.05587900	-4.00589700
H	5.21618700	0.00789800	-4.42362300
H	4.77472800	1.49156300	-3.57220500
H	5.52370800	0.15724700	-2.69034800
C	0.55882500	2.18808500	-0.29038400
C	-0.28120800	2.90771800	0.75108700
H	0.14956300	2.36746000	-1.29528600
H	1.58741100	2.57807900	-0.29016600
C	-0.28783800	4.41373300	0.55015500
H	-1.31190400	2.52517000	0.71533900
H	0.08340000	2.67903900	1.76541300
C	-1.14486300	5.12871100	1.57617000
H	0.74430000	4.79366600	0.59197200

H	-0.64773600	4.63975300	-0.46470800
H	-1.14593200	6.21338400	1.42658800
H	-2.18643400	4.78857700	1.52876600
H	-0.78818000	4.93697800	2.59569400
C	1.87092900	0.17795500	1.28080900
C	2.22023200	-1.26424900	1.60502000
H	1.45940000	0.67487400	2.17082200
H	2.77148500	0.74485900	1.00077400
C	3.28047300	-1.37452300	2.68793300
H	1.31429400	-1.80184700	1.92172000
H	2.57190100	-1.78558900	0.69997300
C	3.61883700	-2.81417100	3.02105500
H	4.18680000	-0.83898200	2.36621800
H	2.93005300	-0.85122500	3.59014200
H	4.38330900	-2.88622600	3.80152300
H	2.73446700	-3.35775500	3.37462200
H	3.99584300	-3.34836600	2.14024000
C	-3.38369900	-0.62265100	-0.35982600
C	-3.92407000	-1.50995300	-1.46411900
C	-5.37805500	-1.87307200	-1.21654800
H	-3.95989300	0.30270400	-0.25238700
H	-3.45364300	-1.14051700	0.60238700
H	-3.31525800	-2.42186900	-1.53183400
H	-5.77760800	-2.50685000	-2.01604000
H	-5.50140300	-2.41593900	-0.27147000
H	-6.00730600	-0.97630400	-1.16245000
H	-3.82906000	-1.00659000	-2.43507100
C	-0.77498600	-2.35876600	-0.06912000
O	-0.37539800	-3.40363400	-0.31768100

I

Co	0.95934500	-1.16862300	0.26133200
C	1.70197700	0.05379700	1.41162800
O	1.54907800	0.73413700	2.38578500
P	-0.56753600	0.36700900	-0.11007700
C	0.67255700	-2.12111700	-1.23364100
O	0.46454000	-2.69526100	-2.20323600
C	-1.56765000	0.65111500	1.40371900
C	-2.63046800	1.73592200	1.34824500
H	-0.84309600	0.85016500	2.20576300
H	-2.01682300	-0.32231500	1.64977300
C	-3.49302500	1.75099000	2.60008500
H	-2.15675000	2.72166500	1.22719900
H	-3.28128500	1.60553200	0.46855400

