CHEMISTRY
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Supporting Information

Mechanism, Regioselectivity and Kinetics of Phosphine-Catalyzed (3+2) Cycloaddition Reaction of Allenoates and Electron-Deficient Alkenes

Yong Liang,[†] Song Liu,[†] Yuanzhi Xia,[†,‡] Yahong Li,[‡,§]

and Zhi-Xiang Yu*[,†]

[†]*Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of the Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China,*

[‡]*Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, Xining 810008, China,*

[§]*Key Laboratory of Organic Synthesis of Jiangsu Province, Department of Chemistry and Chemical Engineering, Suzhou University, Suzhou 215006, China*

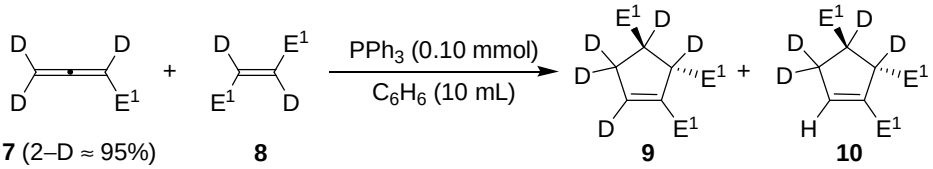
yuzx@pku.edu.cn

Content

1. Experimental Details and Spectroscopic Data

Allenoates,[1] deuterium labeled methyl 2,3–butadienoate (**7**),[1,2] and deuterium labeled dimethyl fumarate (**8**)[3] were prepared according to literature procedures. Phosphine-catalyzed (3+2) cycloaddition reactions were performed according to Lu's procedures.[4,5] Benzene was refluxed with Na and benzophenone, and freshly distilled prior to use. All reactions were performed under nitrogen. For the reactions with additives (water/methanol), the additive was added to the mixture through a syringe before the addition of allenoate. Detailed experimental results were summarized in Schemes S1 and S2. The ratio of deuterium and hydrogen was determined by ^{1}H NMR analysis.

Scheme S1. Isotopic Labeling Experiments ($E^1 = CO_2Me$, $E^2 = CO_2Et$)

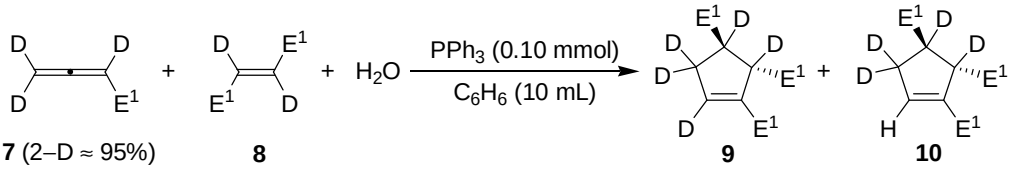


7 (2–D ≈ 95%) **8** **9** : **10**

75 : 25 **(I)**

M	101	146	246.75
m (mg)	101	292	191
n (mmol)	1.00	2.00	0.774
Yield			77%

Note: This reaction was conducted 10 days after the deuterium labeled reactants **7** and **8** were synthesized.

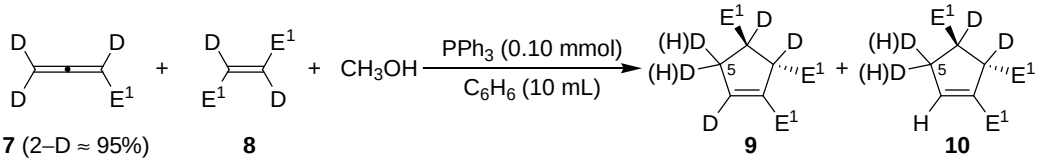


7 (2–D ≈ 95%) **8** **9** : **10** **(II)**

12 : 88

M	101	146	18	246.12
m (mg)	101	292	18	56
n (mmol)	1.00	2.00	1.0	0.228
Yield				23%

[1] R. W. Lang, H. Hansen, *Organic Syntheses* **1990**, *Coll. Vol. 7*, p232.
[2] Y. Xia, Y. Liang, Y. Chen, M. Wang, L. Jiao, F. Huang, S. Liu, Y. Li, Z. -X. Yu, *J. Am. Chem. Soc.* **2007**, *129*, 3470. The ratio of 2–D is about 95%, and the ratio of 4–D is more than 98%.
[3] K. M. Lee, K. Ramalingam, J. K. Son, R. W. Woodard, *J. Org. Chem.* **1989**, *54*, 3195. The ratio of 2(3)–D is more than 98%.
[4] Using electron-deficient alkenes as trappers, see: C. Zhang, X. Lu, *J. Org. Chem.* **1995**, *60*, 2906.
[5] Using electron-deficient imines as trappers, see: Z. Xu, X. Lu, *J. Org. Chem.* **1998**, *63*, 5031.

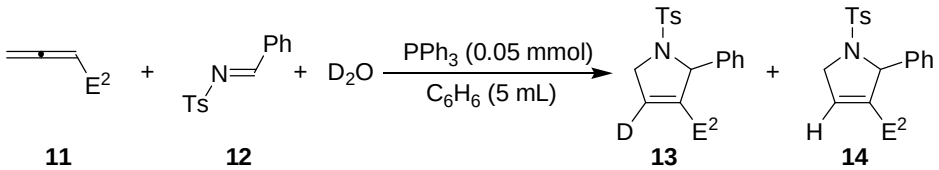


7 (2–D ≈ 95%) **8** **9** : **10** **(III)**

24 : 76

M	101	146	32	246.24
m (mg)	101	292	32	109
n (mmol)	1.00	2.00	1.0	0.443
Yield				44%

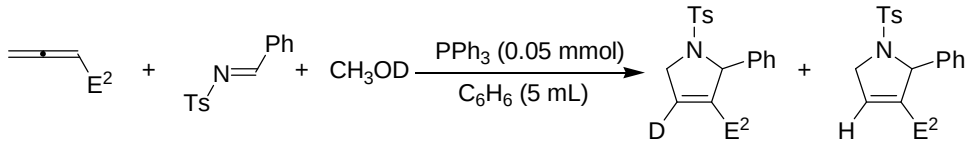
Note: The ratio of H in the 5–position of products **9** and **10** is about 8%.



11 **12** **13** : **14** **(IV)**

69 : 31

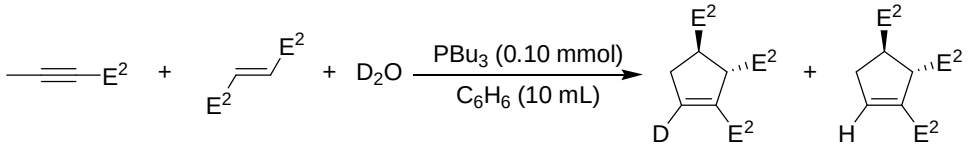
M	112	259	20	371.69
m (mg)	62	119	10	142
n (mmol)	0.55	0.46	0.50	0.382
Yield				83%



11 **12** **13** : **14** **(V)**

46 : 54

M	112	259	33	371.46
m (mg)	59	118	15	96
n (mmol)	0.53	0.46	0.45	0.258
Yield				56%

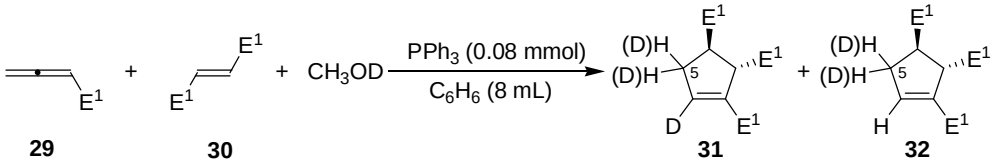


25 **26** **27** : **28** **(VI)**

72 : 28

M	112	172	20	284.72
m (mg)	113	348	22	28
n (mmol)	1.01	2.02	1.1	0.098
Yield				10%

Scheme S2. Additional Isotopic Labeling Experiments ($E^1 = CO_2Me$, $E^2 = CO_2Et$)

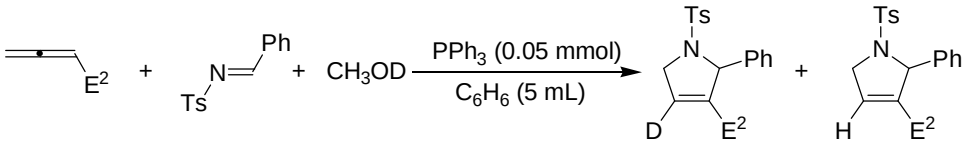


29 **30** **31** **32**

83 : 17 **(VII)**

M	98	144	33		242.83
m (mg)	75	214	250		130
n (mmol)	0.77	1.49	7.6		0.535
Yield					69%

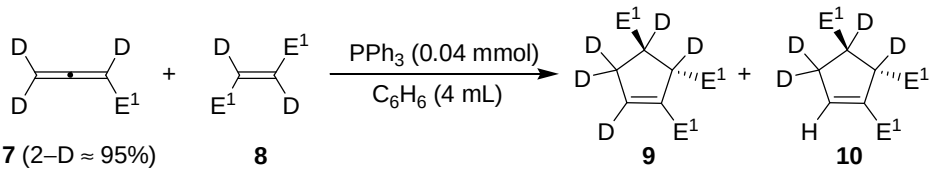
Note: The ratio of D in the 5–position of products **31** and **32** is about 35%.



11 **12** **13** **14**

86 : 14 **(VIII)**

M	112	259	33		371.86
m (mg)	57	119	205		159
n (mmol)	0.51	0.46	6.2		0.428
Yield					93%

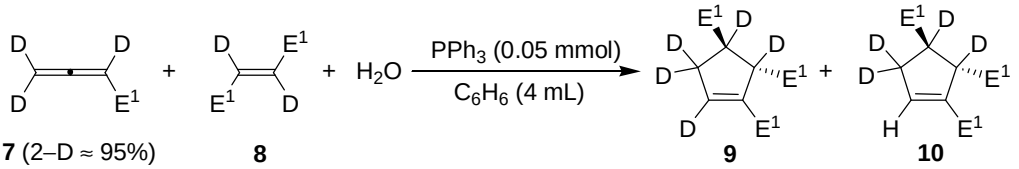


7 (2–D ≈ 95%) **8** **9** **10**

48 : 52 **(IX)**

M	101	146		246.48
m (mg)	37	112		53
n (mmol)	0.37	0.77		0.215
Yield				58%

Note: This reaction was conducted after the deuterium labeled reactants **7** and **8** were stored in the refrigerator for 14 months.



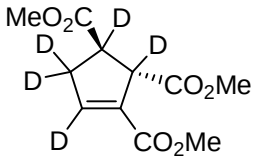
7 (2–D ≈ 95%) **8** **9** **10**

24 : 76 **(X)**

M	101	146	18		246.24
m (mg)	55	120	4.8		48
n (mmol)	0.54	0.82	0.27		0.195
Yield					36%

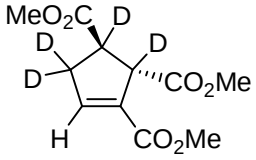
Note: This reaction was conducted after the deuterium labeled reactants **7** and **8** were stored in the refrigerator for 14 months.

***trans*-Trimethyl [1,2,4,5,5-D_5]Cyclopent-3-ene-1, 2, 3-tricarboxylate (9)**



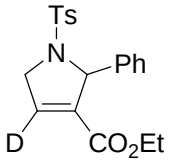
^{1}H NMR (400 MHz, $CDCl_3$): *d* 3.74 (s, 6H), 3.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): *d* 35.1 (m), 45.9 (t, $J_{C–D}$ = 20 Hz), 51.5, 52.1 (t, $J_{C–D}$ = 21 Hz), 52.2, 133.5, 143.5 (t, $J_{C–D}$ = 26 Hz), 163.6, 173.3, 173.4. MS (ESI) m/z: 248 $(M+H)^+$.

***trans*-Trimethyl [1,2,5,5-D_4]Cyclopent-3-ene-1, 2, 3-tricarboxylate (10)**



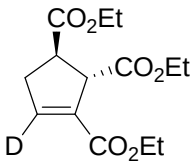
^{1}H NMR (400 MHz, $CDCl_3$): *d* 3.74 (s, 6H), 3.75 (s, 3H), 6.84 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): *d* 35.2 (m), 45.9 (t, $J_{C–D}$ = 20 Hz), 51.6, 52.1 (t, $J_{C–D}$ = 21 Hz), 52.2, 133.7, 143.8, 163.7, 173.3, 173.4. MS (ESI) m/z: 247 $(M+H)^+$.

Ethyl 2-Phenyl-1-tosyl-[4-D]2, 5-dihydro-1*H*-pyrrole-3-carboxylate (13)



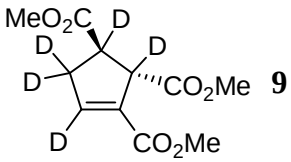
^{1}H NMR (400 MHz, $CDCl_3$): *d* 1.09 (t, *J* = 7.2 Hz, 3H), 2.36 (s, 3H), 4.01 (m, 2H), 4.37 (dd, *J* = 17.2, 5.6 Hz, 1H), 4.50 (dd, *J* = 17.2, 2.4 Hz, 1H), 5.73 (dd, *J* = 5.6, 2.4 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.22 (m, 5H), 7.42 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): *d* 13.7, 21.3, 54.7, 60.6, 68.9, 126.9, 127.7, 127.8, 128.1, 129.3, 135.1 (t, $J_{C–D}$ = 26 Hz), 135.5, 135.7, 139.4, 143.1, 161.6. MS (ESI) m/z: 373 $(M+H)^+$.

***trans*-Triethyl [4-D]Cyclopent-3-ene-1, 2, 3-tricarboxylate** (**27**)



^{1}H NMR (400 MHz, $CDCl_3$): *d* 1.28 (m, 9H), 2.85 (ddd, *J* = 18.8, 6.4, 2.0 Hz, 1H), 2.92 (ddd, *J* = 18.8, 8.8, 2.0 Hz, 1H), 3.38 (ddd, *J* = 8.8, 6.4, 6.4 Hz, 1H), 4.08 (ddd, *J* = 6.4, 2.0, 2.0 Hz, 1H), 4.19 (m, 6H). MS (ESI) m/z: 286 $(M+H)^+$.

2. Copies of ^{1}H, ^{13}C NMR and Mass Spectra



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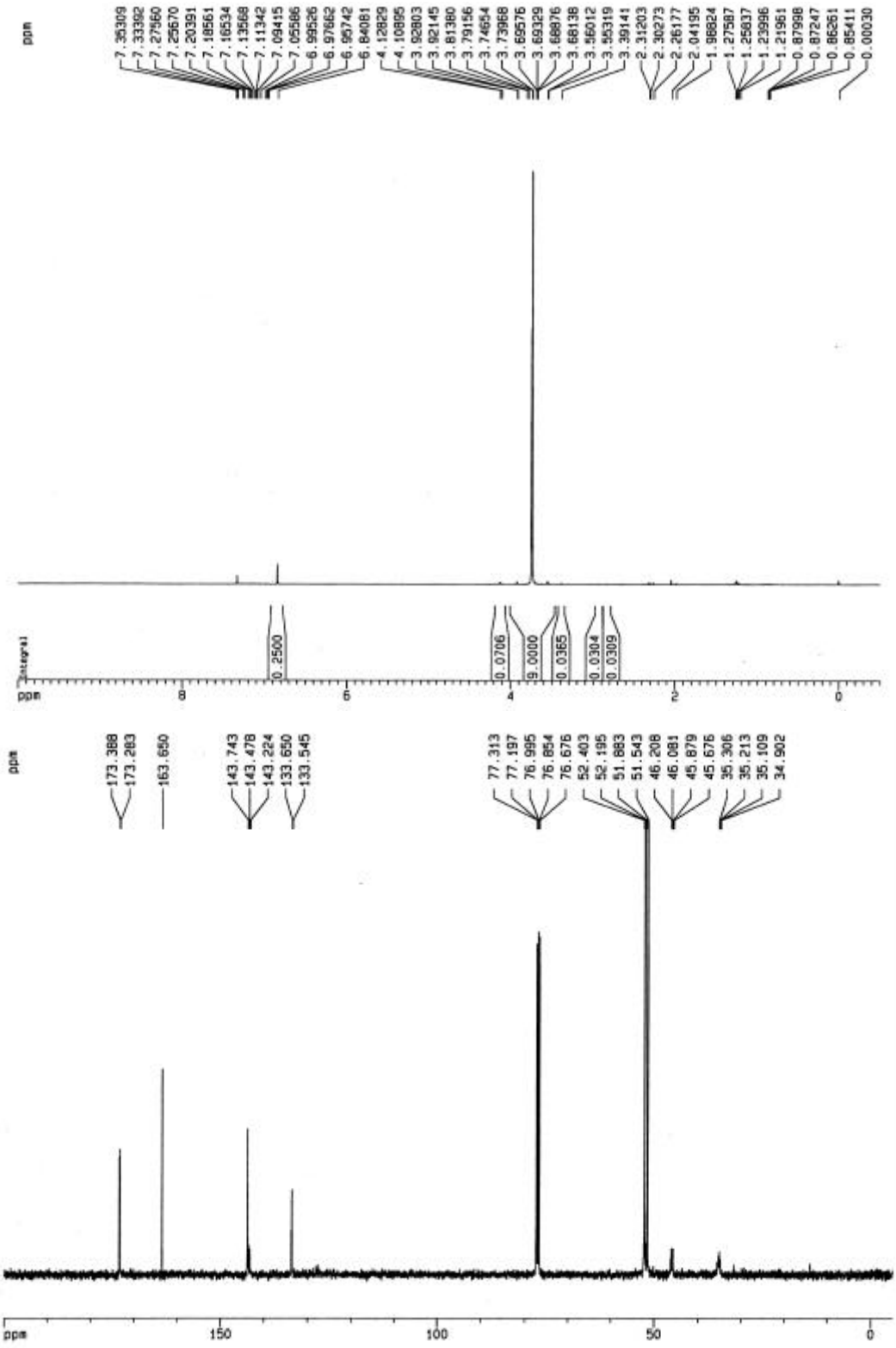

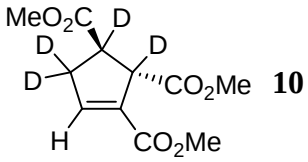
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D
D
D
CO2Me
H
CO2Me

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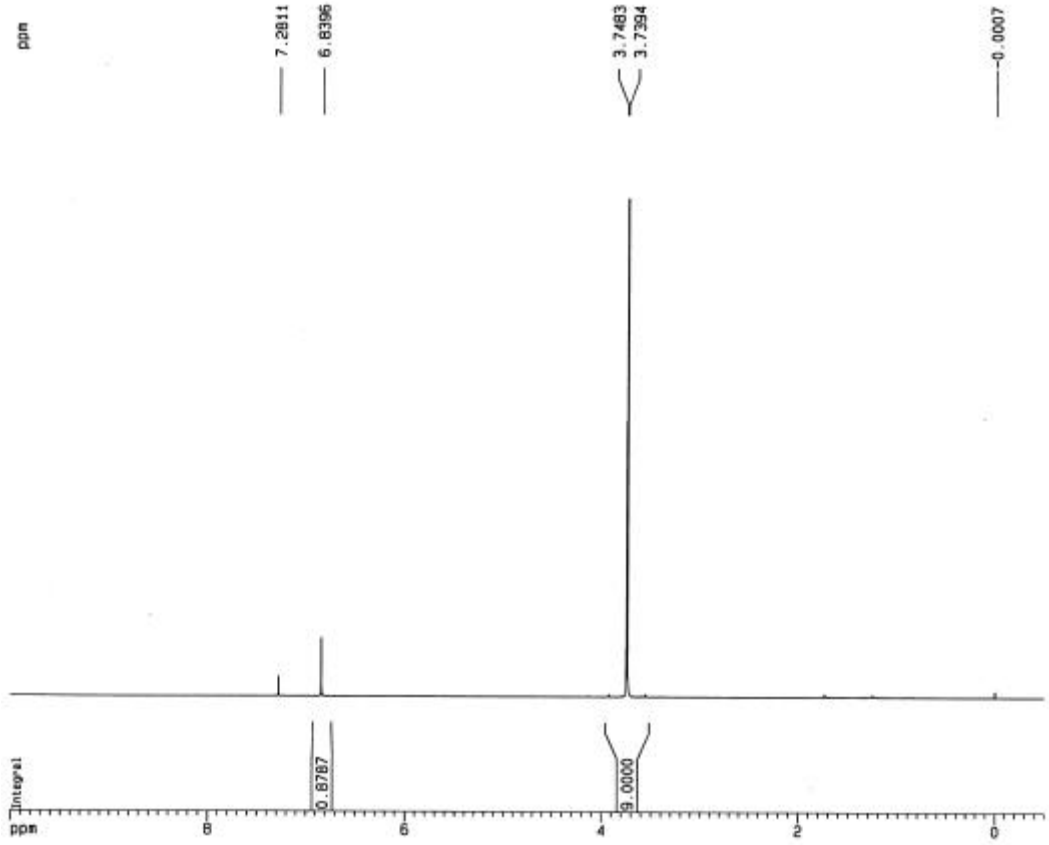
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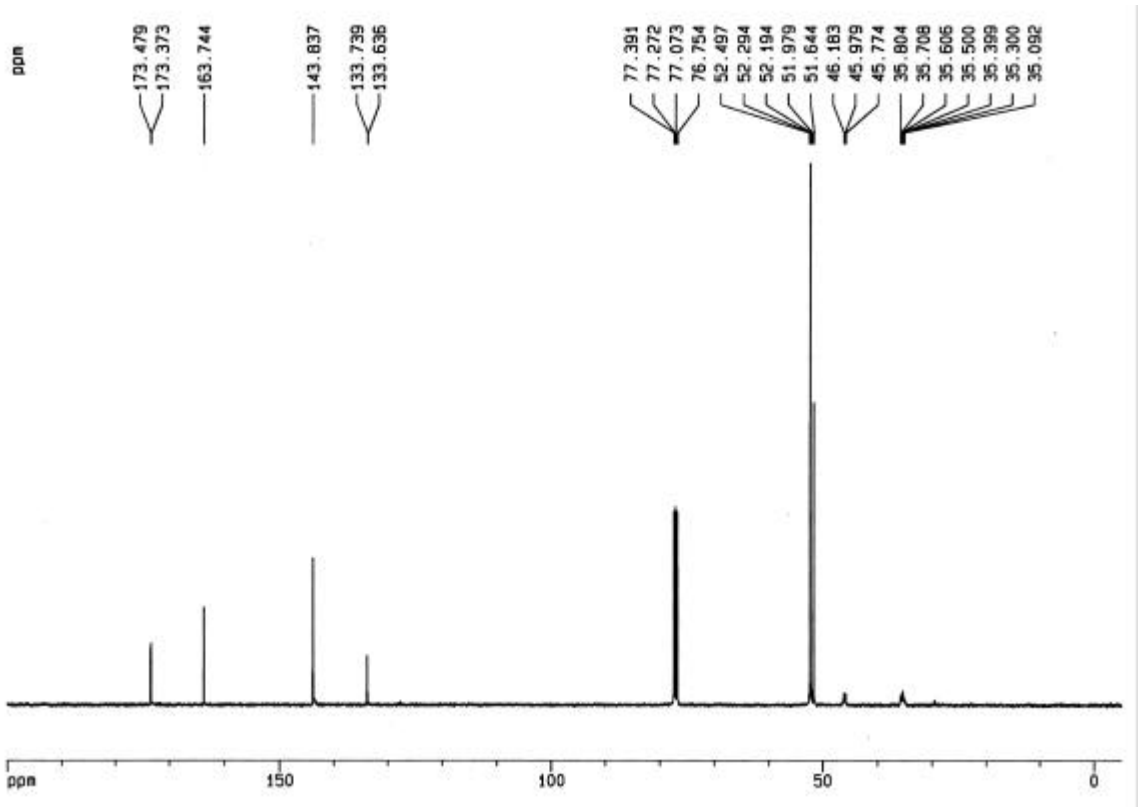
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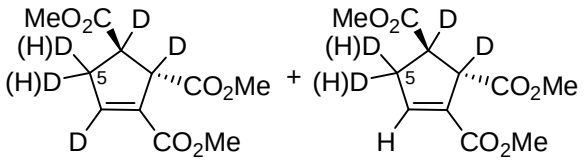
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D
(H)D
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D
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+
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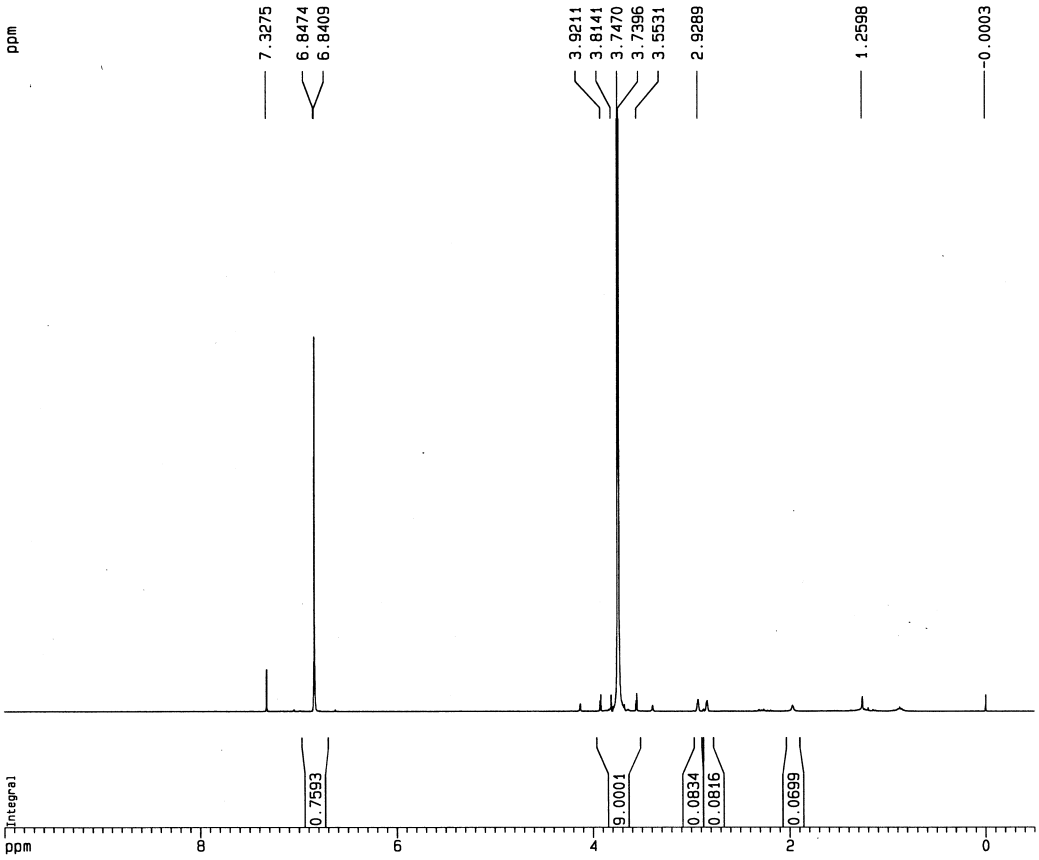
(H)D
5
CO2Me
H
CO2Me

