Supporting Information

Mechanism of the Gold-Catalyzed Cyclopropanation of Alkenes with 1,6-Enynes

Patricia Pérez-Galán, Elena Herrero-Gómez, Daniel T. Hog, Nolwenn J. A. Martin, Feliu Maseras, and Antonio M. Echavarren*

[a] *Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans 16, 43007 Tarragona (Spain). E-mail: aechavarren@iciq.es*

Contents

General methods

All reactions were carried out under Ar atmosphere. Solvents were dried using a Solvent Purification System (SPS). Analytical thin layer chromatography controls were carried out using TLC-aluminum sheets with 0.2 mm of silica gel (Merck GF234). Flash chromatography purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60. NMR spectra were recorded at 23 ºC (except stated) on the following spectrometers: Bruker Avance 400 Ultrashield (400 MHz for ^{1}H, and 100 MHz for ^{13}C) and Bruker Avance 500 Ultrashield (500 MHz for ^{1}H, and 125 MHz for ^{13}C) at the Institut Català d'Investigaciò Química (ICIQ). Mass spectra were recorded on a Waters LCT Premier (ESI) and Waters GCT (EI, CI) spectrometers at the ICIQ. Melting points were determined using a Büchi melting point apparatus.

X-Ray: Crystal structure determination were performed using a Bruker-Nonius diffractometer equipped with a APPEX 2 4K CCD area detector, a FR591 rotating anode with Mo_{K_α} radiation, Montel mirrors as monochromator and a Kryoflex low temperature device (T = 100 K). Fullsphere data collection omega and phi scans. Programs used: Data collection Apex2 V. 1.0-22 (Bruker-Nonius 2004), data reduction Saint + Version 6.22 (Bruker-Nonius 2001) and absorption correction SADABS V. 2.10 (2003). Crystal structure solutions were achieved using direct methods as implemented in SHELXTL Version 6.10 (Sheldrick, Universität Göttingen (Germany), 2000) and visualized using XP program. Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinements on F2 using all measured intensities were carried out using the program SHELXTL Version 6.10 (Sheldrick, Universität Göttingen (Germany), 2000). All non-hydrogen atoms were refined including anisotropic displacement parameters.

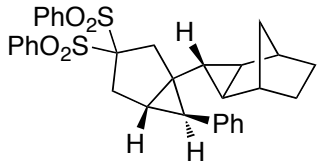
The following compounds were reported before: **5aa**, **5ac**, **5ba**, **5bb**, **7**, **13f**, **13h**, **13i**.[1]

General procedure for the gold(I)-catalyzed cyclopropanation

0.05 eq. of the cationic catalyst were dissolved in 1.5 mL CH_2Cl_2 and cooled down to -40 ºC. A solution of the alkene (5.0 eq.) and the enyne (1.0 eq.) in 0.5 mL CH_2Cl_2 was added. The reaction mixture was stirred for 1 h at -40 ºC and was allowed to warm up to rt in 16 h. The reaction was quenched adding 1 mL of a 0.1 M solution of NEt_3 in hexane. The crude was purified by flash chromatography (hexane:EtOAc, V:V = 10:1).

Cyclopropanation of cyclic alkenes with gold(I9 catalysts A'

(1*R*,2*S*,3*R*,4*R*,5*S*)-3-((5*S*,6*R*)-6-Phenyl-3,3-bis(phenylsulfonyl)bicyclo[3.1.0]hexan-1-yl)tricyclo[3.2.1.0^{2,4}]octane (5ab)



White Solid. Dec. at 177 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18-8.12 (m, 2H), 8.09-8.03 (m, 2H), 7.77-7.69 (m, 2H), 7.67-7.58 (m, 4H), 7.27-7.20 (m, 2H), 7.18-7.07 (m, 3H), 3.14 (dd, J = 16.1, 6.3 Hz, 1H), 2.93 (part A, AB system, J = 16.3 Hz, 1H), 2.89 (part B, AB system, J = 16.3 Hz, 1H), 2.72 (d, J = 16.1 Hz, 1H), 2.22 (d, J = 4.3 Hz, 1H), 2.11-2.08 (m, 1H), 1.80-1.75 (m, 1H), 1.74-1.71 (m, 1H), 1.36-1.20 (m, 2H), 1.19-1.10 (m, 1H), 1.09-1.00 (m, 1H), 0.71 (dd, J = 7.3, 2.9 Hz, 1H), 0.68-0.60 (m, 1H), 0.53 (t, J = 2.8 Hz, 1H), 0.43 (d, J = 10.5 Hz, 1H), 0.27 (dd, J = 7.3, 2.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1 (C), 137.1 (C), 136.4 (C), 134.8 (CH), 134.8 (CH), 132.1 (CH), 131.6 (CH), 129.0 (CH), 128.9 (CH), 128.9 (CH), 127.9 (CH), 125.9 (CH), 97.5 (C), 42.0(CH_2), 39.2 (C), 36.8 (CH_2), 36.1 (CH), 36.0 (CH), 35.8 (CH), 29.9 (CH), 29.6 (CH_2), 29.5 (CH_2), 28.5 (CH_2), 24.6 (CH), 21.6 (CH), 14.2 (CH); HRMS-ESI calcd for $C_{32}H_{32}O_4NaS_2$ $[M+Na]^+$: 567.1640. Found: 567.1664. The structure of **5ab** was confirmed by X-ray diffraction.

(1) S. López, E. Herrero-Gómez, P. Pérez-Galán, C. Nieto-Oberhuber, A. M. Echavarren, *Angew. Chem. Int. Ed*. **2006**, *45*, 6029-6032.

Table 1. Crystal data and structure refinement for **5ab**.

Identification code	**5ab**	
Empirical formula	C32 H32 O4 S2	
Formula weight	544.70	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.0661(9) Å	α= 108.467(5)°.
	b = 11.2303(12) Å	β = 92.142(5)°.
	c = 12.7093(12) Å	γ = 102.893(5)°.
Volume	1319.3(2) $Å^3$	
Z	2	
Density (calculated)	1.371 Mg/m^3	
Absorption coefficient	0.240 mm^{-1}	
F(000)	576	
Crystal size	0.40 x 0.20 x 0.15 mm^3	
Theta range for data collection	2.78 to 36.35 °.	
Index ranges	-16 <=h<=16 ,-18 <=k<=17 ,0 <=l<=21	
Reflections collected	19756	
Independent reflections	16892 [R(int) = 0.0000]	
Completeness to theta = 36.35 °	0.927 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9649 and 0.9102	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19756 / 0 / 344	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0412 , wR2 = 0.1105	
R indices (all data)	R1 = 0.0495 , wR2 = 0.1158	
Largest diff. peak and hole	0.517 and -0.443 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for **5ab**.

Bond lengths----	
S1-O1	1.4383(6)
S1-O2	1.4445(7)
S1-C21	1.7661(9)

S1-C1	1.8402(8)
C1-C5	1.5542(11)
C1-C2	1.5629(12)
C1-S2	1.8345(8)
S2-O3	1.4418(7)
S2-O4	1.4421(7)
S2-C27	1.7610(9)
C2-C3	1.5191(11)
C3-C4	1.5052(12)
C3-C6	1.5125(12)
C4-C13	1.4945(10)
C4-C5	1.5245(11)
C4-C6	1.5286(10)
C6-C7	1.4888(11)
C7-C12	1.3955(12)
C7-C8	1.3957(13)
C8-C9	1.3905(12)
C9-C10	1.3873(15)
C10-C11	1.3886(15)
C11-C12	1.3962(12)
C13-C14	1.5064(12)
C13-C19	1.5177(11)
C14-C19	1.5201(11)
C14-C15	1.5248(11)
C15-C20	1.5373(13)
C15-C16	1.5461(13)
C16-C17	1.5660(13)
C17-C18	1.5469(14)
C18-C19	1.5265(11)
C18-C20	1.5360(13)
C21-C26	1.3920(12)
C21-C22	1.3954(11)
C22-C23	1.3884(13)
C23-C24	1.3899(15)
C24-C25	1.3878(14)
C25-C26	1.3907(14)
C27-C28	1.3914(12)
C27-C32	1.3987(12)

C28-C29	1.3881(13)
C29-C30	1.3912(14)
C30-C31	1.3807(16)
C31-C32	1.3898(14)

Angles----------

O1-S1-O2	118.75(4)
O1-S1-C21	109.51(4)
O2-S1-C21	106.20(4)
O1-S1-C1	108.21(4)
O2-S1-C1	104.06(4)
C21-S1-C1	109.82(4)
C5-C1-C2	107.82(6)
C5-C1-S2	108.00(6)
C2-C1-S2	111.86(5)
C5-C1-S1	109.76(5)
C2-C1-S1	106.84(6)
S2-C1-S1	112.47(4)
O3-S2-O4	119.23(5)
O3-S2-C27	108.76(4)
O4-S2-C27	106.49(4)
O3-S2-C1	107.74(4)
O4-S2-C1	104.92(4)
C27-S2-C1	109.41(4)
C3-C2-C1	106.14(6)
C4-C3-C6	60.87(5)
C4-C3-C2	110.07(7)
C6-C3-C2	114.81(7)
C13-C4-C3	126.17(7)
C13-C4-C5	114.88(6)
C3-C4-C5	108.83(6)
C13-C4-C6	122.24(6)
C3-C4-C6	59.80(5)
C5-C4-C6	113.71(6)
C4-C5-C1	106.86(7)
C7-C6-C3	124.25(7)
C7-C6-C4	122.23(6)
C3-C6-C4	59.33(5)

C12-C7-C8	118.59(8)
C12-C7-C6	124.43(8)
C8-C7-C6	116.98(8)
C9-C8-C7	120.80(9)
C10-C9-C8	120.46(9)
C9-C10-C11	119.16(8)
C10-C11-C12	120.63(9)
C7-C12-C11	120.34(8)
C4-C13-C14	121.39(7)
C4-C13-C19	117.01(7)
C14-C13-C19	60.35(5)
C13-C14-C19	60.19(5)
C13-C14-C15	119.36(7)
C19-C14-C15	104.07(6)
C14-C15-C20	103.77(7)
C14-C15-C16	105.08(7)
C20-C15-C16	100.32(7)
C15-C16-C17	102.71(7)
C18-C17-C16	103.28(7)
C19-C18-C20	103.13(6)
C19-C18-C17	105.05(8)
C20-C18-C17	100.57(7)
C13-C19-C14	59.46(5)
C13-C19-C18	120.82(8)
C14-C19-C18	104.06(6)
C18-C20-C15	94.78(7)
C26-C21-C22	121.21(8)
C26-C21-S1	120.59(6)
C22-C21-S1	118.03(7)
C23-C22-C21	119.25(8)
C22-C23-C24	120.05(8)
C25-C24-C23	120.17(9)
C24-C25-C26	120.64(9)
C25-C26-C21	118.68(8)
C28-C27-C32	121.52(8)
C28-C27-S2	119.57(6)
C32-C27-S2	118.72(7)
C29-C28-C27	118.68(8)

C28-C29-C30	120.13(9)
C31-C30-C29	120.79(9)
C30-C31-C32	120.06(9)
C31-C32-C27	118.74(9)

Table 3. Torsion angles [°] for **5ab**.

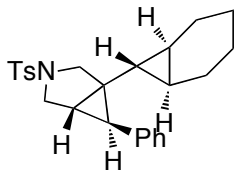
O1-S1-C1-C5	161.37(6)
O2-S1-C1-C5	-71.45(6)
C21-S1-C1-C5	41.88(7)
O1-S1-C1-C2	-81.99(6)
O2-S1-C1-C2	45.19(6)
C21-S1-C1-C2	158.52(5)
O1-S1-C1-S2	41.12(6)
O2-S1-C1-S2	168.30(4)
C21-S1-C1-S2	-78.37(5)
C5-C1-S2-O3	-78.24(6)
C2-C1-S2-O3	163.27(6)
S1-C1-S2-O3	43.02(6)
C5-C1-S2-O4	49.77(6)
C2-C1-S2-O4	-68.72(7)
S1-C1-S2-O4	171.03(5)
C5-C1-S2-C27	163.68(5)
C2-C1-S2-C27	45.19(7)
S1-C1-S2-C27	-75.06(5)
C5-C1-C2-C3	4.81(8)
S2-C1-C2-C3	123.41(6)
S1-C1-C2-C3	-113.11(6)
C1-C2-C3-C4	-2.47(8)
C1-C2-C3-C6	-68.76(8)
C6-C3-C4-C13	-109.82(8)
C2-C3-C4-C13	142.26(7)
C6-C3-C4-C5	107.05(7)
C2-C3-C4-C5	-0.87(9)
C2-C3-C4-C6	-107.92(7)
C13-C4-C5-C1	-143.86(7)
C3-C4-C5-C1	3.87(8)
C6-C4-C5-C1	68.36(9)

C2-C1-C5-C4	-5.35(8)
S2-C1-C5-C4	-126.40(6)
S1-C1-C5-C4	110.67(6)
C4-C3-C6-C7	110.26(8)
C2-C3-C6-C7	-149.64(7)
C2-C3-C6-C4	100.10(7)
C13-C4-C6-C7	2.56(13)
C3-C4-C6-C7	-113.56(9)
C5-C4-C6-C7	147.68(8)
C13-C4-C6-C3	116.12(9)
C5-C4-C6-C3	-98.76(8)
C3-C6-C7-C12	-3.59(12)
C4-C6-C7-C12	68.94(11)
C3-C6-C7-C8	175.85(7)
C4-C6-C7-C8	-111.62(9)
C12-C7-C8-C9	-1.44(12)
C6-C7-C8-C9	179.09(8)
C7-C8-C9-C10	0.84(14)
C8-C9-C10-C11	0.15(14)
C9-C10-C11-C12	-0.51(13)
C8-C7-C12-C11	1.08(11)
C6-C7-C12-C11	-179.49(7)
C10-C11-C12-C7	-0.11(12)
C3-C4-C13-C14	2.02(11)
C5-C4-C13-C14	143.27(7)
C6-C4-C13-C14	-71.98(11)
C3-C4-C13-C19	-68.14(10)
C5-C4-C13-C19	73.10(10)
C6-C4-C13-C19	-142.14(8)
C4-C13-C14-C19	-105.36(8)
C4-C13-C14-C15	164.68(7)
C19-C13-C14-C15	-89.95(7)
C13-C14-C15-C20	32.03(9)
C19-C14-C15-C20	-31.42(9)
C13-C14-C15-C16	136.92(7)
C19-C14-C15-C16	73.47(8)
C14-C15-C16-C17	-70.42(8)
C20-C15-C16-C17	37.02(8)

C15-C16-C17-C18	-1.45(9)
C16-C17-C18-C19	72.17(8)
C16-C17-C18-C20	-34.65(8)
C4-C13-C19-C14	112.49(8)
C4-C13-C19-C18	-158.87(7)
C14-C13-C19-C18	88.64(8)
C15-C14-C19-C13	116.04(8)
C13-C14-C19-C18	-117.75(8)
C15-C14-C19-C18	-1.71(9)
C20-C18-C19-C13	-28.31(10)
C17-C18-C19-C13	-133.24(8)
C20-C18-C19-C14	34.26(9)
C17-C18-C19-C14	-70.67(8)
C19-C18-C20-C15	-51.45(8)
C17-C18-C20-C15	56.90(7)
C14-C15-C20-C18	50.52(8)
C16-C15-C20-C18	-57.95(7)
O1-S1-C21-C26	-27.71(9)
O2-S1-C21-C26	-157.07(7)
C1-S1-C21-C26	90.99(8)
O1-S1-C21-C22	147.60(7)
O2-S1-C21-C22	18.23(8)
C1-S1-C21-C22	-93.70(7)
C26-C21-C22-C23	-1.37(14)
S1-C21-C22-C23	-176.65(7)
C21-C22-C23-C24	0.71(15)
C22-C23-C24-C25	0.17(17)
C23-C24-C25-C26	-0.42(17)
C24-C25-C26-C21	-0.22(16)
C22-C21-C26-C25	1.13(14)
S1-C21-C26-C25	176.28(8)
O3-S2-C27-C28	-20.58(9)
O4-S2-C27-C28	-150.25(7)
C1-S2-C27-C28	96.86(8)
O3-S2-C27-C32	154.63(7)
O4-S2-C27-C32	24.96(9)
C1-S2-C27-C32	-87.93(8)
C32-C27-C28-C29	1.84(14)

S2-C27-C28-C29	176.92(8)
C27-C28-C29-C30	0.61(15)
C28-C29-C30-C31	-2.16(16)
C29-C30-C31-C32	1.26(16)
C30-C31-C32-C27	1.15(15)
C28-C27-C32-C31	-2.73(15)
S2-C27-C32-C31	-177.84(8)

(5*S*,6*R*)-1-((1*R*,6*S*,7*R*)-Bicyclo[4.1.0]heptan-7-yl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane (5bc)



White Solid. Mp 88-90 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.34 (d, J = 8.2 Hz, 2H), 7.27-7.22 (m, 2H), 7.17-7.12 (m, 1H), 7.07 (d, J = 7.3 Hz, 2H), 3.63 (d, J = 9.2 Hz, 1H), 3.61 (d, J = 9.3 Hz, 1H), 3.14 (dd, J = 9.3, 3.9 Hz, 1H), 3.09 (d, J = 9.3 Hz, 1H), 2.44 (s, 3H), 2.06 (d, J = 3.9 Hz, 1H), 1.68 (sext, J = 6.9 Hz, 1H), 1.60 (t, J = 4.0 Hz, 1H), 1.42-1.31 (m, 2H), 1.10-0.78 (m, 4H), 0.76-0.67 (m, 1H), 0.49 (q, J = 7.1 Hz, 1H), 0.35-0.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6 (C), 137.8 (C), 134.3 (C), 129.8 (CH), 129.1 (CH), 128.1 (CH), 127.7 (CH), 126.0 (CH), 54.4 (CH_2), 50.7 (CH_2), 36.6 (C), 30.4 (CH), 25.1 (CH), 23.4 (CH_2), 22.7 (CH_2), 21.7 (CH_3), 21.5 (CH), 21.4 (CH_2), 21.2 (CH_2), 18.4 (CH), 16.5 (CH); HRMS-ESI calcd for $C_{25}H_{29}NO_2NaS$ $[M+Na]^+$: 430.1817. Found: 430.1828. Elemental analysis (%) calcd for $(C_{25}H_{29}NO_2)_2 \cdot H_2O$: C, 72.08; H, 7.26; N, 3.36; S, 7.70; Found: C, 72.25; H, 7.39; N, 3.25; S, 7.27.

Table 4. Crystal data and structure refinement for **5bc**.

Identification code	**5bc**
Empirical formula	C25.50 H29.50 Cl1.50 N O2 S
Formula weight	467.24
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	C2/c	
Unit cell dimensions	a = 35.8601(11) Å	a= 90.00 °
	b = 6.0216(2) Å	b = 111.9790(10)
°.		
	c = 23.1924(6) Å	g = 90.00 °
Volume	4644.1(2) $Å^3$	
Z	8	
Density (calculated)	1.337 Mg/m^3	
Absorption coefficient	0.335 mm^{-1}	
F(000)	1976	
Crystal size	0.40 x 0.20 x 0.20 mm^3	
Theta range for data collection	3.44 to 31.51 °.	
Index ranges	-52 <=h<=42 ,-6 <=k<=8 ,-32 <=l<=34	
Reflections collected	7482	
Independent reflections	5749 [R(int) = 0.0315]	
Completeness to theta = 31.51 °	0.967 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9360 and 0.8776	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7482 / 0 / 317	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0592 , wR2 = 0.1641	
R indices (all data)	R1 = 0.0770 , wR2 = 0.1786	
Largest diff. peak and hole	1.514 and -0.781 $e.Å^{-3}$	

Table 5. Bond lengths [Å] and angles [°] for **5bc**.

Bond lengths----	
S1-O1	1.4310(14)
S1-O2	1.4369(15)
S1-N1	1.6282(14)
S1-C1	1.7645(18)
C1-C2	1.390(3)

C1-C6	1.397(2)
N1-C12	1.476(2)
N1-C8	1.484(2)
C1S-Cl3S	1.708(7)
C1S-Cl2S	1.745(6)
C1S-Cl1S	1.815(7)
C2-C3	1.393(3)
C3-C4	1.393(3)
C4-C5	1.395(3)
C4-C7	1.506(3)
C5-C6	1.393(2)
C8-C9	1.515(2)
C9-C10	1.511(2)
C9-C11	1.516(2)
C10-C13	1.493(2)
C10-C11	1.522(2)
C11-C19	1.491(2)
C11-C12	1.518(2)
C13-C18	1.391(2)
C13-C14	1.398(2)
C14-C15	1.397(2)
C15-C16	1.386(3)
C16-C17	1.381(3)
C17-C18	1.401(2)
C19-C25	1.500(2)
C19-C20	1.507(2)
C20-C25	1.513(3)
C20-C21	1.521(3)
C21-C22	1.508(5)
C21-C22'	1.594(5)
C22-C23	1.533(7)
C22'-C23'	1.518(6)
C23-C24	1.576(5)
C23'-C24	1.567(5)

C24-C25	1.517(3)

Angles----------

O1-S1-O2	120.25(9)
O1-S1-N1	107.17(8)
O2-S1-N1	106.32(8)
O1-S1-C1	107.35(8)
O2-S1-C1	107.53(9)
N1-S1-C1	107.68(8)
C2-C1-C6	120.75(16)
C2-C1-S1	119.56(14)
C6-C1-S1	119.67(14)
C12-N1-C8	110.06(13)
C12-N1-S1	119.68(12)
C8-N1-S1	119.17(11)
Cl3S-C1S-Cl2S	114.9(3)
Cl3S-C1S-Cl1S	111.7(4)
Cl2S-C1S-Cl1S	107.6(4)
C1-C2-C3	119.11(17)
C2-C3-C4	121.34(18)
C3-C4-C5	118.51(17)
C3-C4-C7	121.15(18)
C5-C4-C7	120.32(18)
C6-C5-C4	121.24(17)
C5-C6-C1	119.01(17)
N1-C8-C9	102.18(13)
C10-C9-C8	115.41(14)
C10-C9-C11	60.38(11)
C8-C9-C11	107.96(14)
C13-C10-C9	122.24(14)
C13-C10-C11	118.66(13)
C9-C10-C11	59.97(11)
C19-C11-C9	125.13(14)
C19-C11-C12	117.59(14)

C9-C11-C12	106.93(13)
C19-C11-C10	119.69(13)
C9-C11-C10	59.65(11)
C12-C11-C10	114.96(13)
N1-C12-C11	102.89(14)
C18-C13-C14	118.32(15)
C18-C13-C10	123.07(16)
C14-C13-C10	118.60(15)
C15-C14-C13	120.97(17)
C16-C15-C14	120.01(18)
C17-C16-C15	119.62(16)
C16-C17-C18	120.48(18)
C13-C18-C17	120.59(18)
C11-C19-C25	122.75(15)
C11-C19-C20	121.79(14)
C25-C19-C20	60.41(13)
C19-C20-C25	59.56(12)
C19-C20-C21	119.93(17)
C25-C20-C21	119.97(16)
C22-C21-C20	112.9(2)
C22-C21-C22'	30.9(2)
C20-C21-C22'	111.9(2)
C21-C22-C23	104.8(4)
C23'-C22'-C21	111.3(3)
C22-C23-C24	110.0(3)
C22'-C23'-C24	105.0(3)
C25-C24-C23'	113.4(2)
C25-C24-C23	109.4(2)
C23'-C24-C23	35.5(2)
C19-C25-C20	60.04(12)
C19-C25-C24	119.54(19)
C20-C25-C24	120.32(17)

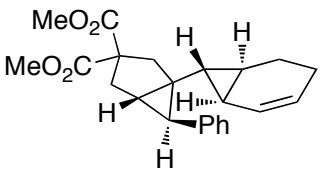
Table 6. Torsion angles [°] for **5bc**.