C	-4.53315800	2.85349100	2.57612300
H	-3.98350600	0.77199000	2.71073100
H	-2.84612600	1.85969900	3.48284100
H	-5.15397900	2.85233600	3.47799900
H	-4.06315200	3.84200300	2.50268300
H	-5.20486700	2.74892200	1.71482200
C	0.00802000	2.04601200	-0.60005000
C	0.85288200	2.03204100	-1.86484700
H	0.58732900	2.44041200	0.24835800
H	-0.85747600	2.71186700	-0.72560800
C	1.54584400	3.35951800	-2.12129500
H	1.60906200	1.23251100	-1.80321200
H	0.22562000	1.77479500	-2.73249900
C	2.36559900	3.34900800	-3.39629000
H	0.79444500	4.16241700	-2.16136200
H	2.18948900	3.59926200	-1.26083700
H	2.86917000	4.30560600	-3.56931300
H	3.13855400	2.57112300	-3.36480500
H	1.73712600	3.14517900	-4.27194500
C	-1.81108300	-0.01993400	-1.41579400
C	-2.70203000	-1.20486600	-1.07856500
H	-1.24488300	-0.22694200	-2.33534800
H	-2.41621400	0.87599400	-1.62070500
C	-3.50076100	-1.69219900	-2.27572200
H	-2.09544200	-2.03543400	-0.68398900
H	-3.39358700	-0.93409600	-0.26557700
C	-4.42289200	-2.84331300	-1.92605800
H	-4.08224100	-0.85495500	-2.69125200
H	-2.80404300	-1.99617400	-3.07122300
H	-4.98835700	-3.19495500	-2.79512700
H	-3.85823600	-3.69765600	-1.53343800
H	-5.14903700	-2.55283000	-1.15669800
C	2.99895500	0.03939400	0.57200600
C	4.18346700	-0.38280100	1.42834000
C	5.48380800	-0.38003300	0.65003000
H	3.13167600	1.05674400	0.17315500
H	2.92457200	-0.62746900	-0.31594400
H	3.98626900	-1.38275500	1.84014700
H	6.33161200	-0.67640000	1.27655600
H	5.44434500	-1.07345000	-0.19906600
H	5.70477900	0.61645400	0.24818200
H	4.24387100	0.29432000	2.29044900
C	0.88331600	-2.41408800	1.51176000
O	0.72635200	-3.20056500	2.32968600

TS_{acyl-iso}-(anti-ma)

Co	0.95008000	-0.94358400	-0.45840400
C	1.66249800	-0.38192200	-2.05510500
O	2.18147900	0.08354600	-2.96401100
P	-0.78768100	0.33925500	0.03237700
C	1.13448300	-2.52317500	0.36077900
O	1.18806500	-3.52094600	0.92693400
C	-1.67697100	-0.12755500	1.57732800
C	-2.98810700	0.57684400	1.88072200
H	-0.94751700	0.03576400	2.38303600
H	-1.82517700	-1.21630000	1.53260100
C	-3.59754100	0.11972900	3.19679600
H	-2.83781500	1.66665100	1.91560000
H	-3.71428900	0.39884500	1.07163800
C	-4.90870200	0.81679900	3.50199600
H	-3.74769800	-0.96990900	3.16715500
H	-2.87745500	0.29733300	4.00912600
H	-5.34123500	0.48241200	4.45068300
H	-4.77537400	1.90380500	3.56695000
H	-5.65206400	0.62787100	2.71745500
C	-0.62902400	2.16945900	0.17214900
C	0.29744500	2.77607900	-0.86742000
H	-0.25482900	2.38095600	1.18306900
H	-1.63182200	2.61661800	0.09996600
C	0.36957900	4.29058000	-0.77240400
H	1.30690700	2.35245600	-0.75074600
H	-0.02296400	2.49140400	-1.88280800
C	1.31399000	4.89014500	-1.79566200
H	-0.63913800	4.71236300	-0.89863500
H	0.68475300	4.57296100	0.24330100
H	1.36135600	5.98164400	-1.72219000
H	2.33352600	4.50663000	-1.66709800
H	1.00268200	4.64171000	-2.81780500
C	-2.04630400	0.14326000	-1.30186400
C	-2.35896600	-1.31724800	-1.58579500
H	-1.62468600	0.61747000	-2.20053700
H	-2.96083600	0.70206500	-1.05415400
C	-3.33521700	-1.50292100	-2.73445600
H	-1.42381800	-1.85953600	-1.81034400
H	-2.76662500	-1.79836100	-0.68217200
C	-3.64221800	-2.96241700	-3.00599600
H	-4.26424500	-0.95714000	-2.50975500
H	-2.92355000	-1.02914100	-3.63813700