9 **10**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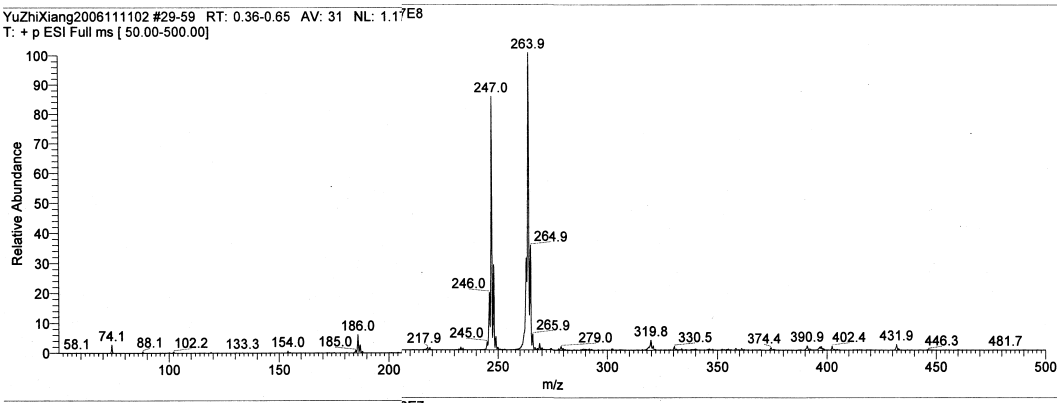
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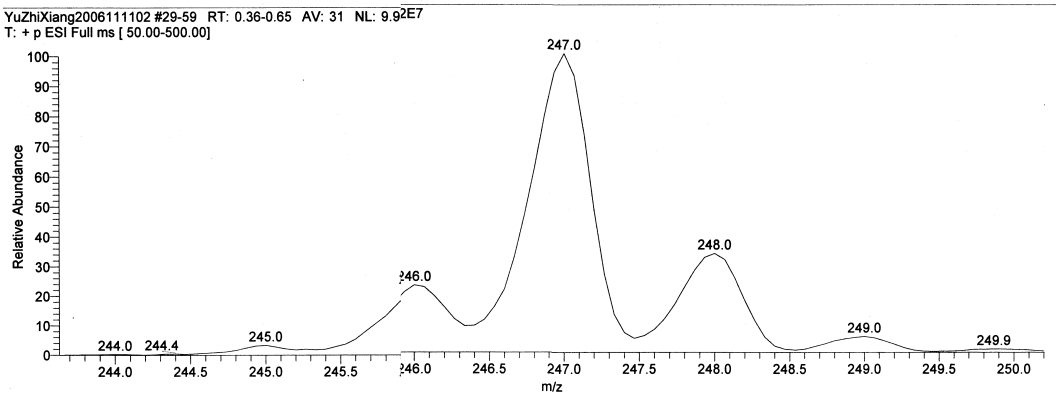
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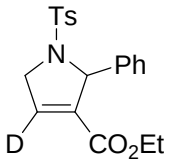
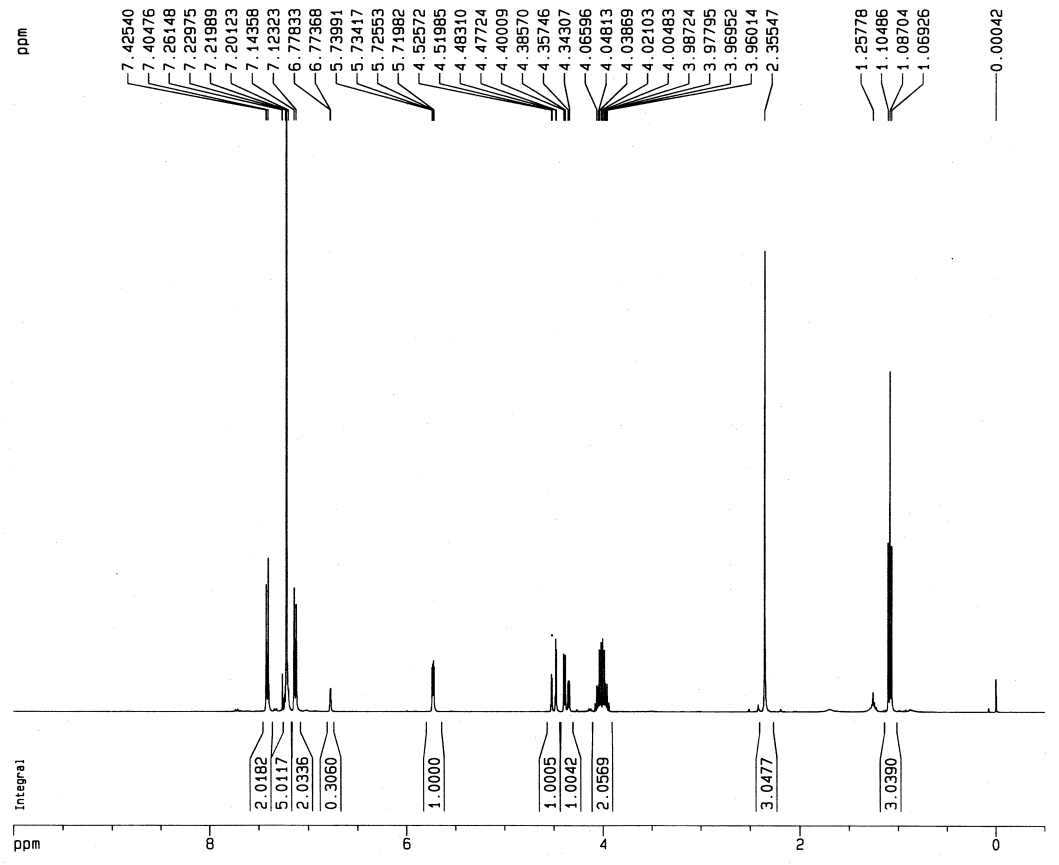
245.0


Ts
N
Ph
D
CO2Et

13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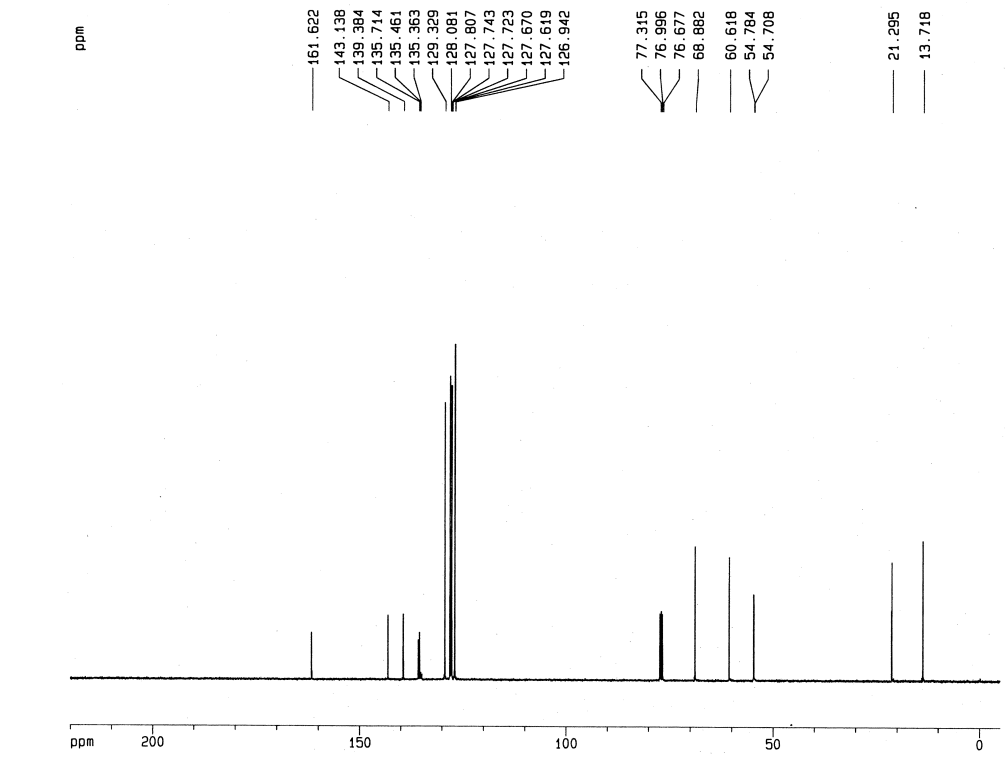
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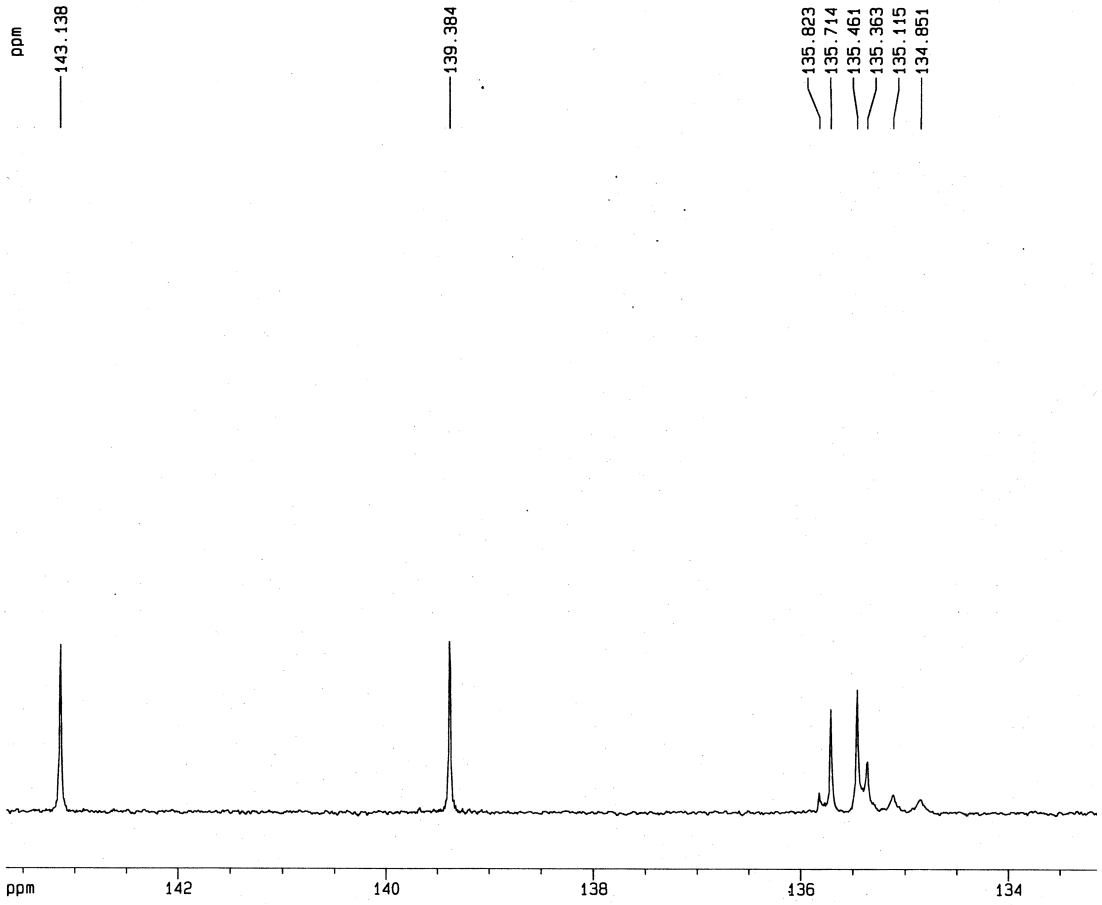
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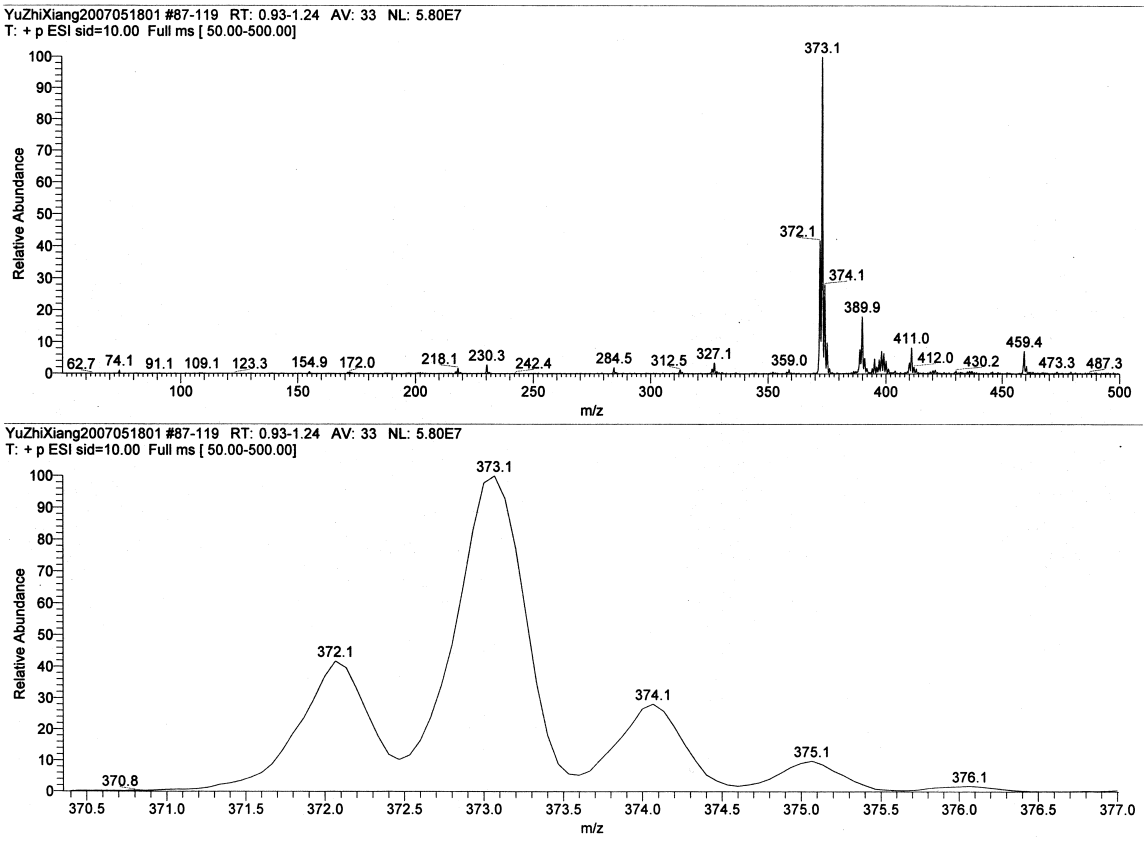
140
138
136
134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74.1
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154.9
172.0
218.1
230.3
242.4
284.5
312.5
327.1
359.0

YuZhiXiang2007051801 #87-119 RT: 0.93-1.24 AV: 33 NL: 5.80E7
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Relative Abundance
m/z
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372.1
374.1
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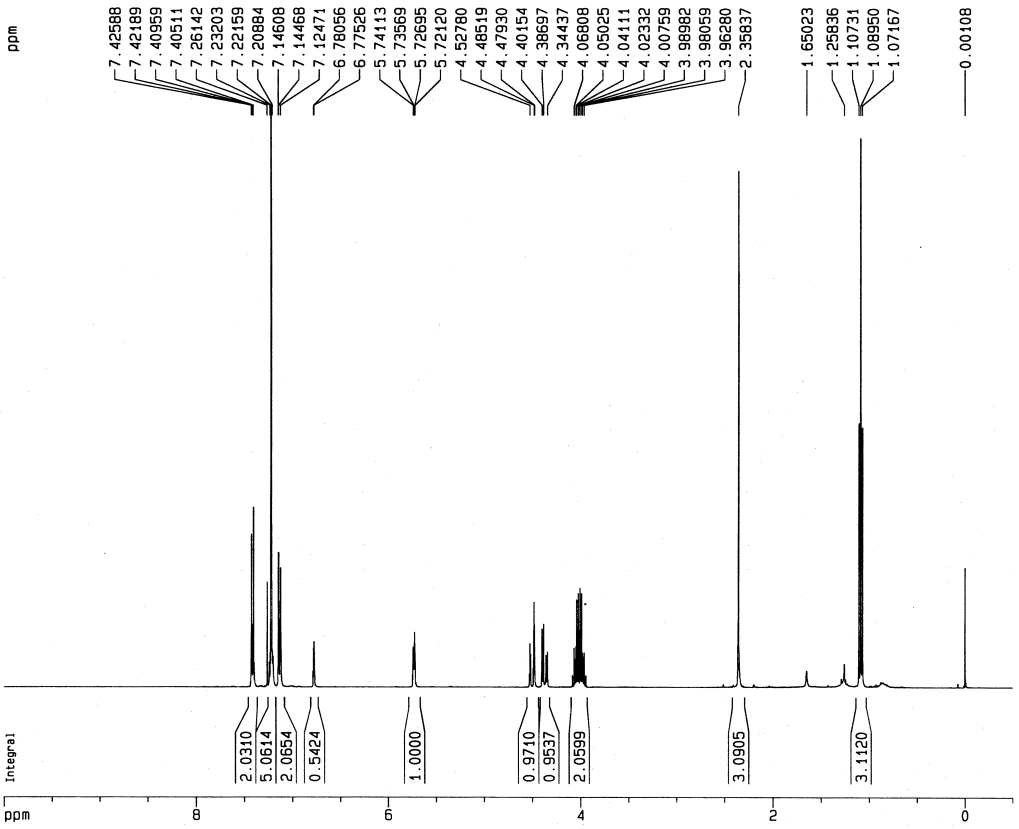
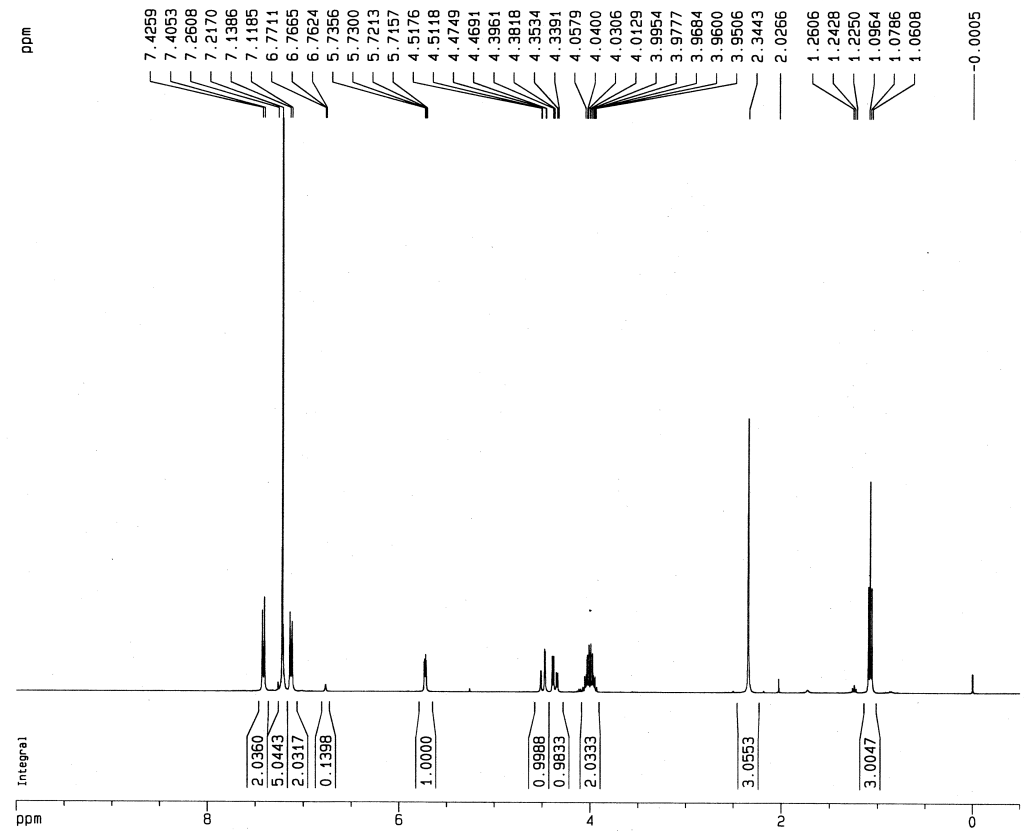
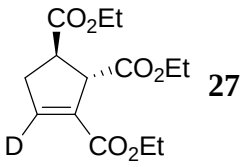
376.1
370.8