O1-S1-C1-C2	156.06(13)
O2-S1-C1-C2	25.36(15)
N1-S1-C1-C2	-88.84(15)
O1-S1-C1-C6	-22.46(15)
O2-S1-C1-C6	-153.17(13)
N1-S1-C1-C6	92.63(14)
O1-S1-N1-C12	-168.46(13)
O2-S1-N1-C12	-38.68(16)
C1-S1-N1-C12	76.32(15)
O1-S1-N1-C8	51.16(15)
O2-S1-N1-C8	-179.06(13)
C1-S1-N1-C8	-64.06(15)
C6-C1-C2-C3	1.4(2)
S1-C1-C2-C3	-177.14(13)
C1-C2-C3-C4	-0.3(3)
C2-C3-C4-C5	-1.3(3)
C2-C3-C4-C7	177.04(17)
C3-C4-C5-C6	2.0(2)
C7-C4-C5-C6	-176.35(16)
C4-C5-C6-C1	-1.0(2)
C2-C1-C6-C5	-0.7(2)
S1-C1-C6-C5	177.82(12)
C12-N1-C8-C9	31.31(18)
S1-N1-C8-C9	175.17(12)
N1-C8-C9-C10	46.86(19)
N1-C8-C9-C11	-18.23(17)
C8-C9-C10-C13	156.07(15)
C11-C9-C10-C13	-106.88(17)
C8-C9-C10-C11	-97.05(16)
C10-C9-C11-C19	106.85(17)
C8-C9-C11-C19	-143.61(16)
C10-C9-C11-C12	-109.44(14)
C8-C9-C11-C12	0.10(18)

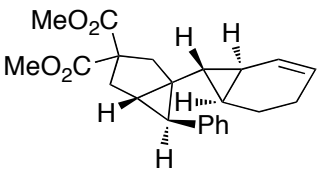
C8-C9-C11-C10	109.54(15)
C13-C10-C11-C19	-3.0(2)
C9-C10-C11-C19	-115.70(17)
C13-C10-C11-C9	112.73(17)
C13-C10-C11-C12	-151.55(15)
C9-C10-C11-C12	95.72(15)
C8-N1-C12-C11	-31.45(17)
S1-N1-C12-C11	-175.10(11)
C19-C11-C12-N1	165.13(14)
C9-C11-C12-N1	18.23(17)
C10-C11-C12-N1	-45.60(18)
C9-C10-C13-C18	-28.9(2)
C11-C10-C13-C18	-99.7(2)
C9-C10-C13-C14	152.47(16)
C11-C10-C13-C14	81.7(2)
C18-C13-C14-C15	-0.5(3)
C10-C13-C14-C15	178.18(16)
C13-C14-C15-C16	0.8(3)
C14-C15-C16-C17	-0.1(3)
C15-C16-C17-C18	-0.9(3)
C14-C13-C18-C17	-0.4(3)
C10-C13-C18-C17	-179.09(16)
C16-C17-C18-C13	1.2(3)
C9-C11-C19-C25	-0.2(3)
C12-C11-C19-C25	-140.47(18)
C10-C11-C19-C25	71.8(2)
C9-C11-C19-C20	72.8(2)
C12-C11-C19-C20	-67.5(2)
C10-C11-C19-C20	144.77(17)
C11-C19-C20-C25	-112.33(19)
C11-C19-C20-C21	138.38(19)
C25-C19-C20-C21	-109.3(2)
C19-C20-C21-C22	48.6(3)
C25-C20-C21-C22	-21.4(4)

C19-C20-C21-C22'	82.0(3)
C25-C20-C21-C22'	12.0(3)
C20-C21-C22-C23	56.1(4)
C22'-C21-C22-C23	-38.6(4)
C22-C21-C22'-C23'	49.4(5)
C20-C21-C22'-C23'	-49.0(4)
C21-C22-C23-C24	-74.9(5)
C21-C22'-C23'-C24	70.2(4)
C22'-C23'-C24-C25	-55.7(4)
C22'-C23'-C24-C23	35.2(4)
C22-C23-C24-C25	53.5(4)
C22-C23-C24-C23'	-49.9(4)
C11-C19-C25-C20	110.80(18)
C11-C19-C25-C24	-139.14(19)
C20-C19-C25-C24	110.1(2)
C21-C20-C25-C19	109.2(2)
C19-C20-C25-C24	-108.8(2)
C21-C20-C25-C24	0.4(3)
C23'-C24-C25-C19	-48.5(3)
C23-C24-C25-C19	-86.5(3)
C23'-C24-C25-C20	22.0(3)
C23-C24-C25-C20	-16.0(3)

(5*S*,6*R*)-Dimethyl 1-((1*R*, 6*S*, 7*R*)-bicyclo[4.1.0]hept-2-en-7-yl)-6-phenylbicyclo [3.1.0]hexane-3,3-dicarboxylate (5ca) and (5*S*,6*R*)-dimethyl 1-((7*S*)-bicyclo[4.1.0]hept-2-en-7-yl)-6-phenylbicyclo[3.1.0]hexane-3,3-dicarboxylate (5ca')



5ca

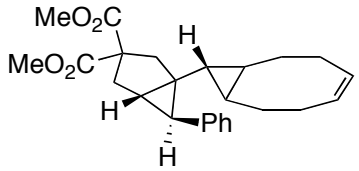


5ca'

Colorless oil, mixture of at least two diastereoisomers (**5ca**/**5ca'**, ratio 1.0 : 0.7). Each diastereoisomer was assigned based on the chemical shift of the olefin protons. Due to

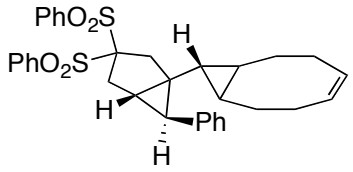
extensive overlapping the assigment of ^{1}H is temptative (The structure was studied by COSY, HSQC, HMBC, and NOESY experiments). ^{1}H NMR (400 MHz, $CDCl_3$) 7.28-7.20 (m, 2H major, 2H minor), 7.17-7.09 (m, 3H major, 3H minor), 6.00-5.93 (m, 1H major), 5.50-5.41 (m, 1H minor), 5.31-5.24 (m, 1H major), 5.24-5.17 (m, 1H minor), 3.75-3.71 (m, 6H major, 6H minor), 2.83 (d, J = 13.8 Hz, 1H major), 2.72 (d, J = 13.9 Hz, 1H minor), 2.66-2.57 (m, 2H major, 2H minor), 2.48 (d, J = 13.9 Hz, 1H major), 2.39 (d, J = 13.8 Hz, 1H minor), 1.87-1.59 (m, 4H major, 3H minor), 1.53-1.32 (m, 2H major, 1H minor), 1.16-1.04 (m, 2H minor), 1.04-0.86 (m, 1H major, 2H minor), 0.84-0.73 (m, 1H major, 1H minor), 0.72-0.64 (m, 1H major); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3 (C), 172.7 (C), 138.7 (C), 138.7 (C), 129.3 (CH), 129.2 (CH), 128.1 (CH), 127.8 (CH), 127.8 (CH), 127.6 (CH), 125.7 (CH), 122.9 (CH), 122.4 (CH), 60.7 (C), 60.6 (C), 53.0 (CH_3), 52.9 (CH_3), 42.4 (CH_2), 41.3 (CH_2), 37.0 (CH_2), 37.0 (CH_2), 32.6 (CH), 27.6 (CH), 26.6 (CH), 24.6 (CH), 24.4 (CH), 22.9 (CH), 20.8 (CH_2), 20.8 (CH_2), 20.0 (CH), 18.0 (CH_2), 17.6 (CH), 17.2 (CH_2), 16.5 (CH); HRMS-ESI calcd for $C_{23}H_{26}O_4Na$ $[M+Na]^+$: 389.1729. Found: 389.1720.

(1*S*,5*S*,6*R*)-Dimethyl 1-((1*R*,8*S*,9*r*,*Z*)-bicyclo [6.1.0]non-4-en-9-yl)-6-phenylbicyclo[3.1.0]hexane-3,3-dicarboxylate (5da)



Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.21 (m, 2H), 7.13-7.10 (m, 3H), 5.57-5.45 (m, 2H), 3.73 (s, 3H), 3.71 (s, 3H), 2.80 (d, J = 13.8 Hz, 1H), 2.58 (d, J = 2.9 Hz, 2H), 2.42 (d, J = 13.8 Hz, 1H), 2.20-2.12 (m, 1H), 2.10-1.91 (m, 3H), 1.80-1.79 (d, J = 4.0 Hz, 1H), 1.80-1.78 (m, 1H), 1.59-1.56 (m, 1H), 1.24-1.10 (m, 2H), 0.77-0.68 (m, 1H), 0.77-0.68 (m, 1H), 0.35-0.28 (m, 1H), 0.22 (t, J = 5.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3 (C_q), 172.2 (C_q), 139.0 (C_q, C-11), 130.3 (CH), 130.2 (CH), 129.3 (CH), 128.0 (CH), 125.7 (CH), 60.8 (C_q), 53.1 (CH_3), 53.0 (CH_3), 43.5 (CH_2), 38.2 (C_q), 37.1 (CH_2), 32.8 (CH), 29.7 (CH_2), 28.7 (CH_2), 27.2 (CH), 27.2 (CH_2), 26.9 (CH_2), 26.8 (CH), 25.3 (CH), 23.1 (CH); HRMS- ESI calcd for $C_{25}H_{30}NaO_4$ $[M+Na]^+$ 417.2042. Found: 417.2028.

(1*R*,8*S*,9*r*,*Z*)-9-((1*S*,5*S*,6*R*)-6-phenyl-3,3-bis(phenylsulfonyl)bicyclo[3.1.0]hexan-1-yl)bicyclo[6.1.0]non-4-ene (5db)



Pale yellow solid. Mp: 191-192 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.04 (m, 4H), 7.76-7.69 (m, 2H), 7.65-7.57 (m, 4H), 7.29-7.20 (m, 2H), 7.17-7.10 (m, 1H), 7.10-7.05 (m, 2H), 5.57-5.46 (m, 2H), 3.13 (dd, *J* = 16.2 Hz, 6.5 Hz, 1H), 3.03 (d, *J* = 16.2 Hz, 1H), 2.89 (d, *J* = 16.2 Hz, 1H), 2.69 (d, *J* = 5.3 Hz, 1H), 2.30 (d, *J* = 4.1 Hz, 1H), 2.23-1.92 (m, 4H), 1.86-1.80 (m, 1H), 1.86-1.71 (m, 1H), 1.24-1.05 (m, 2H), 0.94-0.84 (m, 1H), 0.73-0.61 (m, 1H), 0.40-0.30 (m, 1H), 0.19 (t, *J* = 5.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1 (C_q), 137.0 (C_q), 136.3 (C_q), 134.8 (CH), 134.7 (CH), 132.0 (CH), 131.6 (CH), 130.6 (CH), 130.2 (CH), 129.0 (CH), 128.9 (CH), 128.8 (CH), 128.1 (CH), 125.9 (CH), 97.6 (C_q), 42.2 (CH_2), 41.4 (C_q), 36.6 (CH_2), 36.2 (CH), 29.9 (CH_2), 28.9 (CH), 28.8 (CH_2), 27.7 (CH), 27.0 (CH_2), 26.8 (CH_2), 26.2 (CH), 22.9 (CH); HRMS-ESI calcd for $C_{33}H_{34}O_4NaS_2$ $[M+Na]^+$ 581.1796. Found 581.1780. Elemental analysis (%) calcd for $C_{33}H_{34}O_2 \cdot H_2O$: C, 68.72; H, 6.29; found: C, 69.11; H, 6.29.

Table 7. Crystal data and structure refinement for **5db**.

Identification code	**5db**	
Empirical formula	C33 H34 O4 S2	
Formula weight	558.72	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.7285(12) Å	α= 111.389(5) °
	b = 10.9833(12) Å	β=92.772(5) °
	c = 13.0463(12) Å	γ = 103.536(6) °
Volume	1376.4(2) Å^3	
Z	2	
Density (calculated)	1.348 Mg/m^3	
Absorption coefficient	0.232 mm^{-1}	
Crystal size	0.20 x 0.10 x 0.10 mm^3	
Theta range for data collection	2.79 to 2.79 °	

Index ranges	-15 <=h<=12 ,-10 <=k<=15 ,-18 <=l<=18
Reflections collected	7467
Independent reflections	5081 [R(int) = 0.0825]
Completeness to theta = 30.29 °	0.905 %
Absorption correction	Empirical
Max. and min. transmission	0.9772 and 0.9551
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7467 / 0 / 352
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 =0.0729 , wR2 = 0.1838
R indices (all data)	R1 = 0.1108 , wR2 =0.2100
Largest diff. peak and hole	0.539 and -0.600 e.$Å^{-3}$

Table 8. Bond lengths [Å] and angles [°] for **5db**.

S1-O2	1.439(2)
S1-O1	1.442(2)
S1-C16	1.765(3)
S1-C1	1.840(3)
C1-C6	1.558(4)
C1-C2	1.563(4)
C1-S2	1.833(3)
S2-O4	1.439(2)
S2-O3	1.440(2)
S2-C22	1.764(4)
C2-C3	1.519(4)
C3-C5	1.506(5)
C3-C4	1.515(4)
C4-C28	1.498(4)
C4-C5	1.525(4)
C5-C7	1.494(4)
C5-C6	1.531(4)
C7-C8	1.515(4)
C7-C15	1.519(4)
C8-C15	1.507(4)
C8-C9	1.513(4)
C9-C10	1.547(4)
C10-C11	1.513(5)

C11-C12	1.323(4)
C12-C13	1.501(5)
C13-C14	1.558(5)
C14-C15	1.518(4)
C16-C17	1.390(4)
C16-C21	1.395(4)
C17-C18	1.383(5)
C18-C19	1.390(5)
C19-C20	1.386(5)
C20-C21	1.388(5)
C22-C23	1.394(4)
C22-C27	1.407(4)
C23-C24	1.384(6)
C24-C25	1.386(6)
C25-C26	1.394(5)
C26-C27	1.379(5)
C28-C33	1.392(4)
C28-C29	1.396(4)
C29-C30	1.396(4)
C30-C31	1.386(5)
C31-C32	1.389(5)
C32-C33	1.392(4)
O2-S1-O1	118.63(15)
O2-S1-C16	109.47(14)
O1-S1-C16	105.86(14)
O2-S1-C1	108.63(13)
O1-S1-C1	103.94(12)
C16-S1-C1	110.04(14)
C6-C1-C2	107.4(2)
C6-C1-S2	108.54(19)
C2-C1-S2	111.1(2)
C6-C1-S1	109.42(19)
C2-C1-S1	107.14(19)
S2-C1-S1	113.08(14)
O4-S2-O3	119.28(14)
O4-S2-C22	107.16(14)
O3-S2-C22	108.42(15)
O4-S2-C1	104.11(13)

O3-S2-C1	108.34(13)
C22-S2-C1	109.19(14)
C3-C2-C1	106.2(3)
C5-C3-C4	60.64(19)
C5-C3-C2	109.8(2)
C4-C3-C2	115.1(2)
C28-C4-C3	123.6(2)
C28-C4-C5	121.1(3)
C3-C4-C5	59.40(19)
C7-C5-C3	124.8(2)
C7-C5-C4	120.6(2)
C3-C5-C4	60.0(2)
C7-C5-C6	116.3(3)
C3-C5-C6	108.8(2)
C4-C5-C6	114.4(2)
C5-C6-C1	106.4(2)
C5-C7-C8	124.5(3)
C5-C7-C15	121.1(3)
C8-C7-C15	59.55(18)
C15-C8-C9	123.2(3)
C15-C8-C7	60.39(18)
C9-C8-C7	119.6(3)
C8-C9-C10	114.0(3)
C11-C10-C9	113.4(3)
C12-C11-C10	126.0(3)
C11-C12-C13	125.4(3)
C12-C13-C14	111.8(3)
C15-C14-C13	112.5(3)
C8-C15-C14	121.6(3)
C8-C15-C7	60.06(18)
C14-C15-C7	122.0(3)
C17-C16-C21	121.0(3)
C17-C16-S1	117.8(2)
C21-C16-S1	120.9(3)
C18-C17-C16	119.9(3)
C17-C18-C19	119.6(3)
C20-C19-C18	120.2(3)
C19-C20-C21	121.0(3)

C20-C21-C16	118.3(3)
C23-C22-C27	120.6(3)
C23-C22-S2	119.6(3)
C27-C22-S2	119.8(2)
C24-C23-C22	118.7(3)
C23-C24-C25	121.0(3)
C24-C25-C26	120.2(4)
C27-C26-C25	119.7(3)
C26-C27-C22	119.7(3)
C33-C28-C29	118.6(3)
C33-C28-C4	117.9(3)
C29-C28-C4	123.5(3)
C28-C29-C30	120.3(3)
C31-C30-C29	120.5(3)
C30-C31-C32	119.4(3)
C31-C32-C33	120.0(3)
C32-C33-C28	121.1(3)

Table 9. Torsion angles [°] for **5db**.

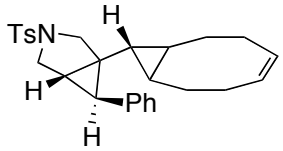
O2-S1-C1C6	-159.12(19)
O1-S1-C1C6	73.7(2)
C16-S1-C1C6	-39.3(2)
O2-S1-C1C2	84.7(2)
O1-S1-C1C2	-42.5(2)
C16-S1-C1C2	-155.5(2)
O2-S1-C1S2	-38.0(2)
O1-S1-C1S2	-165.22(17)
C16-S1-C1S2	81.8(2)
C6-C1-S2O4	-55.1(2)
C2-C1-S2O4	62.8(2)
S1-C1-S2O4	-176.73(17)
C6-C1-S2O3	72.8(2)
C2-C1-S2O3	-169.3(2)
S1-C1-S2O3	-48.8(2)
C6-C1-S2C22	-169.30(18)
C2-C1-S2C22	-51.4(2)
S1-C1-S2C22	69.09(19)

C6-C1-C2C3	-10.9(3)
S2-C1-C2C3	-129.5(2)
S1-C1-C2C3	106.6(2)
C1-C2-C3C5	6.5(3)
C1-C2-C3C4	72.5(3)
C5-C3-C4C28	-109.1(3)
C2-C3-C4C28	151.3(3)
C2-C3-C4C5	-99.6(3)
C4-C3-C5C7	108.3(3)
C2-C3-C5C7	-143.4(3)
C2-C3-C5C4	108.4(2)
C4-C3-C5C6	-107.9(2)
C2-C3-C5C6	0.5(3)
C28-C4-C5C7	-1.8(4)
C3-C4-C5C7	-115.1(3)
C28-C4-C5C3	113.3(3)
C28-C4-C5C6	-148.3(3)
C3-C4-C5C6	98.4(3)
C7-C5-C6C1	140.0(2)
C3-C5-C6C1	-7.3(3)
C4-C5-C6C1	-72.1(3)
C2-C1-C6C5	11.2(3)
S2-C1-C6C5	131.42(19)
S1-C1-C6C5	-104.8(2)
C3-C5-C7C8	-7.7(4)
C4-C5-C7C8	65.0(4)
C6-C5-C7C8	-149.2(3)
C3-C5-C7C15	64.6(4)
C4-C5-C7C15	137.3(3)
C6-C5-C7C15	-76.9(4)
C5-C7-C8C15	108.8(3)
C5-C7-C8C9	-137.5(3)
C15-C7-C8C9	113.7(3)
C15-C8-C9C10	-74.3(4)
C7-C8-C9C10	-146.4(3)
C8-C9-C10C11	102.4(4)
C9-C10-C11C12	-73.1(5)
C10-C11-C12C13	1.0(6)

C11-C12-C13C14	74.6(5)
C12-C13-C14C15	-107.6(3)
C9-C8-C15C14	3.4(5)
C7-C8-C15C14	111.3(3)
C9-C8-C15C7	-107.9(3)
C13-C14-C15C8	71.4(4)
C13-C14-C15C7	143.6(3)
C5-C7-C15C8	-114.4(3)
C5-C7-C15C14	134.8(3)
C8-C7-C15C14	-110.7(3)
O2-S1-C16C17	-139.6(2)
O1-S1-C16C17	-10.6(3)
C1-S1-C16C17	101.1(3)
O2-S1-C16C21	35.0(3)
O1-S1-C16C21	163.9(2)
C1-S1-C16C21	-84.4(3)
C21-C16-C17C18	1.0(5)
S1-C16-C17C18	175.5(3)
C16-C17-C18C19	-0.6(5)
C17-C18-C19C20	0.2(5)
C18-C19-C20C21	0.0(5)
C19-C20-C21C16	0.3(5)
C17-C16-C21C20	-0.8(5)
S1-C16-C21C20	-175.1(2)
O4-S2-C22C23	150.4(2)
O3-S2-C22C23	20.4(3)
C1-S2-C22C23	-97.5(3)
O4-S2-C22C27	-26.8(3)
O3-S2-C22C27	-156.8(2)
C1-S2-C22C27	85.3(3)
C27-C22-C23C24	-1.8(5)
S2-C22-C23C24	-179.0(3)
C22-C23-C24C25	-0.1(5)
C23-C24-C25C26	1.6(5)
C24-C25-C26C27	-1.2(5)
C25-C26-C27C22	-0.7(5)
C23-C22-C27C26	2.2(5)
S2-C22-C27C26	179.4(3)

C3-C4-C28C33	170.7(3)
C5-C4-C28C33	98.9(3)
C3-C4-C28C29	-10.2(5)
C5-C4-C28C29	-81.9(4)
C33-C28-C29C30	-1.4(4)
C4-C28-C29C30	179.5(3)
C28-C29-C30C31	1.9(5)
C29-C30-C31C32	-1.3(5)
C30-C31-C32C33	0.1(5)
C31-C32-C33C28	0.4(5)
C29-C28-C33C32	0.2(5)
C4-C28-C33C32	179.4(3)

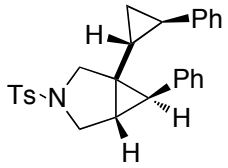
(5*S*,6*R*)-1-((1*R*,8*S*,9*R*,*Z*)-bicyclo[6.1.0]non-4-en-9-yl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane (5dc)



Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.69 (m, 2H), 7.36-7.31 (m, 2H), 7.27-7.22 (m, 2H), 7.17-7.11 (m, 1H), 7.09-7.04 (m, 2H), 5.55-5.43 (m, 2H), 3.66 (d, J = 9.4 Hz, 1H), 3.60 (d, J = 9.2 Hz, 1H), 3.14 (dd, J = 9.2, 4.0 Hz, 1H), 3.09 (d, J = 9.4 Hz, 1H), 2.44 (s, 3H), 2.19-1.85 (m, 4H), 2.09 (d, J = 4.0 Hz, 1H), 1.81-1.71 (m, 1H), 1.61-1.59 (m, J = 4.0 Hz, 1H), 1.24-1.11 (m, 2H), 0.80-0.69 (m, 1H), 0.51-0.42 (m, 1H), 0.32-0.24 (m, 1H), 0.16 (t, J = 5.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6 (C_q), 137.6 (C_q), 134.2 (C_q), 130.3 (CH), 130.1 (CH), 129.8 (CH), 129.1 (CH), 128.2 (CH), 127.6 (CH), 126.1 (CH), 54.5 (CH_2), 50.6 (CH_2), 36.5 (C_q), 30.4 (CH), 29.4 (CH_2), 28.5 (CH_2), 27.0 (CH_2), 26.8 (CH_2), 25.1 (CH), 25.0 (CH), 24.5 (CH), 23.0 (CH), 21.7 (CH_3); HRMS-ESI calcd for $C_{27}H_{31}NO_2NaS$ $[M+Na]^+$: 456.1973. Found 456.1966.

Cyclopropanation of acyclic alkenes

(1*R*,5*S*,6*R*)-6-Phenyl-1-((1*R*,2*R*)-2-phenylcyclopropyl)-3-tosyl-3-azabicyclo[3.1.0]hexane (13a)



Catalyst: **A** or **D**. White solid. Mp: 178-179 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.69 (m, 2H), 7.36 (t, J = 6.6 Hz, 2H), 7.25-7.19 (m, 2H), 7.18-7.12 (m, 3H), 7.12-7.07 (m, 3H), 6.76 (dd, J = 5.2, 3.3 Hz, 2H), 3.70 (dd, J = 11.5, 9.4 Hz, 2H), 3.23 (dd, J = 9.3, 3.9 Hz, 1H), 3.17 (d, J = 9.4 Hz, 1H), 2.46 (s, 3H), 2.18 (d, J = 4.2 Hz, 1H), 1.73 (t, J = 4.1 Hz, 1H), 1.49-1.42 (m, 1H), 1.02-0.94 (m, 1H), 0.67-0.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 142.3, 137.1, 133.8, 129.9, 129.1, 128.3, 127.7, 126.3, 125.8, 125.8, 54.6, 50.7, 36.0, 30.6, 25.2, 22.3, 21.7, 21.3,16.0; Significant signals for the minor diastereoisomer: δ 7.61 (d, J = 8.5 Hz, 2H), 7.29 (t, J = 7.4 Hz, 3H), 6.83 (d, J = 7.9 Hz, 2H), 6.43 (dd, J = 7.4, 2.4 Hz, 3H), 3.72 (d, J = 9.3 Hz, 2H), 3.41 (dd, J = 13.0, 9.6 Hz, 2H) 3.20 (d, J = 4.0 Hz, 1H) 3.13 (d, J = 9.2 Hz, 1H), 2.74 (d, J = 9.6 Hz, 1H), 2.62 (dd, J = 8.9, 4.0 Hz, 1H), 2.45 (s, 3H), 2.23 (d, J = 4.0 Hz, 1H), 1.96 (d, J = 4.6 Hz, 1H), 1.38 (m, J = 4.8 Hz, 2H); HRMS-ESI calcd for $C_{27}H_{27}NO_2NaS$ [M+Na]: 452.1660. Found: 452.1640.

Elemental analysis (%) calcd $C_{27}H_{27}NO_2S$: C, 75.49; H, 6.34; N, 3.26; O, 7.45; S, 7.46. Found: C, 74.96; H, 6.33; N, 3.17.

Table 10. Crystal data and structure refinement for **13a** (Major diastereoisomer).

Identification code	**13a**	
Empirical formula	C27 H27 N O2 S	
Formula weight	429.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.6368(12) Å	a= 90.00 °
	b = 7.9693(8) Å	b = 97.724(2) °

	c = 21.2530(17) Å g = 90.00 °
Volume	2288.7(4) $Å^3$
Z	4
Density (calculated)	1.247 Mg/m^3
Absorption coefficient	0.165 mm^{-1}
F(000)	912
Crystal size	0.60 x 0.60 x 0.60 mm^3
Theta range for data collection	1.51 to 1.51 °
Index ranges	-18 <=h<=20 ,-12 <=k<=11 ,-32 <=l<=16
Reflections collected	8536
Independent reflections	7333 [R(int) = 0.0234]
Completeness to theta = 33.17 °	0.976 %
Absorption correction	Empirical
Max. and min. transmission	0.9075 and 0.9074
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8536 / 0 / 281
Goodness-of-fit on F^2	1.109
Final R indices [I>2sigma(I)]	R1 = 0.0483 , wR2 = 0.1327
R indices (all data)	R1 = 0.0563 , wR2 = 0.1393
Largest diff. peak and hole	0.546 and -0.362 $e.Å^{-3}$

Table 11. Bond lengths [Å] and angles [°] for **13a**.

Bond lengths----	
C1-C2	1.386(2)
C1-C6	1.389(2)
C2-C3	1.3936(18)
C3-C4	1.3966(17)
C4-C5	1.3969(17)
C4-C7	1.4861(16)
C5-C6	1.3903(17)
C7-C8	1.5107(16)
C7-C9	1.5236(16)
C8-C9	1.502(16)
C9-C10	1.4884(16)
C10-C18	1.5084(15)
C10-C20	1.5212(15)
C10-C11	1.5302(16)

C11-C12	1.4888(16)
C11-C18	1.5095(16)
C12-C17	1.3934(17)
C12-C13	1.3979(17)
C13-C14	1.39(2)
C14-C15	1.382(3)
C15-C16	1.386(3)
C16-C17	1.3984(19)
C18-C19	1.5094(16)
C19-N1	1.4829(15)
C20-N1	1.4816(15)
C21-C22	1.393(17)
C21-C27	1.3969(17)
C21-S1	1.7621(13)
C22-C23	1.3897(19)
C23-C24	1.3949(19)
C24-C26	1.3993(19)
C24-C25	1.503(2)
C26-C27	1.39(19)
N1-S1	1.6263(10)
O1-S1	1.4348(10)
O2-S1	1.4345(10)

Angles----------

C2-C1-C6	119.56(12)
C1-C2-C3	120.17(12)
C2-C3-C4	120.73(12)
C3-C4-C5	118.58(11)
C3-C4-C7	119.12(11)
C5-C4-C7	122.24(10)
C6-C5-C4	120.53(12)
C1-C6-C5	120.43(13)
C4-C7-C8	122.76(10)
C4-C7-C9	120.17(10)
C8-C7-C9	59.34(8)
C9-C8-C7	60.76(8)
C10-C9-C8	123.27(9)
C10-C9-C7	118.95(9)

C8-C9-C7	59.90(8)
C9-C10-C18	125.47(9)
C9-C10-C20	116.35(9)
C18-C10-C20	106.91(9)
C9-C10-C11	122.09(9)
C18-C10-C11	59.57(7)
C20-C10-C11	114.07(9)
C12-C11-C18	122.62(10)
C12-C11-C10	121.12(9)
C18-C11-C10	59.50(7)
C17-C12-C13	118.59(12)
C17-C12-C11	123.84(11)
C13-C12-C11	117.56(11)
C14-C13-C12	120.77(14)
C15-C14-C13	120.02(15)
C14-C15-C16	120.19(13)
C15-C16-C17	119.81(15)
C12-C17-C16	120.62(14)
C10-C18-C19	108.07(9)
C10-C18-C11	60.93(7)
C19-C18-C11	115.82(10)
N1-C19-C18	102.33(9)
N1-C20-C10	102.85(8)
C22-C21-C27	120.41(12)
C22-C21-S1	119.41(10)
C27-C21-S1	120.15(9)
C23-C22-C21	119.28(12)
C22-C23-C24	121.41(12)
C23-C24-C26	118.40(12)
C23-C24-C25	120.44(13)
C26-C24-C25	121.16(13)
C27-C26-C24	121.04(12)
C26-C27-C21	119.44(12)
C20-N1-C19	109.40(9)
C20-N1-S1	119.22(7)
C19-N1-S1	118.29(8)
O2-S1-O1	120.32(6)
O2-S1-N1	106.94(5)

O1-S1-N1	105.93(6)
O2-S1-C21	107.72(6)
O1-S1-C21	107.98(6)
N1-S1-C21	107.31(6)

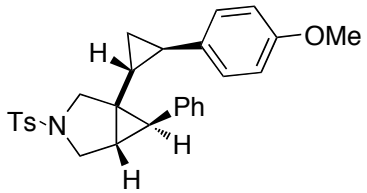
Table 12. Torsion angles [°] for **13a**.