H	-4.34577900	-3.08694700	-3.83556000
H	-2.73191900	-3.51902300	-3.26005600
H	-4.08256900	-3.44663900	-2.12566000
C	1.94905500	-0.11488200	0.86514500
O	1.58696500	0.54332100	1.79870500
C	3.43788500	-0.36124700	0.59332400
C	4.11694800	-0.92678300	1.83384200
H	3.59626700	-1.02038000	-0.26544300
H	3.63472700	-1.87677100	2.10678800
H	3.94490100	-0.24534000	2.67607400
H	3.86304500	0.62075100	0.33312900
C	5.60045800	-1.14076100	1.60758500
H	6.10506400	-0.19919500	1.35845200
H	6.08951600	-1.55059400	2.49749500
H	5.78391600	-1.83776600	0.78103500

n

Co	-1.14691700	0.23665100	-0.19583000
C	-1.46470700	0.64494000	1.48390600
O	-1.63590500	1.05686200	2.54465600
P	1.07901000	0.17222900	-0.08202100
C	-2.77213800	-0.61184000	-0.46632000
O	-2.36538300	-1.74137300	-0.62371500
C	1.77152400	-0.86721900	-1.43574500
C	3.27156600	-1.10698200	-1.44129200
H	1.45427000	-0.37623700	-2.36827400
H	1.21997100	-1.81860200	-1.41058400
C	3.71535700	-1.95452500	-2.62308000
H	3.81035500	-0.14713400	-1.46545800
H	3.58367600	-1.60219200	-0.50890400
C	5.21167500	-2.19747000	-2.63269700
H	3.17730700	-2.91391000	-2.60201600
H	3.40719000	-1.46245100	-3.55752100
H	5.52305000	-2.80829100	-3.48626800
H	5.76796400	-1.25331100	-2.68430600
H	5.53658100	-2.71591100	-1.72208300
C	1.97490000	1.76909800	-0.25186200
C	1.42397800	2.85527100	0.65877900
H	1.87897000	2.07506800	-1.30512100
H	3.04693300	1.61120700	-0.06229700
C	2.17751600	4.16728500	0.52293600
H	0.35854000	3.01436000	0.43440300
H	1.45723400	2.52504500	1.70950500
C	1.61536500	5.25189000	1.42068300

H	3.24156400	4.00297300	0.75162500
H	2.14560400	4.49394000	-0.52737900
H	2.16214800	6.19488100	1.31740100
H	0.56299600	5.45358800	1.18729500
H	1.66170400	4.95787900	2.47647700
C	1.77085600	-0.55038900	1.46155100
C	1.26988600	-1.96406600	1.71059000
H	1.45166500	0.10908300	2.28203800
H	2.87015900	-0.51525000	1.43981800
C	1.65604500	-2.49149400	3.08212500
H	0.17356800	-1.99361600	1.59908900
H	1.66093900	-2.64423700	0.93752500
C	1.17900000	-3.91226800	3.30974700
H	2.74918700	-2.43702000	3.19989900
H	1.23971600	-1.82610800	3.85307100
H	1.45166500	-4.28296000	4.30326400
H	0.08845200	-3.98321100	3.21860000
H	1.61053200	-4.59990300	2.57191000
C	-4.20481000	-0.18703000	-0.51176300
C	-5.20436200	-1.29786200	-0.77977400
C	-6.62697600	-0.77424800	-0.80768100
H	-4.41248700	0.32567800	0.44072900
H	-4.27335300	0.61230400	-1.26647200
H	-6.90028000	-0.30665300	0.14649400
H	-6.75893100	-0.01534800	-1.58899400
H	-7.35151600	-1.57214900	-1.00063000
H	-5.09703600	-2.07595600	-0.01282200
H	-4.95708900	-1.78731300	-1.73075400
C	-1.22581100	1.23674600	-1.63677200
O	-1.24781300	2.02572700	-2.47488100

TS_{H2}-(anti-ma)