Add 1 equiv. CH_3OD



Add 13.5 equiv. CH_3OD




CO2Et
CO2Et
D
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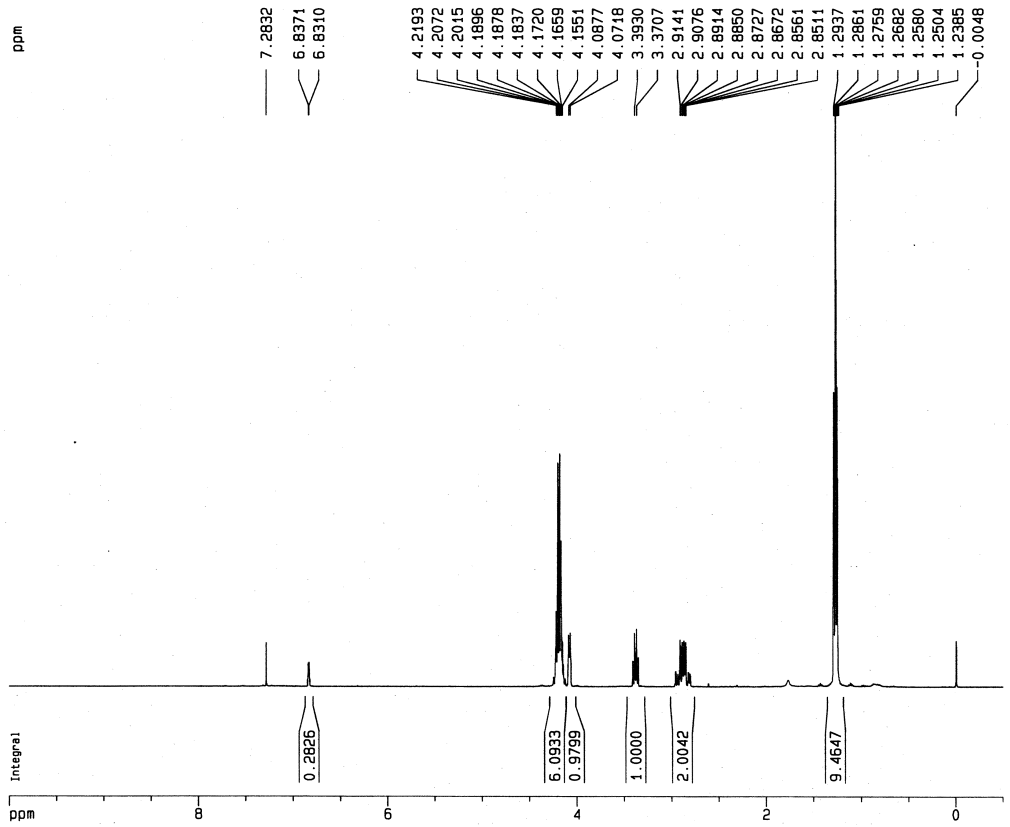
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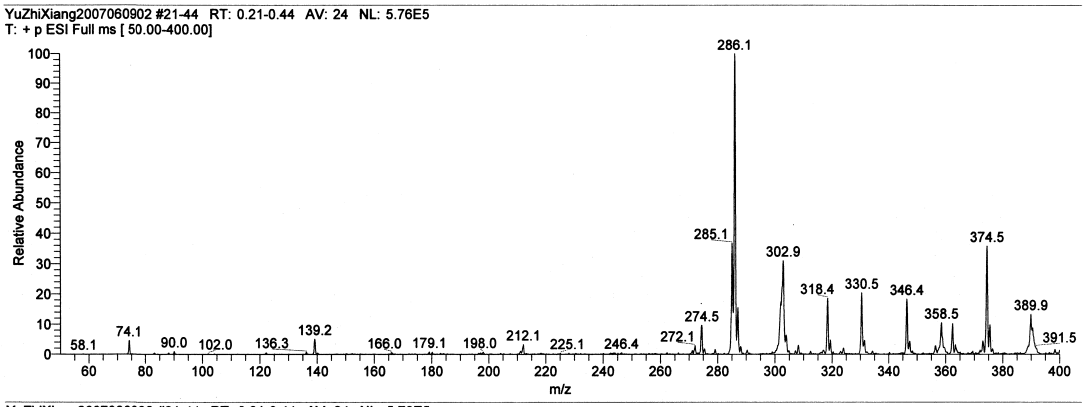
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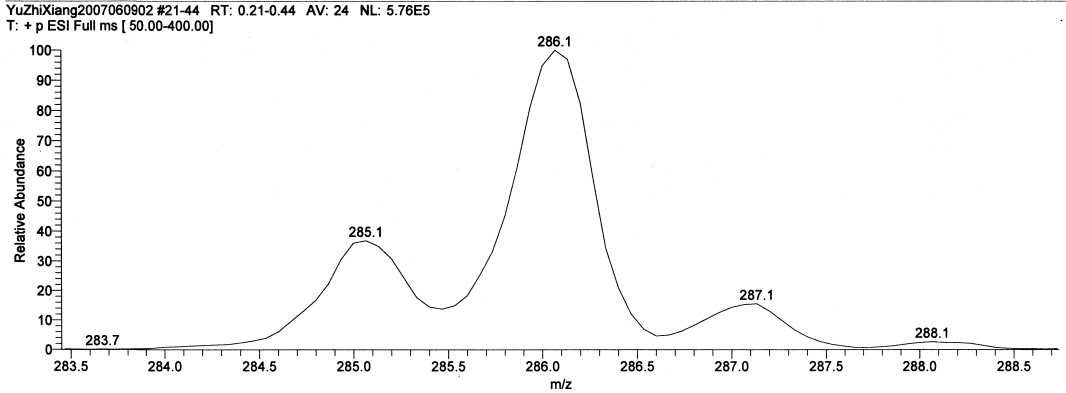
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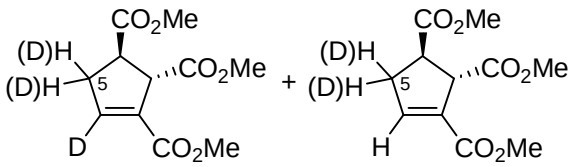
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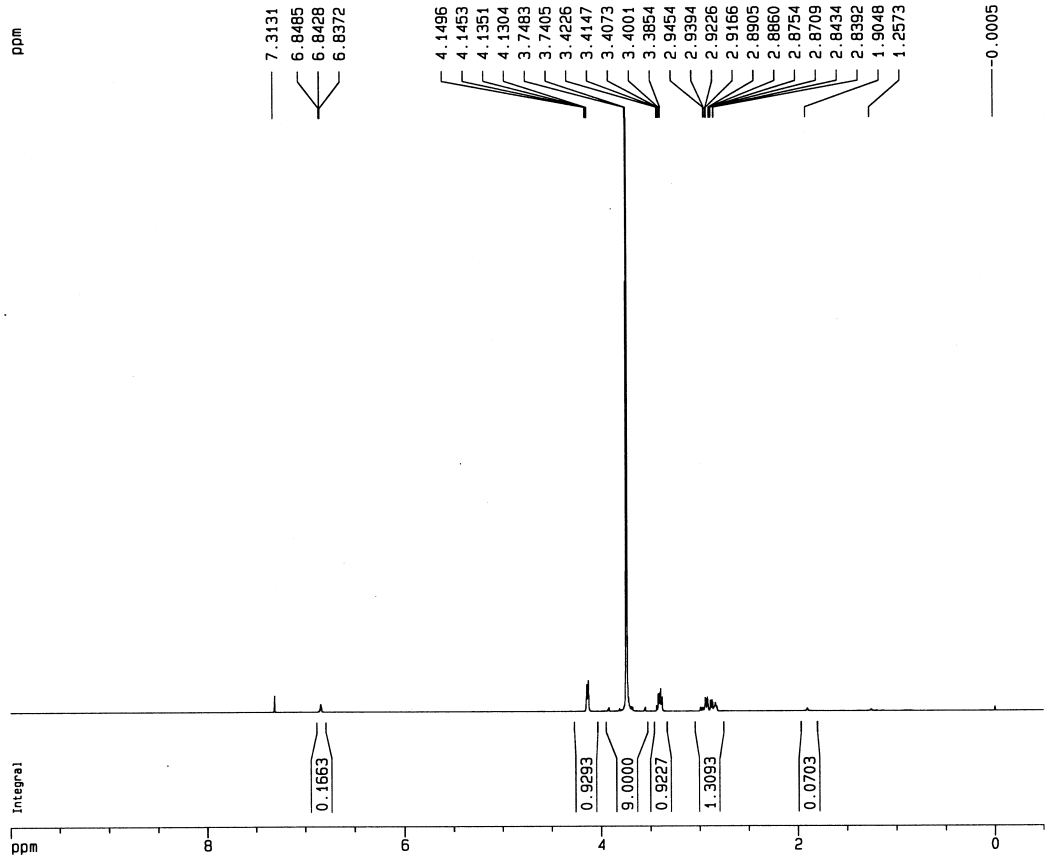
31 **32**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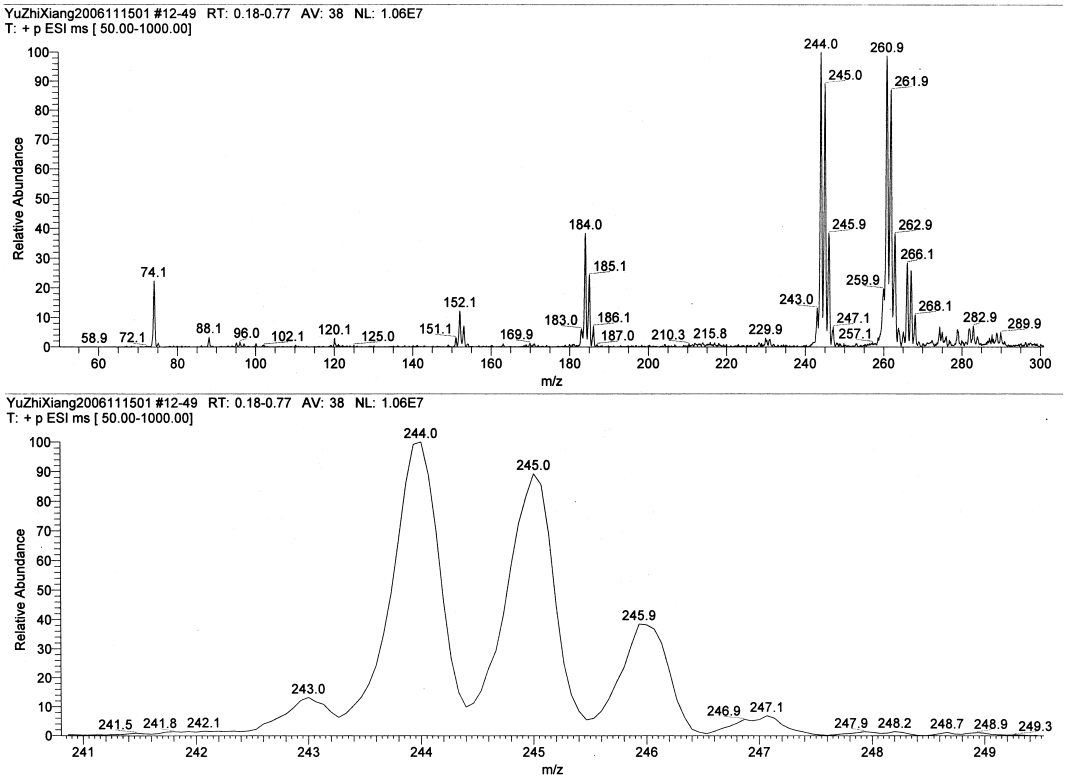
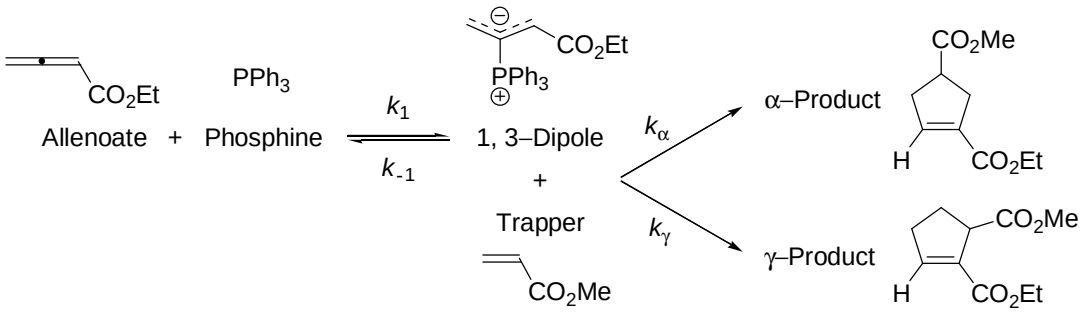


3. Details of Kinetic Studies

Scheme S3. The Simplified Kinetic Model for the Experimentally Measured (3+2) Cycloaddition Reaction



Derivation of the rate law:

? $[a\text{-Product}] = k_a \int [1,3\text{-Dipole}][\text{Trapper}]dt$

$[g\text{-Product}] = k_g \int [1,3\text{-Dipole}][\text{Trapper}]dt$

? $\dfrac{[a\text{-Product}]}{[g\text{-Product}]} = \dfrac{k_a}{k_g}$ (Eq. 1)

It is defined: $v_{\text{initial}} = \dfrac{d[a\text{-Product}]}{dt} = k_a[1,3\text{-Dipole}][\text{Trapper}]$

In the phosphine-catalyzed (3+2) cycloaddition reaction of allenoates and activated alkenes,

the generation of 1,3-dipole is endergonic by 11.5 kcal/mol in gas phase and 9.7 kcal/mol in benzene according to the computational results (Figure 1), so the concentration of 1,3-dipole is believed to be very low compared with the concentration of phosphine ([Phosphine] >> [1,3-Dipole]). That is to say, the concentration of phosphine in the reaction process nearly equals the total concentration of the added phosphine catalyst.

Thus, $$\frac{d[\text{1,3-Dipole}]}{dt} = k_1[\text{Allenoate}][\text{Phosphine}] - k_{-1}[\text{1,3-Dipole}] - (k_a + k_g)[\text{1,3-Dipole}][\text{Trapper}]$$

Using the steady state approximation: $\frac{d[\text{1,3-Dipole}]}{dt} = 0$

? $$[\text{1,3-Dipole}] = \frac{k_1[\text{Allenoate}][\text{Phosphine}]}{k_{-1} + (k_a + k_g)[\text{Trapper}]}$$

? $$v_{\text{initial}} = \frac{d[a\text{-Product}]}{dt} = \frac{k_a k_1[\text{Allenoate}][\text{Phosphine}][\text{Trapper}]}{k_{-1} + (k_a + k_g)[\text{Trapper}]}$$ (Eq. 2)

Eq. 2 can be reformatted to Eq. 3:

$$\frac{[\text{Allenoate}][\text{Phosphine}]}{v_{\text{initial}}} = \frac{k_{-1} + (k_a + k_g)[\text{Trapper}]}{k_a k_1[\text{Trapper}]} = \frac{k_{-1}}{k_a k_1} \times \frac{1}{[\text{Trapper}]} + \frac{k_a + k_g}{k_a k_1}$$ (Eq. 3)

Let $Y = \frac{[\text{Allenoate}][\text{Phosphine}]}{v_{\text{initial}}}$, $X = \frac{1}{[\text{Trapper}]}$

? $$Y = \frac{k_{-1}}{k_a k_1} X + \frac{k_a + k_g}{k_a k_1}$$ (Eq. 4)

Standard kinetic protocol:

All kinetic experiments were conducted similarly to the procedure described here. To a 10 mL volumetric flask, ethyl allenoate, methyl acrylate, and *n*–hexadecane (as the internal standard) were added. Benzene was added so that the whole solution was exactly 10.0 mL. Then a stir bar was added to the solution. The volumetric flask was placed in a water bath at a specified temperature and allowed to stir for several minutes before triphenylphosphine was added. Monitoring the process of the reaction began immediately after triphenylphosphine catalyst was added to the solution. After every period of time, the reaction mixture was sampled by microsyringe, and was submitted to GC for analysis immediately. Compared with

the concentration of internal standard, the concentrations of (3+2) α–Product and γ–Product were obtained. In all kinetic experiments, the initial reaction rates (the formation rate of α–product, Eq. 2) were determined at a low conversion of ethyl allenoate (< 15% conversion of allenoate). The concentration of allenoate used for calculating *Y* equals [(1−conversion/2)×(initial concentration of ethyl allenoate)].

Table S1. Kinetic studies conducted at 284 K

1	*t* / s	540	1260	1980	2700	4140
	[α–Product]/mol·L^{-1}	0.000601	0.001616	0.002586	0.003429	0.004773
2	*t* / s	480	1200	1980	2700	3420
	[α–Product]/mol·L^{-1}	0.000471	0.001364	0.002323	0.003152	0.004030
3	*t* / s	900	1620	2340	3030	3720
	[α–Product]/mol·L^{-1}	0.000747	0.001495	0.002323	0.003010	0.003596
4	*t* / s	960	1680	2400	3120	3840
	[α–Product]/mol·L^{-1}	0.000970	0.001737	0.002621	0.003318	0.004141

For entry 1, [Trapper] = 0.852 mol·L^{-1}, *X* = 1.17

? [α–Product] = 1.207×10^{-6} *t*, R^2 = 0.99.

? $v_{initial} = 1.207\times10^{-6}$ mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0480 mol·L^{-1}, [Phosphine] = 0.0255 mol·L^{-1}

? *Y* = 1014

For entry 2, [Trapper] = 0.499 mol·L^{-1}, *X* = 2.00

? [α–Product] = 1.170×10^{-6} *t*, R^2 = 0.999.

? $v_{initial} = 1.170\times10^{-6}$ mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0474 mol·L^{-1}, [Phosphine] = 0.0265 mol·L^{-1}

? *Y* = 1074

For entry 3, [Trapper] = 0.364 mol·L^{-1}, *X* = 2.75

? [α–Product] = 9.718×10^{-7} *t*, R^2 = 0.994.

? $v_{initial} = 9.718\times10^{-7}$ mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0456 mol·L^{-1}, [Phosphine] = 0.0231 mol·L^{-1}

? *Y* = 1084

For entry 4, [Trapper] = 0.227 mol·L^{-1}, *X* = 4.41

? [α–Product] = 1.071×10^{-6} *t*, $R^2 = 0.998$.

? $v_{initial} = 1.071\times10^{-6}$ mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0468 mol·L^{-1}, [Phosphine] = 0.0264 mol·L^{-1}

? $Y = 1154$

The relationship between *X* and *Y* at 284 K:

$Y = 40.8X + 976$, $R^2 = 0.96$.

? $\frac{k_a + k_g}{k_a k_1} = 976 \pm 17$, $\frac{k_{-1}}{k_a k_1} = 40.8 \pm 5.8$

And $k_\alpha/k_\gamma = 3.09$ at 284 K,

? $k_1 = (1.36 \pm 0.02)\times10^{-3}$ mol^{-1}·L·s^{-1}

$k_\alpha/k_{-1} = 18.0 \pm 2.6$

$k_\gamma/k_{-1} = 5.83 \pm 0.83$

Table S2. Kinetic studies conducted at 290 K

1	*t* / s	900	1710	2400	3120	3840
	[α–Product]/mol·L^{-1}	0.000546	0.001273	0.001955	0.002667	0.003182
2	*t* / s	900	1620	2340	3060	3780
	[α–Product]/mol·L^{-1}	0.000566	0.001217	0.001884	0.002455	0.003071
3	*t* / s	1260	1980	2730	3480	4320
	[α–Product]/mol·L^{-1}	0.001076	0.001591	0.002359	0.002990	0.003747
4	*t* / s	1290	1980	2700	3420	4140
	[α–Product]/mol·L^{-1}	0.000955	0.001505	0.002030	0.002551	0.003354

For entry 1, [Trapper] = 0.830 mol·L^{-1}, X = 1.20

? [α–Product] = 8.211×10^{-7} t, R^2 = 0.99.

? $v_{initial}$ = 8.211×10^{-7} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0480 mol·L^{-1}, [Phosphine] = 0.0114 mol·L^{-1}

? Y = 666.4

For entry 2, [Trapper] = 0.498 mol·L^{-1}, X = 2.01

? [α–Product] = 7.987×10^{-7} t, R^2 = 0.992.

? $v_{initial}$ = 7.987×10^{-7} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0497 mol·L^{-1}, [Phosphine] = 0.0118 mol·L^{-1}

? Y = 734.3

For entry 3, [Trapper] = 0.294 mol·L^{-1}, X = 3.40

? [α–Product] = 8.583×10^{-7} t, R^2 = 0.997.

? $v_{initial}$ = 8.583×10^{-7} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0473 mol·L^{-1}, [Phosphine] = 0.0140 mol·L^{-1}

? Y = 771.5

For entry 4, [Trapper] = 0.191 mol·L^{-1}, X = 5.24

? [α–Product] = 7.744×10^{-7} *t*, $R^2 = 0.99$.

? $v_{initial} = 7.744\times10^{-7}$ mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0478 mol·L^{-1}, [Phosphine] = 0.0138 mol·L^{-1}

? $Y = 851.8$

The relationship between *X* and *Y* at 290 K:

$Y = 43.0X + 629$, $R^2 = 0.97$.

? $\frac{k_a + k_g}{k_a k_1} = 629 \pm 18$, $\frac{k_{-1}}{k_a k_1} = 43.0 \pm 5.5$

And $k_\alpha/k_\gamma = 2.88$ at 290 K,

? $k_1 = (2.14 \pm 0.06)\times10^{-3}$ mol^{-1}·L·s^{-1}

$k_\alpha/k_{-1} = 10.9 \pm 1.4$

$k_\gamma/k_{-1} = 3.78 \pm 0.48$

Table S3. Kinetic studies conducted at 297 K

1	*t* / s	720	1440	2160	2880	4260
	[α–Product]/mol·L^{-1}	0.000446	0.001152	0.001919	0.002742	0.004010
2	*t* / s	1260	1980	2700	3420	4140
	[α–Product]/mol·L^{-1}	0.000944	0.001672	0.002207	0.002909	0.003525
3	*t* / s	1200	1920	2640	3360	4080
	[α–Product]/mol·L^{-1}	0.000838	0.001434	0.002045	0.002525	0.003015
4	*t* / s	1320	2040	2760	3480	4200
	[α–Product]/mol·L^{-1}	0.000808	0.001465	0.001949	0.002500	0.002985

For entry 1, [Trapper] = 0.856 mol·L^{-1}, X = 1.17

? [α–Product] = 9.230×10^{-7} t, R^2 = 0.99.

? $v_{initial}$ = 9.230×10^{-7} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0470 mol·L^{-1}, [Phosphine] = 0.00740 mol·L^{-1}

? Y = 376.8

For entry 2, [Trapper] = 0.493 mol·L^{-1}, X = 2.03

? [α–Product] = 8.407×10^{-7} t, R^2 = 0.995.

? $v_{initial}$ = 8.407×10^{-7} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0482 mol·L^{-1}, [Phosphine] = 0.00718 mol·L^{-1}

? Y = 411.7

For entry 3, [Trapper] = 0.298 mol·L^{-1}, X = 3.36

? [α–Product] = 7.481×10^{-7} t, R^2 = 0.997.

? $v_{initial}$ = 7.481×10^{-7} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0487 mol·L^{-1}, [Phosphine] = 0.00718 mol·L^{-1}

? Y = 467.4

For entry 4, [Trapper] = 0.213 mol·L^{-1}, X = 4.69

? [α–Product] = 7.088×10^{-7} *t*, $R^2 = 0.994$.

? $v_{initial} = 7.088\times10^{-7}$ mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0485 mol·L^{-1}, [Phosphine] = 0.00752 mol·L^{-1}

? $Y = 514.6$

The relationship between *X* and *Y* at 297 K:

$Y = 39.4X + 332$, $R^2 = 0.999$.

? $\frac{k_a + k_g}{k_a k_1} = 332 \pm 3$, $\frac{k_{-1}}{k_a k_1} = 39.4 \pm 1.0$

And $k_\alpha/k_\gamma = 2.56$ at 297 K,

? $k_1 = (4.19 \pm 0.04)\times10^{-3}$ mol^{-1}·L·s^{-1}

$k_\alpha/k_{-1} = 6.06 \pm 0.15$

$k_\gamma/k_{-1} = 2.37 \pm 0.06$

Table S4. Kinetic studies conducted at 304 K

1	*t* / s	780	1560	2340	3120	3840
	[α–Product]/mol·L^{-1}	0.000702	0.001682	0.002747	0.003682	0.004561
2	*t* / s	930	1710	2430	3210	3900
	[α–Product]/mol·L^{-1}	0.000909	0.001843	0.002818	0.003919	0.004455
3	*t* / s	900	1620	2340	3060	3780
	[α–Product]/mol·L^{-1}	0.000556	0.001111	0.001722	0.002222	0.002763
4	*t* / s	900	1680	2490	3180	3900
	[α–Product]/mol·L^{-1}	0.000586	0.001152	0.001944	0.002429	0.002949

For entry 1, [Trapper] = 0.888 mol·L^{-1}, X = 1.13

? [α–Product] = 1.170×10^{-6} t, R^2 = 0.993.

? $v_{initial}$ = 1.170×10^{-6} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0474 mol·L^{-1}, [Phosphine] = 0.00504 mol·L^{-1}

? Y = 204.2

For entry 2, [Trapper] = 0.527 mol·L^{-1}, X = 1.90

? [α–Product] = 1.159×10^{-6} t, R^2 = 0.99.

? $v_{initial}$ = 1.159×10^{-6} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0488 mol·L^{-1}, [Phosphine] = 0.00550 mol·L^{-1}

? Y = 231.6

For entry 3, [Trapper] = 0.320 mol·L^{-1}, X = 3.12

? [α–Product] = 7.239×10^{-7} t, R^2 = 0.995.

? $v_{initial}$ = 7.239×10^{-7} mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0481 mol·L^{-1}, [Phosphine] = 0.00424 mol·L^{-1}

? Y = 281.7

For entry 4, [Trapper] = 0.221 mol·L^{-1}, X = 4.52

? [α–Product] = 7.547×10^{-7} *t*, $R^2 = 0.993$.

? $v_{initial} = 7.547\times10^{-7}$ mol·L^{-1}·s^{-1}

? [Allenoate] = 0.0476 mol·L^{-1}, [Phosphine] = 0.00485 mol·L^{-1}

? $Y = 305.9$

The relationship between *X* and *Y* at 304 K:

$Y = 30.7X + 174$, $R^2 = 0.97$.