C6-C1-C2-C3	0.1(2)
C1-C2-C3-C4	-0.2(2)
C2-C3-C4-C5	0.35(18)
C2-C3-C4-C7	-176.88(11)
C3-C4-C5-C6	-0.34(18)
C7-C4-C5-C6	176.81(11)
C2-C1-C6-C5	-0.1(2)
C4-C5-C6-C1	0.21(19)
C3-C4-C7-C8	-155.09(11)
C5-C4-C7-C8	27.78(17)
C3-C4-C7-C9	134.02(12)
C5-C4-C7-C9	-43.11(16)
C4-C7-C8-C9	-108.26(12)
C7-C8-C9-C10	-106.79(12)
C4-C7-C9-C10	-133.66(11)
C8-C7-C9-C10	113.82(11)
C4-C7-C9-C8	112.52(12)
C8-C9-C10-C18	1.65(17)
C7-C9-C10-C18	-69.53(14)
C8-C9-C10-C20	140.37(11)
C7-C9-C10-C20	69.18(13)
C8-C9-C10-C11	-71.65(15)
C7-C9-C10-C11	-142.84(10)
C9-C10-C11-C12	3.17(15)
C18-C10-C11-C12	-112.04(12)
C20-C10-C11-C12	151.82(10)
C9-C10-C11-C18	115.21(11)
C20-C10-C11-C18	-96.15(10)
C18-C11-C12-C17	5.56(17)
C10-C11-C12-C17	77.05(14)
C18-C11-C12-C13	-176.12(10)
C10-C11-C12-C13	-104.64(13)

C17-C12-C13-C14	-0.52(19)
C11-C12-C13-C14	-178.93(12)
C12-C13-C14-C15	0.1(2)
C13-C14-C15-C16	0.2(2)
C14-C15-C16-C17	-0.1(2)
C13-C12-C17-C16	0.61(18)
C11-C12-C17-C16	178.91(12)
C15-C16-C17-C12	-0.3(2)
C9-C10-C18-C19	140.19(11)
C20-C10-C18-C19	-1.63(13)
C11-C10-C18-C19	-110.05(11)
C9-C10-C18-C11	-109.76(12)
C20-C10-C18-C11	108.41(10)
C12-C11-C18-C10	109.58(11)
C12-C11-C18-C19	-153.23(10)
C10-C11-C18-C19	97.19(10)
C10-C18-C19-N1	19.95(12)
C11-C18-C19-N1	-45.85(12)
C9-C10-C20-N1	-163.25(9)
C18-C10-C20-N1	-17.43(12)
C11-C10-C20-N1	46.21(12)
C27-C21-C22-C23	-1.05(19)
S1-C21-C22-C23	-179.09(10)
C21-C22-C23-C24	1.5(2)
C22-C23-C24-C26	-0.8(2)
C22-C23-C24-C25	179.87(13)
C23-C24-C26-C27	-0.4(2)
C25-C24-C26-C27	178.97(13)
C24-C26-C27-C21	0.79(19)
C22-C21-C27-C26	-0.08(19)
S1-C21-C27-C26	177.94(10)
C10-C20-N1-C19	31.48(12)
C10-C20-N1-S1	172.08(8)
C18-C19-N1-C20	-32.36(12)
C18-C19-N1-S1	-173.37(8)
C20-N1-S1-O2	47.58(11)
C19-N1-S1-O2	-175.25(9)
C20-N1-S1-O1	177.06(9)

C19-N1-S1-O1	-45.77(11)
C20-N1-S1-C21	-67.77(10)
C19-N1-S1-C21	69.39(10)
C22-C21-S1-O2	-19.07(12)
C27-C21-S1-O2	162.88(10)
C22-C21-S1-O1	-150.44(10)
C27-C21-S1-O1	31.52(12)
C22-C21-S1-N1	95.77(11)
C27-C21-S1-N1	-82.28(11)

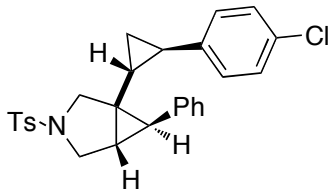
(1*R*,5*S*,6*R*)-1-((1*R*,2*R*)-2-(4-Methoxyphenyl)cyclopropyl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane (13b)



Catalyst: **A** or **D**. White solid. Major diastereoisomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.6 Hz, 3H), 7.36 (d, J = 8.6 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 7.19-7.13 (m, 3H), 7.10 (d, J = 8.0 Hz, 3H), 3.74 (s, 3H), 3.68 (d, J = 9.6 Hz , 2H), 3.23 (dd, J = 9.5, 4.2 Hz, 1H), 3.17 (d, J = 9.5 Hz, 1H), 2.46 (s, 3H), 2.17 (d, J = 4.2 Hz, 1H), 1.72 (t, J = 4.1 Hz, 1H), 1.45-1.40 (m, 1H), 0.94-0.83 (m, 2H), 0.56-0.45 (m, 1H); Minor diastereoisomer: δ 7.60 (d, J = 8.1 Hz, 2H), 7.36 (d, J = 14.1 Hz, 2H), 7.29 (d, J = 7.3 Hz, 2H), 6.99 (d, J = 7.7 Hz, 2H), 6.59-6.56 (m, 3H), 6.32 (d, J = 8.6 Hz, 2H), 3.77 (s, 3H), 3.43 (dd, J = 12.1, 9.2 Hz, 2H), 3.18 (dd, J = 9.2, 4.1 Hz, 1H), 3.12 (d, J = 9.2 Hz, 1H), 2.50 (s, 3H), 2.23 (d, J = 4.4 Hz, 1H), 1.91-1.84 (m, 1H), 1.45-1.40 (m, 1H), 0.94-0.83 (m, 2H), 0.56-0.45 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 143.8, 137.2, 134.2, 133.9, 129.9, 129.1, 128.3, 127.7, 127.1, 126.3, 113.8, 55.5, 54.6, 50.8, 36.1, 30.6, 25.3, 21.8, 21.5, 20.6, 15.5; HRMS-ES calcd for $C_{28}H_{29}NO_3NaS$ $[M+Na]^+$: 482.1766. Found: 482.1765.

Elemental analysis (%) calcd $C_{28}H_{29}NO_3S \cdot 1/2H_2O$: C, 71.77; H, 6.45; N, 2.99; O, 11.95; S, 6.84. Found: C, 71.75; H, 6.55; N, 2.88.

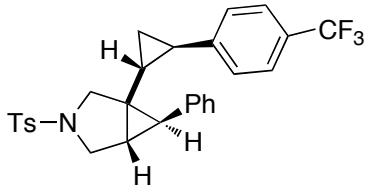
(1*R*,5*S*,6*R*)-1-((1*R*,2*R*)-2-(4-Chlorophenyl)cyclopropyl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane (13c)



Catalyst: **A** or **D**. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.24-7.15 (m, 3H), 7.09 (t, *J* = 7.6 Hz, 4H), 6.64 (d, *J* = 8.4 Hz, 2H), 3.68 (dd, *J* = 9.3, 4.8 Hz, 2H), 3.24 (dd, *J* = 9.4, 3.9 Hz, 1H), 3.13 (d, *J* = 9.4 Hz, 1H), 2.46 (s, 3H), 2.17 (d, *J* = 4.2 Hz, 1H), 1.75 (t, *J* = 4.0 Hz, 1H), 1.43 (q, *J* = 7.3 Hz, 1H), 1.00-0.77 (m, 1H), 0.58 (dt, *J* = 12.9, 6.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 143.8, 140.8, 137.0, 133.9, 131.4, 129.9, 128.4, 127.7, 127.2, 126.4, 54.3, 50.7, 35.8, 30.6, 25.4, 21.8, 21.5, 15.9; HRMS-ES calcd for $C_{27}H_{26}NO_2NaS^{35}Cl$ $[M+Na]^+$: 486.1270. Found: 486.1252.

Elemental analysis (%) calcd $C_{27}H_{26}NO_2S^{35}Cl \cdot 1/2H_2O$: C, 68.56; H, 5.75; Cl, 7.49; N, 2.96; O, 8.46; S, 6.78. Found: C, 68.79; H, 5.52; N, 2.86.

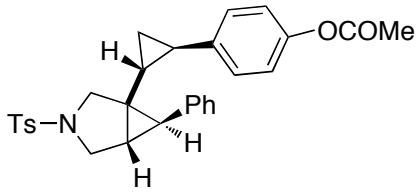
(1*R*,5*S*,6*R*)-6-Phenyl-3-tosyl-1-((1*R*,2*R*)-2-(4-(trifluoromethyl)phenyl)cyclopropyl)-3-azabicyclo[3.1.0]hexane (13d)



Catalyst: **A** or **D**. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.78 (d, *J* = 8.2 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 4H), 7.29-7.18 (m, 3H), 7.13 (d, *J* = 6.9 Hz, 2H), 6.85 (d, *J* = 8.1 Hz, 2H), 3.74 (dd, *J* = 9.4, 2.4 Hz, 2H), 3.31 (dd, *J* = 9.4, 3.9 Hz, 1H), 3.18 (d, *J* = 9.4 Hz, 1H), 2.52 (s, 3H), 2.25 (d, *J* = 4.2 Hz, 1H), 1.83 (t, *J* = 4.0 Hz, 1H), 1.59-1.51 (m, 1H), 1.07 (dd, *J* = 13.2, 6.3 Hz, 1H), 0.78-0.69 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 146.6, 143.9, 137.0, 133.9, 129.9, 129.0, 128.5, 127.8, 126.5, 125.8, 125.9, 125.3, 54.3, 50.7, 35.8, 30.6, 25.4, 22.3, 21.8,16.4; HRMS-ES calcd for $C_{28}H_{26}NO_2NaSF_3$ $[M+Na]^+$: 520.1534. Found: 520.1514.

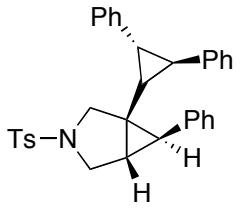
Elemental analysis (%) calcd $C_{28}H_{26}NO_2SF_3 \cdot 1/2H_2O$: C, 66.39; H, 5.37; F, 11.25; N, 2.76; O, 7.90; S, 6.33; found: C, 66.17; H, 5.39; N, 2.71.

4-((1*R*)-2-((1*R*,5*S*,6*R*)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexan-1-yl)cyclopropyl)phenyl acetate (13e)



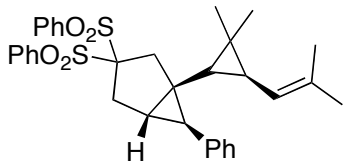
Catalyst: **A** or **D**. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.5 Hz, 2H), 7.36 (d, J = 8.8 Hz, 2H), 7.27-7.06 (m, 5H), 6.86 (d, J = 8.8 Hz, 2H), 6.74 (d, J = 8.8 Hz, 2H), 3.69 (dd, J = 9.8, 6.8 Hz, 2H), 3.23 (dd, J = 9.2, 4.4 Hz, 1H), 3.13 (d, J = 9.2 Hz, 1H), 2.46 (s, 3H), 2.26 (s, 3H), 2.19 (d, J = 4.8 Hz, 1H), 1.74 (t, J = 4.4 Hz, 1H), 1.50-1.42 (m, 1H), 0.99-0.90 (m, 1H), 0.65-0.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 148.7, 143.8, 139.8, 137.0, 133.8, 129.9, 129.0, 128.3, 127.7, 126.9, 126.4, 121.4, 54.5, 50.7, 35.9, 30.6, 25.2, 21.8, 21.3, 15.9; HRMS-ES calcd for $C_{29}H_{29}NO_4NaS$ $[M+Na]^+$: 510.1715. Found: 510.1714.

(1*R*,5*S*,6*R*)-1-((2*R*,3*R*)-2,3-Diphenylcyclopropyl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane (13g)



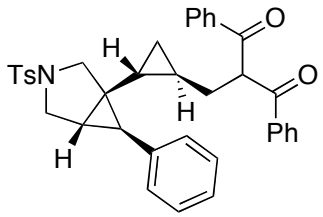
Catalyst: **A**. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 8.2 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 7.26 (dd, J = 8.0, 6.6 Hz, 3H), 7.20 (t, J = 7.3 Hz, 2H), 7.16-7.08 (m, 4H), 6.98-6.89 (m, 6H), 3.46 (dd, J = 14.2, 9.5 Hz, 2H), 2.95 (d, J = 9.7 Hz, 1H), 2.88 (dd, J = 9.2, 3.8 Hz, 1H), 2.50 (s, 3H), 2.26 (s, 1H), 2.24 (d, J = 1.7 Hz, 1H), 1.92 (d, J = 4.6 Hz, 1H), 1.38 (t, J = 4.1 Hz, 1H), 0.91-0.82 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 141.6, 138.1, 137.1, 133.9, 130.1, 128.7, 128.2, 127.9, 126.9, 126.6, 126.2, 54.7, 50.9, 33.7, 32.1, 31.1, 28.1, 27.7; HRMS-ESI calcd for $C_{33}H_{31}NO_2NaS$ $[M+Na]^+$: 528.1973. Found: 528.1978.

(1*S*,5*S*,6*R*)-1-((1*S*,3*S*)-2,2-Dimethyl-3-(2-methylprop-1-enyl)cyclopropyl)-6-phenyl-3,3-bis(phenylsulfonyl)bicyclo[3.1.0]hexane (13j)



Catalyst: **A**. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.03 (m, 4H), 7.76-7.51 (m, 6H), 7.25-7.18 (m, 2H), 7.17-7.11 (m, 1H), 7.02-6.96 (m, 2H), 4.72 (d, J = 8.2 Hz, 1H), 3.11 (dd, J = 16.2, 6.4 Hz, 1H), 3.02 (d, J = 16.2 Hz, 1H), 2.94 (d, J = 16.2 Hz, 1H), 2.74 (d, J = 16.2 Hz, 1H), 2.23 (d, J = 4.4 Hz, 1H), 1.79-1.69 (m, 1H), 1.74 (s, 3H), 1.72 (s, 3H), 1.20 (dd, J = 8.2, 5.7 Hz, 1H), 0.68 (s, 3H), 0.43 (d, J = 5.6 Hz, 1H), 0.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.8 (C_q), 137.5, (C_q), 136.4 (C_q), 134.8 (CH), 134.6 (CH), 133.1 (C_q), 131.8 (CH), 131.5 (CH), 129.0 (CH), 128.9 (CH), 128.2 (CH), 128.0 (CH), 125.9 (CH), 124.8 (CH), 97.9 (C_q), 42.3 (CH_2), 39.3 (C_q), 38.5 (CH), 37.4 (CH_2), 36.0 (CH), 34.5 (CH), 30.0 (CH), 25.9 (CH_3), 23.3 (C_q), 23.0 (CH_3), 21.7 (CH_3), 18.7 (CH_3); HRMS-ESI calcd for $C_{33}H_{36}O_4NaS_2$ $[M+Na]^+$: 583.1953. Found: 583.1957.

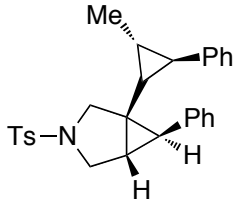
1,3-Diphenyl-2-(((1*S*,2*R*)-2-((1*R*,5*S*,6*R*)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexan-1-yl)cyclopropyl)methyl)propane-1,3-dione (13k)



Catalyst: **A**. White foam solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.86 (m, 2H), 7.82-7.77 (m, 2H), 7.61-7.55 (m, 4H), 7.48-7.41 (m, 4H), 7.28-7.20 (m, 4H), 7.18-7.13 (m, 1H), 7.10-7.06 (m, 2H), 5.03 (t, J = 6.6 Hz, 1H), 3.60 (d, J = 9.4 Hz, 1H), 3.51 (d, J = 9.4 Hz, 1H), 3.06 (dd, J = 9.2, 3.9 Hz, 1H), 2.85 (d, J = 9.4 Hz, 1H), 2.43 (s, 3H), 2.16 (d, J = 4.1 Hz, 1H), 1.89-1.82 (m, 1H), 1.76-1.69 (m, 1H), 1.64 (t, J = 3.9 Hz, 1H), 0.61-0.49 (m, 2H), 0.18-0.14 (dt, J = 8.4, 5.2 Hz, 1H), 0.08-0.03 (dt, J = 8.8, 5.3 Hz, 1H). Significant signals for the minor diastereoisomer: δ 4.81 (t, J = 6.6 Hz, 1H), 3.24 (dd, J = 9.4, 3.7 Hz, 1H), 2.95 (d, J = 9.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.8 (C_q), 143.7 (C_q), 137.3 (C_q), 136.2 (CH), 135.9 (C_q), 133.8 (CH), 133.7 (C_q), 129.9 (CH), 129.1 (CH), 129.0 (CH), 128.7 (CH), 128.3 (CH), 127.6 (CH), 126.3 (CH), 57.3 (CH), 53.5 (CH_2), 50.5 (CH_2), 35.3 (C_q), 34.0 (CH_2), 30.3 (CH), 25.4 (CH), 21.7 (CH_3),

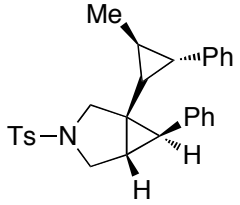
17.2 (CH), 16.5 (CH), 12.6 (CH_2); HRMS-ESI calcd for $C_{37}H_{35}NO_4NaS$ $[M+Na]^+$ 612.2185. Found: 612.2178.

(1*R,5*S**,*6*R*)-1-((2*R**,3*R**)-2-Methyl-3-phenylcyclopropyl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane (13l$_1$)**



Catalyst: **A**. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.31-7.20 (m, 3H), 7.08-7.02 (m, 3H), 6.96 (d, J = 8.4 Hz, 2H), 6.78 (dd, J = 7.6, 0.8 Hz, 2H), 3.39 (dd, J = 9.2, 6.0 Hz, 2H), 2.85 (d, J = 10.0 Hz, 1H), 2.73 (dd, J = 9.2, 3.6 Hz, 1H), 2.51 (s, 3H), 1.87 (d, J = 4.4 Hz, 1H), 1.64 (dd, J = 8.8, 5.6 Hz, 1H), 1.18 (t, J = 4.0 Hz, 1H), 1.14-1.10 (m, J = 5.6 Hz, 1H), 1.01 (d, J = 5.6 Hz, 3H), 0.66-0.63 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 129.6, 128.1, 128.1, 127.9, 127.9, 127.6, 126.0, 125.8, 125.4, 54.4, 50.7, 31.8, 30.7, 28.0, 26.0, 21.6, 19.0, 17.5; HRMS-ESI calcd. for $C_{28}H_{30}NO_2S$ $[M+H]^+$: 444.1997. Found: 444.2016.

(1*R*,5*S*,6*R*)-1-((1*R*,2*S*,3*S*)-2-methyl-3-phenylcyclopropyl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane (13l$_3$)



Catalyst: **B**. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, J = 8.4 Hz, 2H), 7.33-7.25 (m, 5H or 6H), 7.21-7.16 (m, 4H or 3H), 6.87 (d, J = 4.4 Hz, 3H), 3.46 (dd, J = 8.4, 6.0 Hz, 2H), 2.57 (d, J = 8.8 Hz, 1H), 2.50 (s, 3H), 2.30 (dd, J = 8.4, 3.6 Hz, 1H), 2.17 (d, J = 2.4 Hz, 1H), 1.68-1.62 (m, 2H), 0.88-0.85 (m, 1H), 0.66-0.62 (m, 1H), 0.39 (d, J = 6.0 Hz, 3H).

Table 13. Crystal data and structure refinement for **13l$_3$**.

Identification code	**$13l_3$**	
Empirical formula	C28 H29 N O2 S	
Formula weight	443.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.9620(7) Å	α= 90.00 °
	b = 10.4716(7) Å	β = 100.903(3) °
	c = 12.3795(10) Å	γ = 90.00 °
Volume	1140.80(15) $Å^3$	
Z	2	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.168 mm^{-1}	
F(000)	472	
Crystal size	0.50 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.68 to 36.43 °	
Index ranges	-12 <=h<=14 ,-17 <=k<=7 ,-20 <=l<=19	
Reflections collected	6325	
Independent reflections	5682 [R(int) = 0.0306]	
Completeness to theta = 36.43 °	0.879 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9834 and 0.9208	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6325 / 1 / 291	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0432 , wR2 = 0.1153	
R indices (all data)	R1 = 0.0493 , wR2 = 0.1227	
Absolute Structure Flack parameter	x =0.04(5)	
Largest diff. peak and hole	0.733 and -0.401 $e.Å^{-3}$	

Table 14. Bond lengths [Å] and angles [°] for **$13l_3$**.

Bond lengths----	
C1-C2	1.505(2)
C2-C3	1.398(2)
C2-C7	1.405(2)

C3-C4	1.387(3)
C4-C5	1.394(2)
C5-C6	1.398(2)
C5-S1	1.7599(15)
C6-C7	1.386(3)
C8-N1	1.4738(19)
C8-C9	1.524(2)
C9-C19	1.496(2)
C9-C10	1.513(2)
C9-C12	1.533(2)
C10-C12	1.510(2)
C10-C11	1.517(2)
C11-N1	1.4757(19)
C12-C13	1.490(2)
C13-C18	1.394(2)
C13-C14	1.398(2)
C14-C15	1.397(3)
C15-C16	1.396(3)
C16-C17	1.377(3)
C17-C18	1.397(2)
C19-C20	1.5027(19)
C19-C21	1.535(2)
C20-C22	1.507(2)
C20-C21	1.518(2)
C21-C23	1.482(3)
C23-C28	1.400(3)
C23-C24	1.405(2)
C24-C25	1.394(3)
C25-C26	1.402(3)
C26-C27	1.378(4)
C27-C28	1.398(3)
N1-S1	1.6222(12)
O1-S1	1.4368(12)
O2-S1	1.4381(12)

Angles----------

C3-C2-C7	118.18(15)
C3-C2-C1	121.32(17)

C7-C2-C1	120.49(16)
C4-C3-C2	121.54(15)
C3-C4-C5	118.98(15)
C4-C5-C6	120.98(14)
C4-C5-S1	119.63(13)
C6-C5-S1	119.39(13)
C7-C6-C5	119.01(15)
C6-C7-C2	121.31(15)
N1-C8-C9	102.42(12)
C19-C9-C10	126.35(12)
C19-C9-C8	118.89(13)
C10-C9-C8	106.97(12)
C19-C9-C12	118.73(13)
C10-C9-C12	59.45(10)
C8-C9-C12	112.57(12)
C12-C10-C9	60.94(10)
C12-C10-C11	115.42(12)
C9-C10-C11	107.76(12)
N1-C11-C10	101.61(12)
C13-C12-C10	123.46(12)
C13-C12-C9	120.89(11)
C10-C12-C9	59.61(10)
C18-C13-C14	118.13(15)
C18-C13-C12	123.91(15)
C14-C13-C12	117.95(13)
C15-C14-C13	120.92(15)
C16-C15-C14	119.91(18)
C17-C16-C15	119.64(17)
C16-C17-C18	120.37(15)
C13-C18-C17	121.03(16)
C9-C19-C20	123.92(13)
C9-C19-C21	124.13(14)
C20-C19-C21	59.96(10)
C19-C20-C22	120.05(14)
C19-C20-C21	61.08(10)
C22-C20-C21	120.17(14)
C23-C21-C20	123.71(14)
C23-C21-C19	124.69(13)

C20-C21-C19	58.97(10)
C28-C23-C24	118.04(18)
C28-C23-C21	118.36(16)
C24-C23-C21	123.60(16)
C25-C24-C23	121.04(19)
C24-C25-C26	119.9(2)
C27-C26-C25	119.5(2)
C26-C27-C28	120.7(2)
C27-C28-C23	120.7(2)
C8-N1-C11	110.38(11)
C8-N1-S1	120.10(10)
C11-N1-S1	119.73(10)
O1-S1-O2	119.96(7)
O1-S1-N1	106.22(7)
O2-S1-N1	106.58(7)
O1-S1-C5	108.07(8)
O2-S1-C5	107.94(8)
N1-S1-C5	107.49(7)

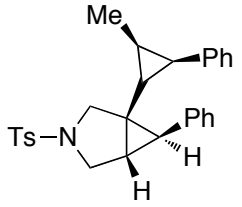
Table 15. Torsion angles [°] for **13l$_3$**.

C7-C2-C3-C4	0.1(2)
C1-C2-C3-C4	-179.22(14)
C2-C3-C4-C5	-0.3(2)
C3-C4-C5-C6	0.2(2)
C3-C4-C5-S1	179.65(11)
C4-C5-C6-C7	-0.1(2)
S1-C5-C6-C7	-179.53(11)
C5-C6-C7-C2	0.0(2)
C3-C2-C7-C6	0.0(2)
C1-C2-C7-C6	179.34(14)
N1-C8-C9-C19	167.60(14)
N1-C8-C9-C10	16.42(16)
N1-C8-C9-C12	-46.93(16)
C19-C9-C10-C12	104.99(18)
C8-C9-C10-C12	-106.61(13)
C19-C9-C10-C11	-145.27(16)
C8-C9-C10-C11	3.13(18)

C12-C9-C10-C11	109.74(13)
C12-C10-C11-N1	44.38(17)
C9-C10-C11-N1	-21.26(17)
C9-C10-C12-C13	-109.01(15)
C11-C10-C12-C13	153.97(13)
C11-C10-C12-C9	-97.02(14)
C19-C9-C12-C13	-4.3(2)
C10-C9-C12-C13	113.20(15)
C8-C9-C12-C13	-149.81(13)
C19-C9-C12-C10	-117.48(14)
C8-C9-C12-C10	96.99(14)
C10-C12-C13-C18	-3.0(2)
C9-C12-C13-C18	-74.87(19)
C10-C12-C13-C14	178.16(13)
C9-C12-C13-C14	106.30(17)
C18-C13-C14-C15	0.2(2)
C12-C13-C14-C15	179.09(14)
C13-C14-C15-C16	0.0(3)
C14-C15-C16-C17	0.0(3)
C15-C16-C17-C18	-0.3(3)
C14-C13-C18-C17	-0.4(2)
C12-C13-C18-C17	-179.27(15)
C16-C17-C18-C13	0.5(3)
C10-C9-C19-C20	10.9(3)
C8-C9-C19-C20	-134.16(17)
C12-C9-C19-C20	82.5(2)
C10-C9-C19-C21	85.1(2)
C8-C9-C19-C21	-60.0(2)
C12-C9-C19-C21	156.64(13)
C9-C19-C20-C22	-136.81(17)
C21-C19-C20-C22	110.10(17)
C9-C19-C20-C21	113.09(18)
C19-C20-C21-C23	-113.39(16)
C22-C20-C21-C23	136.69(16)
C22-C20-C21-C19	-109.92(17)
C9-C19-C21-C23	-1.0(2)
C20-C19-C21-C23	111.79(17)
C9-C19-C21-C20	-112.75(16)

C20-C21-C23-C28	-152.12(14)
C19-C21-C23-C28	134.85(16)
C20-C21-C23-C24	27.8(2)
C19-C21-C23-C24	-45.2(2)
C28-C23-C24-C25	-1.7(2)
C21-C23-C24-C25	178.35(14)
C23-C24-C25-C26	2.2(2)
C24-C25-C26-C27	-0.6(3)
C25-C26-C27-C28	-1.4(3)
C26-C27-C28-C23	1.9(3)
C24-C23-C28-C27	-0.3(2)
C21-C23-C28-C27	179.65(15)
C9-C8-N1-C11	-31.78(17)
C9-C8-N1-S1	-177.58(11)
C10-C11-N1-C8	33.52(17)
C10-C11-N1-S1	179.46(11)
C8-N1-S1-O1	-39.72(14)
C11-N1-S1-O1	177.64(12)
C8-N1-S1-O2	-168.72(12)
C11-N1-S1-O2	48.65(14)
C8-N1-S1-C5	75.76(13)
C11-N1-S1-C5	-66.87(14)
C4-C5-S1-O1	-155.75(11)
C6-C5-S1-O1	23.66(12)
C4-C5-S1-O2	-24.62(13)
C6-C5-S1-O2	154.79(11)
C4-C5-S1-N1	89.99(12)
C6-C5-S1-N1	-90.59(12)

(1*R,5*S**,6*R**)-1-((1*R**,2*S**,3*R**)-2-Methyl-3-phenylcyclopropyl)-6-phenyl-3-tosyl-3-azabicyclo[3.1.0]hexane ($13m_1$)**



Catalyst: **A**. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 7.6 Hz, 2H), 7.20-7.13 (m, 6H), 6.93 (d, J =

7.2 Hz, 2H), 3.77 (d, *J* = 9.2 Hz, 1H), 3.69 (d, *J* = 10.4 Hz, 1H), 3.20-3.14 (m, 2H), 2.42 (s, 3H), 2.25 (d, *J* = 4.0 Hz, 1H), 1.75-1.68 (m, 2H), 0.84 (t, *J* = 5.4 Hz, 1H), 0.60-0.54 (m, 1H), 0.17 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 138.3, 137.1, 134.0, 129.7, 129.0, 129.0, 128.2, 127.9, 127.4, 126.1, 125.8, 54.1, 50.4, 35.9, 30.1, 27.4, 24.4, 22.8, 21.5, 21.2, 12.3; HRMS-ESI calcd for $C_{28}H_{29}NO_2NaS$ $[M+Na]^+$: 466.1817. Found: 466.1833.