Co	1.19308700	-0.06189000	0.07285200
C	1.06455500	-1.80979700	-0.07071900
O	0.98036200	-2.92819900	-0.32263100
C	1.56186300	1.32576100	-0.93455200
O	1.76368900	2.15376200	-1.70667400
C	3.09139600	-0.26132300	0.38884500
O	3.43402400	0.03539300	1.50656300
C	4.06423400	-0.73921300	-0.66178100
C	5.51333900	-0.80769300	-0.21771400
H	3.94583800	-0.08224500	-1.53848000
H	3.70912900	-1.72128200	-1.01330000
C	6.41850000	-1.29651700	-1.33186200

H	5.83423600	0.18267600	0.13045000
H	5.59443200	-1.46420600	0.65822000
H	7.46568000	-1.34735600	-1.01510100
H	6.12994700	-2.29924600	-1.67168700
H	6.37233900	-0.63408600	-2.20551400
H	0.57705800	0.40887000	2.49038800
H	1.32689600	0.41343100	2.40829400
P	-1.03678800	0.29030600	-0.03118300
C	-1.77335700	-0.52900900	-1.50884800
C	-1.57244700	2.04222200	-0.22644300
C	-2.07987000	-0.27318900	1.38114200
C	-3.27722600	-0.43440800	-1.70101900
H	-1.45568600	-1.58088200	-1.48331500
H	-1.24381700	-0.09163200	-2.36947600
C	-1.02098500	2.96812200	0.84602600
H	-2.67060600	2.09343500	-0.24682900
H	-1.22358000	2.36592500	-1.21918100
C	-1.95855500	-1.75489600	1.69163800
H	-3.12546600	0.00022500	1.17317500
H	-1.78079600	0.31820000	2.25831000
C	-3.73603100	-1.11465200	-2.98126000
H	-3.79921500	-0.89300900	-0.84669300
H	-3.59840800	0.61804000	-1.72030900
C	-1.32729400	4.42941900	0.56385100
H	-1.43232900	2.69427600	1.83041500
H	0.06831800	2.83502300	0.93280600
C	-2.87722900	-2.18717300	2.82238700
H	-2.18391300	-2.35480100	0.79526000
H	-0.91706800	-1.99462900	1.95309400
C	-5.23730200	-1.03252100	-3.17484200
H	-3.21987000	-0.65781700	-3.83866400
H	-3.41429600	-2.16660600	-2.96762400
C	-0.80215300	5.35027500	1.64740900
H	-0.89016500	4.70395200	-0.40796800
H	-2.41425100	4.56077100	0.45082300
C	-2.74443500	-3.66273000	3.14354400
H	-2.65717800	-1.58537800	3.71696800
H	-3.91867800	-1.95180000	2.55454500
H	-5.55935200	-1.52353500	-4.09880200
H	-5.77236500	-1.51094800	-2.34520200
H	-5.57628700	0.00977900	-3.22147500
H	-1.01781000	6.40185800	1.43216200
H	-1.24956400	5.11534200	2.62111700
H	0.28455300	5.25293900	1.75798400

H	-3.41055400	-3.96700400	3.95737500
H	-2.98522000	-4.28280100	2.27132400
H	-1.72011200	-3.91276800	3.44478500

12. Structures in Figure S1

TS_{co-ma}

Co	-0.28839200	0.42192100	0.15031800
C	2.79550400	-0.25511000	-1.29802400
O	3.41987600	-1.12670100	-0.95213700
C	-1.58725200	1.44124900	-0.50370500
O	-2.47081100	2.07789400	-0.83810900
C	0.30859700	-0.65656300	1.44467300
O	0.62517300	-1.28245400	2.34214900
C	0.88672900	1.74762200	0.43828100
O	1.63668600	2.58883500	0.60209900
C	-1.44185100	-1.10716400	-0.52073200
H	-2.28444200	-0.71557100	-1.10528700
C	-1.99791500	-2.14497500	0.42905900
H	-2.64989400	-1.70482800	1.19150800
H	-1.21139900	-2.70350600	0.95105400
H	-2.59866900	-2.88624000	-0.12031500
C	-0.41537400	-1.67752900	-1.48289900
H	0.07094100	-0.90975700	-2.10305800
H	0.37121100	-2.23587000	-0.95872200
H	-0.88920700	-2.38184900	-2.18571500