? $\frac{k_a + k_g}{k_a k_1} = 174 \pm 12$, $\frac{k_{-1}}{k_a k_1} = 30.7 \pm 4.0$

And $k_\alpha/k_\gamma = 2.52$ at 304 K,

? $k_1 = (8.03 \pm 0.55)\times10^{-3}$ mol^{-1}·L·s^{-1}

$k_\alpha/k_{-1} = 4.06 \pm 0.53$

$k_\gamma/k_{-1} = 1.61 \pm 0.21$

Derivation of the activation parameters:

TS-1:

$$\ln\frac{k_1}{T} = -\frac{\Delta H_{\text{TS-1}}}{RT} + \frac{\Delta S_{\text{TS-1}}}{R} + \ln\frac{k_B}{h}$$

? $\ln\frac{k_1}{T} = -(7450 \pm 360)\frac{1}{T} + (13.9 \pm 1.2)$, $R^2 = 0.996$ (Figure S1)

? $\Delta H_{\text{TS-1}} = (14.8 \pm 0.7)$ kcal/mol, $\Delta S_{\text{TS-1}} = -(19.6 \pm 1.7)$ cal/mol·K
$\Delta G_{\text{TS-1}}(298\ \text{K}) = 20.6$ kcal/mol

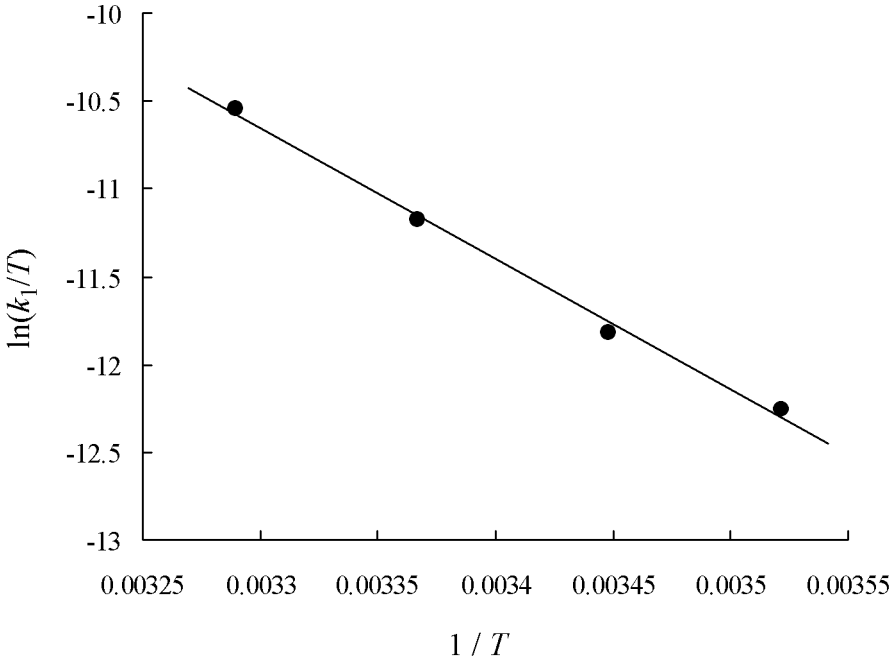


Figure S1. Eyring Plot for k_1.

a-**TS:**

$$\ln\frac{k_a}{k_{-1}} = -\frac{\Delta H_{\text{a-TS}} - \Delta H_{\text{TS-1}}}{RT} + \frac{\Delta S_{\text{a-TS}} - \Delta S_{\text{TS-1}}}{R}$$

? $\ln\frac{k_a}{k_{-1}} = (6510 \pm 320)\frac{1}{T} - (20.1 \pm 1.1)$, $R^2 = 0.995$ (Figure S2)

? $\Delta H_{\text{a-TS}} - \Delta H_{\text{TS-1}} = -(12.9 \pm 0.6)$ kcal/mol, $\Delta S_{\text{a-TS}} - \Delta S_{\text{TS-1}} = -(40.0 \pm 2.2)$ cal/mol·K

? $\Delta H_{\text{a-TS}} = (1.9 \pm 0.6)$ kcal/mol, $\Delta S_{\text{a-TS}} = -(59.6 \pm 2.2)$ cal/mol·K
$\Delta G_{\text{a-TS}}(298\text{ K}) = 19.6$ kcal/mol

g-**TS:**

$$\ln\frac{k_g}{k_{-1}} = -\frac{\Delta H_{\text{?-TS}} - \Delta H_{\text{TS-1}}}{RT} + \frac{\Delta S_{\text{?-TS}} - \Delta S_{\text{TS-1}}}{R}$$

? $\ln\frac{k_g}{k_{-1}} = (5570 \pm 160)\frac{1}{T} - (17.9 \pm 0.5)$, $R^2 = 0.999$ (Figure S2)

? $\Delta H_{\text{?-TS}} - \Delta H_{\text{TS-1}} = -(11.1 \pm 0.3)$ kcal/mol, $\Delta S_{\text{?-TS}} - \Delta S_{\text{TS-1}} = -(35.6 \pm 1.0)$ cal/mol·K

? $\Delta H_{\text{?-TS}} = (3.7 \pm 0.3)$ kcal/mol, $\Delta S_{\text{?-TS}} = -(55.2 \pm 1.0)$ cal/mol·K
$\Delta G_{\text{?-TS}}(298\text{ K}) = 20.1$ kcal/mol

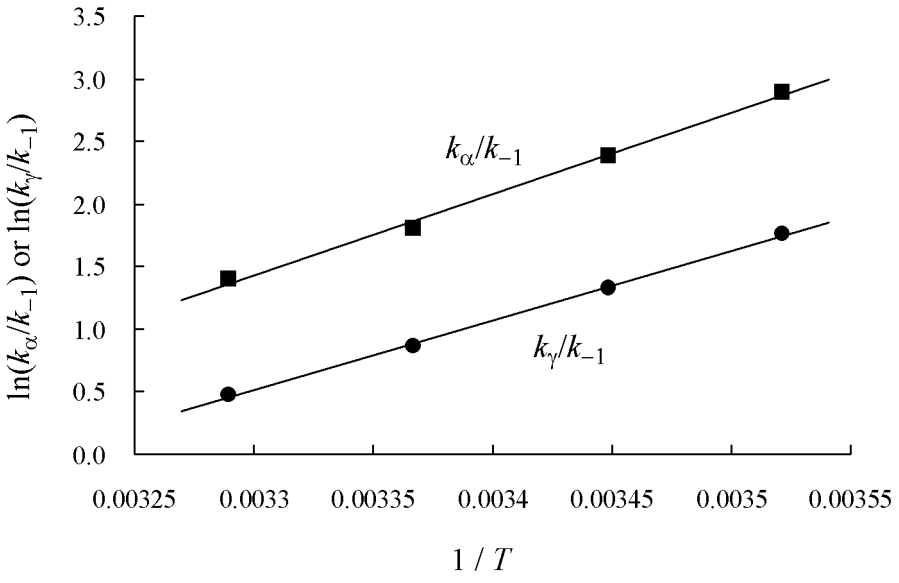


Figure S2. Eyring Plot for k_α/k_{-1} and k_γ/k_{-1}.

4. Further Regioselectivity Discussions of the (3+2) Cycloaddition

There are four possible approaches for addition of 1,3-dipole **3** to methyl acrylate (**4**) considering their relative orientations (α–**TS2**, α–**TS2'**, γ–**TS2** and γ–**TS2'**, see Figure S3). Calculations indicate that α–**TS2'** and γ–**TS2'** are generally disfavored than α–**TS2** and γ–**TS2** by more than 4 kcal/mol (Figure S3). The AIM analysis shows the higher energies of α–**TS2'** and γ–**TS2'** with respect to α–**TS2** and γ–**TS2** are due to the absence of H-bonding interaction between carbonyl oxygen of the alkenoate moiety and hydrogen of the phosphine moiety (Figure S4), although the formers are less sterically hindered than the latters.

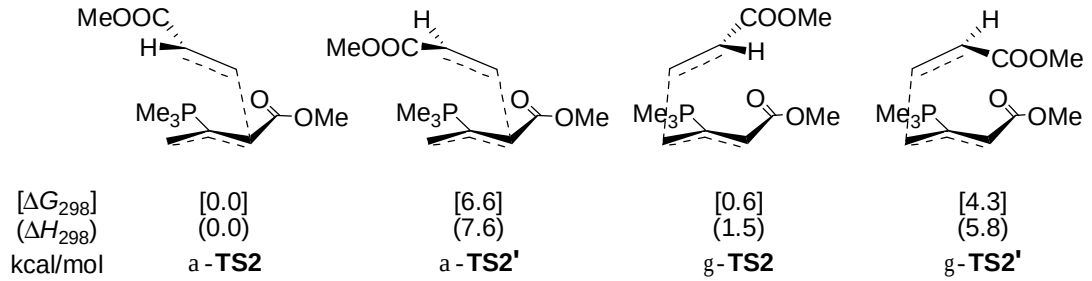


Figure S3. Four possible (3+2) addition modes between 1,3-dipole **3** and methyl acrylate (**4**).

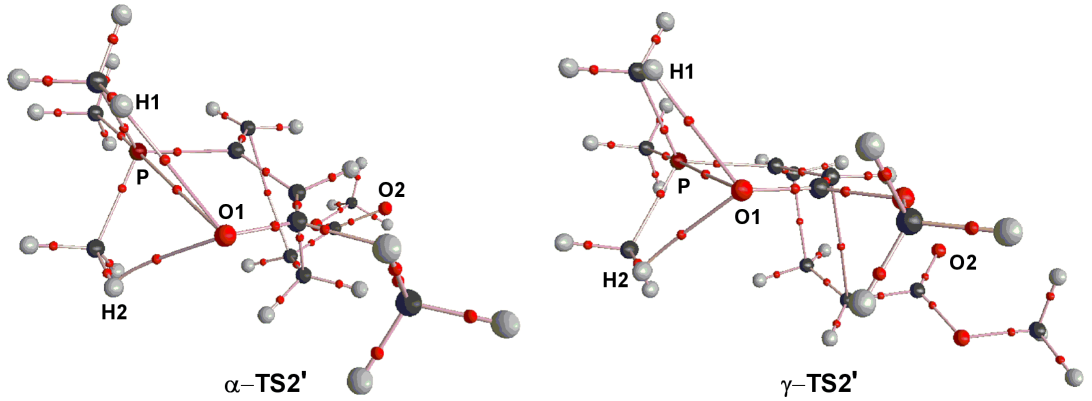


Figure S4. The bond critical points (small red spheres) in the transition states α–**TS2'** and γ–**TS2'**.

5. Further Discussions of the H-D Exchange between Allenoate and Water/Methanol

Previous control experiment revealed that there was no deuterium and hydrogen exchange (H–D exchange) between deuterium labeled allenoate **7** and water in the presence of triphenylphosphine in benzene.[6] It was observed that only dimer and other unidentifiable products were formed. Hydrogen incorporation in **7** could not be detected in the reaction mixture by ^{1}H NMR. In final (3+2) cycloadducts, there was no 5-H substituted product found (reactions **I** and **II**, Scheme S1). However, about 8% 5-H substituted products **9** and **10** were generated in the reaction between **7** and **8** with 1 equiv. CH_3OH as the additive (reaction **III**, Scheme S1). This indicated that some deuterium and hydrogen exchange occurred between deuterium labeled allenoate **7** and the added methanol. This hypothesis was further supported experimentally by the reaction between **29** and **30** with 10 equiv. CH_3OD as the additive (reaction **VII**, Scheme S2), where about 35% 5-D substituted products **31** and **32** were formed. However, when we used a more electron-deficient trapper, *N*-tosyl imine, there were no 5-D substituted products **13** and **14** found in the reaction between **11** and **12** using 1 equiv. CH_3OD as the additive (reaction **V**, Scheme S1). Adding more CH_3OD (13.5 equiv.) still gave the same results (reaction **VIII**, Scheme S2). For comparison, we have also done the H–D exchange reaction between deuterium labeled allenoate **7** and methanol in the presence of triphenylphosphine in benzene. In this case, hydrogen incorporation in **7** could not be detected in the reaction mixture by ^{1}H NMR either.

The above experimental results suggest that during the (3+2) cycloaddition of 1,3-dipole and the trapper, there is a competitive H–D exchange reaction between the 1,3-dipole and the protic additive, which could lead to hydrogen incorporation in the α– and/or γ–position of allenoate **7**. Whether this H–D exchange occurs or not depends on the added additives and the trappers. When water is the additive, there is no H–D exchange reaction using either electron-deficient alkene or imine (reactions **II** and **IV**, Scheme S1). However, when methanol is the additive, the involvement of H–D exchange reaction depends on the trappers used: in the case of electron-deficient alkene, there is H–D exchange competing with the (3+2)

[6] Details see the Supporting Information of *J. Am. Chem. Soc.* **2007**, *129*, 3470.

cycloaddition (reaction **III**, Scheme S1); in the case of electron-deficient imine, the (3+2) cycloaddition is favored and the H–D exchange is suppressed (reaction **V**, Scheme S1). No matter whether the H–D exchange occurs or not, it is still evident from all reactions shown in Schemes S1 and S2 that the [1,2]-proton shift has to be catalyzed by a protic source such as water or methanol.

To better understand the H–D exchange between allenoate and water/methanol, we computed the proton exchange between 1,3-dipole **3** and water or methanol, respectively. The computed energy surfaces are shown in Figures S5 and S6, and relative energies of transition states are listed in Table S5.

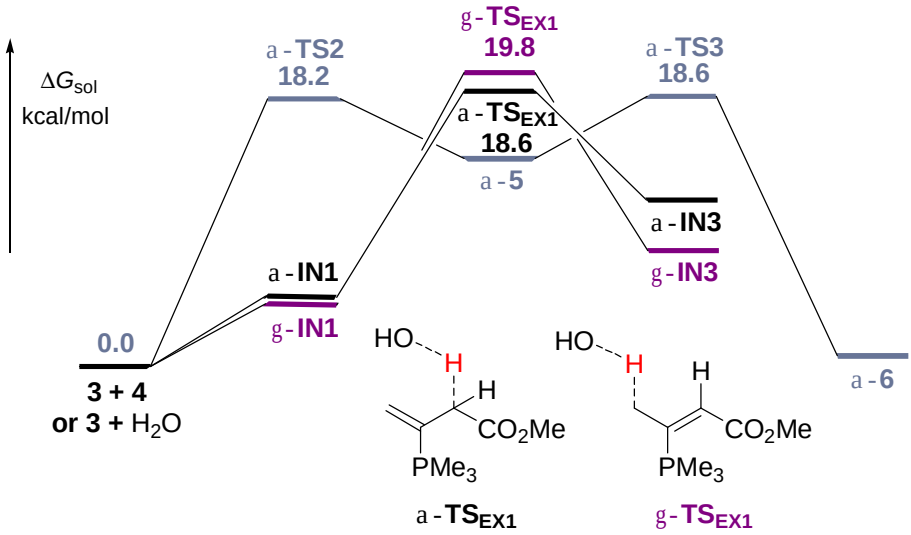


Figure S5. The DFT computed energy surfaces of the proton exchange between 1,3-dipole **3** and water. The α–addition mode of (3+2) cycloaddition is also given for reference.

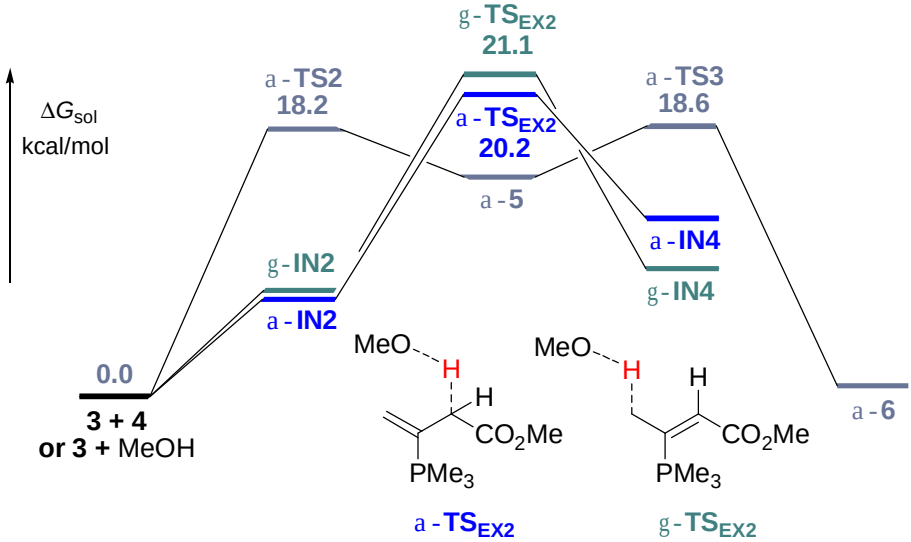


Figure S6. The DFT computed energy surfaces of the proton exchange between 1,3-dipole **3**

and methanol. The α–addition mode of (3+2) cycloaddition is also given for reference.

Table S5. The DFT computed energies of transition states in the proton exchange between 1,3-dipole **3** and water/methanol. Energies of transition states in the α–addition mode of (3+2) cycloaddition are also listed for reference. Energies are in kcal/mol.

	a-$\mathbf{TS_{EX1}}$	g-$\mathbf{TS_{EX1}}$	a-$\mathbf{TS_{EX2}}$	g-$\mathbf{TS_{EX2}}$	a-**TS2**	g-**TS2**
$D\boldsymbol{G}_{sol}$	18.6	19.8	20.2	21.1	18.2	18.6
$D\boldsymbol{G}_{298}$	18.2	19.3	18.1	18.5	19.0	19.8
$D\boldsymbol{H}_{298}$	6.8	7.2	6.4	6.6	4.0	3.7

Calculations indicate that the energies of the proton exchange between 1,3-dipole **3** and water/methanol are 1–3 kcal/mol higher than those of the α–addition mode of (3+2) cycloaddition (Table S5), suggesting the (3+2) cycloaddition is more facile than the proton exchange in theory. Why H–D exchange between **3** and methanol happens (its extent depends on the concentration of added methanol), whereas H–D exchange between **3** and water does not? It is known that a reaction's rate is proportional to both the rate constant and the concentration of the reactant(s) that appears in the reaction rate equation. We reason that the concentrations of protic source (water or methanol) and the trapping reagent are critical in determining the competition between H–D exchange and (3+2) cycloaddition. In the case of water, the concentration of saturated water in benzene at room temperature (0.035 mol/L at 298 K) is far less than that of the trapping reagent in phosphine-catalyzed (3+2) reaction (usually 2–0.2 mol/L[4,5]). Therefore, the H–D exchange is disfavored with respect to (3+2) cycloaddition. Consequently, in all isotopic labeling experiments using water (H_2O or D_2O), no H–D exchange occurred at the 5–position of final (3+2) products. In contrary, in the case of methanol, methanol can form a miscible solution with benzene, so its concentration can be adjusted to be higher than the trapper's concentration (Scheme S2, reactions **VII** and **VIII**), making H–D exchange very competitive. Consequently, H–D exchange can be observed in some cases. When the energy difference between the proton exchange and the (3+2) cycloaddition is small, the extent of H–D exchange will be increased as the concentration of methanol is increased (e.g. reactions **III** and **VII**). When the energy difference between the

proton exchange and the (3+2) cycloaddition is large, the H–D exchange will be hardly observed (e.g. reactions **V** and **VIII**).

6. MeOH - Catalyzed [1,2] - Proton and [1,3] - Proton Shifts

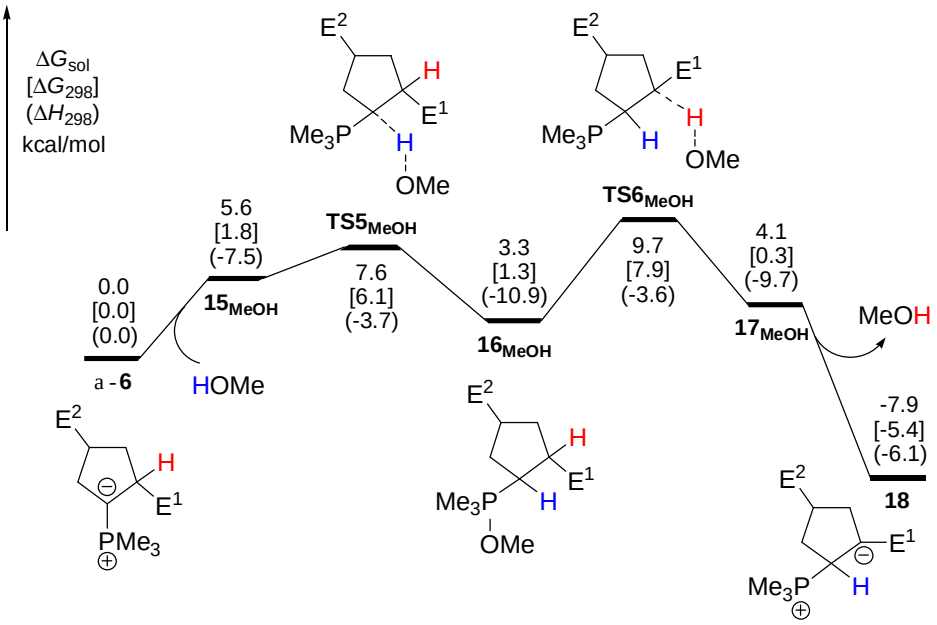


Figure S7. The DFT computed energy surface of MeOH–catalyzed [1,2]–proton shift ($E^1 = E^2 = CO_2Me$).

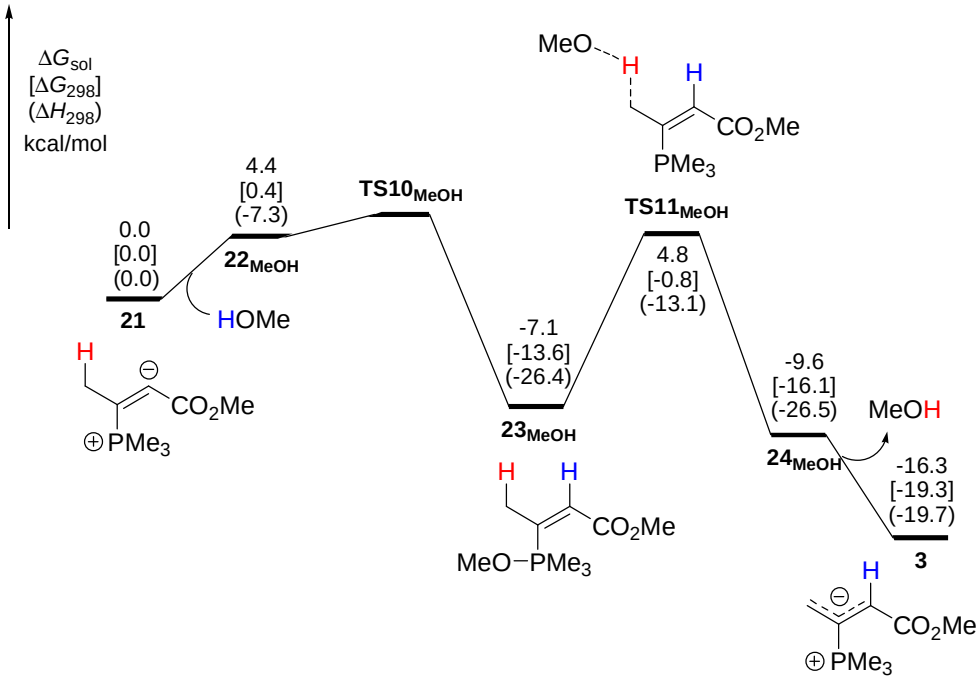


Figure S8. The DFT computed energy surface of MeOH–catalyzed [1,3]–proton shift.[7]

[7] After many attempts, the transition state **TS10$_{MeOH}$** can not be located. However, the reaction between olefinic anion and methanol is expected to be very facile with a very low activation barrier.

7. Colour Versions of the Figures 2, 5, 7, 9, 11, and 16

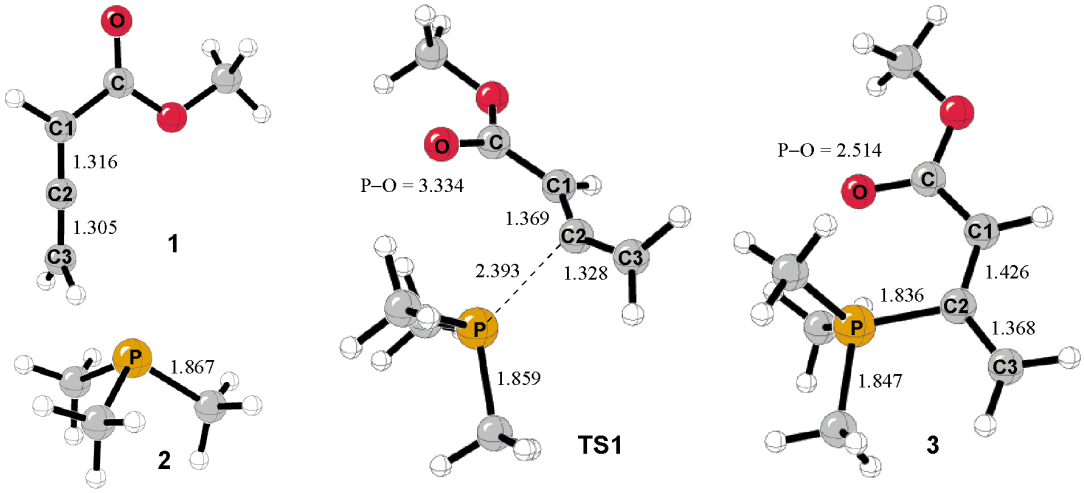


Figure 2. The DFT optimized structures of **1**, **2**, transition state **TS1**, and 1,3-dipole **3**. Distances are in Å.

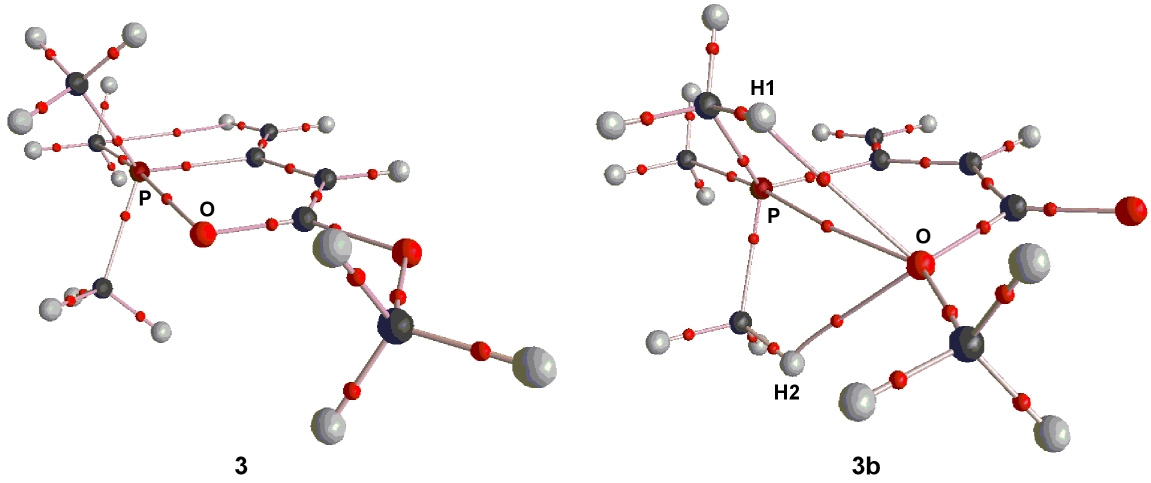


Figure 5. The bond critical points (small red spheres) in the 1,3-dipole **3** and its isomer **3b**.