Table 16. Crystal data and structure refinement for **13m$_1$**.

Identification code	**13m$_1$**	
Empirical formula	C28 H29 N O2 S	
Formula weight	443.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pccn	
Unit cell dimensions	a = 34.3459(17) Å	a= 90.00 °
	b = 11.0908(6) Å	b = 90.00 °
	c = 12.4392(5) Å	g = 90.00 °
Volume	4738.4(4) Å^3	
Z	8	
Density (calculated)	1.244 Mg/m^3	
Absorption coefficient	0.162 mm^{-1}	
F(000)	1888	
Crystal size	0.40 x 0.40 x 0.35 mm^3	
Theta range for data collection	1.19 to 36.38 °	
Index ranges	-56 <=h<=50 ,-14 <=k<=17 ,-20 <=l<=8	
Reflections collected	10549	
Independent reflections	8021 [R(int) = 0.0434]	
Completeness to theta = 36.38 °	0.913 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9456 and 0.9382	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10549 / 0 / 291	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0480 , wR2 = 0.1260	

R indices (all data)	R1 = 0.0676 , wR2 = 0.1386
Largest diff. peak and hole	0.695 and -0.344 e.Å^{-3}

Table 17. Bond lengths [Å] and angles [°] for **13m$_1$**.

Bond lengths----	
C1-C2	1.5035(17)
C2-C7	1.3920(16)
C2-C3	1.4002(17)
C3-C4	1.3869(15)
C4-C5	1.3965(13)
C5-C6	1.3911(14)
C5-S1	1.7608(10)
C6-C7	1.3909(15)
C8-N1	1.4790(14)
C8-C9	1.5141(14)
C9-C12	1.5061(15)
C9-C10	1.5096(13)
C10-C19	1.4926(14)
C10-C11	1.5174(14)
C10-C12	1.5231(13)
C11-N1	1.4740(12)
C12-C13	1.4961(14)
C13-C14	1.3943(17)
C13-C18	1.3958(17)
C14-C15	1.3981(16)
C15-C16	1.381(2)
C16-C17	1.384(2)
C17-C18	1.3949(17)
C19-C20	1.4986(18)
C19-C21	1.5076(16)
C20-C22	1.5041(17)
C20-C21	1.5236(16)
C21-C23	1.4951(14)
C23-C24	1.3916(17)
C23-C28	1.4005(17)
C24-C25	1.3908(15)
C25-C26	1.383(2)

C26-C27	1.382(2)
C27-C28	1.3963(18)
N1-S1	1.6140(9)
O1-S1	1.4374(8)
O2-S1	1.4363(8)

Angles----------

C7-C2-C3	118.61(10)
C7-C2-C1	121.35(11)
C3-C2-C1	120.04(11)
C4-C3-C2	120.96(10)
C3-C4-C5	119.33(10)
C6-C5-C4	120.68(9)
C6-C5-S1	119.61(7)
C4-C5-S1	119.71(8)
C7-C6-C5	119.11(9)
C6-C7-C2	121.31(10)
N1-C8-C9	102.11(7)
C12-C9-C10	60.67(6)
C12-C9-C8	115.57(10)
C10-C9-C8	107.61(8)
C19-C10-C9	124.98(10)
C19-C10-C11	117.69(8)
C9-C10-C11	107.02(7)
C19-C10-C12	119.02(8)
C9-C10-C12	59.55(6)
C11-C10-C12	115.64(9)
N1-C11-C10	102.39(7)
C13-C12-C9	121.00(10)
C13-C12-C10	118.42(9)
C9-C12-C10	59.78(6)
C14-C13-C18	118.50(10)
C14-C13-C12	122.46(10)
C18-C13-C12	119.03(10)
C13-C14-C15	120.59(12)
C16-C15-C14	120.36(13)
C15-C16-C17	119.55(11)
C16-C17-C18	120.45(14)

C17-C18-C13	120.54(13)
C10-C19-C20	122.79(9)
C10-C19-C21	121.11(9)
C20-C19-C21	60.90(8)
C19-C20-C22	120.55(12)
C19-C20-C21	59.84(7)
C22-C20-C21	122.25(9)
C23-C21-C19	122.28(10)
C23-C21-C20	123.16(9)
C19-C21-C20	59.25(8)
C24-C23-C28	117.88(10)
C24-C23-C21	123.25(10)
C28-C23-C21	118.75(11)
C25-C24-C23	121.18(12)
C26-C25-C24	120.25(13)
C27-C26-C25	119.72(11)
C26-C27-C28	120.06(13)
C27-C28-C23	120.90(13)
C11-N1-C8	109.50(8)
C11-N1-S1	122.47(7)
C8-N1-S1	120.67(6)
O2-S1-O1	119.76(5)
O2-S1-N1	107.08(5)
O1-S1-N1	106.54(4)
O2-S1-C5	106.93(4)
O1-S1-C5	108.13(5)
N1-S1-C5	107.92(5)

Table 18. Torsion angles [°] for **13m$_1$**.

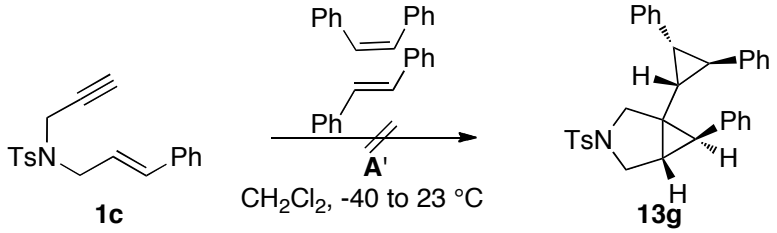
C7-C2-C3-C4	0.3(2)
C1-C2-C3-C4	179.81(13)
C2-C3-C4-C5	-0.13(18)
C3-C4-C5-C6	-0.32(17)
C3-C4-C5-S1	179.65(9)
C4-C5-C6-C7	0.58(18)
S1-C5-C6-C7	-179.39(10)
C5-C6-C7-C2	-0.4(2)

C3-C2-C7-C6	0.0(2)
C1-C2-C7-C6	-179.54(14)
N1-C8-C9-C12	-46.10(11)
N1-C8-C9-C10	19.20(11)
C12-C9-C10-C19	-105.99(10)
C8-C9-C10-C19	144.07(10)
C12-C9-C10-C11	110.18(9)
C8-C9-C10-C11	0.24(12)
C8-C9-C10-C12	-109.94(10)
C19-C10-C11-N1	-166.57(9)
C9-C10-C11-N1	-19.67(11)
C12-C10-C11-N1	44.17(11)
C10-C9-C12-C13	107.01(10)
C8-C9-C12-C13	-156.34(9)
C8-C9-C12-C10	96.65(9)
C19-C10-C12-C13	4.49(15)
C9-C10-C12-C13	-111.26(11)
C11-C10-C12-C13	153.33(9)
C19-C10-C12-C9	115.75(11)
C11-C10-C12-C9	-95.42(9)
C9-C12-C13-C14	31.70(15)
C10-C12-C13-C14	101.67(12)
C9-C12-C13-C18	-148.29(11)
C10-C12-C13-C18	-78.32(15)
C18-C13-C14-C15	-0.38(18)
C12-C13-C14-C15	179.63(11)
C13-C14-C15-C16	-0.2(2)
C14-C15-C16-C17	0.6(2)
C15-C16-C17-C18	-0.4(2)
C16-C17-C18-C13	-0.3(2)
C14-C13-C18-C17	0.6(2)
C12-C13-C18-C17	-179.36(13)
C9-C10-C19-C20	-1.13(15)
C11-C10-C19-C20	139.27(11)
C12-C10-C19-C20	-72.52(14)
C9-C10-C19-C21	-74.46(13)
C11-C10-C19-C21	65.94(13)
C12-C10-C19-C21	-145.85(10)

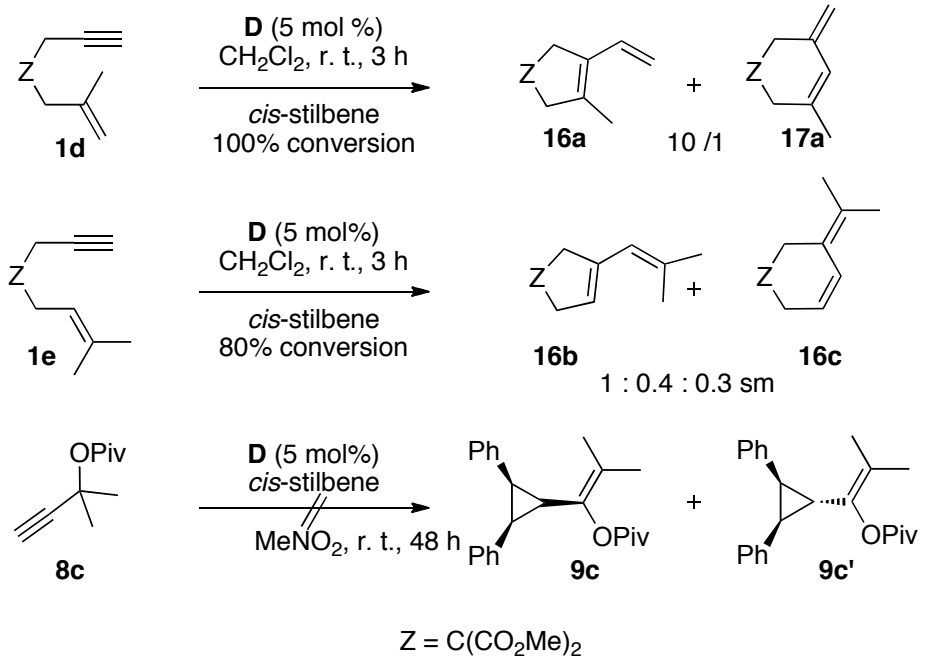
C10-C19-C20-C22	137.88(11)
C21-C19-C20-C22	-111.94(12)
C10-C19-C20-C21	-110.17(11)
C10-C19-C21-C23	-135.02(11)
C20-C19-C21-C23	112.15(12)
C10-C19-C21-C20	112.83(11)
C19-C20-C21-C23	-110.70(12)
C22-C20-C21-C23	-1.5(2)
C22-C20-C21-C19	109.18(15)
C19-C21-C23-C24	8.60(17)
C20-C21-C23-C24	80.57(16)
C19-C21-C23-C28	-175.35(11)
C20-C21-C23-C28	-103.39(14)
C28-C23-C24-C25	0.06(18)
C21-C23-C24-C25	176.14(11)
C23-C24-C25-C26	-0.9(2)
C24-C25-C26-C27	1.0(2)
C25-C26-C27-C28	-0.1(2)
C26-C27-C28-C23	-0.8(2)
C24-C23-C28-C27	0.78(19)
C21-C23-C28-C27	-175.48(12)
C10-C11-N1-C8	33.51(10)
C10-C11-N1-S1	-176.40(7)
C9-C8-N1-C11	-33.28(10)
C9-C8-N1-S1	176.00(7)
C11-N1-S1-O2	158.39(8)
C8-N1-S1-O2	-54.74(9)
C11-N1-S1-O1	29.12(10)
C8-N1-S1-O1	176.00(8)
C11-N1-S1-C5	-86.81(9)
C8-N1-S1-C5	60.06(9)
C6-C5-S1-O2	17.62(11)
C4-C5-S1-O2	-162.35(9)
C6-C5-S1-O1	147.82(9)
C4-C5-S1-O1	-32.14(11)
C6-C5-S1-N1	-97.29(10)
C4-C5-S1-N1	82.74(10)

Inhibition of cyclopropanation in the presence of *cis*-stilbene

Whereas the reaction of **1a** with *trans*-stilbene gave **13g** in nearly quantitative yield after 15 h, when the same reaction was carried out with a 1:1 mixture of *trans*- and *cis*-stilbenes, no reaction was observed after 24 h.



The skeletal rearrangement of **1d** was reported to proceed in 1 min with 100% conversion,[2] whereas in the presence of *cis*-stilbene the reaction required 3 h. Similarly, enyne **1c** was reported to react in 5 min (100% conversion), but in presence of *cis*-stilbene after 3 h, the conversion was 80%.[2]

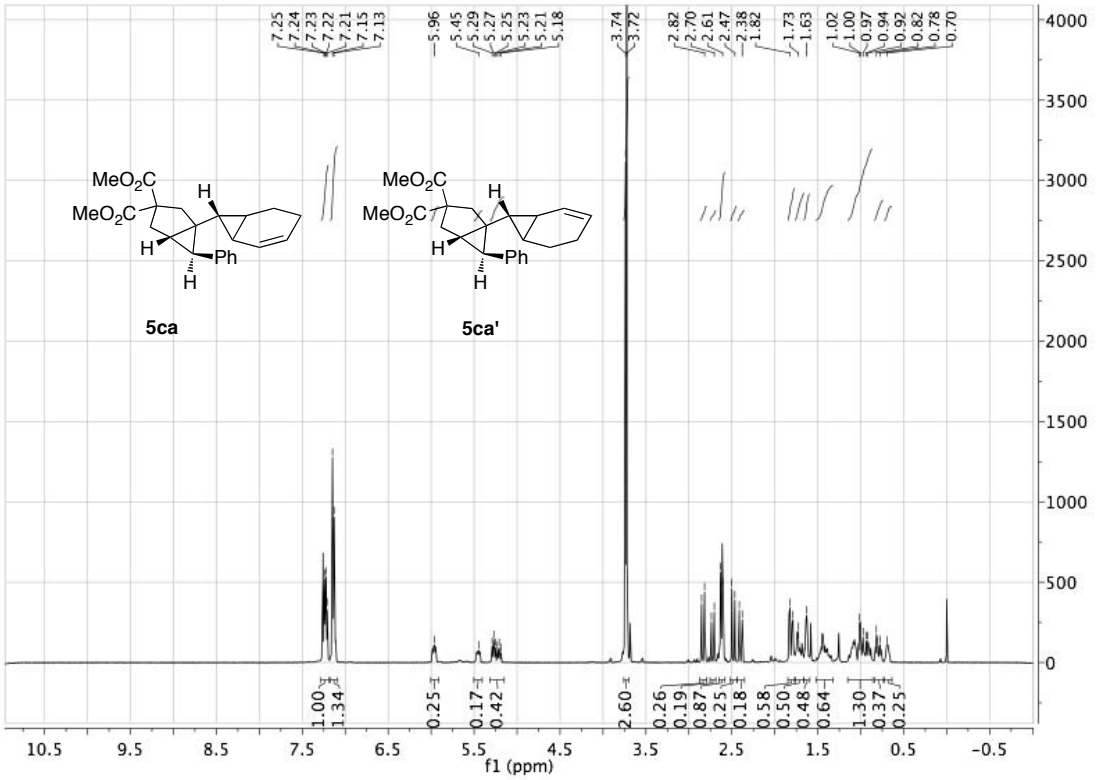


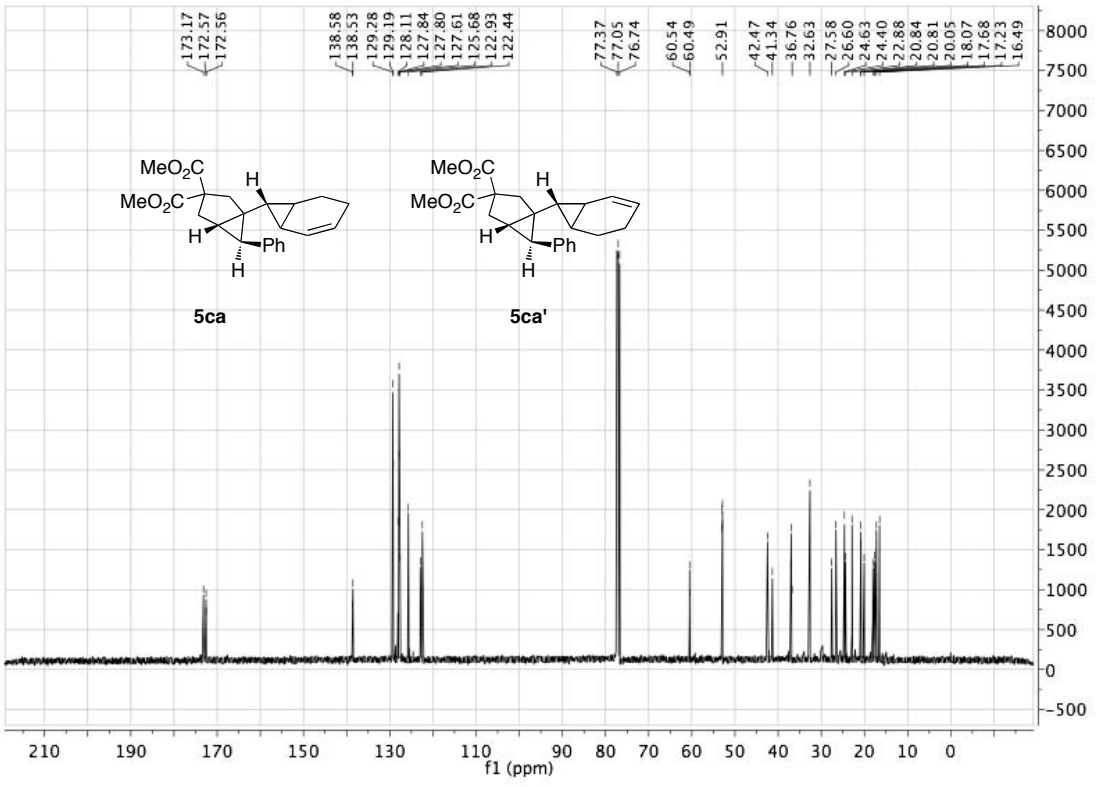
Finally, whereas the cyclopropanation of **8c** with *trans*-stilbene[3] proceed in 81% yield, no reaction was observed after 48 h in the presence of *cis*-stilbene.

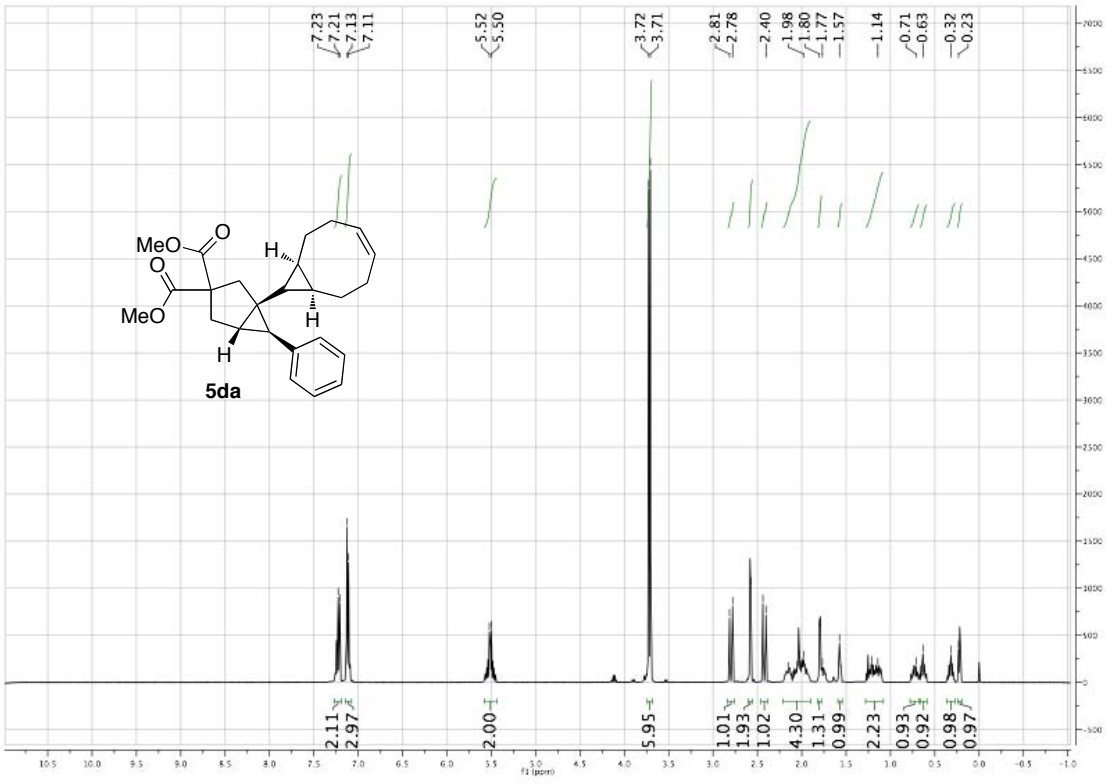
(2) (a) C. Nieto-Oberhuber, M. P. Muñoz, E. Buñuel, C. Nevado, D. J. Cárdenas and A. M. Echavarren, *Angew. Chem. Int. Ed.* **2004**, *43*, 2402-2406. (b) C. Nieto-Oberhuber, M. P. Muñoz, S. López, E. Jiménez-Núñez, C. Nevado, E. Herrero-Gómez, M. Raducan and A. M. Echavarren, *Chem. Eur. J.* **2006**, *12*, 1677-1693.

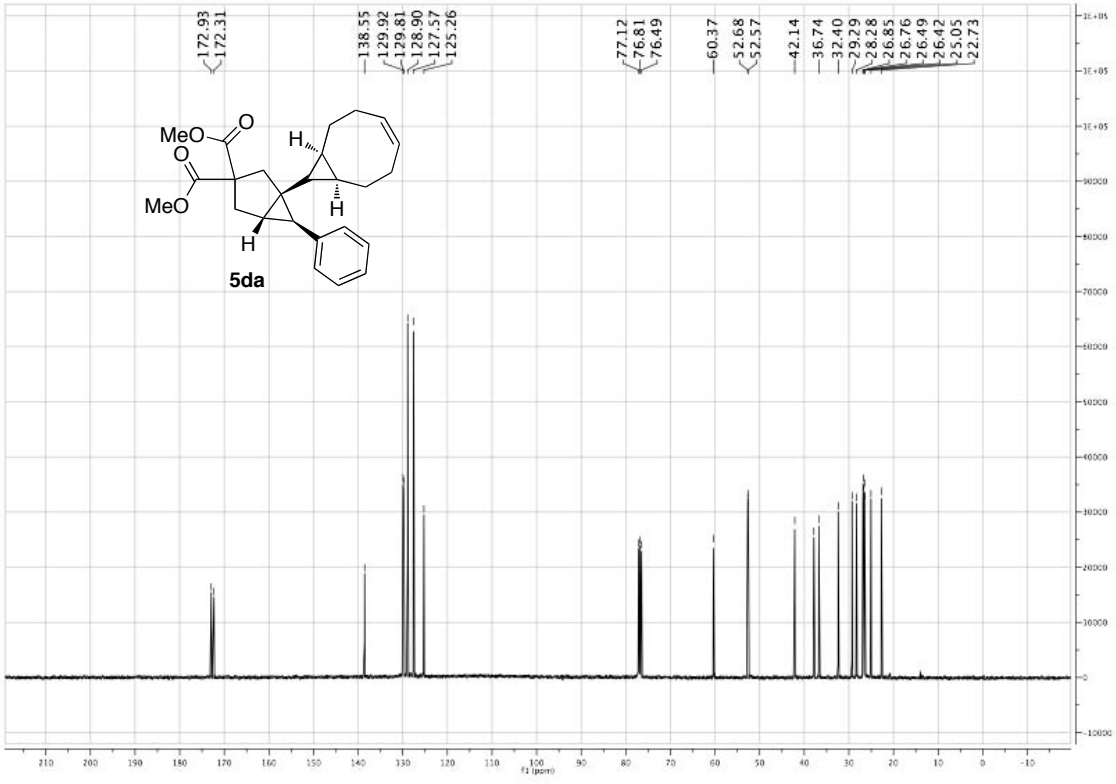
(3) M. J. Johansson, D. J. Gorin, S. T. Staben, E. D. Toste *J. Am. Chem. Soc.* **2005**, *127*, 18002-18003.