TS_{co-(anti-ma)}

Co	-0.82657100	-0.01979400	0.16152100
C	-0.17618800	-1.41510000	1.05087800
O	0.22833400	-2.25948800	1.69830200
C	-1.47218500	1.64089500	0.00553300
O	-1.88075300	2.70229800	0.01904700
C	0.83123300	0.93170000	0.82807200
C	1.50096700	1.50522400	-0.41461900
C	2.94514400	1.90398100	-0.15148700
H	1.52633200	0.25648100	1.34459500
H	0.59789200	1.72494200	1.55013800
H	0.94180100	2.37874100	-0.77970800
H	3.41253200	2.35548700	-1.03408900
H	3.00674400	2.63016600	0.66806800
H	3.55022500	1.03619100	0.13834600
H	1.47262500	0.78322700	-1.24727700
C	2.03131600	-1.75588000	-1.25411400
O	3.01581400	-1.79420300	-0.70742400

C	-2.16853000	-0.87815100	-0.65199500
O	-3.00605200	-1.42696000	-1.19426800

i

Co	0.38471400	-0.00007800	0.01370800
C	-0.23740600	-0.00730800	1.70609100
O	-0.65092000	-0.01194100	2.76789600
C	0.47146600	-1.52235400	-0.97309300
O	0.49996800	-2.45748100	-1.62161100
C	0.47207300	1.52882600	-0.96239500
O	0.50090700	2.46828600	-1.60462600
C	2.13087900	-0.00163100	0.49239500
O	3.22438900	-0.00229700	0.80139700
C	-1.66297900	0.00278200	-0.50840700
H	-1.61717400	0.00693800	-1.60539400
C	-2.39362500	1.24400400	-0.03802700
H	-1.94957400	2.18015300	-0.38845300
H	-2.45786600	1.30009700	1.05539700
H	-3.42985000	1.22308300	-0.40961300
C	-2.39475600	-1.24144100	-0.04773500
H	-1.95124000	-2.17522300	-0.40518300
H	-2.45942400	-1.30590500	1.04522500
H	-3.43080900	-1.21683600	-0.41952500

j

Co	-0.55465300	0.00000900	0.01001800
C	-0.11635700	-1.58957000	-0.73822000
O	0.20098000	-2.59527100	-1.16723700
C	-0.90307100	0.00055400	1.79396400
O	-1.03947200	0.00104600	2.92327300
C	-0.11633000	1.58910300	-0.73926700
O	0.20103200	2.59454200	-1.16887800
C	-2.27467500	-0.00014000	-0.54614700
O	-3.35458900	-0.00037100	-0.89925800
C	1.42584500	0.00017400	0.63914100
H	1.54018100	0.88183500	1.28255600
H	1.54019400	-0.88112900	1.28304600
C	2.48949100	-0.00011800	-0.44004800
C	3.88256600	-0.00001100	0.17164800
H	2.38163800	0.87428200	-1.09587800
H	2.38159400	-0.87481200	-1.09547600
H	4.66199800	-0.00022600	-0.59839900
H	4.04083600	0.88346200	0.80180500
H	4.04077600	-0.88317800	0.80224600

TS_{insert}-ma

Co	-0.11557900	0.35186200	0.25833100
C	0.60418500	0.10169200	-1.30282100
O	1.10375800	0.17625300	-2.34285600
C	-1.59223600	-0.07036400	1.25370100
O	-2.53292700	-0.34632300	1.83165200
C	-0.61010500	2.02877700	-0.07695700
O	-0.89824100	3.10609500	-0.30958400
C	0.06802100	-1.68060900	-0.66850600
H	-0.28742900	-1.96875700	0.32404200
C	-0.96840900	-2.04899000	-1.70410100
H	-1.10785200	-3.13929000	-1.71766700
H	-1.94042000	-1.59052300	-1.49896900
H	-0.66174600	-1.75241100	-2.71388300
C	1.40696400	-2.35602800	-0.88090100
H	2.15594400	-2.04120900	-0.14653200
H	1.81195800	-2.16869200	-1.88086900
H	1.28119800	-3.44227300	-0.77670300
C	1.30165300	0.35849700	1.44366500
O	2.19117800	0.42585700	2.14892800