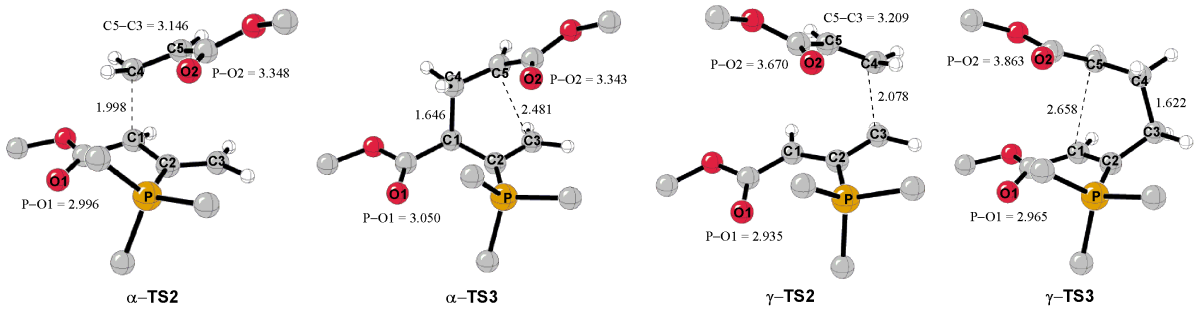


Figure 7. The DFT optimized structures of the transition states in the (3+2) cycloaddition

process. Distances are in Å. For clarity, each methyl group is represented by a carbon atom.

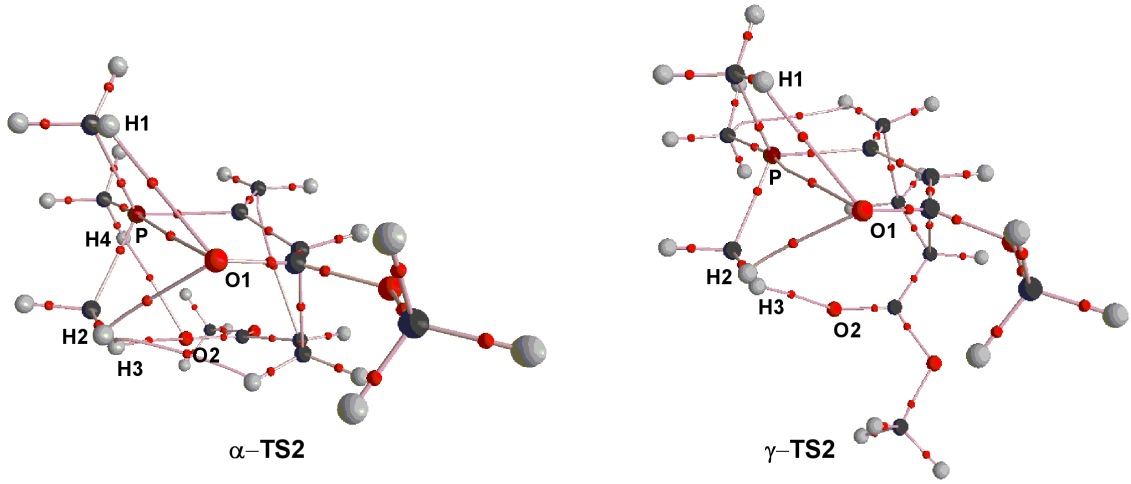


Figure 9. The bond critical points (small red spheres) in the transition states α–**TS2** and γ–**TS2**.

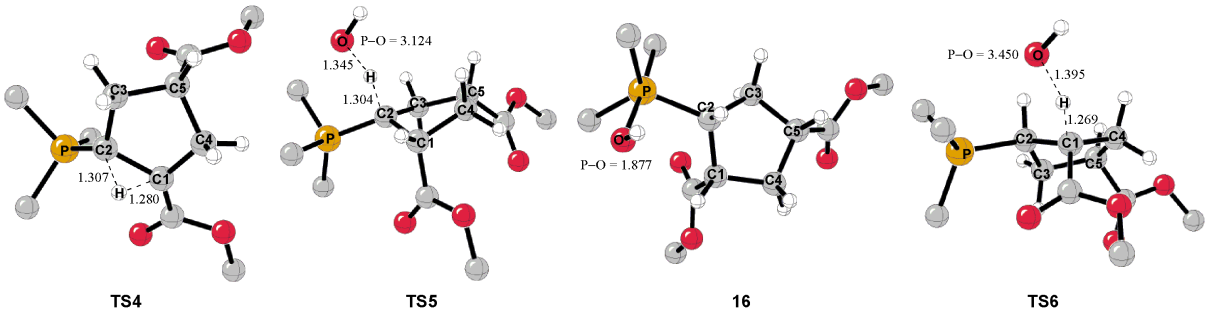


Figure 11. The DFT optimized structures of the transition states and intermediate **16** in the [1,2]-proton shift. Distances are in Å. For clarity, each methyl group is represented by a carbon atom.

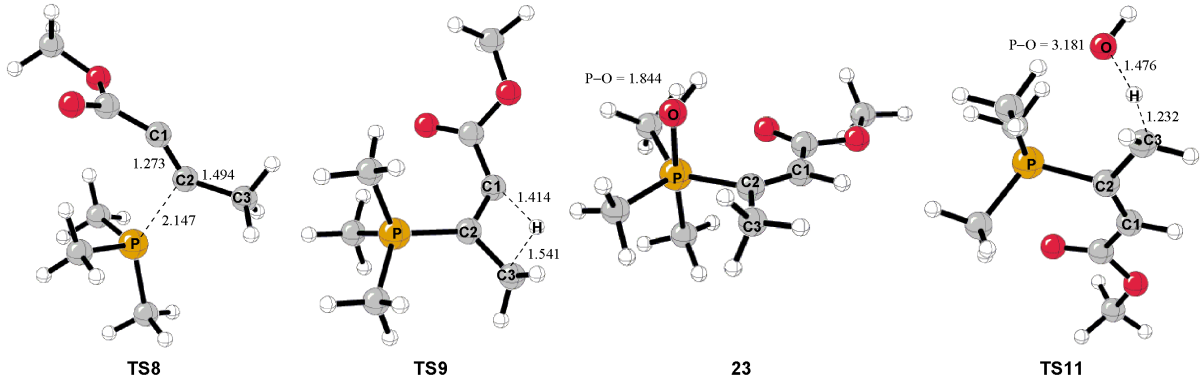
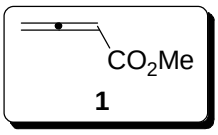


Figure 16. The DFT optimized geometries of the transition states and intermediate **23** in the 1,3-dipole formation between PMe_3 and alkynoate. Distances are in Å.

8. Coordinates of All Stationary Points



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	1	0	3.320267	-1.054402	0.930193
4	1	0	3.320857	-1.054400	-0.929455
5	6	0	0.864078	0.974797	-0.000526
6	1	0	1.036251	2.048757	0.000741
7	6	0	-0.568363	0.585412	0.000013
8	8	0	-1.477016	1.395538	0.000243
9	8	0	-0.756465	-0.751884	-0.000220
10	6	0	-2.127014	-1.190238	0.000050
11	1	0	-2.079608	-2.279654	-0.000192
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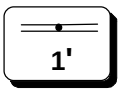
13	1	0	-2.644658	-0.825450	-0.891345



Standard orientation:

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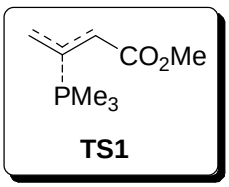
5	1	0	-1.877033	-0.477806	0.796395
6	1	0	1.877176	-0.796311	-0.477712
7	1	0	1.876976	0.796429	0.477833

PMe_3
2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000524	-0.000549	-0.605642
2	6	0	0.459499	1.577630	0.279874
3	1	0	1.464428	1.892352	-0.024061
4	1	0	-0.235590	2.376423	-0.003128
5	1	0	0.442065	1.467894	1.372459
6	6	0	1.138131	-1.185734	0.280334
7	1	0	0.899553	-2.214844	-0.011709
8	1	0	2.175594	-0.991610	-0.015164
9	1	0	1.063949	-1.104634	1.373003
10	6	0	-1.596898	-0.391177	0.280738
11	1	0	-2.369749	0.326646	-0.017192
12	1	0	-1.945666	-1.389199	-0.008584
13	1	0	-1.491116	-0.359109	1.373332



Standard orientation:

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1	6	0	0.212786	1.613678	-0.061829
2	15	0	1.675320	-0.280288	-0.070219
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4	1	0	0.740280	-1.321686	1.898774
5	1	0	2.276971	-0.519151	2.281834
6	1	0	2.297527	-2.110180	1.474483
7	1	0	-0.034738	-1.812915	-0.857640
8	6	0	0.958660	-1.531619	-1.216665
9	1	0	1.588718	-2.426899	-1.276136
10	1	0	3.928001	-1.188098	-0.589053
11	1	0	0.855253	-1.100492	-2.218206
12	6	0	3.454970	-0.197265	-0.600379
13	1	0	4.013465	0.462665	0.072245
14	1	0	3.521014	0.214850	-1.612797
15	1	0	2.036310	2.560171	0.509938
16	6	0	0.957975	2.612754	0.397116
17	6	0	-1.029270	1.287398	-0.536747
18	1	0	-1.381989	1.740460	-1.459781
19	1	0	0.469917	3.541516	0.690316
20	6	0	-1.826836	0.254292	0.069184

21	8	0	-1.479402	-0.495853	0.986117
22	1	0	-3.500385	-1.848358	-0.075407
23	6	0	-3.930023	-0.847942	0.039191
24	1	0	-4.111528	-0.661004	1.102018
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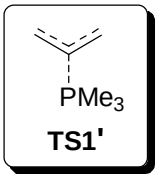
26	8	0	-3.063011	0.148561	-0.512617



Standard orientation:

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5	1	0	3.012534	1.716793	-0.252885
6	6	0	2.115728	-1.074686	-0.028784
7	1	0	2.890836	-1.276380	0.705936
8	1	0	1.843426	-1.885589	-0.697963
9	6	0	-0.934086	-0.643637	1.643661
10	6	0	-1.013431	-1.259042	-1.192117
11	1	0	-0.934597	-0.881699	-2.217052
12	1	0	-0.977150	0.158169	2.387736
13	1	0	-1.891177	-1.176992	1.633703
14	1	0	-0.133520	-1.338659	1.917956

15	1	0	-0.346690	-2.118310	-1.082892
16	1	0	-2.043255	-1.586282	-1.010559
17	6	0	-1.814639	1.366939	-0.295868
18	1	0	-1.652124	1.823122	-1.278130
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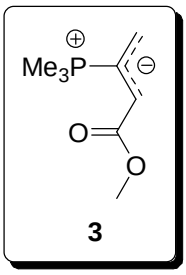

3

Standard orientation:

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4	1	0	2.636341	2.186230	-0.000167
5	6	0	-0.777436	1.472904	0.000082
6	1	0	-1.211101	2.466873	0.000220
7	6	0	-1.601841	0.347762	-0.000053
8	8	0	-1.175345	-0.844999	-0.000240
9	8	0	-2.949878	0.592747	0.000093
10	6	0	-3.802651	-0.552552	-0.000009
11	1	0	-4.820137	-0.155610	-0.000078
12	1	0	-3.639374	-1.168646	-0.890674

13	1	0	-3.639526	-1.168686	0.890661
14	15	0	1.296351	-0.384892	0.000020
15	6	0	0.993646	-1.329651	-1.547003
16	1	0	0.531289	-2.289787	-1.311472
17	1	0	0.297384	-0.767571	-2.171865
18	1	0	1.936690	-1.481674	-2.081898
19	6	0	0.993318	-1.329574	1.547023
20	1	0	0.296876	-0.767487	2.171678
21	1	0	0.531077	-2.289754	1.311444
22	1	0	1.936238	-1.481511	2.082161
23	6	0	3.139656	-0.261670	0.000206
24	1	0	3.506501	0.255190	-0.890678
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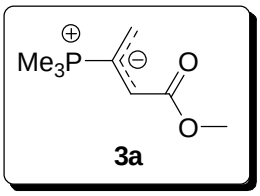
26	1	0	3.542640	-1.281126	0.000309



Standard orientation:

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6	8	0	-2.545574	1.324742	0.000064

7	8	0	-2.995971	-0.914395	-0.000042
8	6	0	-4.380493	-0.571112	0.000044
9	1	0	-4.919146	-1.522162	-0.000020
10	1	0	-4.644120	0.012080	0.889141
11	1	0	-4.644191	0.012242	-0.888926
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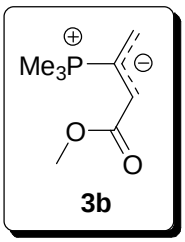
13	1	0	-0.543237	2.595196	-0.000071
14	1	0	1.315357	2.580603	-0.000058
15	6	0	2.096015	-1.261525	1.469071
16	1	0	2.030363	-0.642592	2.369109
17	1	0	3.056251	-1.787606	1.453377
18	1	0	1.279843	-1.988106	1.493931
19	6	0	2.096080	-1.261910	-1.468760
20	1	0	1.279836	-1.988413	-1.493549
21	1	0	3.056257	-1.788089	-1.452820
22	1	0	2.030610	-0.643194	-2.368962
23	1	0	3.333289	1.570474	0.889290
24	6	0	3.350740	0.935161	-0.000119
25	1	0	4.271290	0.342716	-0.000111
26	1	0	3.333223	1.570351	-0.889615



3b

Standard orientation:

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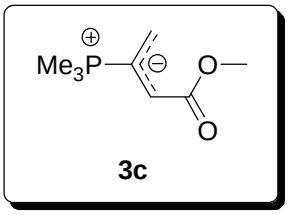
4	1	0	-2.660719	2.083128	-0.196843
5	6	0	0.772703	1.577326	0.053388
6	1	0	1.024749	2.632697	0.113325
7	6	0	1.918760	0.749014	0.033747
8	8	0	3.093847	1.109737	0.127657
9	8	0	1.647445	-0.635377	-0.113130
10	6	0	2.806111	-1.475345	-0.111255
11	1	0	2.434708	-2.498357	-0.226096
12	1	0	3.475169	-1.222066	-0.939019
13	1	0	3.362565	-1.378000	0.826157
14	15	0	-1.298062	-0.369074	0.026610
15	6	0	-0.803254	-1.256698	1.542831
16	1	0	-1.266141	-2.249093	1.563454
17	1	0	0.282539	-1.345845	1.571131
18	1	0	-1.145596	-0.679206	2.407480
19	6	0	-0.936337	-1.370005	-1.457447
20	1	0	-1.385978	-0.873681	-2.323434
21	1	0	0.143456	-1.433215	-1.591510
22	1	0	-1.366302	-2.371729	-1.350347
23	6	0	-3.128676	-0.349782	0.105263
24	1	0	-3.474757	0.207496	0.979103
25	1	0	-3.554527	0.095422	-0.797063
26	1	0	-3.475647	-1.385650	0.183719

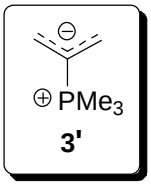


3c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.900086	-0.046160	0.000014
2	6	0	2.272516	-1.065931	1.469522
3	1	0	2.094207	-0.470115	2.369932
4	1	0	1.604423	-1.930538	1.494902
5	1	0	3.313295	-1.406234	1.454113
6	6	0	3.113624	1.316720	-0.000274
7	1	0	4.123999	0.895424	-0.000209
8	1	0	2.984786	1.938500	-0.890033
9	1	0	2.984822	1.938836	0.889254
10	6	0	2.272594	-1.066625	-1.468994
11	1	0	1.604318	-1.931096	-1.494146
12	1	0	2.094593	-0.471151	-2.369693
13	1	0	3.313296	-1.407146	-1.453236
14	6	0	0.181190	0.497501	-0.000151
15	6	0	0.002969	1.863771	-0.000134
16	1	0	-0.996670	2.278665	-0.000132
17	1	0	0.833025	2.560199	-0.000151
18	6	0	-0.697188	-0.620535	-0.000143
19	1	0	-0.286357	-1.625786	-0.000162
20	6	0	-2.124816	-0.618669	-0.000090
21	8	0	-2.846381	-1.621159	0.000007

22	8	0	-2.681597	0.649249	-0.000027
23	6	0	-4.110436	0.687358	0.000113
24	1	0	-4.516586	0.194140	0.889083
25	1	0	-4.374589	1.747703	0.000471
26	1	0	-4.516737	0.194732	-0.889125

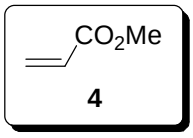


3'

Standard orientation:

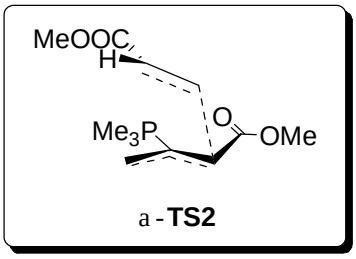
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.448223	0.000108	0.001542
2	6	0	1.342145	0.000046	-0.117989
3	6	0	1.888631	1.282708	-0.038433
4	1	0	1.306084	2.185103	-0.177390
5	1	0	2.961327	1.409441	0.080281
6	6	0	1.889928	-1.281868	-0.043164
7	1	0	2.963079	-1.408192	0.071503
8	1	0	1.305156	-2.185120	-0.166505
9	6	0	-1.020907	-0.015605	1.739413
10	6	0	-1.228459	-1.442652	-0.810295
11	1	0	-0.937225	-1.473847	-1.864047
12	1	0	-0.622791	0.865142	2.250365
13	1	0	-2.114868	-0.012225	1.791590
14	1	0	-0.629296	-0.910029	2.231207
15	1	0	-0.902403	-2.368922	-0.331528

16	1	0	-2.318253	-1.367511	-0.735082
17	6	0	-1.227023	1.457578	-0.785190
18	1	0	-0.932840	1.509490	-1.837269
19	1	0	-0.903558	2.374376	-0.286915
20	1	0	-2.316954	1.379430	-0.715388



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.500131	-0.018631	-0.000308
2	1	0	2.553737	1.066939	-0.001022
3	1	0	3.434008	-0.573250	-0.000264
4	6	0	1.318444	-0.643954	0.000346
5	1	0	1.236754	-1.727292	0.001064
6	6	0	0.044921	0.120731	-0.000055
7	8	0	-0.060263	1.333047	0.000322
8	8	0	-1.017561	-0.719603	-0.000096
9	6	0	-2.313523	-0.093813	-0.000160
10	1	0	-3.030850	-0.914918	-0.001206
11	1	0	-2.435871	0.526692	0.891737
12	1	0	-2.435025	0.528280	-0.891057

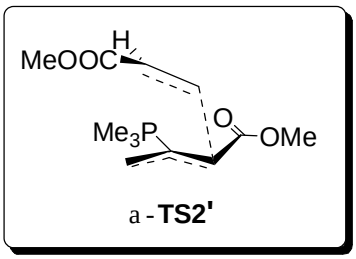


a-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.261143	0.348148	1.067606
2	6	0	0.694135	0.298497	2.033481
3	1	0	0.727373	-0.545887	2.715089
4	1	0	1.445250	1.063315	2.186723
5	6	0	-1.083508	-0.825486	0.795566
6	1	0	-1.110042	-1.516711	1.634615
7	6	0	-2.372922	-0.699699	0.137919
8	8	0	-2.749618	0.244857	-0.565523
9	8	0	-3.141903	-1.809675	0.304602
10	6	0	-4.403573	-1.817675	-0.379082
11	1	0	-4.860447	-2.776389	-0.129349
12	1	0	-5.034639	-0.992595	-0.035580
13	1	0	-4.258913	-1.732562	-1.459892
14	15	0	-0.252540	1.806872	-0.018292
15	6	0	-1.609631	2.954237	0.412250
16	1	0	-2.565072	2.468797	0.204476
17	1	0	-1.546657	3.207856	1.475046
18	1	0	-1.520096	3.869396	-0.183270
19	6	0	-0.286842	1.492708	-1.811380
20	1	0	0.568835	0.851608	-2.045351

21	1	0	-1.228160	1.018314	-2.087680
22	1	0	-0.188751	2.455512	-2.325935
23	6	0	1.291959	2.745751	0.250453
24	1	0	1.383544	3.091172	1.283251
25	1	0	2.136296	2.103110	-0.016061
26	1	0	1.278935	3.619300	-0.409722
27	6	0	0.046630	-1.991081	-0.369450
28	1	0	-0.584693	-2.873527	-0.282532
29	1	0	-0.093095	-1.456539	-1.307234
30	6	0	1.369573	-2.094415	0.105511
31	1	0	1.648186	-2.867772	0.814417
32	6	0	2.378166	-1.182471	-0.310127
33	8	0	2.238849	-0.181420	-1.043574
34	8	0	3.629473	-1.512521	0.173966
35	6	0	4.704711	-0.667704	-0.225966
36	1	0	5.607029	-1.126564	0.185083
37	1	0	4.775727	-0.603042	-1.316577
38	1	0	4.587755	0.345328	0.178399



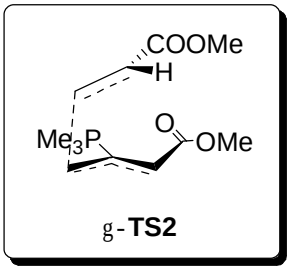
a-**TS2'**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.410939	-0.636305	-0.668440

2	6	0	0.682506	-1.328581	-1.110816
3	1	0	1.525140	-0.783223	-1.521084
4	1	0	0.736512	-2.408699	-1.177095
5	6	0	-0.266236	0.805896	-0.451521
6	1	0	0.392572	1.260148	-1.189721
7	6	0	-1.448986	1.616160	-0.178441
8	8	0	-2.507117	1.202746	0.313868
9	8	0	-1.245624	2.930167	-0.422821
10	6	0	-2.309652	3.825139	-0.063422
11	1	0	-1.944525	4.820993	-0.317140
12	1	0	-3.216047	3.593762	-0.630547
13	1	0	-2.526380	3.757013	1.006374
14	15	0	-1.778765	-1.603411	-0.014728
15	6	0	-3.356453	-1.392846	-0.913112
16	1	0	-3.710503	-0.368945	-0.791078
17	1	0	-3.188157	-1.604340	-1.973834
18	1	0	-4.098424	-2.096005	-0.518852
19	6	0	-2.073056	-1.413379	1.779780
20	1	0	-1.134434	-1.594929	2.312579
21	1	0	-2.425131	-0.402059	1.985384
22	1	0	-2.820553	-2.144755	2.106091
23	6	0	-1.397565	-3.385067	-0.212747
24	1	0	-1.249214	-3.641202	-1.265073
25	1	0	-0.501847	-3.655000	0.352595
26	1	0	-2.244846	-3.961758	0.172093
27	6	0	0.891063	1.051593	1.028538
28	1	0	1.162550	2.080067	0.791094
29	1	0	0.204037	0.995861	1.875649
30	6	0	1.966095	0.119216	1.058736
31	1	0	1.950537	-0.739465	1.721753

32	6	0	3.108665	0.309699	0.227321
33	8	0	3.239913	1.160241	-0.663811
34	8	0	4.122020	-0.600975	0.485148
35	6	0	5.296490	-0.455319	-0.312025
36	1	0	5.978780	-1.240187	0.023908
37	1	0	5.072655	-0.580123	-1.377342
38	1	0	5.753627	0.529352	-0.167016

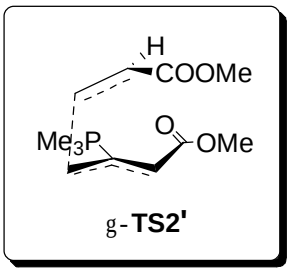


g-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.962984	-0.357136	1.045488
2	6	0	0.851887	-1.470519	1.916335
3	1	0	0.633581	-1.218850	2.951288
4	1	0	1.524744	-2.316289	1.819754
5	6	0	0.214480	0.797289	1.277271
6	1	0	-0.388821	0.829553	2.178133
7	6	0	0.278639	2.002046	0.503434
8	8	0	1.031983	2.211506	-0.460899
9	8	0	-0.577119	2.961732	0.953864
10	6	0	-0.562741	4.205166	0.243925
11	1	0	-1.288799	4.838538	0.756205

12	1	0	0.431829	4.660828	0.275360
13	1	0	-0.855582	4.059885	-0.800571
14	15	0	1.932727	-0.581748	-0.477221
15	6	0	3.497267	0.360222	-0.398436
16	1	0	3.260417	1.425671	-0.373201
17	1	0	4.045834	0.078720	0.505526
18	1	0	4.109143	0.135996	-1.279113
19	6	0	1.119084	-0.263246	-2.077771
20	1	0	0.156857	-0.786252	-2.077476
21	1	0	0.964569	0.808063	-2.201956
22	1	0	1.766689	-0.650306	-2.873066
23	6	0	2.434471	-2.339553	-0.590370
24	1	0	3.053314	-2.641546	0.257725
25	1	0	1.546798	-2.975983	-0.642535
26	1	0	3.014273	-2.469325	-1.509969
27	6	0	-0.974644	-2.408885	1.596803
28	1	0	-0.612797	-3.067460	0.811562
29	1	0	-0.987810	-2.854765	2.588913
30	6	0	-1.998477	-1.527025	1.257067
31	1	0	-2.623160	-1.052628	2.006583
32	6	0	-2.226937	-1.202179	-0.121453
33	8	0	-1.543919	-1.588720	-1.083233
34	8	0	-3.333608	-0.414585	-0.310115
35	6	0	-3.630492	-0.056915	-1.660252
36	1	0	-3.766368	-0.947224	-2.282564
37	1	0	-4.557454	0.518315	-1.612907
38	1	0	-2.829983	0.556223	-2.088550