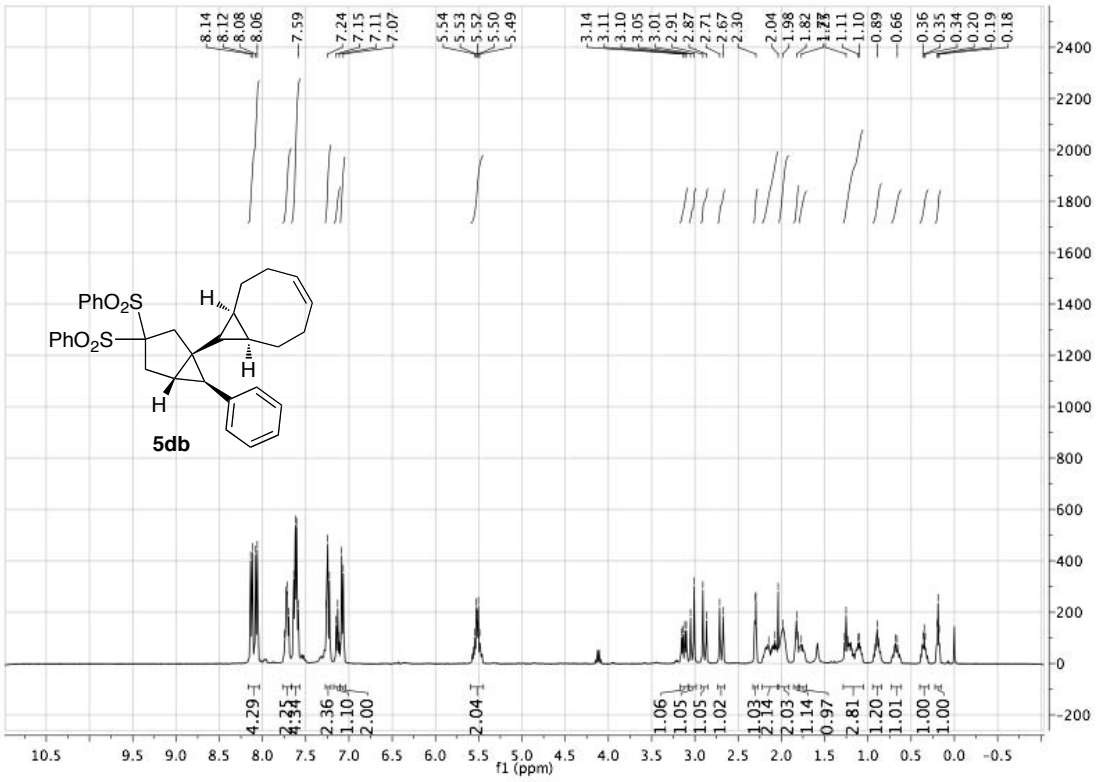
NMR Spectra

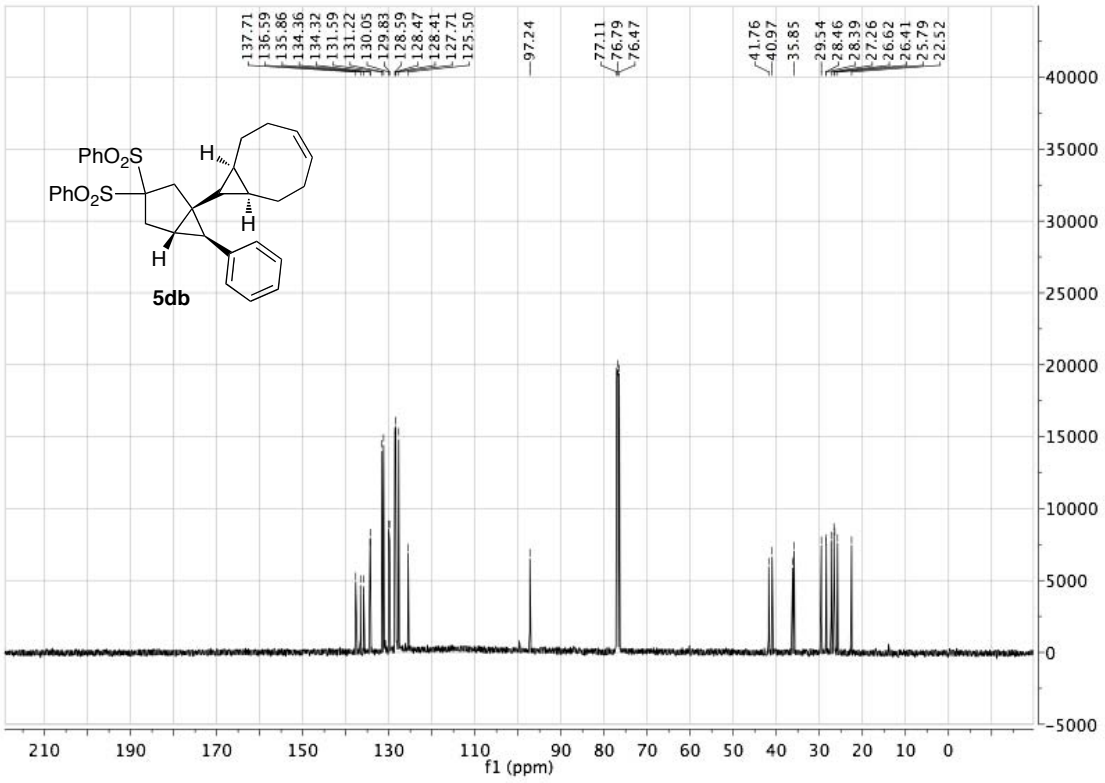

7.25
7.24
7.23
7.22
7.21
7.15
7.13
5.96
5.45
5.29
5.27
5.25
5.23
5.21
5.18
3.74
3.72
2.82
2.70
2.61
2.47
2.38
1.82
1.73
1.63
1.02
1.00
0.97
0.94
0.92
0.82
0.78
0.70
MeO2C
MeO2C
H
H
H
Ph
H
5ca
5ca'
1.00
1.34
0.25
0.17
0.42
2.60
0.26
0.19
0.87
0.25
0.18
0.58
0.50
0.48
0.64
1.30
0.37
0.25
f1 (ppm)

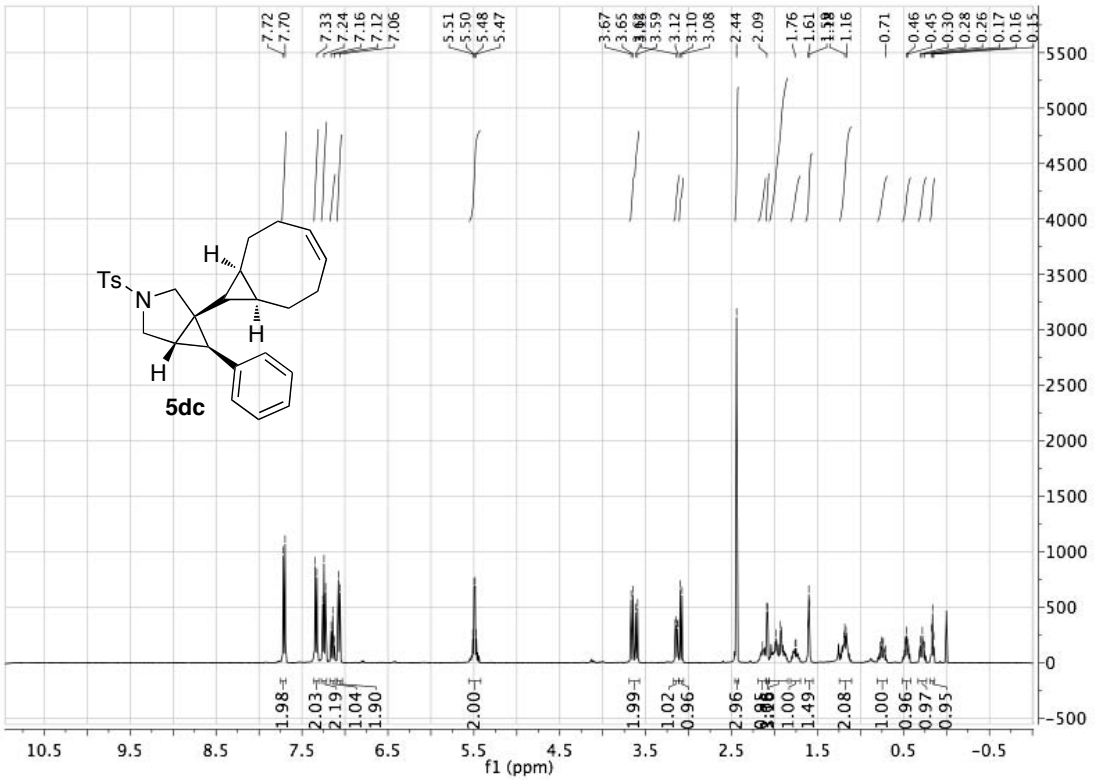

173.17
172.57
172.56
138.58
138.53
129.28
129.19
128.11
127.84
127.80
127.61
125.68
122.93
122.44
77.37
77.05
76.74
60.54
60.49
52.91
42.47
41.34
36.76
32.63
27.58
26.60
24.63
24.40
22.88
20.84
20.81
20.05
18.07
17.68
17.23
16.49
MeO2C
MeO2C
H
H
H
Ph
H
5ca
5ca'
f1 (ppm)

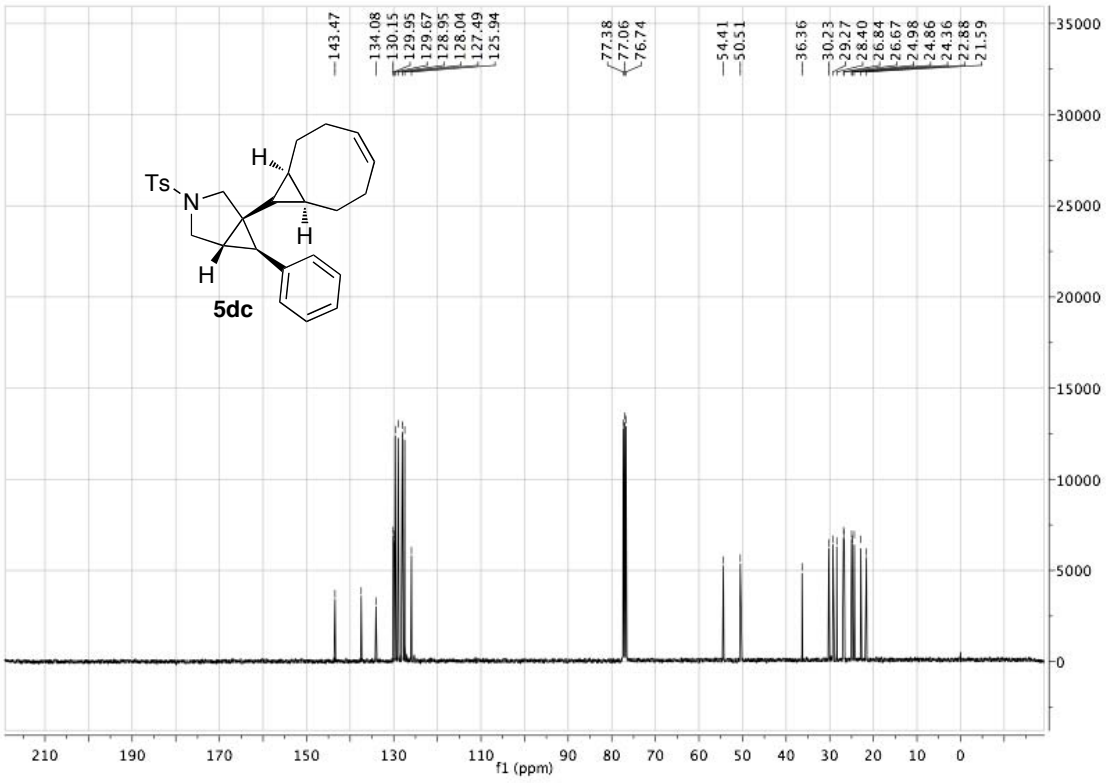

7.23
7.21
7.13
7.11
5.52
5.50
3.72
3.71
2.81
2.78
2.40
1.98
1.80
1.77
1.57
1.14
0.71
0.63
0.32
0.23
MeO
O
O
MeO
H
H
H
5da
2.11
2.97
2.00
5.95
1.01
1.93
1.02
4.30
1.31
0.99
2.23
0.93
0.92
0.98
0.97

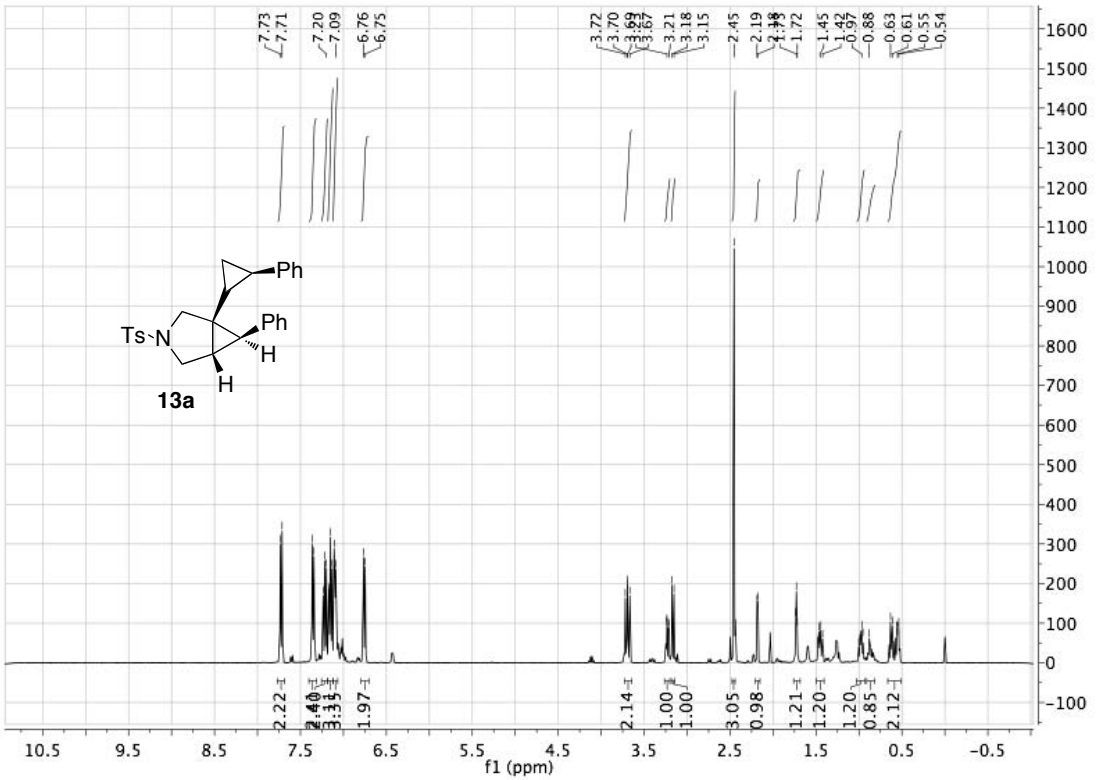

172.93
172.31
138.55
129.92
129.81
128.90
127.57
125.26
77.12
76.81
76.49
60.37
52.68
52.57
42.14
36.74
32.40
29.29
28.28
26.85
26.76
26.49
26.42
25.05
22.73
MeO
O
O
MeO
H
H
H
5da

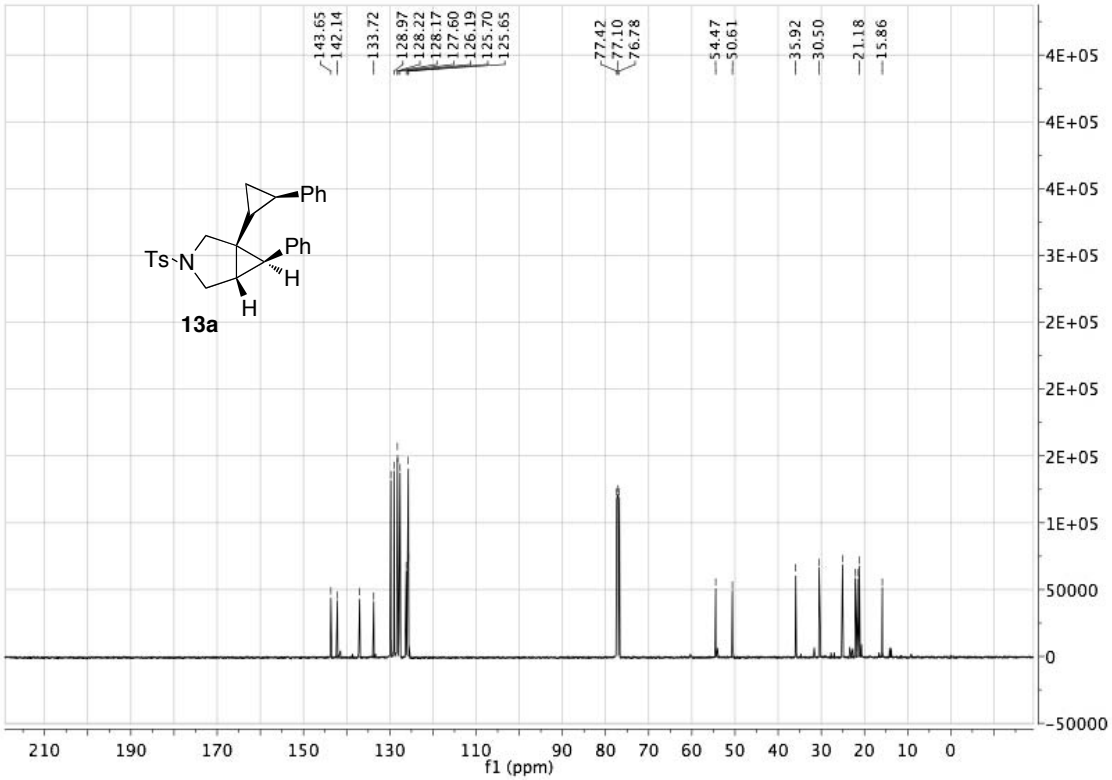

PhO2S
PhO2S
H
H
H
5db
f1 (ppm)

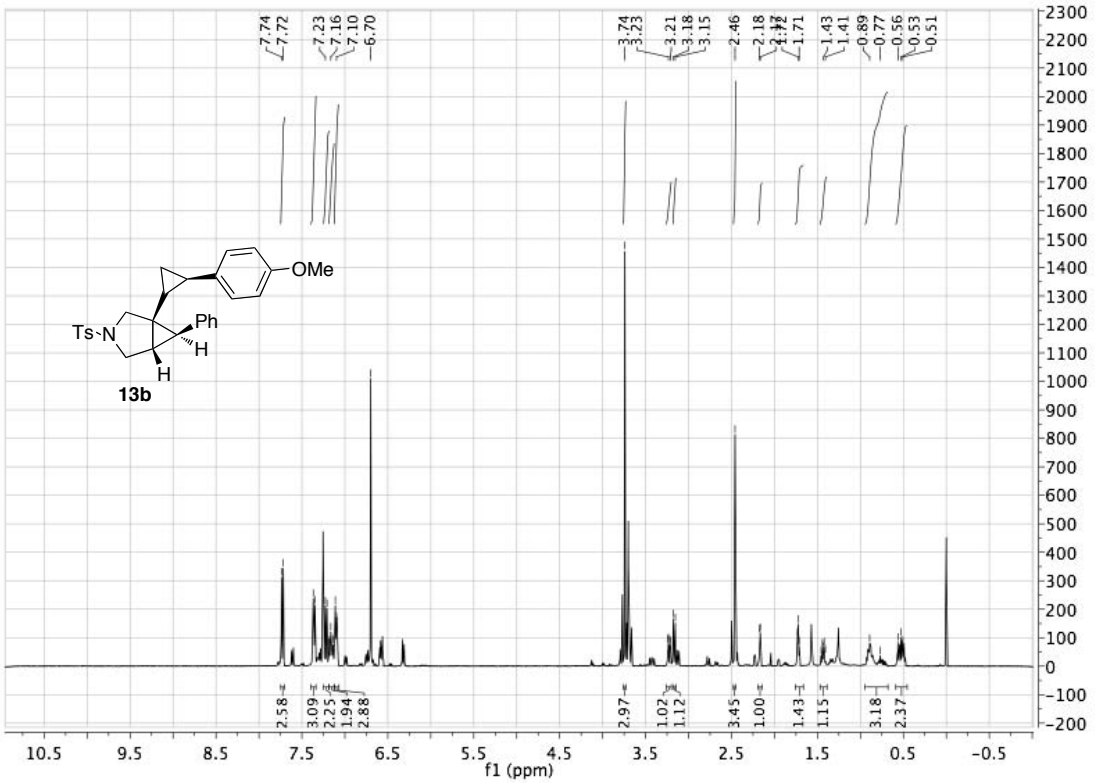

PhO2S
PhO2S
H
H
H
5db
f1 (ppm)

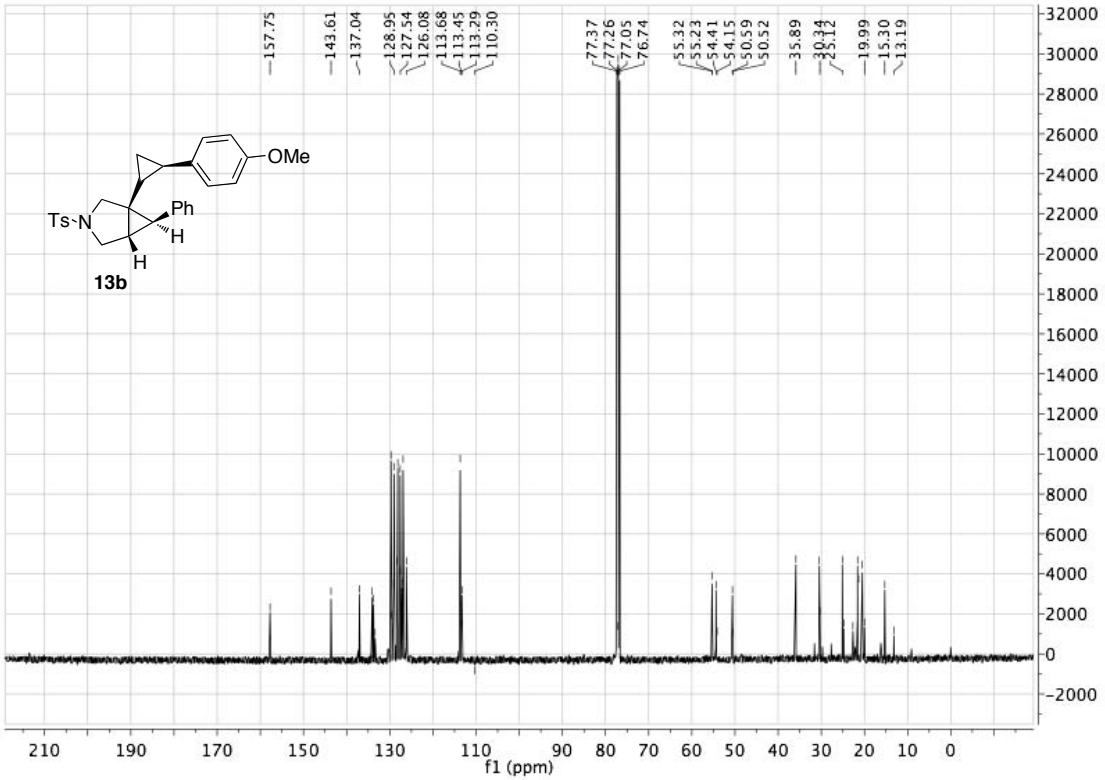

Ts
N
H
H
H
5dc
f1 (ppm)

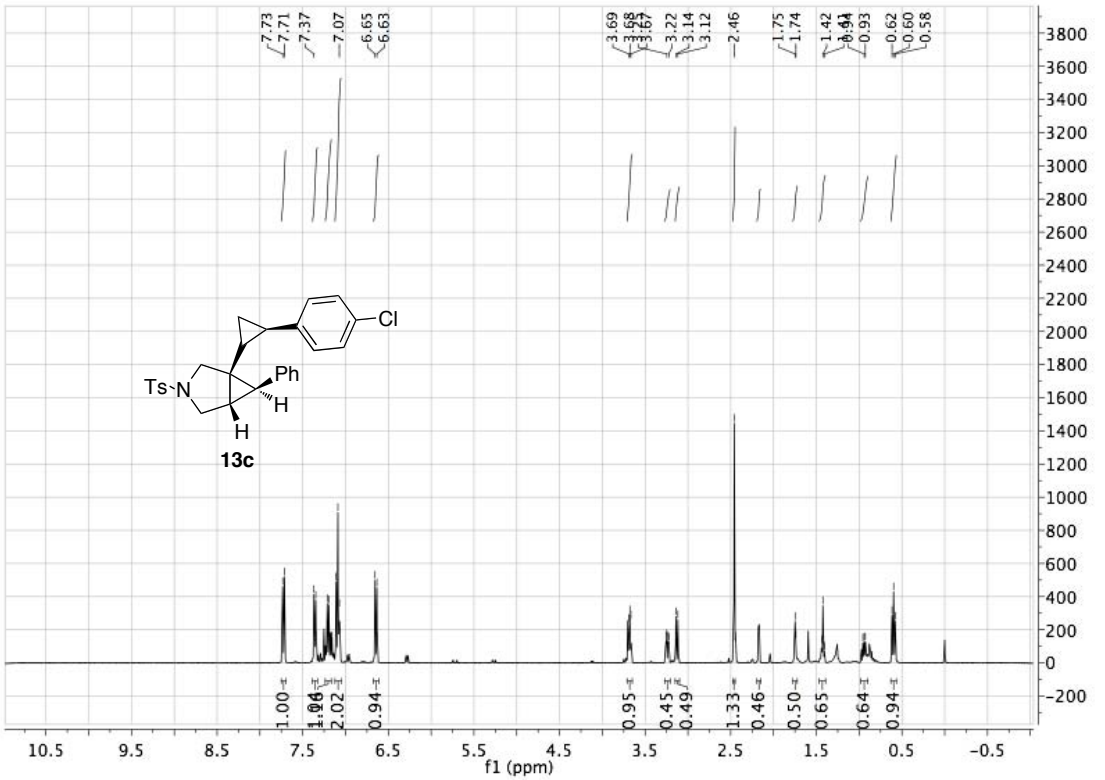

Ts
N
H
H
H
5dc
f1 (ppm)

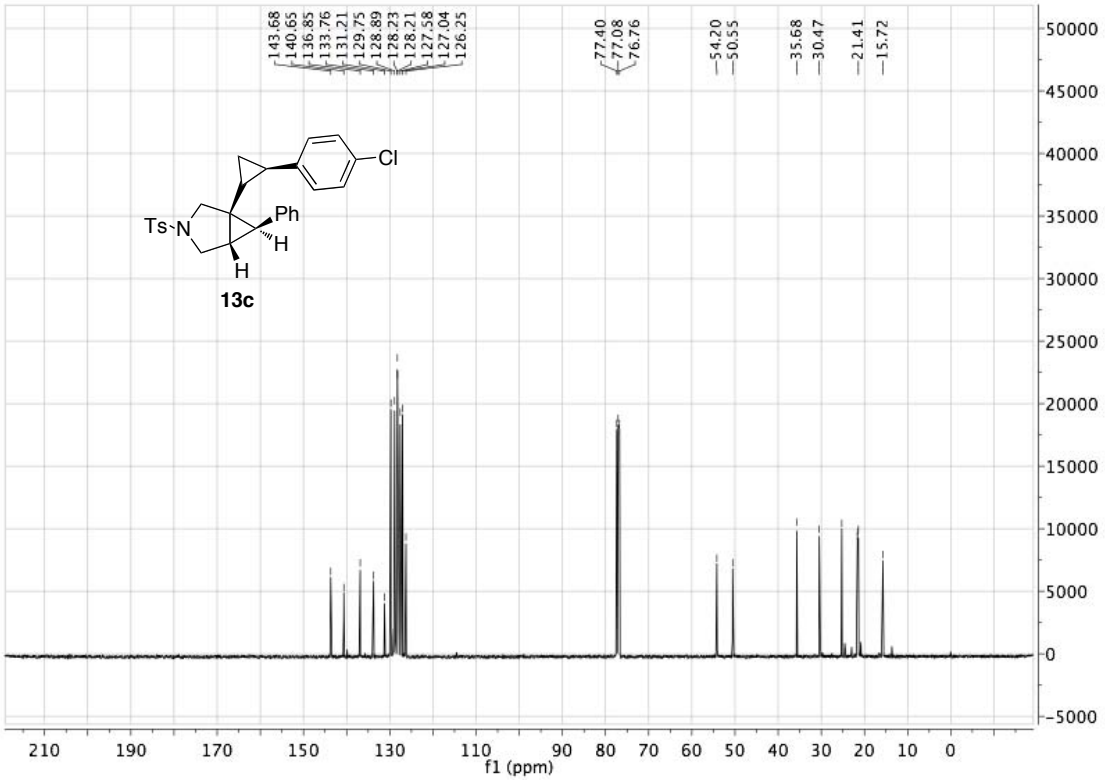

7.73
7.71
7.20
7.09
6.76
6.75
3.72
3.70
3.69
3.67
3.21
3.18
3.15
2.45
2.19
1.72
1.45
1.42
0.97
0.88
0.63
0.61
0.55
0.54
Ph
Ts-N
Ph
H
H
13a
2.22
1.97
2.14
1.00
1.00
3.05
0.98
1.21
1.20
1.20
0.85
2.12
f1 (ppm)