TS_{insert}-(anti-ma)

Co	3.31317100	-0.23023800	0.22367000
C	2.21499400	-1.59572200	0.64700400
O	1.51188700	-2.44066900	0.94390100
C	4.75120200	-1.25227500	-0.21269700
O	5.64296200	-1.88067900	-0.53424700
C	2.04077300	0.87281400	-0.21082900
O	1.10368300	1.53277600	-0.34118900
C	4.00435900	0.67738600	1.64631100
O	4.40158200	1.22545800	2.56072100
C	3.33861900	0.80896000	-1.70386100
H	4.42961100	0.73076400	-1.73218800
H	3.13646100	1.88255600	-1.78965300
C	2.68383300	0.02387800	-2.81936500
H	2.97817300	-1.03209100	-2.75150500
H	1.59100200	0.03650500	-2.70250200
C	3.05692100	0.58229900	-4.18272500
H	2.59342200	0.01050100	-4.99376300
H	2.73298200	1.62475400	-4.28680200
H	4.14200600	0.55942100	-4.34065700

k

Co	-0.59138900	0.00008000	-0.00634000
C	-0.86350900	-1.59550600	-0.76115100
O	-1.08866000	-2.56527800	-1.31589300
C	-1.96098100	-0.00035500	1.20632400
O	-2.81491500	-0.00067300	1.95713500
C	1.14631800	0.00033500	-0.66595200
O	1.80733800	0.00077800	-1.64791100
C	-0.86352100	1.59611500	-0.76013800
O	-1.08861700	2.56621800	-1.31432600
C	1.66591500	-0.00026800	0.78734200
H	0.81362100	-0.00015000	1.51002000
C	2.47720700	-1.26796800	1.00350500
H	1.87948700	-2.17080400	0.84059800
H	3.32215700	-1.29144500	0.30587500
C	2.47820400	1.26667100	1.00424600
H	1.88113100	2.17006500	0.84207500
H	2.87514000	1.30037400	2.02485000
H	3.32306400	1.29000100	0.30650300
H	2.87394800	-1.30269000	2.02414900

I

Co	0.66811300	-0.07139300	-0.01508000
C	1.69771100	1.13874600	-0.82936000
O	2.40501100	1.92161900	-1.25986100
C	0.57421600	-0.34787200	1.74876000
O	0.60095100	-0.46650700	2.88183000
C	1.54649100	-1.59704200	-0.51762600
O	2.09626100	-2.54251500	-0.82844000
C	-0.69748900	1.17499700	0.11705300
O	-1.02066100	2.21338300	0.58300400
C	-1.56638600	0.23959200	-0.73950900
H	-1.02727000	-0.68337100	-1.05590500
H	-1.78533500	0.77919200	-1.66986500
C	-2.83273200	-0.14242200	0.01505000
H	-3.35624500	0.78072500	0.29533700
H	-2.55452000	-0.63285400	0.95857800
C	-3.73191500	-1.04511200	-0.80499500
H	-4.64569600	-1.30336900	-0.26054100
H	-4.03316600	-0.56206400	-1.74213900
H	-3.22868500	-1.98380700	-1.06681300

TS_{acy-iso}-(anti-ma)