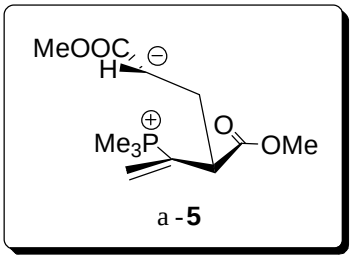


g-**TS2'**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.849954	-0.596428	-0.712336
2	6	0	-0.306256	-1.873686	-1.002626
3	1	0	0.530193	-1.874782	-1.698095
4	1	0	-0.956365	-2.736593	-1.117642
5	6	0	-0.028979	0.537803	-0.752567
6	1	0	0.917578	0.453104	-1.273781
7	6	0	-0.369642	1.823624	-0.224391
8	8	0	-1.424146	2.110490	0.372058
9	8	0	0.593757	2.759160	-0.441606
10	6	0	0.346989	4.061994	0.098546
11	1	0	1.222614	4.655596	-0.168856
12	1	0	-0.557627	4.499573	-0.335029
13	1	0	0.236097	4.016653	1.186398
14	15	0	-2.493225	-0.560149	0.031163
15	6	0	-3.665062	0.548774	-0.825099
16	1	0	-3.334163	1.581488	-0.710671
17	1	0	-3.694051	0.279428	-1.885510
18	1	0	-4.664292	0.424025	-0.393521
19	6	0	-2.550332	-0.245360	1.833701
20	1	0	-1.921672	-0.983210	2.341897

21	1	0	-2.178406	0.760013	2.033507
22	1	0	-3.581317	-0.344654	2.191262
23	6	0	-3.254979	-2.219470	-0.141317
24	1	0	-3.315053	-2.513818	-1.192278
25	1	0	-2.684733	-2.973162	0.408029
26	1	0	-4.268225	-2.178342	0.271840
27	6	0	1.731811	-1.331168	0.929516
28	1	0	1.511227	-0.674975	1.764240
29	6	0	0.886919	-2.383961	0.571814
30	1	0	0.133745	-2.694024	1.295121
31	1	0	1.321257	-3.206060	0.006409
32	6	0	2.916184	-1.055888	0.152520
33	8	0	3.238880	-1.610502	-0.900040
34	8	0	3.690439	-0.067945	0.709316
35	6	0	4.872477	0.277090	-0.017774
36	1	0	5.353694	1.065511	0.564646
37	1	0	5.538820	-0.586135	-0.114267
38	1	0	4.622570	0.643043	-1.018880



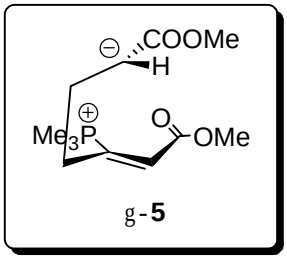
a-**5**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.230972	0.316421	1.018943

2	6	0	0.536775	0.265469	2.126317
3	1	0	0.483315	-0.595065	2.786563
4	1	0	1.245305	1.036719	2.409069
5	6	0	-1.005765	-0.910246	0.626303
6	1	0	-1.109592	-1.534379	1.517472
7	6	0	-2.377200	-0.655973	0.077471
8	8	0	-2.724216	0.334162	-0.556791
9	8	0	-3.202128	-1.699624	0.295559
10	6	0	-4.519746	-1.608275	-0.277647
11	1	0	-5.017730	-2.537805	-0.000877
12	1	0	-5.054626	-0.747106	0.131994
13	1	0	-4.456631	-1.512870	-1.364790
14	15	0	-0.070206	1.787689	-0.038359
15	6	0	-1.368225	3.003778	0.405336
16	1	0	-2.349817	2.586114	0.173258
17	1	0	-1.310669	3.228552	1.474934
18	1	0	-1.216653	3.927679	-0.163798
19	6	0	-0.155258	1.538183	-1.838514
20	1	0	0.660719	0.864374	-2.114124
21	1	0	-1.126989	1.126029	-2.112009
22	1	0	-0.024053	2.516555	-2.315115
23	6	0	1.513263	2.626984	0.299349
24	1	0	1.572454	2.968956	1.335968
25	1	0	2.312829	1.915907	0.070970
26	1	0	1.587620	3.500007	-0.358084
27	6	0	-0.154993	-1.841882	-0.422727
28	1	0	-0.760043	-2.749789	-0.526755
29	1	0	-0.172209	-1.312326	-1.382501
30	6	0	1.221593	-2.149937	0.009090
31	1	0	1.438765	-3.073942	0.534202

32	6	0	2.249522	-1.261902	-0.280025
33	8	0	2.136161	-0.131626	-0.847308
34	8	0	3.516938	-1.693730	0.110179
35	6	0	4.599937	-0.829965	-0.198294
36	1	0	5.501905	-1.365073	0.111954
37	1	0	4.648194	-0.606652	-1.270269
38	1	0	4.533375	0.119382	0.350589

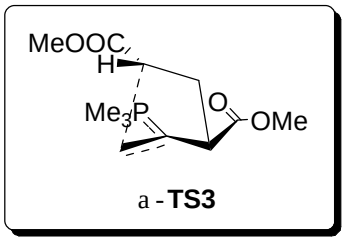


g-**5**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.131589	0.791934	-1.008614
2	6	0	-1.260760	0.786077	-1.995512
3	1	0	-0.820897	0.595990	-2.979862
4	1	0	-1.764185	1.757059	-2.060356
5	6	0	0.911646	-0.055063	-1.249823
6	1	0	0.863759	-0.676158	-2.138759
7	6	0	2.143325	-0.158909	-0.475668
8	8	0	2.501257	0.615568	0.411320
9	8	0	2.907270	-1.196357	-0.884774
10	6	0	4.162748	-1.368906	-0.208685
11	1	0	4.623948	-2.238871	-0.677087

12	1	0	4.791931	-0.483093	-0.334926
13	1	0	4.001343	-1.548097	0.858028
14	15	0	-0.293538	1.823115	0.477352
15	6	0	0.699383	3.347158	0.232848
16	1	0	1.757055	3.075253	0.188574
17	1	0	0.409870	3.836209	-0.702325
18	1	0	0.534368	4.038824	1.066380
19	6	0	0.142006	1.189056	2.132410
20	1	0	-0.462964	0.297832	2.310328
21	1	0	1.204974	0.957105	2.181171
22	1	0	-0.102896	1.978003	2.853808
23	6	0	-2.027960	2.369051	0.626711
24	1	0	-2.362499	2.911636	-0.260439
25	1	0	-2.645677	1.480519	0.783425
26	1	0	-2.106605	3.032336	1.494345
27	6	0	-2.398614	-0.335541	-1.768316
28	1	0	-3.113171	0.101982	-1.059844
29	1	0	-2.904522	-0.421273	-2.737707
30	6	0	-1.929167	-1.649263	-1.283709
31	1	0	-1.824472	-2.505114	-1.940702
32	6	0	-1.619055	-1.739133	0.066347
33	8	0	-1.655772	-0.758519	0.873754
34	8	0	-1.240186	-2.992608	0.524583
35	6	0	-0.910934	-3.089662	1.902812
36	1	0	-1.733396	-2.744620	2.540010
37	1	0	-0.717639	-4.149988	2.086122
38	1	0	-0.011978	-2.507732	2.145662

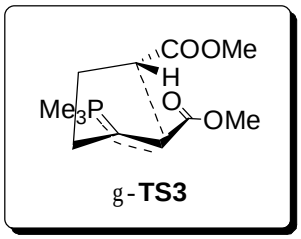


a-**TS3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.264937	0.337486	1.056954
2	6	0	0.824608	0.010338	1.840420
3	1	0	0.738385	-0.788106	2.568911
4	1	0	1.686975	0.654730	1.975341
5	6	0	-1.067870	-0.881240	0.722555
6	1	0	-1.231282	-1.457045	1.639688
7	6	0	-2.405409	-0.692629	0.071373
8	8	0	-2.770433	0.295591	-0.551301
9	8	0	-3.180875	-1.788190	0.204274
10	6	0	-4.462256	-1.751632	-0.450866
11	1	0	-4.920505	-2.718058	-0.239268
12	1	0	-5.073000	-0.938730	-0.048850
13	1	0	-4.335689	-1.611888	-1.527724
14	15	0	-0.187580	1.803248	0.047433
15	6	0	-1.504858	2.995173	0.501245
16	1	0	-2.479824	2.545505	0.302909
17	1	0	-1.424992	3.235042	1.566041
18	1	0	-1.399359	3.913800	-0.086934
19	6	0	-0.251126	1.619227	-1.769619
20	1	0	0.566139	0.952517	-2.060091
21	1	0	-1.216171	1.209140	-2.069388

22	1	0	-0.115888	2.607304	-2.224737
23	6	0	1.378932	2.687017	0.373796
24	1	0	1.496755	2.909881	1.437580
25	1	0	2.207786	2.067672	0.020115
26	1	0	1.367831	3.630226	-0.182236
27	6	0	-0.097100	-1.849989	-0.188240
28	1	0	-0.575070	-2.835286	-0.193845
29	1	0	-0.117585	-1.450644	-1.207886
30	6	0	1.287667	-1.906069	0.333619
31	1	0	1.574013	-2.706580	1.008675
32	6	0	2.319724	-1.165311	-0.284291
33	8	0	2.186499	-0.241780	-1.118248
34	8	0	3.587971	-1.522584	0.152245
35	6	0	4.673901	-0.795395	-0.413635
36	1	0	4.645921	0.262201	-0.122521
37	1	0	5.578596	-1.262024	-0.015840
38	1	0	4.667702	-0.854522	-1.507056



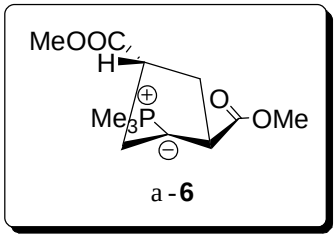
g-**TS3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.181920	-0.119619	-1.039112
2	6	0	-1.287597	-1.415561	-1.769639

3	1	0	-1.098627	-1.242216	-2.835594
4	1	0	-2.255338	-1.919595	-1.696160
5	6	0	0.000068	0.552029	-1.317465
6	1	0	0.476349	0.379452	-2.274332
7	6	0	0.547067	1.661074	-0.545010
8	8	0	0.044286	2.132296	0.475605
9	8	0	1.684000	2.149831	-1.085395
10	6	0	2.328004	3.209608	-0.362266
11	1	0	3.224930	3.445441	-0.935903
12	1	0	1.673211	4.083391	-0.294011
13	1	0	2.593486	2.877358	0.645224
14	15	0	-2.170259	0.161975	0.420165
15	6	0	-3.037291	1.773163	0.358560
16	1	0	-2.297671	2.575718	0.368165
17	1	0	-3.635750	1.832378	-0.555199
18	1	0	-3.692722	1.870350	1.231241
19	6	0	-1.413173	0.006096	2.081155
20	1	0	-0.731406	-0.851169	2.074200
21	1	0	-0.832265	0.903444	2.296382
22	1	0	-2.208039	-0.121248	2.825686
23	6	0	-3.514532	-1.083133	0.424508
24	1	0	-4.090893	-1.045159	-0.503484
25	1	0	-3.104975	-2.089192	0.553462
26	1	0	-4.182191	-0.869449	1.265278
27	6	0	-0.124705	-2.423357	-1.258023
28	1	0	-0.459234	-2.852788	-0.307506
29	1	0	-0.106650	-3.228343	-2.004617
30	6	0	1.203802	-1.806956	-1.090129
31	1	0	1.885599	-1.719448	-1.930032
32	6	0	1.716375	-1.577485	0.212764

33	8	0	1.098477	-1.705251	1.287987
34	8	0	3.040761	-1.174022	0.215411
35	6	0	3.617246	-0.946731	1.499353
36	1	0	4.656513	-0.667741	1.308543
37	1	0	3.102108	-0.138553	2.031115
38	1	0	3.577191	-1.849842	2.118023

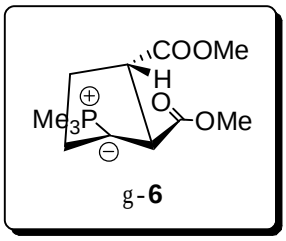


a-**6**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.349967	0.460933	-1.019280
2	6	0	-1.039808	0.148719	-1.541219
3	1	0	-1.009609	-0.105692	-2.612997
4	1	0	-1.767786	0.960610	-1.445559
5	6	0	0.937422	-0.923087	-0.794041
6	1	0	1.142763	-1.399509	-1.765645
7	6	0	2.196141	-1.063636	0.023555
8	8	0	2.565090	-0.314738	0.913217
9	8	0	2.885893	-2.177156	-0.312897
10	6	0	4.069693	-2.451095	0.457950
11	1	0	4.472927	-3.377353	0.047228
12	1	0	4.791392	-1.636550	0.351899
13	1	0	3.817843	-2.574515	1.514848

14	15	0	0.631959	1.857315	-0.068252
15	6	0	2.308999	2.579265	-0.292134
16	1	0	3.062349	1.865494	0.047286
17	1	0	2.466310	2.795287	-1.352923
18	1	0	2.405867	3.502314	0.291580
19	6	0	0.401026	1.924061	1.778729
20	1	0	-0.602818	1.559004	2.018316
21	1	0	1.135902	1.267462	2.250684
22	1	0	0.526282	2.944574	2.162813
23	6	0	-0.505172	3.183069	-0.640032
24	1	0	-0.464318	3.277572	-1.728347
25	1	0	-1.533465	2.968392	-0.335045
26	1	0	-0.204039	4.131958	-0.184286
27	6	0	-0.234304	-1.733354	-0.130124
28	1	0	-0.134334	-2.815914	-0.273797
29	1	0	-0.247532	-1.523945	0.944608
30	6	0	-1.516496	-1.172449	-0.788641
31	1	0	-1.935196	-1.877106	-1.512649
32	6	0	-2.593177	-0.833523	0.209362
33	8	0	-2.424123	-0.280898	1.283197
34	8	0	-3.827692	-1.160206	-0.252871
35	6	0	-4.933636	-0.812301	0.597622
36	1	0	-4.976797	0.270323	0.747883
37	1	0	-5.823488	-1.162656	0.073073
38	1	0	-4.838911	-1.305090	1.569167

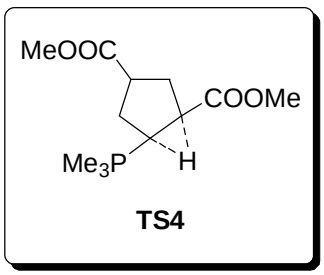


g-**6**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.162795	-0.331406	-0.863082
2	6	0	-1.231162	-1.832419	-1.206525
3	1	0	-1.988923	-2.074378	-1.967655
4	1	0	-1.442704	-2.473944	-0.338444
5	6	0	0.220030	0.173381	-1.230721
6	1	0	0.275553	0.492588	-2.284351
7	6	0	0.822678	1.318426	-0.441451
8	8	0	0.527834	1.649330	0.694328
9	8	0	1.767692	1.962538	-1.161093
10	6	0	2.474208	3.017109	-0.485850
11	1	0	3.180688	3.407226	-1.219379
12	1	0	1.780533	3.799330	-0.165348
13	1	0	3.002793	2.622159	0.385903
14	15	0	-2.223152	0.289974	0.308424
15	6	0	-2.590190	2.084453	0.151635
16	1	0	-1.690720	2.667643	0.361644
17	1	0	-2.934278	2.297529	-0.864549
18	1	0	-3.368185	2.369206	0.869320
19	6	0	-1.942976	0.095305	2.145735
20	1	0	-1.763439	-0.963207	2.362488
21	1	0	-1.050782	0.661102	2.423831

22	1	0	-2.801245	0.444339	2.734262
23	6	0	-3.843418	-0.553923	0.099444
24	1	0	-4.213390	-0.402772	-0.918442
25	1	0	-3.731645	-1.628351	0.275165
26	1	0	-4.570436	-0.158152	0.816490
27	6	0	0.177409	-2.178592	-1.755284
28	1	0	0.485671	-3.197353	-1.499002
29	1	0	0.190334	-2.090858	-2.848672
30	6	0	1.134737	-1.119830	-1.183471
31	1	0	2.027274	-0.971247	-1.799769
32	6	0	1.589383	-1.456045	0.223819
33	8	0	1.019506	-2.189829	1.006915
34	8	0	2.748182	-0.817289	0.529917
35	6	0	3.241576	-1.018345	1.866246
36	1	0	4.177644	-0.460634	1.916799
37	1	0	2.523987	-0.635038	2.596665
38	1	0	3.415950	-2.081491	2.053168



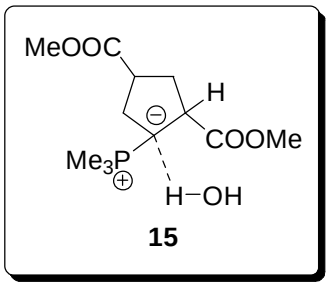
TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.692223	-0.574697	1.042497

2	6	0	-0.493621	-1.312856	1.673576
3	1	0	-0.378418	-1.388732	2.764389
4	1	0	-0.613659	-2.332028	1.297999
5	6	0	0.222515	0.948494	1.006682
6	1	0	1.087197	0.422057	1.789501
7	6	0	0.861146	1.898232	0.175253
8	8	0	1.929985	1.717102	-0.444598
9	8	0	0.207322	3.111533	0.118564
10	6	0	0.857759	4.131105	-0.643158
11	1	0	0.200551	5.001581	-0.583839
12	1	0	1.839824	4.369656	-0.221665
13	1	0	0.987669	3.824971	-1.686252
14	15	0	1.701286	-1.295597	-0.189188
15	6	0	3.475372	-0.897237	0.033258
16	1	0	3.594874	0.186348	-0.034210
17	1	0	3.800736	-1.247118	1.017625
18	1	0	4.071411	-1.387414	-0.745487
19	6	0	1.370756	-1.006398	-1.980431
20	1	0	0.317768	-1.217588	-2.186220
21	1	0	1.588520	0.041602	-2.200069
22	1	0	2.005144	-1.656358	-2.595693
23	6	0	1.609048	-3.118215	0.007736
24	1	0	1.771020	-3.397281	1.052759
25	1	0	0.630498	-3.482845	-0.317079
26	1	0	2.382824	-3.588085	-0.608287
27	6	0	-1.213455	1.011991	1.499061
28	1	0	-1.295224	1.328341	2.547751
29	1	0	-1.805015	1.720738	0.912082
30	6	0	-1.743093	-0.450266	1.385103
31	1	0	-2.547492	-0.623366	2.110074

32	6	0	-2.318381	-0.738168	0.011381
33	8	0	-1.819181	-1.452070	-0.841658
34	8	0	-3.496785	-0.102332	-0.173950
35	6	0	-4.128500	-0.286434	-1.453859
36	1	0	-4.339559	-1.345245	-1.627296
37	1	0	-5.054157	0.287787	-1.403731
38	1	0	-3.485151	0.089779	-2.253982

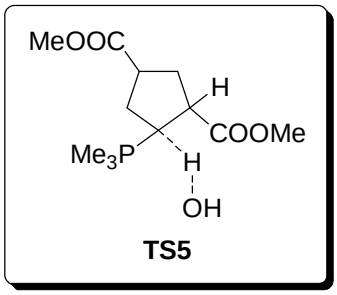


15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.918821	-0.451545	0.470780
2	6	0	0.008185	-1.691816	0.541287
3	1	0	0.427291	-2.488627	1.175489
4	1	0	-0.208208	-2.170700	-0.427313
5	6	0	0.201544	0.757193	1.071750
6	1	0	0.859666	1.329151	1.749472
7	6	0	-0.299630	1.836701	0.106225
8	8	0	0.127346	2.015378	-1.021256
9	8	0	-1.180454	2.675885	0.687148
10	6	0	-1.685920	3.737703	-0.140623
11	1	0	-2.378489	4.293728	0.492742

12	1	0	-0.870179	4.382856	-0.479109
13	1	0	-2.205324	3.320078	-1.006960
14	15	0	2.080564	-0.359217	-0.794093
15	6	0	3.231133	1.039698	-0.547298
16	1	0	2.692795	1.981746	-0.676650
17	1	0	3.654200	0.985263	0.460082
18	1	0	4.039134	0.988215	-1.284703
19	6	0	1.602224	-0.278657	-2.587681
20	1	0	0.944813	-1.123134	-2.823688
21	1	0	1.059570	0.650264	-2.771686
22	1	0	2.487383	-0.335376	-3.233180
23	6	0	3.110178	-1.881952	-0.752552
24	1	0	3.593179	-1.968493	0.224982
25	1	0	2.476345	-2.761367	-0.910397
26	1	0	3.868324	-1.855697	-1.542881
27	6	0	-0.919980	0.109853	1.925944
28	1	0	-0.504466	-0.159147	2.903959
29	1	0	-1.761327	0.785507	2.094231
30	6	0	-1.319758	-1.187746	1.197099
31	1	0	-1.712330	-1.938905	1.889295
32	6	0	-2.373374	-0.957212	0.134630
33	8	0	-2.538185	0.068610	-0.498658
34	8	0	-3.123605	-2.068662	-0.066785
35	6	0	-4.118212	-1.981009	-1.103014
36	1	0	-3.647683	-1.770057	-2.067426
37	1	0	-4.607085	-2.955793	-1.117622
38	1	0	-4.839024	-1.191157	-0.874674
39	1	0	2.252181	-0.740283	1.875044
40	8	0	3.017021	-0.834760	2.521808
41	1	0	2.622526	-1.028693	3.385062

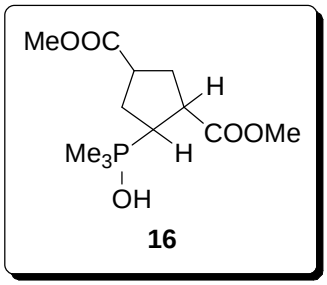


TS5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.896187	-0.541730	0.381239
2	6	0	-0.263616	-1.379539	-0.179428
3	1	0	-0.027823	-2.448626	-0.221486
4	1	0	-0.566810	-1.069188	-1.190781
5	6	0	0.265124	0.696139	1.028035
6	1	0	0.929879	1.114886	1.797048
7	6	0	-0.089701	1.861349	0.109929
8	8	0	0.273599	1.985287	-1.047928
9	8	0	-0.811060	2.799522	0.749719
10	6	0	-1.231001	3.932113	-0.033980
11	1	0	-1.788707	4.567447	0.654670
12	1	0	-0.363472	4.463764	-0.434415
13	1	0	-1.870300	3.599905	-0.855773
14	15	0	2.359965	-0.425234	-0.632677
15	6	0	3.537888	0.712464	0.165431
16	1	0	3.168241	1.741066	0.120176
17	1	0	3.634903	0.384765	1.206772
18	1	0	4.510411	0.659400	-0.334550

19	6	0	2.226931	0.034435	-2.405108
20	1	0	1.523546	-0.640218	-2.904478
21	1	0	1.854783	1.054924	-2.499948
22	1	0	3.207779	-0.065901	-2.883783
23	6	0	3.144266	-2.074805	-0.624732
24	1	0	3.246756	-2.372266	0.427295
25	1	0	2.509332	-2.795812	-1.150444
26	1	0	4.118627	-2.031573	-1.123207
27	6	0	-0.977518	0.071998	1.721617
28	1	0	-0.661730	-0.318757	2.693062
29	1	0	-1.769696	0.804445	1.887238
30	6	0	-1.437755	-1.110386	0.828850
31	1	0	-1.608417	-2.006339	1.431334
32	6	0	-2.711985	-0.812477	0.065876
33	8	0	-3.086277	0.289866	-0.287671
34	8	0	-3.389259	-1.947290	-0.227117
35	6	0	-4.587610	-1.786443	-1.008903
36	1	0	-4.354650	-1.330626	-1.975127
37	1	0	-4.982418	-2.794107	-1.142532
38	1	0	-5.306707	-1.157023	-0.477813
39	1	0	1.482798	-1.131450	1.385647
40	8	0	2.391569	-1.584405	2.267902
41	1	0	2.058367	-1.812766	3.149054