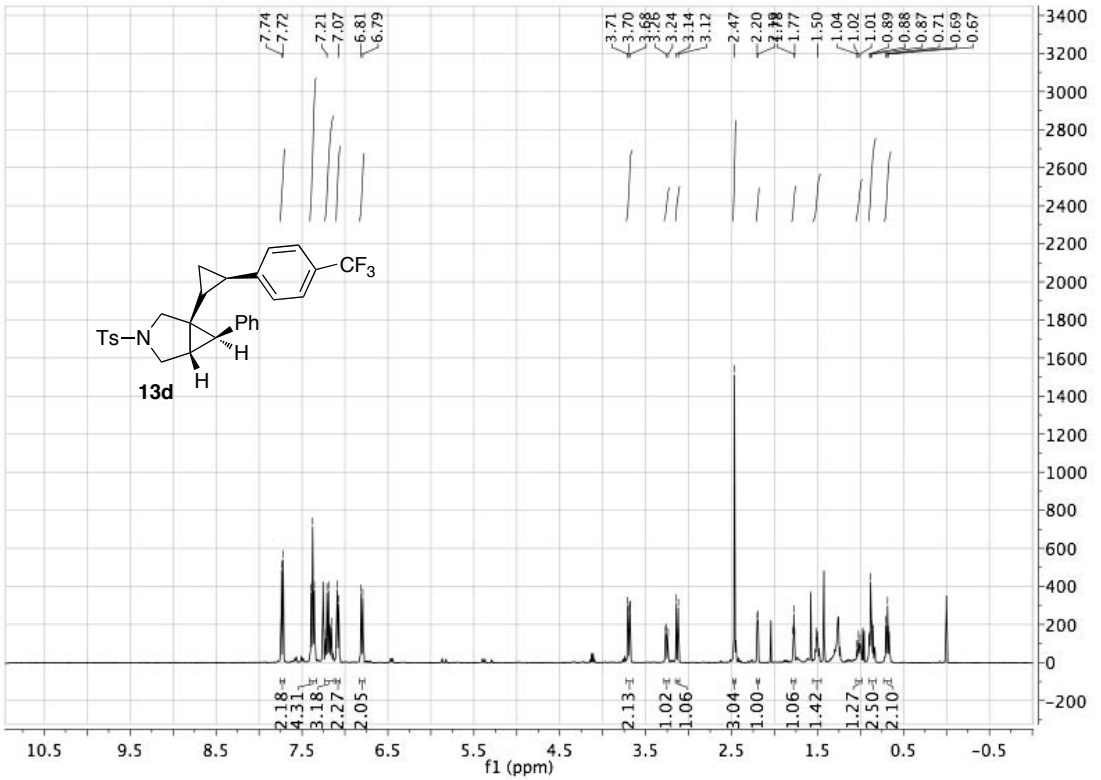

143.65
142.14
133.72
128.97
128.22
128.17
127.60
126.19
125.70
125.65
77.42
77.10
76.78
54.47
50.61
35.92
30.50
21.18
15.86
Ph
Ts-N
Ph
H
H
13a
f1 (ppm)

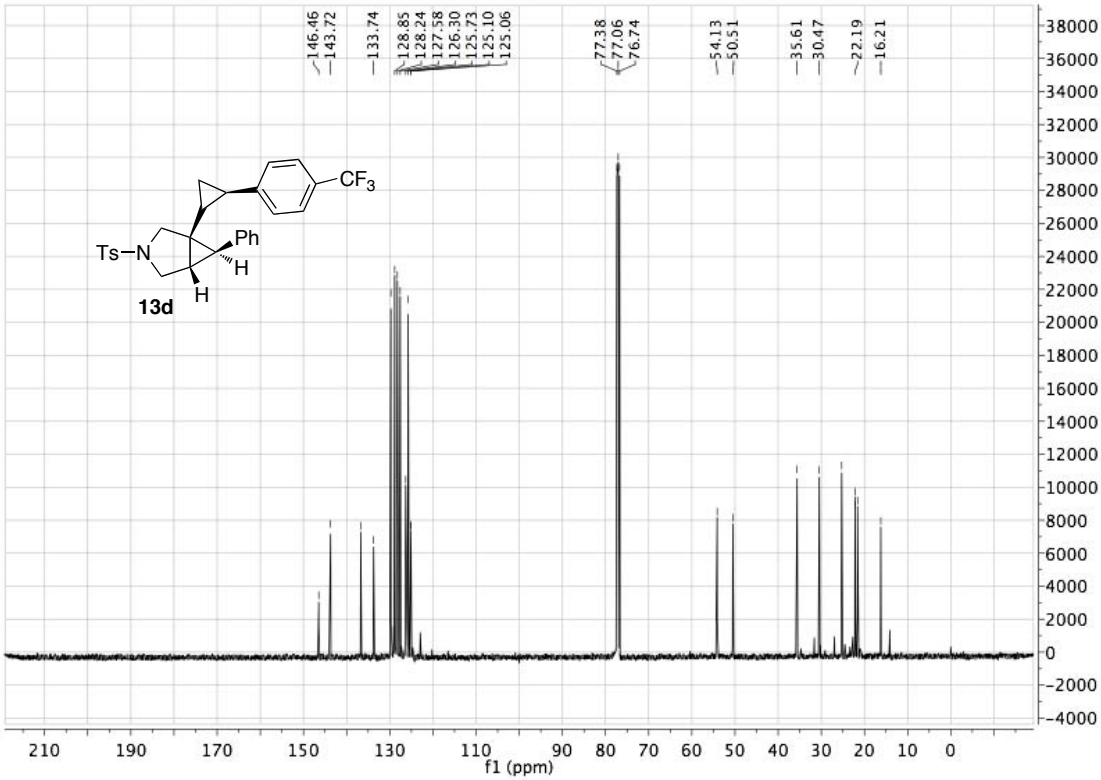

7.74
7.72
7.23
7.16
7.10
6.70
3.74
3.23
3.21
3.18
3.15
2.46
2.18
1.71
1.43
1.41
0.89
0.77
0.56
0.53
0.51
OMe
Ts-N
Ph
H
H
13b
2.58
3.09
2.25
1.94
2.88
2.97
1.02
1.12
3.45
1.00
1.43
1.15
3.18
2.37
f1 (ppm)

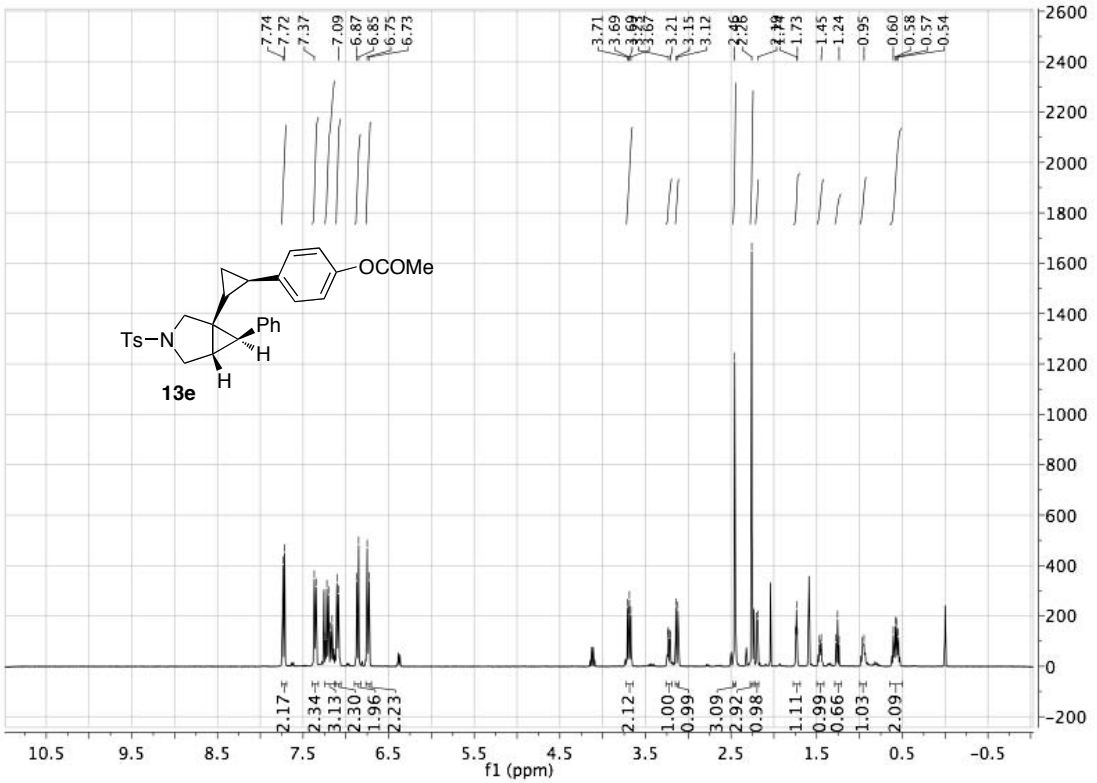

157.75
143.61
137.04
128.95
127.54
126.08
113.68
113.45
113.29
110.30
77.37
77.26
77.05
76.74
55.32
55.23
54.41
54.15
50.59
50.52
35.89
30.34
25.12
19.99
15.30
13.19
OMe
Ts-N
Ph
H
H
13b
f1 (ppm)

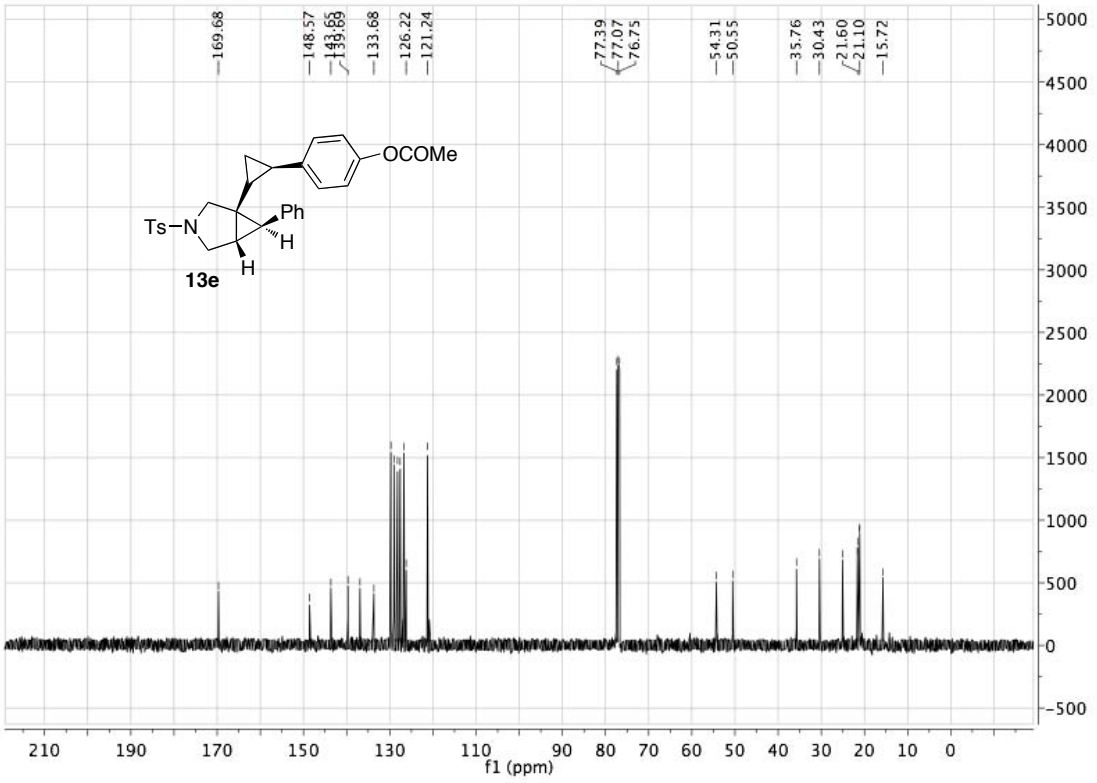

7.73
7.71
7.37
7.07
6.65
6.63
3.69
3.68
3.67
3.22
3.14
3.12
2.46
1.75
1.74
1.42
0.93
0.62
0.60
0.58
Cl
Ph
H
Ts
N
H
13c
1.00
1.06
2.02
0.94
0.95
0.45
0.49
1.33
0.46
0.50
0.65
0.64
0.94
f1 (ppm)

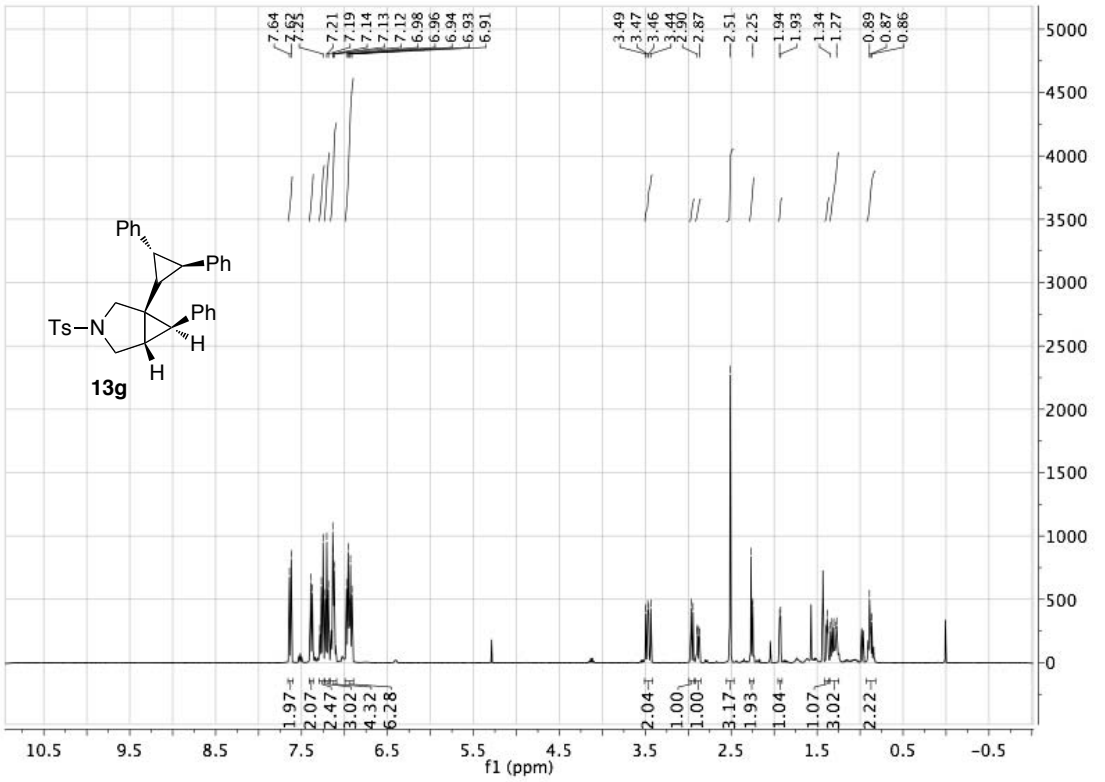

143.68
140.65
136.85
133.76
131.21
129.75
128.89
128.23
128.21
127.58
127.04
126.25
77.40
77.08
76.76
54.20
50.55
35.68
30.47
21.41
15.72
Cl
Ph
H
Ts
N
H
13c
f1 (ppm)

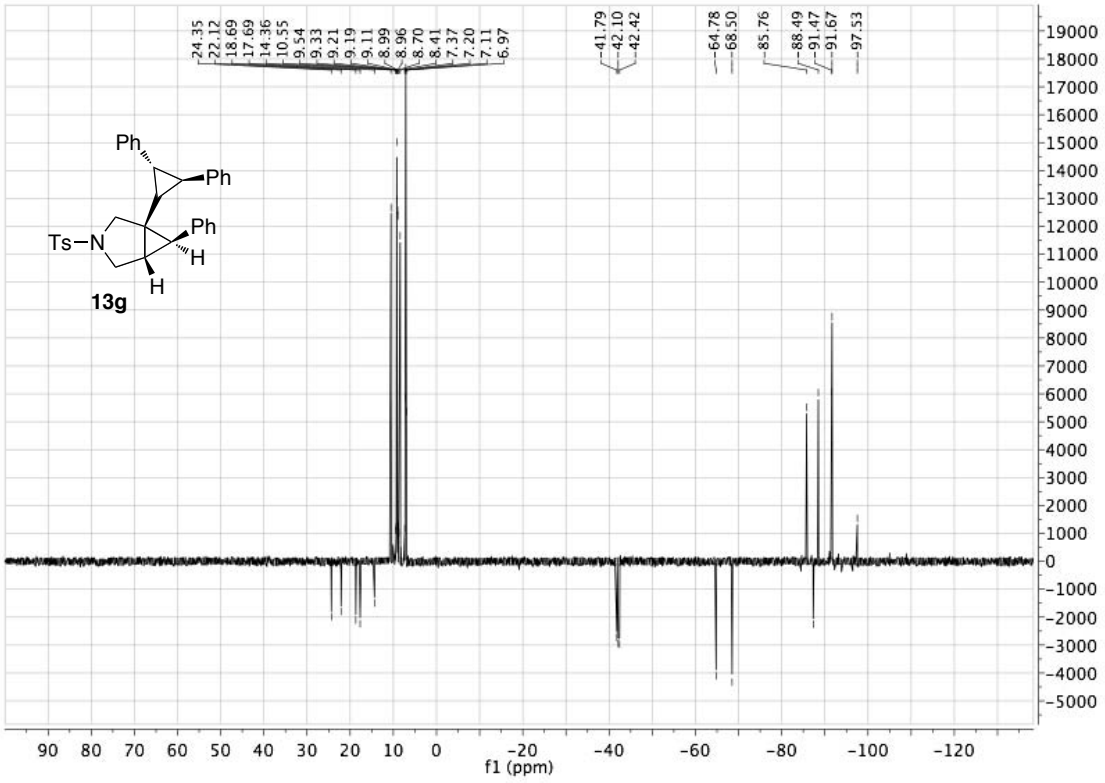

7.74
7.72
7.21
7.07
6.81
6.79
3.71
3.70
3.24
3.14
3.12
2.47
2.20
1.77
1.50
1.04
1.02
1.01
0.89
0.88
0.87
0.71
0.69
0.67
CF3
Ts–N
Ph
H
H
13d
2.18
4.31
3.18
2.27
2.05
2.13
1.02
1.06
3.04
1.00
1.06
1.42
1.27
2.50
2.10
f1 (ppm)

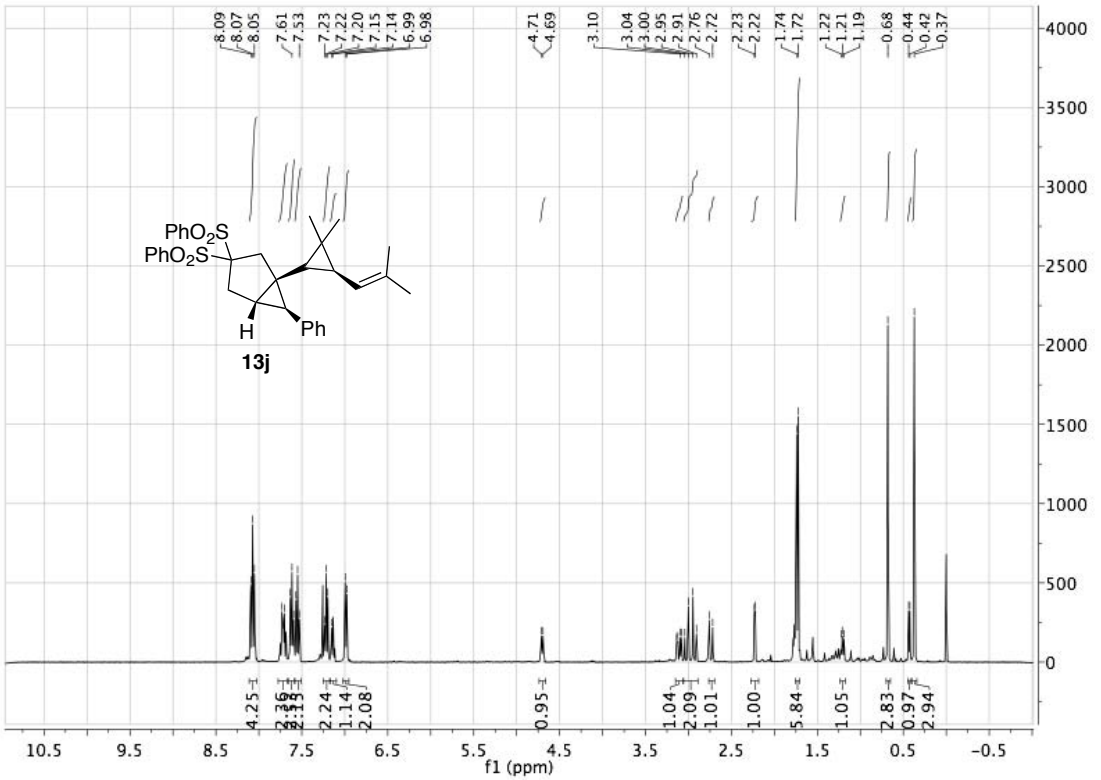

146.46
143.72
133.74
128.85
128.24
127.58
126.30
125.73
125.10
125.06
77.38
77.06
76.74
54.13
50.51
35.61
30.47
22.19
16.21
CF3
Ts–N
Ph
H
H
13d
f1 (ppm)

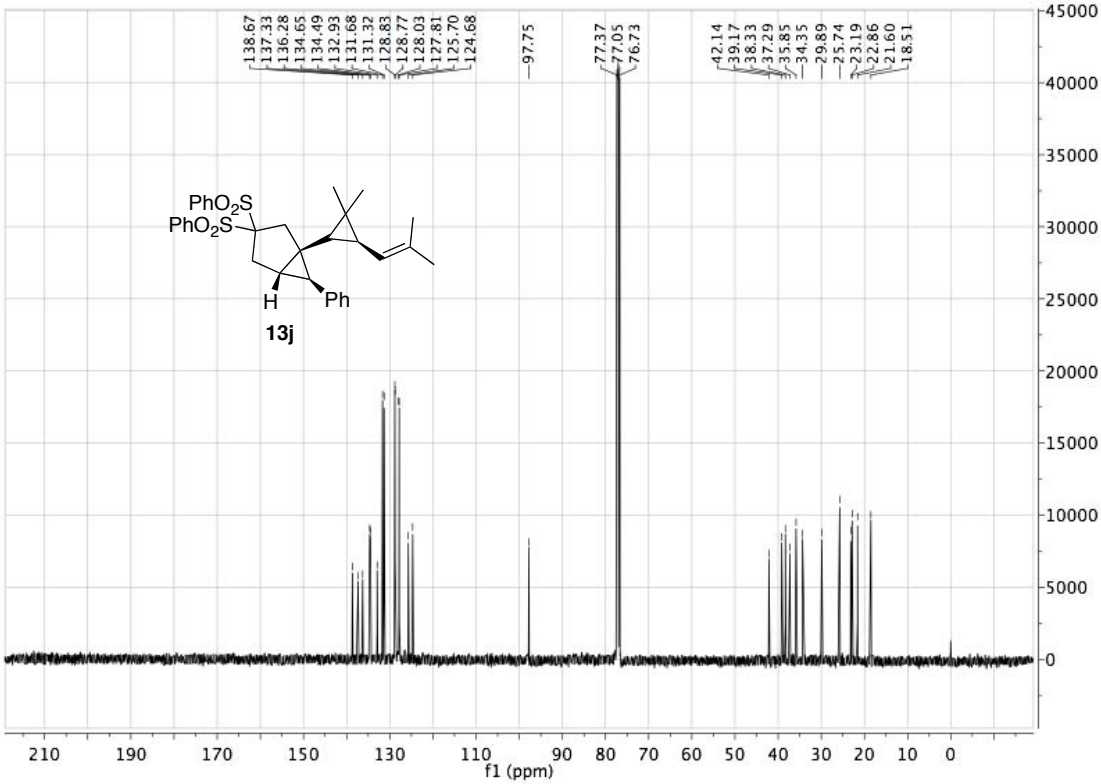

OCOMe
Ts–N
Ph
H
H
13e
f1 (ppm)

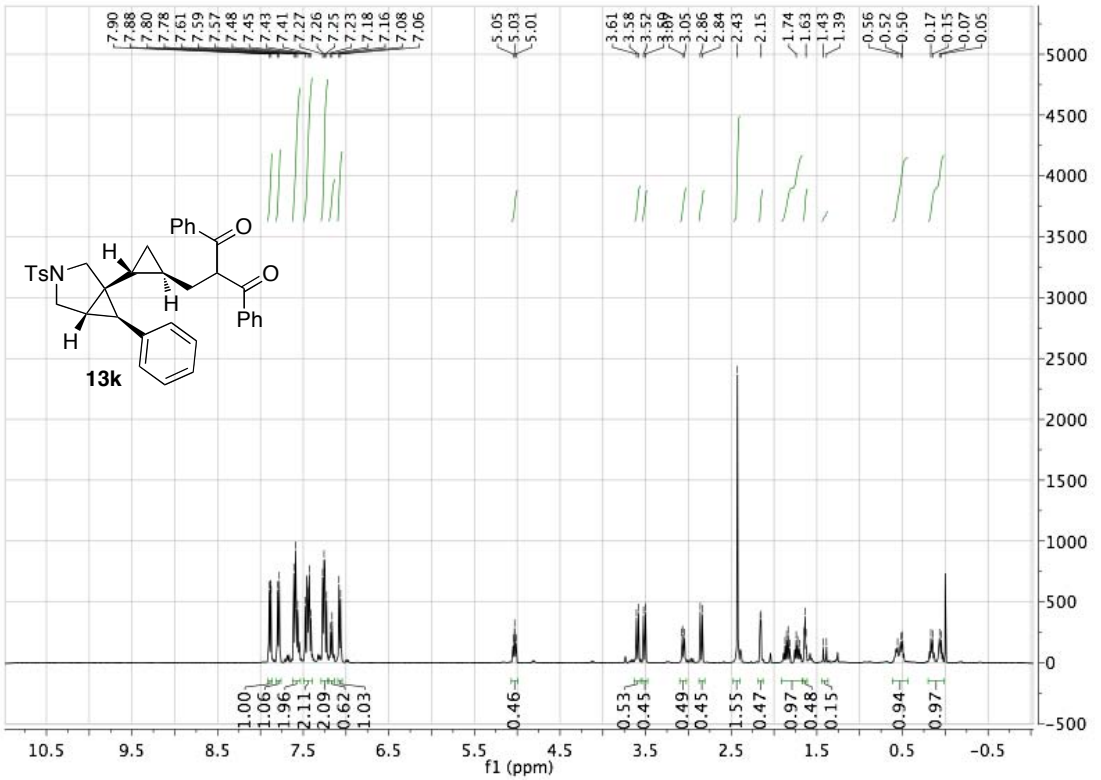

OCOMe
Ts–N
Ph
H
H
13e
f1 (ppm)