Co	0.95069500	0.15726500	0.29918600
C	1.10909500	1.97048200	-0.10879000

O	1.17310400	3.05310500	-0.45242700
C	0.11855500	-0.38547300	1.81215700
O	-0.33243600	-0.78495100	2.78195500
C	-0.36660800	-0.63283200	-0.77235700
O	-0.31686100	-1.62337900	-1.41771500
C	-1.59320400	0.28706700	-0.71745600
C	-2.81902300	-0.52070900	-0.30506600
H	-1.45429700	1.14244200	-0.05055700
H	-2.64848600	-0.96400600	0.68627100
H	-2.93893600	-1.36192500	-0.99857000
H	-1.71053200	0.68163600	-1.73695700
C	-4.06357000	0.34432900	-0.28364300
H	-4.26513100	0.77835500	-1.27024100
H	-4.94623600	-0.23367400	0.00766400
H	-3.96483600	1.17411200	0.42617300
C	2.21450700	-0.84791800	-0.48888000
O	3.05883700	-1.48887100	-0.90651400

n

Co	0.99784600	0.00017900	0.10062900
C	0.84420600	1.60847300	-0.65039500
O	0.74584500	2.57811500	-1.24546900
C	-0.83060400	0.00082300	0.52468700
O	-0.70422500	0.00229500	1.72070600
C	-2.10471400	-0.00053400	-0.24974400
C	-3.36809000	0.00048300	0.59277500
C	-4.61192200	-0.00103300	-0.27389200
H	-2.06529700	0.86693800	-0.92769700
H	-2.06499300	-0.87002100	-0.92509400
H	-4.64810900	0.88109000	-0.92485900
H	-4.64776600	-0.88508400	-0.92225800
H	-5.52514500	-0.00032300	0.32919200
H	-3.36224800	0.87582500	1.25487500
H	-3.36191700	-0.87288600	1.25746900
C	0.84322700	-1.60817500	-0.64975200
O	0.74439200	-2.57801100	-1.24445300
C	2.78291200	-0.00092200	0.46188500
O	3.88943000	-0.00178300	0.72021500

TS_{H2}-(anti-ma)

Co	-1.03691300	0.00006500	0.12866800
C	-0.74341100	-1.70400100	-0.30679300
O	-0.53233300	-2.76171700	-0.67598500
C	-0.74219500	1.70391500	-0.30672200

O	-0.53027300	2.76145600	-0.67593300
C	-2.82823400	0.00068500	-0.18275400
O	-3.94141200	0.00109100	-0.41263500
C	0.86340100	-0.00045000	0.65666300
O	1.00965400	-0.00014600	1.84725400
C	1.99644700	-0.00122200	-0.33334300
C	3.38412600	0.00050800	0.28057300
H	1.85100400	0.86559600	-0.99812400
H	1.85201700	-0.87048500	-0.99517900
C	4.46415500	-0.00004600	-0.78366300
H	3.49067100	0.87476500	0.93544400
H	3.49189200	-0.87197400	0.93759700
H	5.46687800	0.00112400	-0.34442100
H	4.39066900	-0.88378800	-1.42959400
H	4.38952300	0.88206300	-1.43168900
H	-2.04921400	-0.00009200	2.50470500
H	-1.29759700	-0.00077000	2.54184200

13 Structures in Figure S2

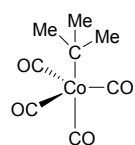
TS_{Co-ma}

Co	-0.03723800	-0.48364100	0.11485900
C	2.47399500	0.88781300	-1.37713100
O	3.33258100	1.36072700	-0.82153600
C	0.63442900	0.39729300	1.49516000
O	0.98384700	0.86057600	2.47833800
C	-1.39330300	-1.61887800	-0.18407000
O	-2.24126700	-2.38033100	-0.21425800
C	1.26961700	-1.72352300	0.01335600
O	2.11473100	-2.48028800	-0.08456000
C	-1.29871500	1.07673200	-0.23959900
C	-1.31875900	0.87557000	-1.74733200
H	-2.03197400	0.10754000	-2.06582800
H	-0.33154400	0.60274200	-2.15567900
H	-1.59683800	1.81406800	-2.25614900
C	-0.66316000	2.42280300	0.07557100
H	-0.63500200	2.63603200	1.14990500
H	0.35754000	2.51750600	-0.31539200
H	-1.25594900	3.22827800	-0.38885800
C	-2.68081800	1.03708900	0.37341300
H	-3.25425500	0.14456500	0.10209900
H	-2.63688600	1.08331100	1.46851200
H	-3.26853600	1.90938600	0.04012100