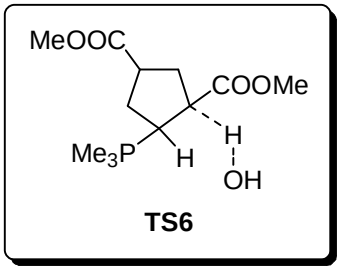


16

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.591764	-0.669450	-0.657449
2	6	0	0.708046	-1.165433	0.002732
3	1	0	0.772811	-2.254258	0.078689
4	1	0	0.809414	-0.747011	1.007282
5	6	0	-0.262788	0.788315	-1.062128
6	1	0	-0.931671	1.136710	-1.850750
7	6	0	-0.357415	1.785503	0.080585
8	8	0	-0.449417	1.519126	1.264351
9	8	0	-0.300001	3.050935	-0.384990
10	6	0	-0.309252	4.094982	0.607164
11	1	0	-0.258078	5.027098	0.043824
12	1	0	-1.228311	4.050252	1.197372
13	1	0	0.554209	3.995600	1.270347
14	15	0	-2.275179	-1.005275	0.137860
15	6	0	-3.334594	0.266953	0.976720
16	1	0	-2.913474	0.544172	1.943695
17	1	0	-3.472550	1.140611	0.340876
18	1	0	-4.316841	-0.197038	1.126385
19	6	0	-1.627890	-1.692960	1.807043
20	1	0	-0.995109	-2.580079	1.682924
21	1	0	-1.063688	-0.936659	2.362090
22	1	0	-2.490045	-1.988175	2.421458
23	6	0	-3.030818	-2.634362	-0.361247
24	1	0	-4.102715	-2.484849	-0.518409
25	1	0	-2.600671	-2.960827	-1.315145

26	1	0	-2.869585	-3.419360	0.382053
27	6	0	1.214084	0.694969	-1.565349
28	1	0	1.225297	0.627218	-2.657877
29	1	0	1.797909	1.575903	-1.288513
30	6	0	1.812840	-0.594056	-0.939089
31	1	0	2.017938	-1.337225	-1.717682
32	6	0	3.110352	-0.361404	-0.188340
33	8	0	3.520578	0.707770	0.217410
34	8	0	3.766003	-1.528203	0.014513
35	6	0	4.988836	-1.443536	0.771083
36	1	0	4.791841	-1.044828	1.769814
37	1	0	5.362666	-2.466132	0.830473
38	1	0	5.707972	-0.797764	0.260102
39	1	0	-0.695568	-1.206599	-1.611437
40	8	0	-3.029247	-0.272479	-1.417396
41	1	0	-2.955218	-0.831946	-2.206932



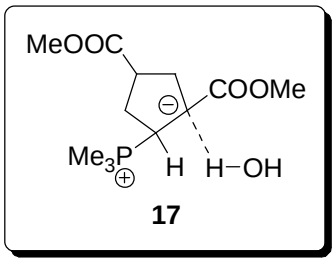
TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.769355	-0.798904	0.451021
2	6	0	-0.406358	-1.513030	-0.249595

3	1	0	-0.289960	-2.602158	-0.316652
4	1	0	-0.551495	-1.121759	-1.261832
5	6	0	0.204185	0.561181	0.889965
6	1	0	1.004634	0.841850	1.834307
7	6	0	0.268371	1.602359	-0.137638
8	8	0	1.081711	1.620467	-1.070287
9	8	0	-0.591670	2.630736	0.062592
10	6	0	-0.492433	3.732261	-0.851997
11	1	0	-1.254157	4.443878	-0.529530
12	1	0	0.501090	4.186825	-0.800532
13	1	0	-0.686034	3.402331	-1.876681
14	15	0	2.394191	-0.837889	-0.409380
15	6	0	3.569051	0.432426	0.133836
16	1	0	3.423170	1.339734	-0.453656
17	1	0	3.343487	0.642356	1.199827
18	1	0	4.588084	0.049352	0.010883
19	6	0	2.277284	-0.926342	-2.229515
20	1	0	1.669859	-1.786792	-2.526927
21	1	0	1.825763	-0.007017	-2.605137
22	1	0	3.284304	-1.043304	-2.644425
23	6	0	3.132177	-2.437243	0.100981
24	1	0	3.313363	-2.413382	1.180377
25	1	0	2.456442	-3.267323	-0.128851
26	1	0	4.083251	-2.601210	-0.415953
27	6	0	-1.186841	0.182908	1.417470
28	1	0	-1.135274	-0.059571	2.484638
29	1	0	-1.903182	0.999573	1.303009
30	6	0	-1.623129	-1.117933	0.623851
31	1	0	-1.857651	-1.908749	1.343169
32	6	0	-2.870803	-0.869641	-0.198003

33	8	0	-2.905884	-0.569735	-1.376463
34	8	0	-3.983802	-0.987737	0.563502
35	6	0	-5.232925	-0.697704	-0.090456
36	1	0	-5.389536	-1.377504	-0.932381
37	1	0	-5.998595	-0.844949	0.671912
38	1	0	-5.242614	0.333706	-0.453415
39	1	0	1.008997	-1.320938	1.388620
40	8	0	2.083647	0.638097	2.693943
41	1	0	1.973560	1.126729	3.524115



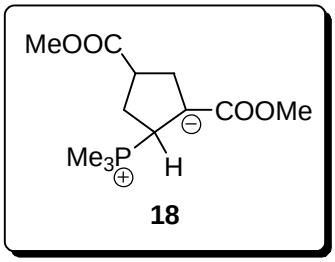
17

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.842176	-0.611229	0.905607
2	6	0	-0.262998	-1.703392	1.175216
3	1	0	-0.006503	-2.281558	2.069767
4	1	0	-0.376701	-2.412490	0.349893
5	6	0	0.116677	0.714777	0.904402
6	1	0	1.659173	1.573301	1.928756
7	6	0	0.237980	1.544201	-0.207698
8	8	0	1.107590	1.399901	-1.116110
9	8	0	-0.649369	2.599229	-0.276936

10	6	0	-0.504623	3.468958	-1.399456
11	1	0	-1.264557	4.242955	-1.266772
12	1	0	0.492248	3.921595	-1.424884
13	1	0	-0.672887	2.936188	-2.341668
14	15	0	1.934752	-0.972305	-0.546388
15	6	0	3.469207	0.022756	-0.587365
16	1	0	3.386588	0.787981	-1.358441
17	1	0	3.572783	0.528820	0.379738
18	1	0	4.333861	-0.625489	-0.764117
19	6	0	1.132486	-1.217747	-2.170240
20	1	0	0.067156	-1.409474	-2.001044
21	1	0	1.226076	-0.304873	-2.757912
22	1	0	1.583896	-2.071000	-2.687520
23	6	0	2.568338	-2.659339	-0.132013
24	1	0	3.064362	-2.647142	0.844330
25	1	0	1.755083	-3.390360	-0.102161
26	1	0	3.294951	-2.978575	-0.886906
27	6	0	-1.135341	0.540296	1.722801
28	1	0	-0.952569	0.591675	2.808076
29	1	0	-1.906196	1.279299	1.489767
30	6	0	-1.584498	-0.929449	1.396175
31	1	0	-2.172881	-1.350304	2.219523
32	6	0	-2.459108	-0.948150	0.158568
33	8	0	-2.110509	-1.277492	-0.962575
34	8	0	-3.712881	-0.527964	0.435914
35	6	0	-4.616016	-0.438320	-0.680647
36	1	0	-4.733694	-1.415653	-1.156673
37	1	0	-5.562539	-0.098108	-0.259262
38	1	0	-4.240892	0.279329	-1.415238
39	1	0	1.583741	-0.679822	1.721986

40	8	0	2.540304	1.657906	2.380364
41	1	0	2.621478	2.595473	2.609218

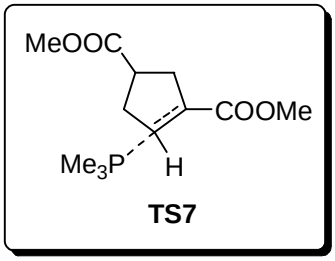


18

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.804298	1.854857	-0.181022
2	6	0	-2.476224	2.551633	0.054446
3	1	0	-3.177498	1.711860	0.056854
4	1	0	-2.528032	3.081991	1.011540
5	1	0	-2.718281	3.251148	-0.752774
6	6	0	-0.712321	1.181597	-1.867122
7	1	0	-0.918798	1.982108	-2.586062
8	1	0	0.285792	0.775227	-2.041675
9	1	0	-1.466223	0.395439	-1.950800
10	6	0	0.338281	3.289681	-0.105271
11	1	0	0.314045	3.739868	0.892609
12	1	0	1.353894	2.954338	-0.327938
13	1	0	0.035150	4.047618	-0.836461
14	6	0	-0.499307	0.563376	1.189313
15	6	0	0.893877	0.623730	1.876980
16	1	0	1.436986	1.562894	1.735228

17	1	0	0.735403	0.504227	2.955328
18	6	0	-0.630102	-0.848120	0.722916
19	6	0	-1.812441	-1.281767	0.142997
20	8	0	-2.785987	-0.542723	-0.181164
21	6	0	0.575433	-1.671657	1.104780
22	1	0	0.441382	-2.249944	2.037119
23	1	0	0.876824	-2.398798	0.341069
24	6	0	1.681403	-0.600234	1.364580
25	1	0	2.405173	-0.958330	2.105310
26	6	0	2.450082	-0.296131	0.098927
27	8	0	2.276436	0.671014	-0.628394
28	1	0	-1.283180	0.879084	1.901714
29	8	0	-1.866613	-2.650091	-0.112877
30	6	0	-3.048132	-3.113315	-0.760036
31	1	0	-3.162000	-2.669046	-1.756092
32	1	0	-2.928449	-4.196561	-0.848460
33	1	0	-3.942890	-2.880422	-0.172881
34	8	0	3.376306	-1.239434	-0.163638
35	6	0	4.130054	-1.081709	-1.379515
36	1	0	4.824313	-1.922174	-1.398576
37	1	0	3.464115	-1.113860	-2.246128
38	1	0	4.671992	-0.132151	-1.372967

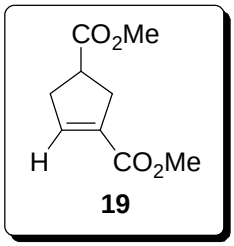


TS7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.429071	1.998824	-0.112469
2	6	0	-2.018739	2.884116	0.111010
3	1	0	-2.817634	2.135990	0.067006
4	1	0	-2.039777	3.371344	1.092552
5	1	0	-2.165213	3.644868	-0.664042
6	6	0	-0.454291	1.363802	-1.823625
7	1	0	-0.604226	2.187154	-2.530369
8	1	0	0.493377	0.862911	-2.034027
9	1	0	-1.275984	0.648770	-1.914645
10	6	0	0.870729	3.309068	-0.059783
11	1	0	0.904094	3.758150	0.938547
12	1	0	1.840004	2.856424	-0.281706
13	1	0	0.657096	4.099320	-0.790653
14	6	0	-0.495920	0.424136	1.228812
15	6	0	0.850460	0.183585	1.930357
16	1	0	1.517023	1.053257	1.952643
17	1	0	0.639250	-0.088441	2.971940
18	6	0	-0.860635	-0.831175	0.609847
19	6	0	-2.158743	-1.052705	0.119651
20	8	0	-3.074917	-0.204597	0.033363
21	6	0	0.279827	-1.825761	0.602437
22	1	0	0.071429	-2.708314	1.225449
23	1	0	0.528297	-2.222248	-0.393979
24	6	0	1.488404	-1.034173	1.218467
25	1	0	2.041939	-1.665767	1.919205
26	6	0	2.449432	-0.627883	0.126872

27	8	0	2.396828	0.406532	-0.521783
28	1	0	-1.257480	0.876033	1.873845
29	8	0	-2.368607	-2.354805	-0.314742
30	6	0	-3.675181	-2.638189	-0.813417
31	1	0	-3.915872	-2.011383	-1.679099
32	1	0	-3.655247	-3.691163	-1.105493
33	1	0	-4.436843	-2.474858	-0.043563
34	8	0	3.390214	-1.570086	-0.089838
35	6	0	4.313296	-1.322426	-1.166495
36	1	0	4.985183	-2.181060	-1.172458
37	1	0	3.777654	-1.246138	-2.116717
38	1	0	4.869006	-0.397933	-0.988193

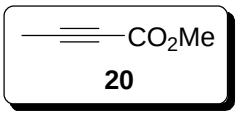


19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.779013	1.820113	-0.098274
2	6	0	-0.719068	1.936884	-0.160418
3	1	0	-1.125042	2.227931	0.818847
4	1	0	-1.059443	2.690426	-0.881562
5	6	0	1.189477	0.541581	-0.106795
6	6	0	2.610715	0.148462	0.004032

7	8	0	3.556842	0.914664	0.044274
8	6	0	0.025391	-0.427426	-0.177294
9	1	0	0.166078	-1.221314	-0.916914
10	1	0	-0.122744	-0.919922	0.793846
11	6	0	-1.176770	0.505125	-0.545976
12	1	0	-1.332801	0.446177	-1.627630
13	6	0	-2.454743	0.068874	0.140965
14	8	0	-2.816035	0.418991	1.247258
15	1	0	1.447746	2.671545	-0.015095
16	8	0	2.747958	-1.200732	0.055559
17	6	0	4.096374	-1.689210	0.169880
18	1	0	4.560848	-1.313538	1.085634
19	1	0	4.008526	-2.775751	0.198944
20	1	0	4.690591	-1.371356	-0.691181
21	8	0	-3.147575	-0.808511	-0.620232
22	6	0	-4.353566	-1.338780	-0.036448
23	1	0	-4.765326	-2.012707	-0.788102
24	1	0	-4.123755	-1.880197	0.885125
25	1	0	-5.055151	-0.530320	0.185187

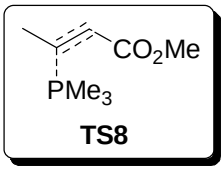


20

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.006726	-0.070434	-0.001284
2	6	0	-0.805425	0.088835	-0.000371
3	6	0	-3.451604	-0.267246	-0.000609

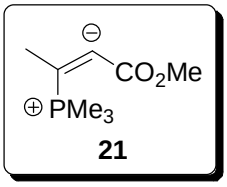
4	6	0	0.611852	0.363623	0.000014
5	8	0	1.098112	1.478712	0.000142
6	8	0	1.336804	-0.776975	0.000131
7	6	0	2.767279	-0.602340	0.000032
8	1	0	-3.805934	-0.512012	1.008104
9	1	0	-3.973640	0.637833	-0.332225
10	1	0	-3.735607	-1.092041	-0.664784
11	1	0	3.177216	-1.612488	0.000228
12	1	0	3.083148	-0.055098	-0.892113
13	1	0	3.083236	-0.054712	0.891909



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.587530	-0.360434	-0.040613
2	6	0	0.471345	1.473354	-0.088032
3	6	0	1.392702	2.633520	-0.282759
4	1	0	1.927334	2.570174	-1.239694
5	1	0	2.146816	2.689776	0.513705
6	1	0	0.809314	3.560562	-0.273299
7	6	0	-0.774962	1.268528	0.073261
8	6	0	-1.849363	0.393276	0.352923
9	8	0	-2.184124	-0.009924	1.469358
10	8	0	-2.552505	0.048278	-0.780094

11	6	0	-3.736192	-0.730092	-0.556155
12	1	0	-4.443251	-0.185444	0.076889
13	1	0	-4.163027	-0.896238	-1.547096
14	1	0	-3.497095	-1.685060	-0.077738
15	6	0	0.780442	-1.446750	-1.287566
16	1	0	1.149267	-1.192496	-2.286920
17	1	0	-0.300461	-1.284350	-1.271337
18	1	0	0.992937	-2.503283	-1.087351
19	1	0	0.079738	-0.975051	1.771588
20	1	0	1.699120	-0.590347	2.379627
21	6	0	1.149940	-1.104651	1.583703
22	1	0	1.403334	-2.171111	1.608474
23	6	0	3.395585	-0.770538	-0.235855
24	1	0	3.745388	-0.443646	-1.220584
25	1	0	3.977828	-0.244575	0.527771
26	1	0	3.575876	-1.849114	-0.136085

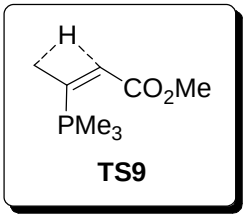


21

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.347207	-0.460127	-0.023842
2	6	0	0.705264	1.241265	-0.072298
3	6	0	1.704378	2.370849	-0.255616
4	1	0	2.241080	2.313223	-1.213902

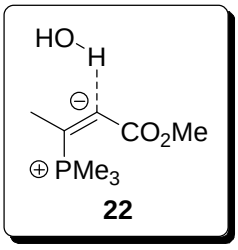
5	1	0	2.460493	2.404742	0.542802
6	1	0	1.150729	3.314106	-0.234974
7	6	0	-0.610970	1.379041	0.091787
8	6	0	-1.680860	0.491341	0.354776
9	8	0	-2.053988	0.100032	1.471230
10	8	0	-2.394982	0.155514	-0.788235
11	6	0	-3.663973	-0.468630	-0.559294
12	1	0	-4.085453	-0.641588	-1.552065
13	1	0	-3.553604	-1.416137	-0.021854
14	1	0	-4.320331	0.188641	0.020068
15	6	0	0.579529	-1.488118	-1.325927
16	1	0	0.931599	-1.150949	-2.306037
17	1	0	-0.505993	-1.361249	-1.289971
18	1	0	0.838266	-2.543776	-1.189873
19	1	0	-0.104926	-1.120594	1.791212
20	1	0	1.526333	-0.735627	2.370457
21	6	0	0.963281	-1.243671	1.580928
22	1	0	1.232746	-2.305704	1.568076
23	6	0	3.163630	-0.631755	-0.259197
24	1	0	3.455293	-0.227639	-1.233550
25	1	0	3.694208	-0.076532	0.520327
26	1	0	3.461551	-1.685301	-0.208009



TS9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.126966	2.555689	-0.095559
2	1	0	-0.375345	2.594324	-0.434947
3	6	0	-0.751964	1.235031	-0.334934
4	6	0	-1.738383	0.167218	-0.273330
5	8	0	-1.635720	-0.946035	-0.807844
6	8	0	-2.883577	0.548609	0.354562
7	6	0	-3.951964	-0.407614	0.358645
8	1	0	-4.258339	-0.648013	-0.663649
9	1	0	-3.651946	-1.330428	0.865619
10	1	0	-4.768378	0.074444	0.898861
11	6	0	0.591419	1.165916	-0.130310
12	1	0	1.126786	3.000716	0.906159
13	1	0	2.062223	2.780350	-0.627408
14	15	0	1.518480	-0.361982	0.081861
15	6	0	0.871420	-1.426452	1.420809
16	1	0	0.834761	-0.857167	2.354310
17	1	0	-0.137297	-1.751196	1.152827
18	1	0	1.514077	-2.303680	1.553727
19	6	0	3.263265	-0.003500	0.486094
20	1	0	3.318360	0.548237	1.428683
21	6	0	1.526513	-1.370418	-1.441760
22	1	0	2.097185	-2.294144	-1.296693
23	1	0	3.836439	-0.933818	0.568464
24	1	0	3.696445	0.622480	-0.299440
25	1	0	1.972914	-0.790393	-2.255639
26	1	0	0.485651	-1.597793	-1.690470

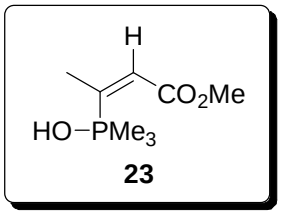


22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.807349	0.777482	0.077361
2	1	0	-1.918353	2.444841	-0.024779
3	8	0	-2.302296	3.359636	-0.072005
4	1	0	-2.938756	3.400354	0.657307
5	6	0	0.492860	1.052587	-0.081280
6	6	0	1.082896	2.440934	-0.269891
7	1	0	1.799011	2.705111	0.522091
8	1	0	0.269415	3.171387	-0.243286
9	1	0	1.603854	2.549004	-1.232084
10	15	0	1.661891	-0.339339	-0.019117
11	6	0	1.277417	-1.592614	-1.292677
12	1	0	0.218120	-1.856523	-1.235371
13	1	0	1.894191	-2.486934	-1.152935
14	1	0	1.469226	-1.168822	-2.283437
15	6	0	3.415793	0.129384	-0.289497
16	1	0	3.734401	0.845822	0.473412
17	1	0	4.057931	-0.756612	-0.234022
18	1	0	3.534076	0.593153	-1.273437
19	6	0	1.594587	-1.173297	1.604737

20	1	0	1.954685	-0.483860	2.375110
21	1	0	0.553240	-1.424871	1.832021
22	1	0	2.216453	-2.075315	1.604199
23	8	0	-2.070045	-0.992354	-0.786878
24	6	0	-3.035198	-2.028851	-0.556823
25	1	0	-3.386282	-2.321507	-1.548294
26	1	0	-3.868510	-1.652817	0.044441
27	1	0	-2.586663	-2.884325	-0.041741
28	6	0	-1.504594	-0.439653	0.344890
29	8	0	-1.706767	-0.930262	1.462211

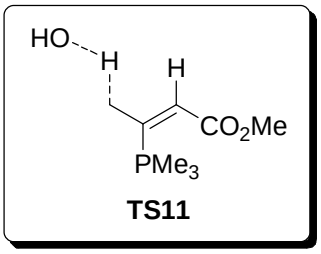


23

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.343546	1.175668	0.026496
2	6	0	-1.158638	2.447577	0.081757
3	1	0	-0.512568	3.330203	0.023512
4	1	0	-1.728505	2.510003	1.018345
5	6	0	1.003464	1.264120	-0.001255
6	1	0	1.468760	2.247619	-0.003236
7	6	0	1.942488	0.136182	-0.026598
8	8	0	1.652710	-1.051035	-0.063425
9	8	0	3.225933	0.573918	-0.000587

10	6	0	4.239975	-0.444680	-0.011868
11	1	0	5.188699	0.092523	0.010246
12	1	0	4.142353	-1.091207	0.864740
13	1	0	4.161878	-1.052738	-0.917474
14	15	0	-1.401638	-0.375101	0.018871
15	6	0	-1.072723	-0.674102	1.884953
16	1	0	-0.042122	-1.012706	2.035593
17	1	0	-1.223972	0.238348	2.476417
18	1	0	-1.747056	-1.447738	2.276768
19	6	0	-1.078777	-2.138724	-0.476855
20	1	0	-0.230934	-2.190944	-1.159719
21	1	0	-0.865335	-2.768347	0.390153
22	1	0	-1.972230	-2.490219	-1.001529
23	6	0	-3.200821	-0.029099	0.255892
24	1	0	-3.353747	0.674206	1.078977
25	1	0	-3.656741	0.346145	-0.659945
26	1	0	-3.677520	-0.974167	0.539022
27	8	0	-1.651265	0.033085	-1.762103
28	1	0	-0.857460	-0.129923	-2.297225
29	1	0	-1.876484	2.476062	-0.743924



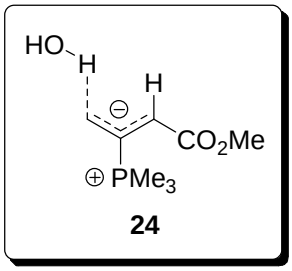
TS11

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-0.392271	-0.820585	-0.703484
2	6	0	-1.383519	-1.842430	-1.045629
3	1	0	-0.917948	-2.776564	-1.373943
4	1	0	-2.147844	-1.524364	-1.762408
5	6	0	0.948214	-1.076721	-0.630184
6	1	0	1.293909	-2.038259	-1.000163
7	6	0	1.978882	-0.222896	-0.059519
8	8	0	1.814758	0.883314	0.454876
9	8	0	3.203292	-0.798063	-0.154280
10	6	0	4.299589	-0.050545	0.395516
11	1	0	5.180623	-0.673229	0.236630
12	1	0	4.408273	0.908120	-0.119801
13	1	0	4.143512	0.130235	1.462765
14	15	0	-1.149187	0.755700	-0.109255
15	6	0	-0.467141	2.222630	-0.962598
16	1	0	0.580359	2.364783	-0.698250
17	1	0	-0.565809	2.088034	-2.044605
18	1	0	-1.051165	3.099363	-0.662234
19	6	0	-1.060006	0.897751	1.699655
20	1	0	-0.020065	0.905643	2.028348
21	1	0	-1.559372	1.822972	2.009441
22	1	0	-1.608339	0.015978	2.068860
23	6	0	-2.923668	0.738286	-0.515796
24	1	0	-3.084016	0.663376	-1.595088
25	1	0	-3.370770	-0.114156	0.018643
26	1	0	-3.360232	1.676658	-0.155620
27	8	0	-2.716135	-1.652894	1.254524
28	1	0	-3.082432	-2.422391	1.717284

29	1	0	-2.016686	-1.993493	0.000255

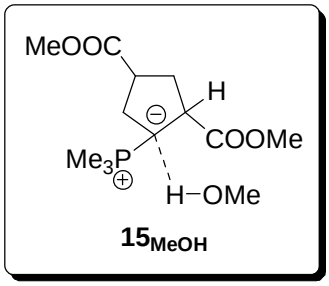


24

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.441840	-0.724091	-0.866882
2	6	0	-1.403511	-1.494814	-1.493258
3	1	0	-1.096479	-2.396310	-2.018734
4	1	0	-2.429734	-1.183575	-1.636855
5	6	0	0.936703	-1.038552	-0.791016
6	1	0	1.263768	-1.938871	-1.302730
7	6	0	1.915971	-0.288049	-0.108249
8	8	0	1.741039	0.777143	0.527186
9	8	0	3.173857	-0.839321	-0.196367
10	6	0	4.218477	-0.126973	0.466827
11	1	0	5.124574	-0.711021	0.291387
12	1	0	4.334154	0.881141	0.054704
13	1	0	4.022911	-0.047499	1.541418
14	15	0	-1.076648	0.800078	-0.064484
15	6	0	-0.388455	2.327037	-0.792219
16	1	0	0.682271	2.367483	-0.589554
17	1	0	-0.571384	2.314134	-1.871600