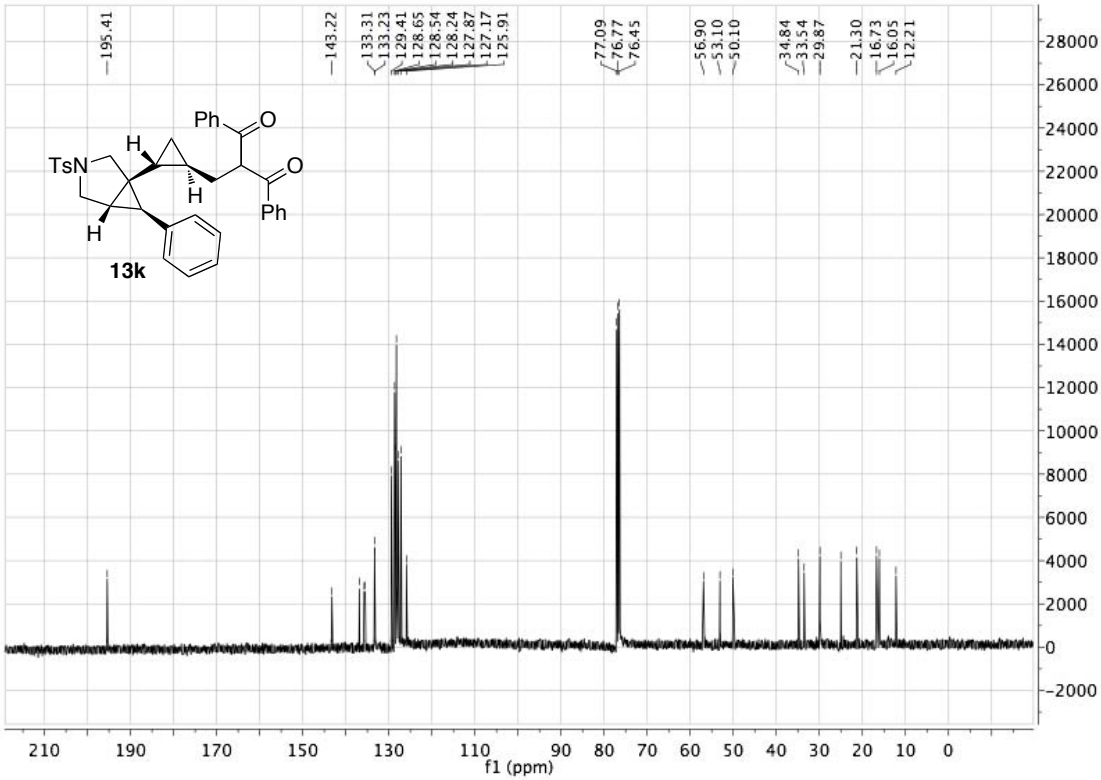

Ph
Ph
Ts–N
Ph
H
H
13g
f1 (ppm)

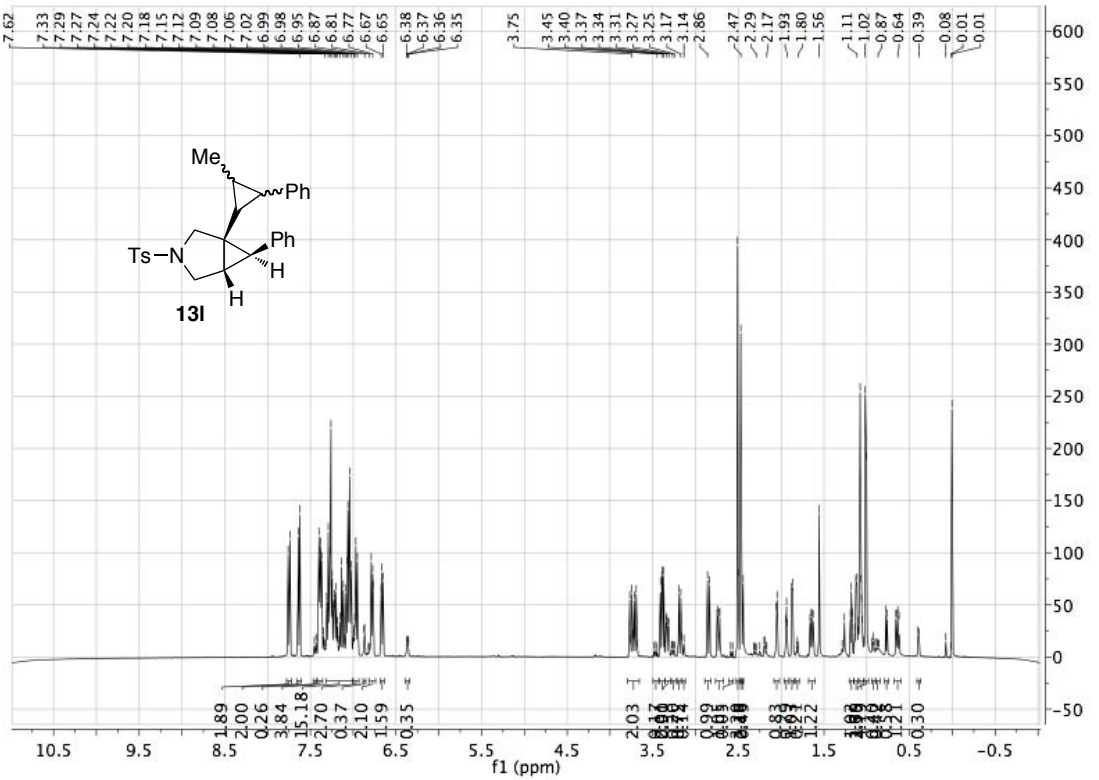

Ph
Ph
Ts–N
Ph
H
H
13g
f1 (ppm)

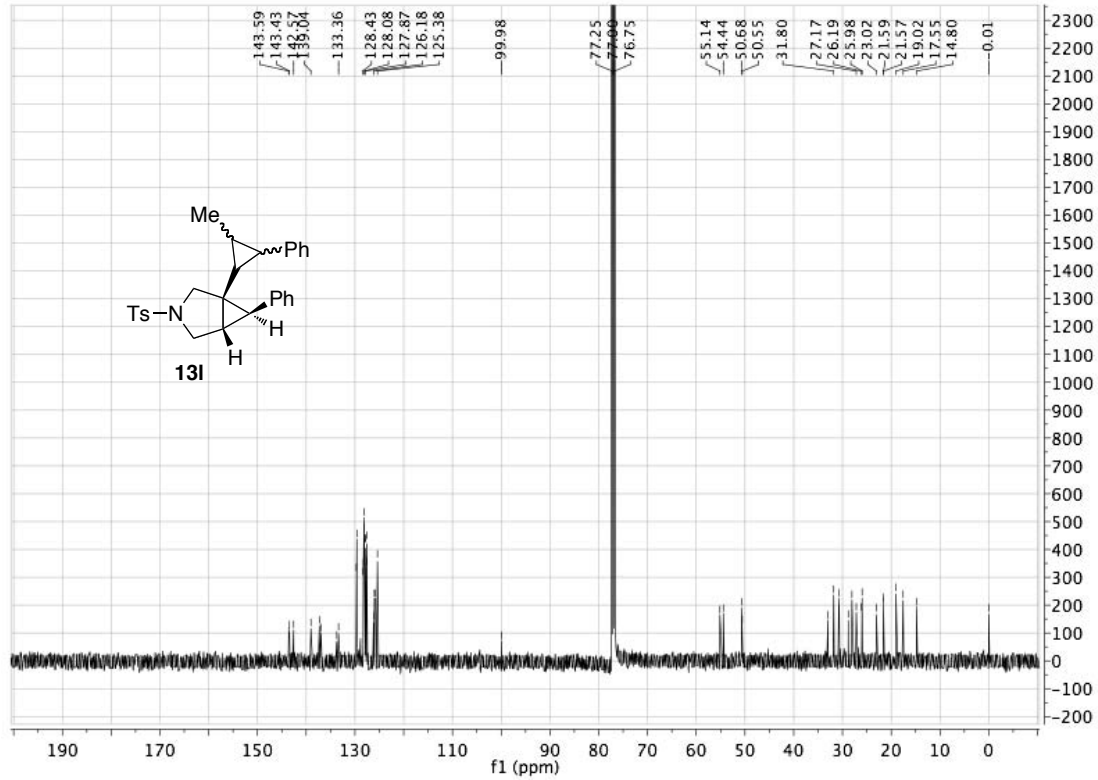

PhO2S
PhO2S
H
Ph
13j
f1 (ppm)

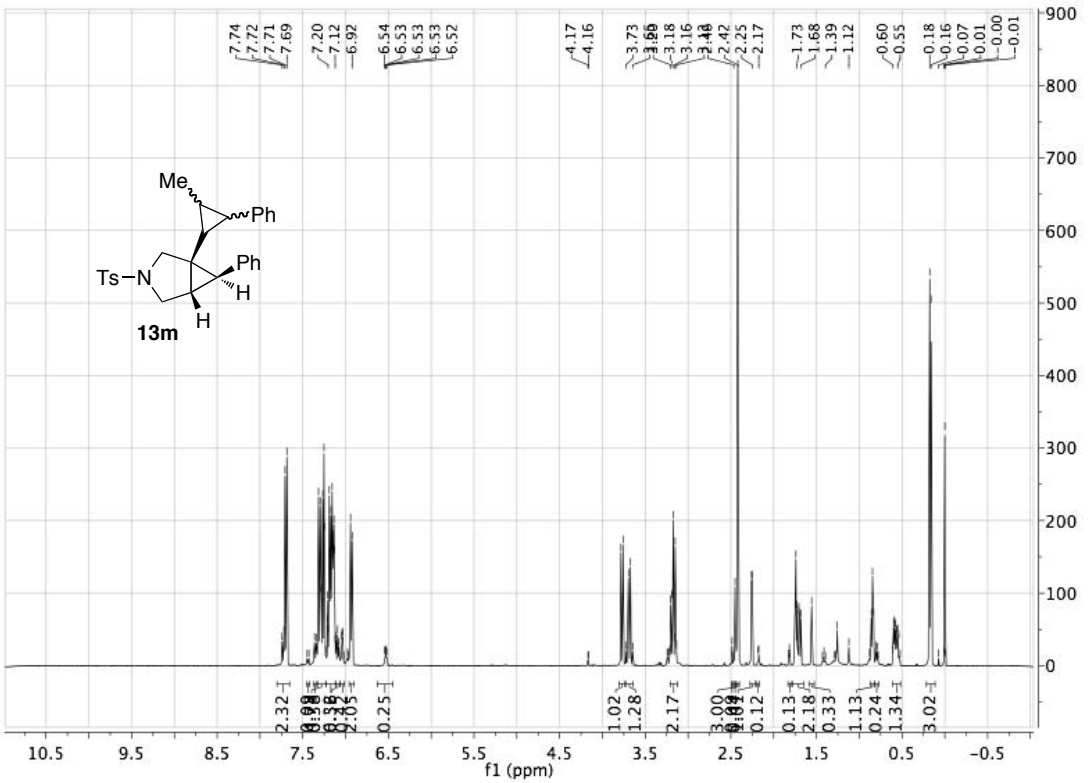

PhO2S
PhO2S
H
Ph
13j
f1 (ppm)

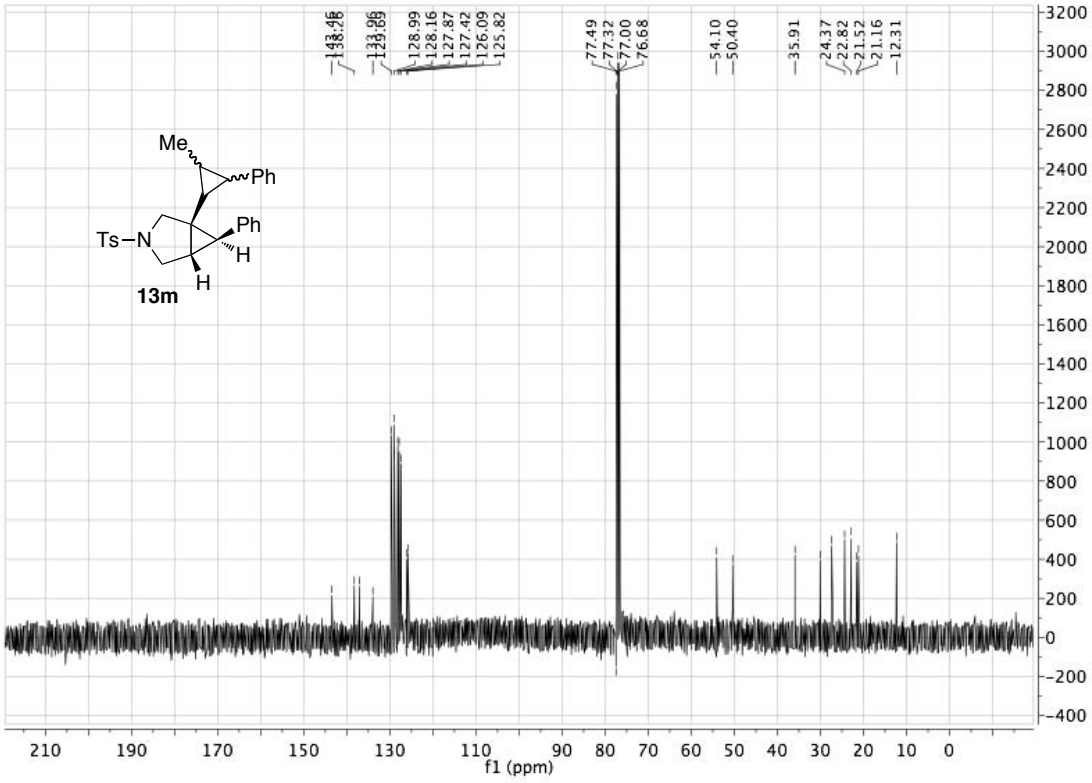

7.90
7.88
7.80
7.78
7.61
7.59
7.57
7.48
7.45
7.43
7.41
7.27
7.26
7.25
7.23
7.18
7.16
7.08
7.06
5.05
5.03
5.01
3.61
3.58
3.52
3.05
2.86
2.84
2.43
2.15
1.74
1.63
1.43
1.39
0.56
0.52
0.50
0.17
0.15
0.07
0.05
Ph
O
H
TsN
H
O
Ph
H
13k
1.00
1.06
1.96
2.11
2.09
0.62
1.03
0.46
0.53
0.45
0.49
0.45
1.55
0.47
0.97
0.48
0.15
0.94
0.97
f1 (ppm)


195.41
143.22
133.31
133.23
129.41
128.65
128.54
128.24
127.87
127.17
125.91
77.09
76.77
76.45
56.90
53.10
50.10
34.84
33.54
29.87
21.30
16.73
16.05
12.21
Ph
O
H
TsN
H
O
Ph
H
13k
f1 (ppm)


Me
Ph
Ts–N
Ph
H
H
13l
f1 (ppm)


Me
Ph
Ts–N
Ph
H
H
13l
f1 (ppm)


Me
Ph
Ts–N
Ph
H
H
13m
f1 (ppm)


Me
Ph
Ts–N
Ph
H
H
13m
f1 (ppm)

Computational Details

All calculations were carried out with DFT method using the B3LYP[4] functional as implemented in Gaussian03.[5] The 6-31G(d) basis set was used for H, C, N, O and P.[6] The inner electrons of Au were described by an effective core potential (SDD), and the associated double-ζ basis set was used for the outer electrons.[7] Frequency calculations were performed to characterize the stationary points. IRC calculations were performed to confirm connection to the minima.

The solvent effect was taken into account by single-point calculations using the polarizable continuum model (PCM),[8,9,10,11] in particular IEF-PCM as implemented in Gaussian 03. Default options were used, except that individual spheres were placed on all hydrogen atoms to get a more accurate cavity. The calculations were performed using dichloromethane ($\varepsilon = 8.93$) as solvent. The standard Gibbs energies in dichloromethane (ΔG_{DCM}) were obtained by adding the solvation energies to the gas-phase Gibbs

(4) (a) C. Lee, R. G Parr, and W. Yang, *Phys. Rev.* **1988**, *37*, 785-789. (b) A. D. Becke, *J. Phys. Chem.* **1993**, *98*, 5648-5652. (c) P. J. Stephens, F. J. Devlin, C. F. Cha-balowski, and M. J. J. Frisch, *Phys. Chem.* **1994**, *98*, 11623-11627.

(5) M .J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challa-combe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. and Pople, "Gaussian 03, Revision C.02", Gaussian, Inc., Wallingford, CT, **2004**.

(6) M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M.S. Gordon, D. J. Defrees and J. A. Pople, *J. Chem. Phys*. **1982**, *77*, 3654-3665.

(7) (a) P. J. Hay and W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 299-310. (b)W. R. Wadt and P. J. Hay, *J. Chem. Phys.* **1985**, *82*, 284-298.

(8) E. Cances, B. Mennucci and J. J. Tomasi, *Chem. Phys.* **1997**, *107*, 3032–3041

(9) M. Cossi, V. Barone, B. Mennucci and J. Tomasi, *Chem. Phys. Lett.* **1998**, *286*, 253-260.

(10) B. Mennucci and J. J. Tomasi, *Chem. Phys.* **1997**, *106,* 5151–5158.

(11) S. Miertus and J. Tomasi, *J. Chem. Phys*. **1982**, *65*, 239–245.

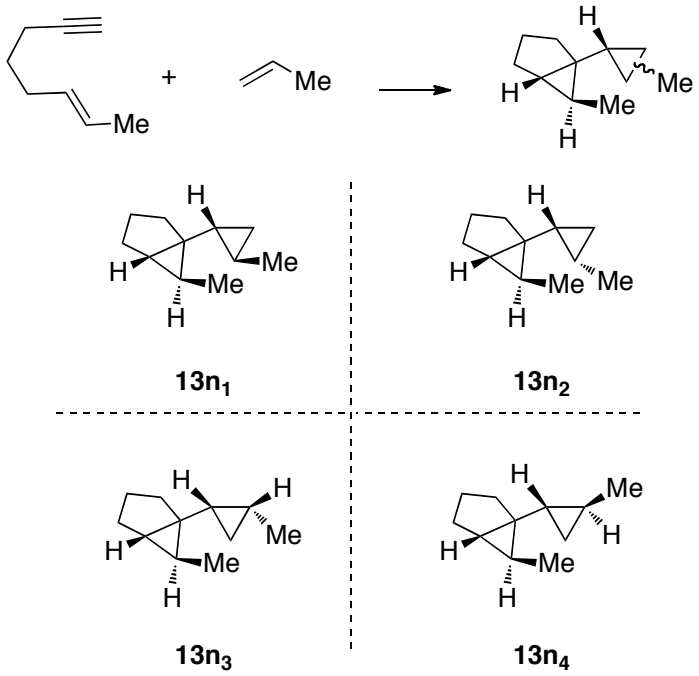
energies computed at 298 K. The same procedure was employed to calcule zero-point corrected energies in dichlorometane.

Molecular graphics images were produced using the UCSF Chimera package from the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco (supported by NIH P41 RR-01081).

Relative Energies and Selected Distances

All relative energies are referred to separated reactants. In this section, the following abbreviations are used: ΔV (potential energy), ΔG (free energy in gas phase), ΔV_{ZPE} (zero-point corrected potential energy in gas phase), ΔV_{DCM} (potential energy including solvation effects in dichloromethane), ΔG_{DCM} (free energy including solvation effects in dichloromethane), $\Delta V_{ZPE+DCM}$ (zero-point corrected potential energy including solvation effects in dichloromethane).

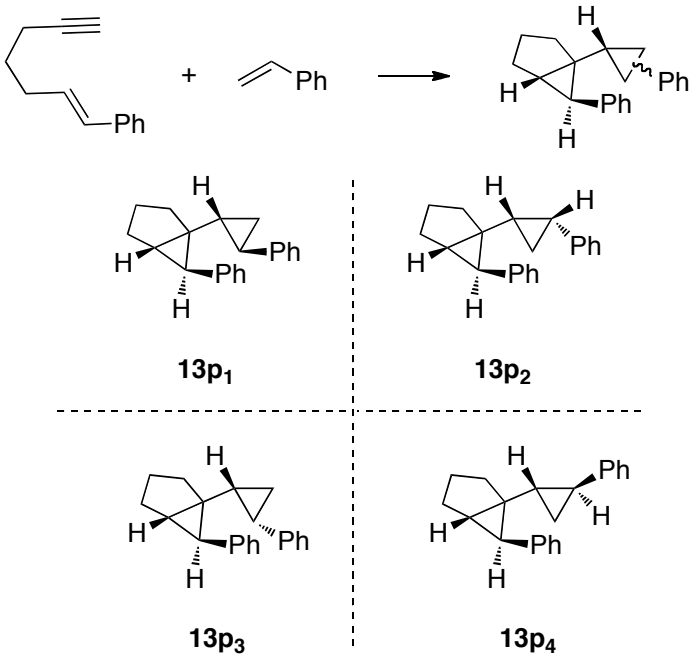
Products $13n_{1-4}$



$13n_1$ **$13n_2$** **$13n_3$** **$13n_4$**

	ΔV (kcal)	ΔG (kcal)	ΔV_{DCM} (kcal)	ΔG_{DCM} (kcal)	$\Delta V_{ZPE+DCM}$ (kcal)
$13n_1$	-40.49	-18.85	-40.00	-18.36	-33.38
$13n_2$	-38.78	-17.08	-38.78	-17.08	-32.25
$13n_3$	-37.88	-15.72	-37.33	-15.17	-30.50
$13n_4$	-40.46	-18.90	-39.90	-18.34	-33.32

Products $13p_{1-4}$.

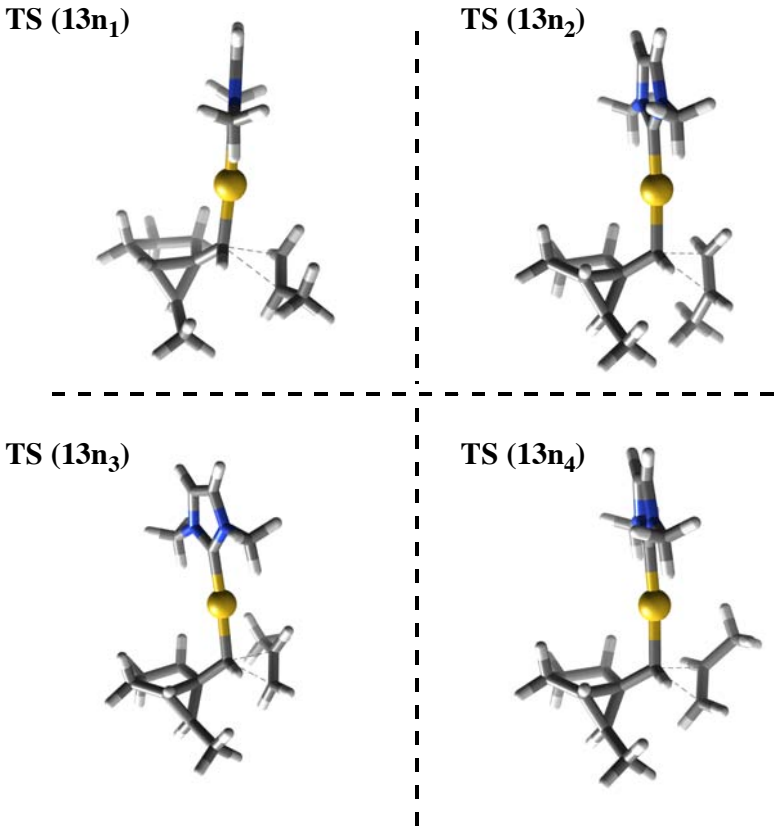


$13p_1$ **$13p_2$**

$13p_3$ **$13p_4$**

	ΔV (kcal)	ΔG (kcal)	ΔV_{DCM} (kcal)	ΔG_{DCM} (kcal)	$\Delta V_{ZPE+DCM}$ (kcal)
13p1	-36.20	-14.27	-33.09	-11.16	-27.22
13p2	-33.04	-10.37	-30.76	-8.10	-24.64
13p3	-34.09	-11.54	-31.32	-8.77	-25.24
13p4	-36.42	-14.73	-34.34	-12.65	-28.43

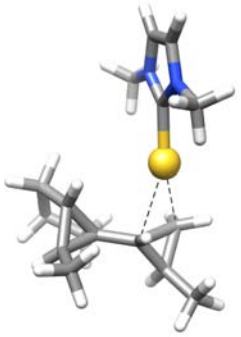
TS(13n$_{1-4}$)a



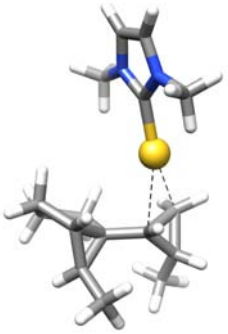
	Ea (V, kcal)	Ea (G, kcal)	Ea (V_{DCM}, kcal)	Ea (G_{DCM}, kcal)	Ea ($V_{ZPE+DCM}$, kcal)
TS (13n$_1$)	4.48	18.92	5.92	20.35	7.49
TS (13n$_2$)	6.88	20.82	7.37	21.32	8.76
TS (13n$_3$)	8,63	23,75	9.48	24.60	11.36
TS (13n$_4$)	8.66	22.87	9.92	24.12	11.47

	d C_{Au}-C1 (Å)	d C_{Au}-C2 (Å)
TS (13n$_1$)	2.12	2.43
TS (13n$_2$)	2.08	2.50
TS (13n$_3$)	2.09	2.20
TS (13n$_4$)	2.15	2.22

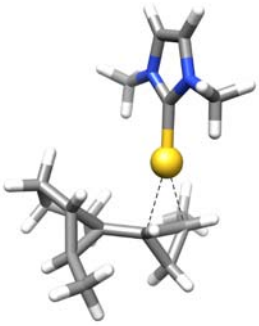
$13n_1$·Au(NHC)$^+$



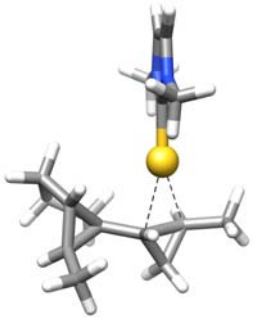
$13n_2$·Au(NHC)$^+$



$13n_3$·Au(NHC)$^+$



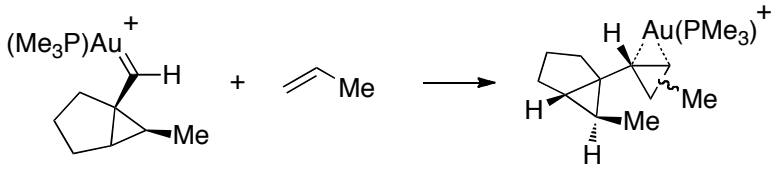
$13n_4$·Au(NHC)$^+$



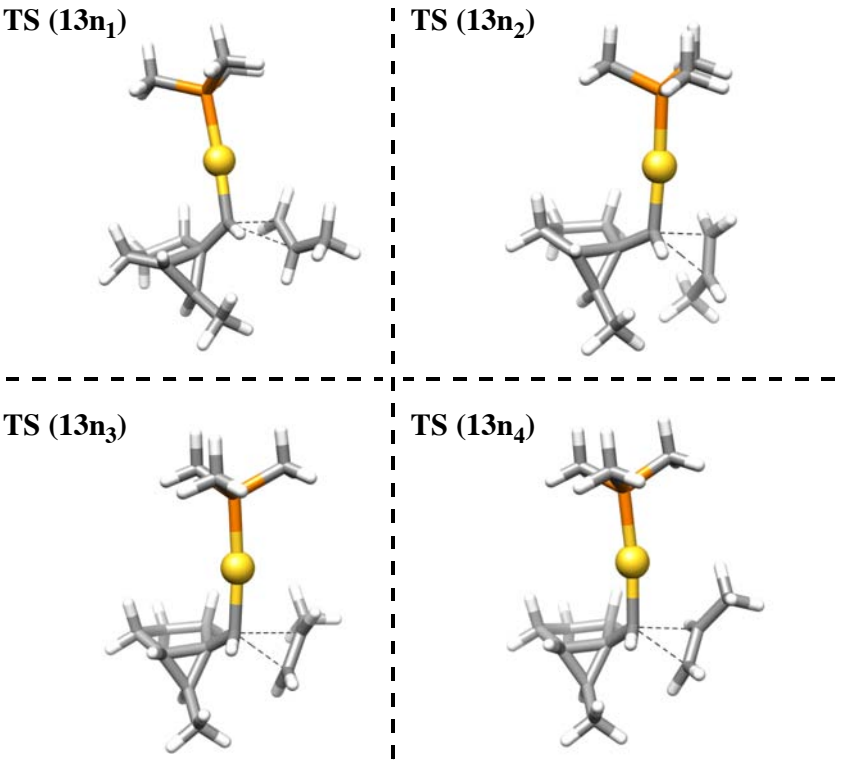
Intermediate	ΔV (kcal)	ΔG (kcal)
$13n_1$·Au(NHC)$^+$	-14.07	2.84
$13n_2$·Au(NHC)$^+$	-11.43	5.95
$13n_3$·Au(NHC)$^+$	-7.45	9.37
$13n_4$·Au(NHC)$^+$	-8.73	7.76

	a (Å)	b (Å)	c (Å)	d (Å)
$13n_1$·Au(NHC)$^+$	2.71	2.32	1.66	1.47
$13n_2$·Au(NHC)$^+$	2.67	2.34	1.65	1.48
$13n_3$·Au(NHC)$^+$	2.46	2.45	1.73	1.50
$13n_4$·Au(NHC)$^+$	2.49	2.45	1.72	1.49

TS($13_{1\text{-}4}$)$_b$



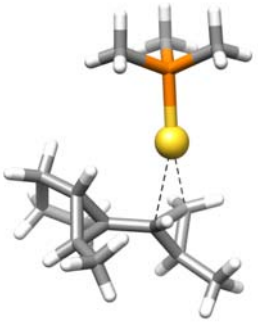
	Ea (V, kcal)	Ea (G, kcal)	Ea (V_{DCM}, kcal)	Ea (G_{DCM}, kcal)	Ea ($V_{ZPE+DCM}$, kcal)
TS ($13n_1$)	3.39	17.11	6.48	20.20	7.90
TS ($13n_2$)	5.57	19.38	8.12	21.93	9.54
TS ($13n_3$)	7.35	22.62	9.40	24.66	11.29
TS ($13n_4$)	7.52	22.00	10.29	24.77	11.93



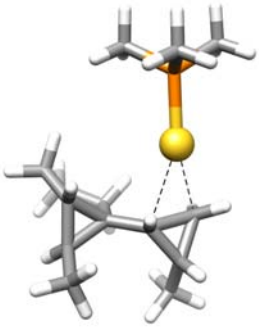
	d C_{Au}-C1 (Å)	d C_{Au}-C2 (Å)
TS ($13n_1$)	2.16	2.46
TS ($13n_2$)	2.09	2.51
TS ($13n_3$)	2.11	2.23
TS ($13n_4$)	2.16	2.24

The corresponding intermediates were obtained following the Internal Reaction Coordinate (IRC) from Transition States.