TS_{Co-(anti-ma)}

Co	0.61801700	-0.49774500	0.33360500
C	0.55360700	1.85827300	-1.93292100
O	0.53023500	2.89929500	-1.50136200
C	0.77449900	0.77302700	1.56762400
O	0.84706400	1.53713400	2.40816700
C	0.22809300	-2.12601600	-0.30858800
O	-0.04780700	-3.17670500	-0.64457100
C	2.26285300	-0.36493500	-0.35093400
O	3.31073100	-0.27581500	-0.78916300
C	-1.31203800	-0.55340200	0.94663300
C	-2.02406300	0.13542600	-0.22599000
H	-1.34913600	0.17875100	-1.10395500
C	-2.40569700	1.56513800	0.12289900
H	-1.54887500	2.14943300	0.47980500
H	-2.83088500	2.09414400	-0.73897100
H	-3.16003400	1.57496600	0.92091000
C	-3.24858100	-0.65853200	-0.65907800
H	-3.96294500	-0.74171200	0.17098500
H	-3.76602000	-0.17937700	-1.49948800
H	-2.98143100	-1.67694900	-0.96691600
H	-1.67596500	-1.57608100	1.09775900
H	-1.50499700	-0.02919800	1.89009900

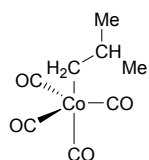
i



Co	0.51051700	0.00024500	-0.00010700
C	0.38222500	1.80589600	0.04947600
O	0.31228100	2.94249000	0.08043600
C	0.38120900	-0.94647200	1.53857400
O	0.30942900	-1.54224700	2.50684700
C	0.38096000	-0.86050700	-1.58832900
O	0.30930800	-1.40270700	-2.58760500
C	2.32080900	0.00002200	-0.00002400
O	3.45729100	-0.00051000	0.00016800
C	-1.64169400	0.00067400	0.00008200
C	-2.16074200	0.74966300	-1.21641700
H	-1.85911900	0.29757800	-2.16699500
H	-1.86152700	1.80271000	-1.23837700
H	-3.26322900	0.73691900	-1.19837700
C	-2.16035700	0.67994900	1.25698100
H	-1.85925600	0.17417700	2.18025600

H	-1.86036000	1.72973800	1.33899700
H	-3.26287400	0.66925800	1.23828500
C	-2.15975300	-1.42747000	-0.04002300
H	-1.85997500	-1.97330500	-0.94054700
H	-1.85779600	-2.02384500	0.82712500
H	-3.26224500	-1.40657200	-0.03815500

j



Co	0.76472500	0.00052900	0.01283900
C	0.24891000	1.57692000	-0.71809400
O	-0.11478900	2.56452300	-1.15222100
C	1.27448600	0.00087800	1.75650900
O	1.51225000	0.00081800	2.86896000
C	0.25103000	-1.57720500	-0.71678500
O	-0.10989500	-2.56593100	-1.15068700
C	2.42907500	0.00084100	-0.68951500
O	3.47370600	0.00084300	-1.13650100
C	-1.15324800	0.00131400	0.82311500
C	-2.33201600	-0.00051500	-0.16100600
H	-1.96051200	0.00012300	-1.19753500
C	-3.18386000	-1.24921000	0.02081700
H	-3.60920000	-1.28092900	1.03309800
H	-4.02041700	-1.27051200	-0.68790700
H	-2.60475100	-2.16848900	-0.12264700
C	-3.18757800	1.24562900	0.02101600
H	-2.61127300	2.16656100	-0.12322100
H	-4.02470900	1.26413000	-0.68710900
H	-3.61225100	1.27637800	1.03360700
H	-1.18753700	-0.87747900	1.47744500
H	-1.18789600	0.88200400	1.47486000