18	1	0	-0.892002	3.195290	-0.353125
19	6	0	-0.949604	0.786549	1.754141
20	1	0	0.100720	0.738345	2.042015
21	1	0	-1.409128	1.699139	2.150267
22	1	0	-1.500163	-0.088419	2.115414
23	6	0	-2.879715	0.941886	-0.364603
24	1	0	-3.101736	0.988681	-1.433751
25	1	0	-3.411158	0.102118	0.090677
26	1	0	-3.222441	1.870387	0.104829
27	8	0	-2.755961	-2.059778	1.273792
28	1	0	-2.828752	-2.940843	1.669895
29	1	0	-2.235341	-2.173667	0.447672



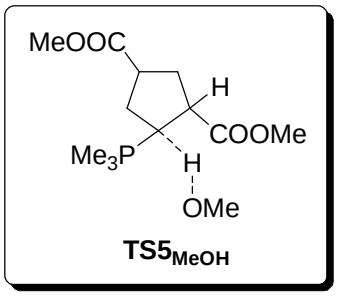
15$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.854109	-0.373156	0.005702
2	1	0	-2.420589	-1.001697	-1.023685
3	8	0	-3.290806	-1.240795	-1.462538
4	6	0	-3.056308	-1.858906	-2.714524
5	1	0	-2.530067	-1.192831	-3.417418
6	1	0	-2.476285	-2.790826	-2.618128

7	1	0	-4.030330	-2.108217	-3.148628
8	6	0	-0.163604	0.466560	-1.068433
9	1	0	-0.880915	0.844724	-1.818531
10	6	0	0.547433	1.748793	-0.619649
11	8	0	0.285957	2.368480	0.396818
12	8	0	1.409598	2.212206	-1.546868
13	6	0	2.098341	3.431382	-1.218832
14	1	0	2.743628	3.638452	-2.073659
15	1	0	2.691934	3.291726	-0.311710
16	1	0	1.385303	4.246768	-1.067373
17	6	0	1.198099	-1.561508	-0.677934
18	1	0	1.608695	-0.083919	-2.274214
19	1	0	1.414770	-2.547000	-1.099978
20	6	0	0.765531	-0.558773	-1.767699
21	6	0	2.430190	-1.105485	0.072120
22	8	0	2.710834	0.046044	0.348651
23	8	0	3.201751	-2.155990	0.445887
24	6	0	4.375885	-1.837316	1.214382
25	1	0	5.039144	-1.181867	0.643401
26	1	0	4.098922	-1.341850	2.149160
27	1	0	4.858950	-2.794475	1.414179
28	1	0	0.184081	-1.101785	-2.520929
29	6	0	-0.025115	-1.638418	0.295942
30	1	0	0.329211	-1.735898	1.335493
31	1	0	-0.580240	-2.565373	0.085900
32	15	0	-1.807858	0.283741	1.279022
33	6	0	-1.057435	0.944246	2.845084
34	1	0	-0.419875	0.173036	3.292084
35	1	0	-0.440990	1.812230	2.605416
36	1	0	-1.834356	1.218108	3.569540

37	6	0	-2.908005	1.613758	0.676469
38	1	0	-2.308009	2.474455	0.371156
39	1	0	-3.489274	1.240179	-0.171844
40	1	0	-3.588799	1.921699	1.477081
41	6	0	-2.913872	-1.035878	1.923822
42	1	0	-2.314339	-1.866299	2.312246
43	1	0	-3.546918	-1.408009	1.113226
44	1	0	-3.536649	-0.648790	2.737577



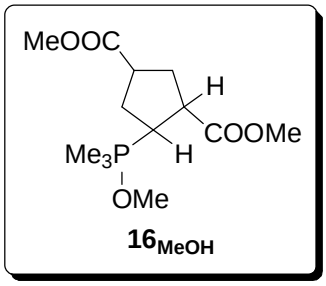
TS5$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.871907	-0.409414	-0.000636
2	1	0	1.657432	-1.144099	0.738200
3	8	0	2.631118	-1.598163	1.531802
4	6	0	2.301476	-2.553355	2.485900
5	1	0	2.997616	-3.416050	2.474714
6	1	0	2.321899	-2.149543	3.519735
7	1	0	1.283772	-2.981253	2.339573
8	6	0	-0.250870	-1.213684	-0.679629
9	1	0	0.083331	-2.201543	-1.015371
10	1	0	-0.674622	-0.698970	-1.554965

11	6	0	0.196032	0.502846	1.030013
12	1	0	0.898984	0.767598	1.831850
13	6	0	-0.376993	1.820445	0.519393
14	8	0	-0.175390	2.296761	-0.585816
15	8	0	-1.091658	2.454114	1.465357
16	6	0	-1.711568	3.694842	1.078593
17	1	0	-2.416526	3.519722	0.262159
18	1	0	-2.233279	4.045522	1.969517
19	1	0	-0.955073	4.418813	0.763565
20	6	0	-0.890797	-0.444374	1.606556
21	1	0	-0.423427	-1.066038	2.374458
22	1	0	-1.717327	0.104360	2.061905
23	6	0	-1.350995	-1.349563	0.435426
24	1	0	-1.421487	-2.392761	0.754529
25	6	0	-2.698367	-0.941611	-0.124755
26	8	0	-3.162742	0.182798	-0.105159
27	8	0	-3.330813	-1.988098	-0.704776
28	6	0	-4.597734	-1.698830	-1.325012
29	1	0	-4.945225	-2.650295	-1.728789
30	1	0	-5.303821	-1.312068	-0.585348
31	1	0	-4.472432	-0.962120	-2.123319
32	15	0	2.169180	0.199607	-1.062117
33	6	0	3.159375	-1.252210	-1.563031
34	1	0	2.559128	-1.922617	-2.187195
35	1	0	3.447636	-1.772771	-0.641239
36	1	0	4.041907	-0.936447	-2.129311
37	1	0	3.539356	0.702804	0.823995
38	6	0	3.282710	1.259684	-0.084465
39	1	0	2.786472	2.199441	0.173751
40	1	0	4.190589	1.479550	-0.655402

41	6	0	1.766889	1.068071	-2.628927
42	1	0	1.255313	2.006936	-2.414406
43	1	0	1.104259	0.439783	-3.233627
44	1	0	2.687302	1.251578	-3.195051

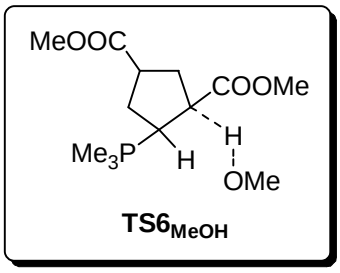


16$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.137177	-0.781159	-0.549373
2	8	0	3.008910	-0.143518	1.038996
3	6	0	3.238422	-0.839519	2.230113
4	1	0	3.485411	-0.116965	3.023198
5	1	0	2.363640	-1.419690	2.588982
6	1	0	4.083708	-1.547995	2.158821
7	6	0	3.065736	-2.376596	-0.340287
8	1	0	2.722079	-2.892100	0.561556
9	1	0	2.931200	-3.038905	-1.198592
10	1	0	4.127276	-2.151108	-0.206167
11	6	0	1.366181	-1.311497	-2.214828
12	1	0	0.809425	-2.253479	-2.139815
13	1	0	2.177487	-1.465245	-2.939662
14	1	0	0.700123	-0.539763	-2.612200

15	6	0	3.025122	0.664152	-1.296996
16	1	0	3.090534	1.486113	-0.585523
17	1	0	2.540461	0.978693	-2.222103
18	1	0	4.046637	0.329429	-1.510857
19	6	0	0.538351	-0.630814	0.441024
20	1	0	0.775112	-1.209210	1.343073
21	6	0	-0.780293	-1.194735	-0.119978
22	1	0	-1.010691	-0.740712	-1.086539
23	1	0	-0.770107	-2.280760	-0.247406
24	6	0	-1.832111	-0.756332	0.947852
25	1	0	-1.943374	-1.564682	1.678797
26	6	0	-3.191809	-0.536094	0.311838
27	8	0	-3.685286	0.538151	0.031450
28	8	0	-3.798416	-1.717538	0.050240
29	6	0	-5.073808	-1.641012	-0.614785
30	1	0	-4.966625	-1.154554	-1.588060
31	1	0	-5.399385	-2.674824	-0.734007
32	1	0	-5.786979	-1.078418	-0.006463
33	6	0	-1.248965	0.513095	1.627872
34	1	0	-1.113742	0.338097	2.699905
35	1	0	-1.919570	1.368445	1.518227
36	6	0	0.143604	0.769998	0.967771
37	1	0	0.867902	1.133244	1.699064
38	6	0	0.017919	1.833764	-0.110884
39	8	0	-0.001670	1.644455	-1.312611
40	8	0	-0.098016	3.060128	0.440588
41	6	0	-0.303488	4.152399	-0.475833
42	1	0	-1.223319	3.999639	-1.046468
43	1	0	0.542074	4.235931	-1.163714
44	1	0	-0.380276	5.041929	0.149958

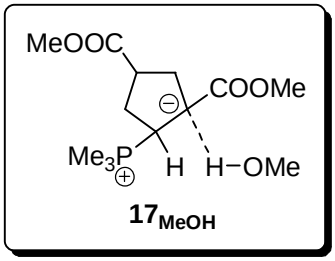


TS6$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.196014	0.721941	-0.417990
2	1	0	-1.105866	1.337926	-1.055888
3	8	0	-2.282094	1.563765	-1.736334
4	6	0	-2.304374	2.780947	-2.412617
5	1	0	-1.503056	3.472528	-2.074816
6	1	0	-3.261258	3.319276	-2.262237
7	15	0	-2.173401	-1.296114	0.274151
8	6	0	-3.452289	-0.028839	0.492200
9	1	0	-3.295025	0.490486	1.438378
10	6	0	-2.907405	-2.541959	-0.854662
11	1	0	-4.436176	-0.510254	0.471830
12	1	0	-3.224330	-2.043061	-1.776224
13	1	0	-3.339625	0.690973	-0.344922
14	1	0	-2.176680	-3.318072	-1.104002
15	1	0	-3.778995	-3.013079	-0.388751
16	6	0	-1.837684	-2.201048	1.824018
17	1	0	-1.171380	-3.047387	1.630585
18	1	0	-2.783975	-2.579826	2.225323

19	1	0	-1.375433	-1.522009	2.541728
20	6	0	-0.660854	-0.731245	-0.609479
21	1	0	-0.980106	-0.799097	-1.660016
22	6	0	-0.186048	1.163742	0.979010
23	8	0	-0.897824	0.682075	1.870050
24	6	0	0.608690	-1.587527	-0.403676
25	1	0	0.543927	-2.590159	-0.844947
26	1	0	0.832489	-1.697322	0.662432
27	1	0	1.946680	-1.101094	-2.072610
28	6	0	1.722794	-0.737945	-1.064837
29	6	0	1.145428	0.734151	-1.164565
30	1	0	0.989907	0.975568	-2.221850
31	1	0	1.832436	1.480596	-0.759601
32	6	0	0.584305	2.762114	2.552013
33	1	0	1.288338	3.595598	2.544526
34	1	0	0.893675	2.005779	3.279003
35	1	0	-0.421069	3.113594	2.800899
36	6	0	3.015471	-0.766508	-0.275257
37	8	0	3.125550	-1.013225	0.910967
38	8	0	4.068824	-0.437026	-1.058405
39	6	0	5.345914	-0.349799	-0.399551
40	1	0	5.319469	0.414164	0.382237
41	1	0	6.055563	-0.076750	-1.181150
42	1	0	5.612024	-1.312346	0.045578
43	8	0	0.616729	2.227313	1.220408
44	1	0	-2.177603	2.664329	-3.508900

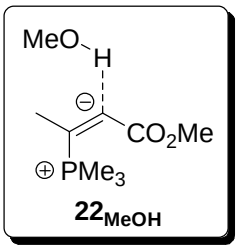


17$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.940910	1.451399	-1.519676
2	1	0	-2.009279	1.444435	-1.179361
3	6	0	-0.197195	0.728583	-0.561682
4	6	0	-0.332782	1.157543	0.756025
5	8	0	0.322790	2.325018	1.087091
6	6	0	0.157220	2.780501	2.429737
7	1	0	-0.896912	2.972131	2.656634
8	1	0	1.569780	1.893352	-1.087698
9	1	0	0.545207	2.051074	3.148875
10	1	0	0.728881	3.709613	2.493323
11	1	0	0.613050	1.386645	-2.483201
12	6	0	0.944489	1.085563	-1.476550
13	6	0	1.728299	-0.267970	-1.631198
14	1	0	2.272634	-0.297304	-2.581923
15	1	0	-3.418062	3.218956	-0.497825
16	6	0	-3.425670	2.785728	-1.509426
17	6	0	2.749066	-0.409860	-0.520234
18	8	0	2.630547	-1.093628	0.482397
19	8	0	3.841926	0.348394	-0.758221
20	6	0	4.850850	0.351505	0.267629

21	1	0	4.439988	0.742223	1.202509
22	1	0	5.640988	1.002986	-0.107205
23	1	0	5.230580	-0.660362	0.433914
24	6	0	-0.375046	-2.156666	1.860151
25	1	0	-0.625320	-1.537006	2.721043
26	1	0	0.671957	-1.969844	1.597452
27	6	0	0.638499	-1.364155	-1.555415
28	1	0	0.394861	-1.728915	-2.559379
29	6	0	-0.626031	-0.678842	-0.908789
30	1	0	-1.436049	-0.694724	-1.659968
31	1	0	1.004360	-2.218154	-0.977882
32	15	0	-1.420618	-1.667325	0.442099
33	6	0	-3.107646	-1.112302	0.882608
34	1	0	-3.086764	-0.621865	1.855274
35	1	0	-3.428502	-0.373775	0.138597
36	1	0	-3.796724	-1.963311	0.885130
37	6	0	-1.746455	-3.274011	-0.414568
38	1	0	-2.363390	-3.109300	-1.304501
39	1	0	-2.282038	-3.952703	0.258120
40	1	0	-0.812727	-3.754768	-0.720960
41	1	0	-0.515306	-3.219455	2.083873
42	1	0	-4.459441	2.759962	-1.868532
43	1	0	-2.843714	3.440211	-2.175821
44	8	0	-1.026150	0.560825	1.631947

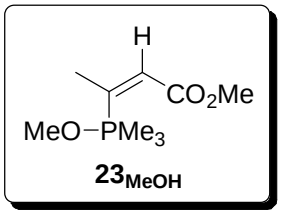


22$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.397333	-1.319670	-0.251617
2	6	0	0.714440	-0.271610	0.005561
3	8	0	3.125731	-1.983858	-0.367733
4	6	0	4.274088	-1.528474	0.323759
5	1	0	4.084563	-1.388293	1.399843
6	1	0	5.050966	-2.291858	0.207863
7	1	0	4.659185	-0.581251	-0.087170
8	6	0	-0.366379	-1.050090	-0.126935
9	6	0	-0.345155	-2.554851	-0.341733
10	1	0	-0.820911	-2.851759	-1.287388
11	1	0	0.695988	-2.888335	-0.369470
12	1	0	-0.852328	-3.102282	0.466365
13	15	0	-1.999639	-0.260543	0.011697
14	6	0	-3.415042	-1.396056	-0.261962
15	1	0	-4.361963	-0.854508	-0.159875
16	1	0	-3.389764	-2.207751	0.471053
17	1	0	-3.359673	-1.830905	-1.264514
18	6	0	-2.231615	0.469218	1.669951
19	1	0	-2.247547	-0.332925	2.414776
20	1	0	-3.170918	1.031048	1.719710

21	1	0	-1.380399	1.122543	1.889349
22	6	0	-2.194854	1.086109	-1.208389
23	1	0	-2.218435	0.658155	-2.215502
24	1	0	-3.121274	1.641385	-1.026058
25	1	0	-1.337729	1.761535	-1.146992
26	6	0	0.857912	1.119445	0.299288
27	8	0	0.854930	1.628826	1.426281
28	8	0	1.137815	1.875855	-0.821121
29	6	0	1.589752	3.214272	-0.570342
30	1	0	0.831377	3.799039	-0.039839
31	1	0	2.507781	3.206121	0.025097
32	1	0	1.781639	3.643493	-1.555681

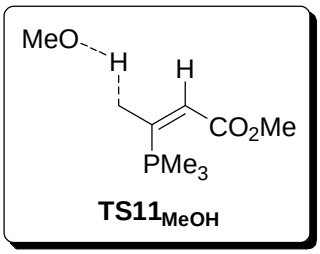


23$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.293176	1.204426	-0.026216
2	6	0	1.094848	2.477537	0.131251
3	1	0	0.439140	3.326242	0.354002
4	1	0	1.645575	2.711854	-0.789349
5	6	0	-1.052339	1.268167	0.070549
6	1	0	-1.518285	2.226681	0.290570
7	6	0	-1.995390	0.157865	-0.116404

8	8	0	-1.718644	-0.996815	-0.406673
9	8	0	-3.273221	0.577337	0.062974
10	6	0	-4.293178	-0.420972	-0.105985
11	1	0	-5.235720	0.095241	0.079423
12	1	0	-4.268251	-0.825518	-1.121752
13	1	0	-4.152698	-1.236229	0.609257
14	15	0	1.361257	-0.301395	-0.336985
15	6	0	1.003176	-0.250072	-2.217015
16	1	0	-0.015322	-0.600524	-2.415318
17	1	0	1.098736	0.768269	-2.615603
18	1	0	1.701689	-0.895248	-2.767038
19	6	0	1.093958	-2.132028	-0.182388
20	1	0	0.101313	-2.331362	0.220783
21	1	0	1.163952	-2.605392	-1.165054
22	1	0	1.850806	-2.534687	0.495515
23	6	0	3.149006	0.123019	-0.513727
24	1	0	3.287276	0.903842	-1.266466
25	1	0	3.581709	0.422359	0.440049
26	1	0	3.659544	-0.778269	-0.871668
27	8	0	1.631590	-0.205370	1.508550
28	1	0	1.828516	2.374417	0.936772
29	6	0	0.699140	-0.636713	2.469288
30	1	0	0.606960	-1.734798	2.504554
31	1	0	1.042902	-0.297063	3.455538
32	1	0	-0.308868	-0.217486	2.305621

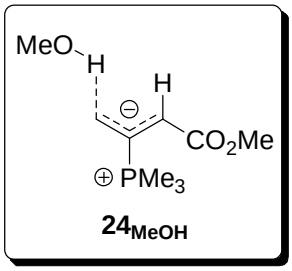


TS11$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.171071	-0.302422	-0.993064
2	6	0	-1.303320	-0.942367	-1.664398
3	1	0	-1.001551	-1.831774	-2.225616
4	1	0	-1.903045	-0.279289	-2.296824
5	6	0	1.074649	-0.864519	-0.926929
6	1	0	1.260073	-1.742561	-1.539733
7	6	0	2.182261	-0.446213	-0.084021
8	8	0	2.182193	0.490926	0.715667
9	8	0	3.272445	-1.230202	-0.273661
10	6	0	4.425834	-0.916905	0.522690
11	1	0	5.180229	-1.650891	0.237421
12	1	0	4.776375	0.097172	0.310104
13	1	0	4.191119	-1.000686	1.587599
14	15	0	-0.655024	1.180180	-0.008751
15	6	0	0.388700	2.639575	-0.361603
16	1	0	1.408716	2.469419	-0.018038
17	1	0	0.383354	2.832615	-1.439225
18	1	0	-0.041083	3.505441	0.153652
19	6	0	-0.740598	0.800851	1.766984
20	1	0	0.237277	0.487548	2.134575

21	1	0	-1.077098	1.692701	2.307916
22	1	0	-1.487799	-0.003386	1.843417
23	6	0	-2.345480	1.663070	-0.483020
24	1	0	-2.402364	1.924965	-1.543345
25	1	0	-3.007432	0.816911	-0.244031
26	1	0	-2.626539	2.537586	0.114433
27	8	0	-2.857696	-1.144600	0.492181
28	1	0	-2.072041	-1.231146	-0.747348
29	6	0	-3.674953	-2.229423	0.786012
30	1	0	-4.232836	-2.070653	1.730435
31	1	0	-4.441352	-2.418015	0.004560
32	1	0	-3.110322	-3.177543	0.911910



24$_{MeOH}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.451831	-1.319690	0.343436
2	8	0	3.024010	-1.327107	-0.453919
3	6	0	3.538250	-2.639241	-0.658647
4	1	0	1.135525	-1.154367	2.725155
5	6	0	1.267714	-0.379279	1.973602
6	1	0	2.163984	0.220827	2.056804

7	15	0	0.554873	1.266615	-0.073637
8	6	0	2.225663	1.956400	0.234179
9	1	0	2.381559	2.775186	-0.476687
10	1	0	2.312225	2.354249	1.248495
11	1	0	2.991486	1.194484	0.065323
12	6	0	0.227534	-0.098889	1.108189
13	1	0	4.169249	-2.599215	-1.550806
14	1	0	-1.160044	-1.572789	1.799260
15	6	0	-1.010809	-0.785394	1.066396
16	1	0	1.416567	-0.027391	-1.891145
17	6	0	0.632842	0.733670	-1.815120
18	1	0	0.894657	1.594197	-2.441046
19	1	0	-0.336637	0.332905	-2.111391
20	8	0	-2.087619	0.334914	-0.741331
21	6	0	-2.062846	-0.532139	0.162684
22	1	0	-1.579513	2.393933	-0.093253
23	6	0	-0.561996	2.692130	0.162090
24	1	0	-0.235178	3.519091	-0.477821
25	1	0	-0.510733	3.006451	1.209577
26	1	0	4.152881	-2.973528	0.189394
27	8	0	-3.146909	-1.358274	0.354617
28	6	0	-4.254901	-1.152277	-0.521939
29	1	0	-5.004073	-1.887599	-0.220339
30	1	0	-3.968420	-1.312443	-1.566766
31	1	0	-4.658207	-0.139215	-0.419274
32	1	0	2.735194	-3.370458	-0.827896

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9. Computed Energies

Table S6. Sum of Electronic and Thermal Enthalpies (H, in a.u.), Sum of Electronic and Thermal Free Energies (G, in a.u.), Thermal Correction to Gibbs Free Energy (TCGFE, in a.u.), Total Free Energy in Solution (G_S, in a.u., solvent = benzene)

Structure	H	G	TCGFE	G_S
1	-344.444080	-344.484881	0.067357	-344.547801
1'	-116.605068	-116.633887	0.031222	-116.660379
2	-460.983860	-461.020947	0.083591	-461.098449
TS1	-805.404400	-805.463512	0.170351	-805.623937
TS1'	-577.541964	-577.588885	0.133908	-577.715425
3	-805.430247	-805.487499	0.175052	-805.654828
3'	-577.553715	-577.601179	0.135165	-577.733553
4	-306.379724	-306.417722	0.065126	-306.479295
a-**TS2**	-1111.803568	-1111.874865	0.265769	-1112.130713
g-**TS2**	-1111.801146	-1111.873854	0.264243	-1112.127243
a-**5**	-1111.806079	-1111.877653	0.267097	-1112.137153
g-**5**	-1111.808464	-1111.880033	0.267650	-1112.139215
a-**TS3**	-1111.804132	-1111.873628	0.268505	-1112.132818
g-**TS3**	-1111.807519	-1111.877329	0.268559	-1112.137094
a-**6**	-1111.831966	-1111.904043	0.269046	-1112.161027
g-**6**	-1111.828336	-1111.899814	0.269397	-1112.156971
TS4	-1111.770760	-1111.841389	0.265510	-1112.094364
15	-1188.242425	-1188.322123	0.288339	-1188.598672
TS5	-1188.235846	-1188.316378	0.282946	-1188.592728
16	-1188.248730	-1188.324880	0.294063	-1188.610886
TS6	-1188.234675	-1188.310266	0.288111	-1188.592672
17	-1188.245629	-1188.323827	0.290225	-1188.603158

18	-1111.841743	-1111.912650	0.269492	-1112.174055
TS7	-1111.841676	-1111.912668	0.268265	-1112.171308
19	-650.890590	-650.947189	0.161229	-651.103487
20	-344.437638	-344.481360	0.065369	-344.541317
TS8	-805.393416	-805.452103	0.171651	-805.615858
21	-805.398824	-805.456716	0.173719	-805.627497
TS9	-805.317501	-805.374815	0.167972	-805.537634
22	-881.808361	-881.875175	0.192208	-882.064953
23	-881.839191	-881.899818	0.200111	-882.092937
TS11	-881.816494	-881.875867	0.195705	-882.068673
24	-881.839202	-881.902743	0.195841	-882.093060
H_2O	-76.397698	-76.419138	0.003435	-76.428114
MeOH	-115.669635	-115.696647	0.028545	-115.726055
15_{MeOH}	-1227.513474	-1227.597885	0.314175	-1227.894813
$TS5_{MeOH}$	-1227.507506	-1227.591012	0.309891	-1227.887273
16_{MeOH}	-1227.518995	-1227.598574	0.320634	-1227.904861
$TS6_{MeOH}$	-1227.507264	-1227.588121	0.312535	-1227.886586
17_{MeOH}	-1227.517052	-1227.600289	0.315748	-1227.898747
22_{MeOH}	-921.080056	-921.152678	0.216780	-921.360999
23_{MeOH}	-921.110558	-921.174991	0.226259	-921.388831
$TS11_{MeOH}$	-921.089407	-921.154682	0.219594	-921.363264
24_{MeOH}	-921.110666	-921.178945	0.221719	-921.388367