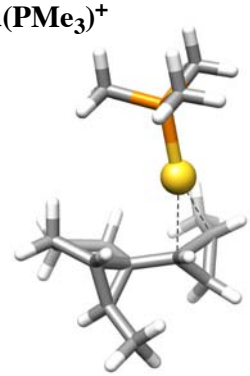
13n$_1$·Au(PMe$_3$)$^+$



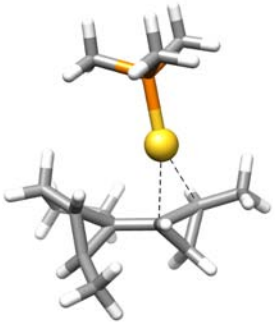
13n$_2$·Au(PMe$_3$)$^+$



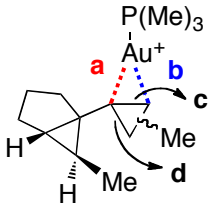
13n$_3$·Au(PMe$_3$)$^+$



13n$_4$·Au(PMe$_3$)$^+$



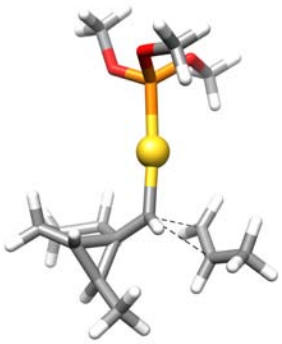
Intermediate	ΔV (kcal)	ΔG (kcal)
13n$_1$·AuL$^+$	-15.76	0.65
13n$_2$·AuL$^+$	-13.13	3.79
13n$_3$·AuL$^+$	-9.15	8.09
13n$_4$·AuL$^+$	-10.38	5.67



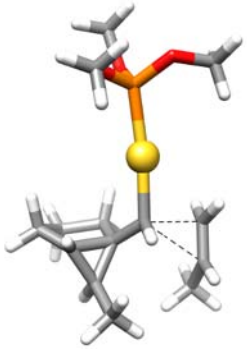
	a (Å)	b (Å)	c (Å)	d (Å)
13n$_1$·Au(PMe$_3$)$^+$	2.74	2.33	1.66	1.47
13n$_2$·Au(PMe$_3$)$^+$	2.70	2.36	1.65	1.48
13n$_3$·Au(PMe$_3$)$^+$	2.47	2.51	1.70	1.50
13n$_4$·Au(PMe$_3$)$^+$	2.51	2.49	1.70	1.50

TS($13n_{1-4}$)$_c$

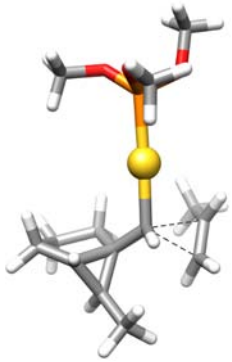
TS ($13n_1$)



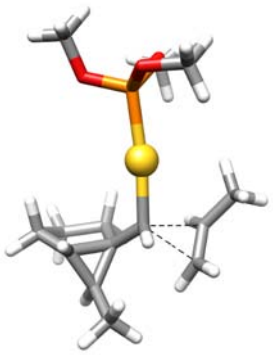
TS ($13n_2$)



TS ($13n_3$)



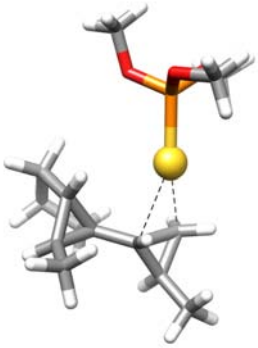
TS ($13n_4$)



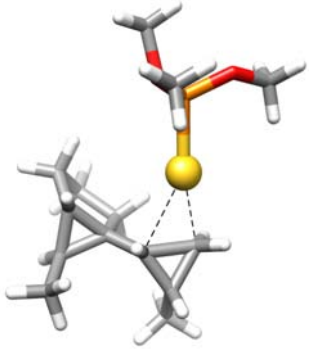
	Ea (V, kcal)	Ea (G, kcal)	Ea (V_{DCM}, kcal)	Ea (G_{DCM}, kcal)	Ea ($V_{ZPE+DCM}$, kcal)
TS ($13n_1$)	3.06	16.71	6.99	20.64	8.41
TS ($13n_2$)	5.08	19.11	8.25	22.28	9.66
TS ($13n_3$)	6.50	21.17	9.37	24.04	11.21
TS ($13n_4$)	7.15	21.27	10.16	24.29	11.72

	d C_{Au}-C1 (Å)	d C_{Au}-C2 (Å)
TS ($13n_1$)	2.15	2.46
TS ($13n_2$)	2.09	2.51
TS ($13n_3$)	2.08	2.26
TS ($13n_4$)	2.16	2.24

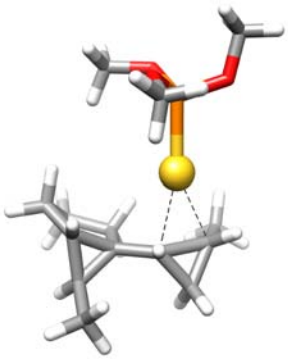
13n$_1$·Au((P(OMe$_3$)$_3$)$^+$



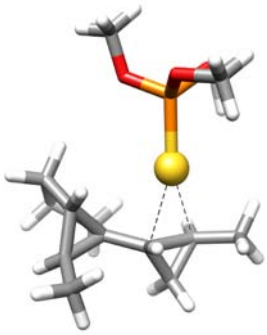
13n$_2$·Au((P(OMe$_3$)$_3$)$^+$



13n$_3$·Au((P(OMe$_3$)$_3$)$^+$



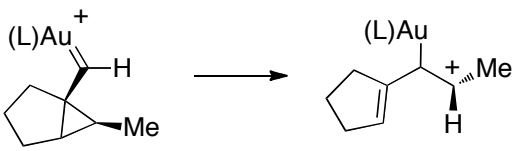
13n$_4$·Au((P(OMe$_3$)$_3$)$^+$



Intermediate	ΔV (kcal)	ΔG (kcal)
13n$_1$·Au(P(OMe$_3$)$_3$)$^+$	-16.02	0.21
13n$_2$·Au(P(OMe$_3$)$_3$)$^+$	-13.29	3.02
13n$_3$·Au(P(OMe$_3$)$_3$)$^+$	-8.91	6.82
13n$_4$·Au(P(OMe$_3$)$_3$)$^+$	-10.92	5.81

	a (Å)	b (Å)	c (Å)	d (Å)
13n$_1$·Au(P(OMe$_3$)$_3$)$^+$	2.72	2.30	1.67	1.46
13n$_2$·Au(P(OMe$_3$)$_3$)$^+$	2.69	2.33	1.66	1.47
13n$_3$·Au(P(OMe$_3$)$_3$)$^+$	2.45	2.50	1.71	1.50
13n$_4$·Au(P(OMe$_3$)$_3$)$^+$	2.51	2.44	1.72	1.49

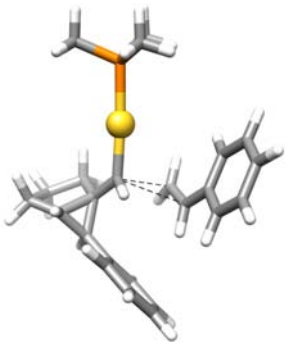
TS14$_{a-c}$



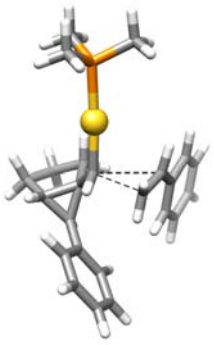
	Ea (V, kcal)	Ea (G, kcal)	Ea (V_{DCM}, kcal)	Ea (G_{DCM}, kcal)	Ea($V_{ZPE+DCM}$, kcal)
$TS14_a$	12.03	12.65	10.03	10.66	9.70
$TS14_b$	10.46	11.62	10.37	11.53	10.22
$TS14_c$	9.67	10.22	9.58	10. 13	9.34

TS($13p_{1-4}$)

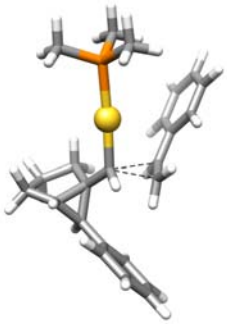
TS ($13p_1$)



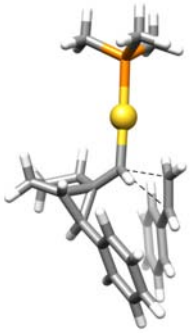
TS ($13p_2$)



TS ($13p_3$)



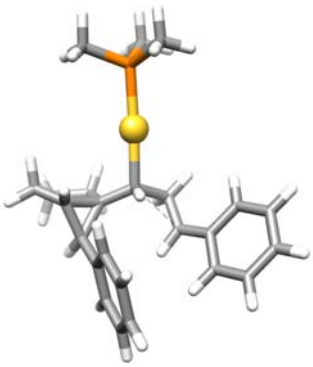
TS ($13p_4$)



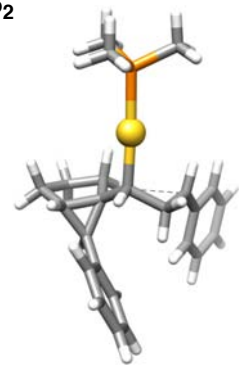
	Ea (V, kcal)	Ea (G, kcal)	Ea (V_{DCM}, kcal)	Ea (G_{DCM}, kcal)	Ea ($V_{ZPE+DCM}$, kcal)
TS ($13p_1$)	0.76	16.22	7.22	22.68	8.71
TS ($13p_2$)	3.84	19.36	9.63	25.15	11.26
TS ($13p_3$)	4.49	20.35	10.24	26,10	11.91
TS ($13p_4$)	3.49	18.32	10.27	25,10	11.72

	d Au-C1 (Å)	d Au-C2 (Å)
TS ($13p_1$)	2.32	2.74
TS ($13p_2$)	2.10	2.79
TS ($13p_3$)	2.20	2.84
TS ($13p_4$)	2.12	2.81

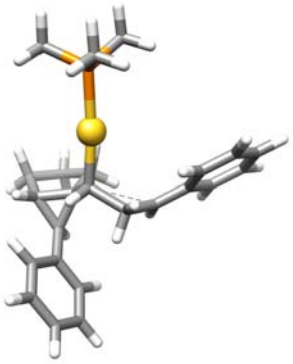
15_1



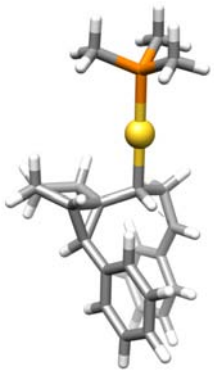
15_2



15_3



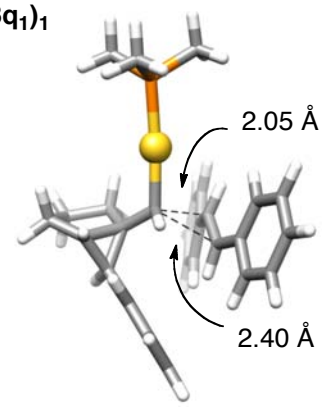
15_4



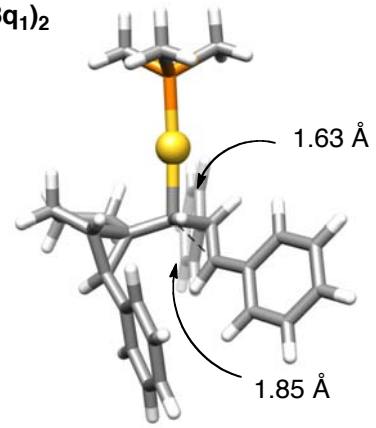
	Ea (V, kcal)	Ea (G, kcal)	Ea (V_{DCM}, kcal)	Ea (G_{DCM}, kcal)	Ea ($V_{ZPE+DCM}$, kcal)
15_1	-8.65	9.05	-3.23	14.48	-0.07
$TS(13p)_2$	-4.86	12.05	-1.47	15.44	1.22
$13p_1 \cdot Au(PMe_3)^+$	-10.89	5.76	-8.02	8.63	-4.9
$TS(13p_1)_{rot}$	2.07	19.43	5.03	22.39	7.23
15_4	-3.79	13.00	1.61	18.40	4.62

Using stilbene as olefin: $TS(13q_1)_{1\text{-}2}$ and 16_1 (Intermediate that connects both TS)

$TS(13q_1)_1$



$TS(13q_1)_2$



	Ea (V, kcal)	Ea (G, kcal)	Ea (V_{DCM}, kcal)	Ea (G_{DCM}, kcal)	Ea ($V_{ZPE+DCM}$, kcal)
$TS(13q_1)_1$	5.94	24.46	14.79	33.31	16.63
16_1	3.20	22.28	12.07	31.15	14.72
$TS(13q_1)_2$	4.85	23.81	12.16	31.12	14.27

Cartesian Coordinates (in Å) and Absolute Energies (in a.u.)

Gold(I)-catalyzed cyclopropanation with (*E*)-oct-6-en-1-yne.

(E)-oct-6-en-1-yne

E = -311.981517792 a.u.

C	-1.998325	1.034190	-0.026079
C	-1.802453	2.225030	0.032288
H	-1.617202	3.273434	0.085756
C	-2.278321	-0.402917	-0.081638
H	-3.215571	-0.588723	0.461321
H	-2.473539	-0.695074	-1.123824
C	-1.184433	-1.327085	0.504426
H	-0.921272	-0.986776	1.512902
H	-1.636523	-2.321783	0.611967
C	0.096990	-1.476249	-0.346420
H	0.654622	-2.345485	0.026427
H	-0.203827	-1.723366	-1.377174
C	1.011898	-0.279346	-0.356822
H	0.604512	0.642940	-0.768911
C	2.263740	-0.283536	0.110838
H	2.666331	-1.209280	0.528509
C	3.192142	0.898089	0.112328
H	3.515902	1.149954	1.131713
H	4.104983	0.690837	-0.463262
H	2.714162	1.784271	-0.318952

Propene

E = -117.905213202 a.u.

C	-1.283180	0.220543	-0.000072
C	-0.133857	-0.455976	0.000002
H	-1.305221	1.308830	0.000249
H	-2.245718	-0.284118	0.000175
C	1.235183	0.162966	0.000047
H	1.812271	-0.148789	0.881173
H	1.812714	-0.151377	-0.879973
H	1.181115	1.256951	-0.001646
H	-0.164037	-1.546696	0.000162

$13n_1$

E = -429.951262424 a.u.

C	2.343688	-1.256143	-0.686944
C	0.800152	-1.247332	-0.806435
C	0.321434	-0.013577	-0.029880
C	-1.100169	0.038237	0.463808
C	2.655130	-0.527294	0.641796
C	1.500398	0.447197	0.820299
C	1.063878	1.272745	-0.371629
C	0.454193	2.646521	-0.166533
C	-2.256563	-0.565310	-0.304667
C	-1.831551	-1.171100	1.013040
H	2.754796	-2.270741	-0.715223
H	2.792867	-0.715118	-1.527139
H	0.388446	-2.151493	-0.340048
H	0.470965	-1.248304	-1.853372
H	-1.347989	0.965420	0.976470
H	2.661108	-1.238750	1.478619
H	3.639106	-0.040827	0.624718
H	1.325012	0.869713	1.808414
H	1.702245	1.227334	-1.254786
H	-0.072960	2.729535	0.789753
H	1.237299	3.414891	-0.169811
H	-0.259683	2.895310	-0.962027
H	-1.978739	-1.142949	-1.185549
H	-1.336868	-2.138606	1.002464
H	-2.474438	-1.018958	1.877540
C	-3.573973	0.170812	-0.432760
H	-3.554357	0.886896	-1.264120
H	-4.405391	-0.523764	-0.608616
H	-3.801122	0.731878	0.482145

$13n_{2a}$

E = -429.948528368 a.u.

C	-2.288431	-1.130138	0.778769
C	-0.763637	-1.329978	0.613266
C	-0.253625	-0.100257	-0.151863
C	1.049673	-0.167403	-0.918566
C	-2.716800	-0.282636	-0.441769
C	-1.487185	0.550233	-0.772067
C	-0.764708	1.244493	0.358007
C	-0.009400	2.532806	0.096460
C	2.425257	-0.093115	-0.272750
C	1.957552	-1.381543	-0.902851
H	-2.826134	-2.082257	0.839677
H	-2.503925	-0.589797	1.707455
H	-0.570001	-2.221241	0.003396
H	-0.267083	-1.488168	1.579601
H	0.999821	0.328496	-1.886895
H	-2.955853	-0.931865	-1.294914
H	-3.609695	0.321220	-0.234463
H	-1.416082	1.001913	-1.760759
H	-1.258852	1.232396	1.330167
H	0.465084	2.537395	-0.890090
H	-0.688620	3.393604	0.140995
H	0.779914	2.693393	0.841097
H	1.706959	-2.197867	-0.230075
H	2.401969	-1.708867	-1.839646
H	3.164812	0.467395	-0.844366
C	2.613956	0.011687	1.226429
H	2.544107	1.052614	1.565096
H	1.858611	-0.563210	1.772139
H	3.599061	-0.370049	1.523190

$13n_{3a}$

E = -429.947099520 a.u.

C	-2.349658	-1.274949	0.414164
C	-0.824776	-1.472285	0.255192
C	-0.245939	-0.111235	-0.177135
C	1.033376	-0.195383	-0.973259
C	-2.708131	-0.127292	-0.557889
C	-1.445067	0.718731	-0.624608
C	-0.728751	1.070032	0.659475
C	-0.029894	2.411471	0.768913
C	2.245552	0.706340	-0.849582
C	2.339519	-0.730000	-0.402438
H	-2.912004	-2.191709	0.207245
H	-2.592400	-0.986228	1.443251
H	-0.618958	-2.197255	-0.544254
H	-0.359822	-1.865551	1.167271
H	0.846278	-0.535561	-1.993482
H	-2.932512	-0.525231	-1.557089
H	-3.592071	0.434690	-0.229479
H	-1.330842	1.420090	-1.449760
H	-1.234744	0.792621	1.585242
H	0.401553	2.729119	-0.184787
H	-0.752961	3.178460	1.074673
H	0.772725	2.401947	1.517156
H	2.888621	-1.399928	-1.063419
C	2.505949	-1.050096	1.069655
H	1.915227	-0.371871	1.695149
H	2.187002	-2.074601	1.297172
H	3.556013	-0.953293	1.373773
H	2.748142	1.012951	-1.763960
H	2.257676	1.459345	-0.069627
C	2.181900	-1.555498	-0.349417
C	0.777408	-1.232740	-0.915526
C	0.328929	0.062126	-0.224696
C	-1.138847	0.393080	-0.165837
C	2.207905	-0.924027	1.063019
C	1.260847	0.262741	0.965597
C	1.370455	1.174604	-0.238360
C	1.002682	2.641257	-0.119310
C	-2.108817	-0.013841	-1.257813
C	-2.214094	-0.634186	0.116153
H	2.383820	-2.631635	-0.331800
H	2.957329	-1.103264	-0.977686
H	0.081663	-2.042229	-0.658970
H	0.785382	-1.152224	-2.009921
H	-1.347123	1.367980	0.270060
H	1.823646	-1.633702	1.808219
H	3.224176	-0.648478	1.373488
H	0.879192	0.700059	1.886864
H	2.224578	1.010488	-0.896193
H	0.234996	2.817734	0.641540
H	1.881660	3.231153	0.168914
H	0.628320	3.043627	-1.069122
H	-2.870864	0.701324	-1.560318
H	-1.737783	-0.632323	-2.070902
C	-3.373586	-0.297068	1.030994
H	-4.253413	-0.913402	0.805883
H	-3.112868	-0.458373	2.084734
H	-1.881098	-1.668703	0.186028

$13n_{4a}$
E = -429.951208919 a.u.

Using $[Au(NHC)]^+$ as catalyst:
$3a_a$
E = -752.470497847 a.u.

C	-3.890011	2.085697	0.510256
C	-2.612825	1.591076	-0.211221
C	-2.662312	0.065554	-0.224087
C	-1.560234	-0.765985	-0.118495
C	-4.298178	0.951496	1.473725
C	-3.943400	-0.355074	0.795466
C	-4.092964	-0.537807	-0.629684
C	-4.222966	-1.909291	-1.257434
H	-3.721002	3.024075	1.044677
H	-4.691359	2.279153	-0.210334
H	-1.712895	1.899769	0.330712
H	-2.536928	1.993348	-1.227916
H	-1.811101	-1.829548	-0.087739
H	-3.756064	1.019490	2.423022
H	-5.369976	0.971430	1.709891
H	-3.774261	-1.235469	1.409945
H	-4.631913	0.243606	-1.164208
H	-3.738086	-2.692767	-0.667963
H	-5.286566	-2.164576	-1.323664
H	-3.808660	-1.924170	-2.269991
Au	0.408604	-0.298399	-0.049509
C	2.444701	0.110097	0.010635
N	3.072728	1.276077	-0.299626
N	3.444862	-0.740263	0.366597
C	4.441341	1.155443	-0.139744
C	2.416866	2.501755	-0.753626
C	4.675642	-0.115102	0.281210
C	3.271241	-2.128498	0.794815
H	5.120157	1.970631	-0.338040
H	2.637679	3.319610	-0.062549
H	1.340964	2.330357	-0.781406
H	2.768044	2.763558	-1.755369
H	5.598019	-0.620272	0.523393
H	3.852876	-2.790412	0.148024
H	3.601705	-2.244266	1.830587
H	2.215100	-2.386927	0.720445

TS($13n_{1a}$)
E = -870.368564316 a.u.

C	2.833755	-3.005700	-0.340683
C	2.302903	-1.728860	-1.036319
C	2.495072	-0.576819	-0.042304
C	1.524564	0.511630	0.022674
C	2.642513	-2.753008	1.169908

C	2.800220	-1.250871	1.345373
C	3.882783	-0.521800	0.619547
C	4.483790	0.731645	1.225116
C	2.501039	2.369399	-1.203448
C	1.639016	1.522692	-1.841770
H	2.313457	-3.905482	-0.681408
H	3.893981	-3.154268	-0.570453
H	1.230982	-1.824359	-1.249920
H	2.811119	-1.546956	-1.992033
H	1.800584	1.286453	0.741219
H	1.636847	-3.049040	1.492712
H	3.358239	-3.314006	1.782786
H	2.410693	-0.787688	2.249504
H	4.621335	-1.144509	0.115589
H	3.738357	1.361077	1.723062
H	5.224308	0.452362	1.982873
H	5.002205	1.340021	0.475315
H	3.542203	2.070916	-1.107723
H	2.002266	0.670839	-2.405537
C	2.124913	3.697564	-0.636387
H	2.490697	3.820016	0.390297
H	2.606004	4.489017	-1.228862
H	1.044217	3.865667	-0.660003
H	0.624500	1.840948	-2.058855
Au	-0.537435	0.217036	-0.029690
C	-2.576111	-0.107257	0.082898
N	-3.323264	-0.989575	-0.633110
N	-3.462687	0.510202	0.909224
C	-4.655171	-0.922791	-0.260717
C	-2.818533	-1.888676	-1.669769
C	-4.742709	0.021275	0.711309
C	-3.134813	1.541503	1.892769
H	-5.412922	-1.542986	-0.714323
H	-3.257492	-1.629478	-2.637205
H	-3.070799	-2.922348	-1.418786
H	-1.735083	-1.783718	-1.723509
H	-5.591248	0.382409	1.271805
H	-3.345754	1.176878	2.901845
H	-2.074316	1.777524	1.807584
H	-3.724755	2.440934	1.697535

TS($13n_{2a}$)
E = -870.364754896 a.u.

C	-2.702778	2.841077	-0.538509
C	-2.323948	1.444654	-1.085723
C	-2.402195	0.474679	0.100259
C	-1.469276	-0.649836	0.196798
C	-2.260983	2.821653	0.939034
C	-2.432767	1.378120	1.384022
C	-3.653185	0.609251	0.983951
C	-4.155844	-0.488473	1.902221
C	-2.822181	-2.364142	-1.007739
C	-1.560779	-1.989420	-1.389354
H	-2.230042	3.647802	-1.106241
H	-3.783694	3.000985	-0.611739
H	-1.291391	1.448262	-1.457790
H	-2.968932	1.142721	-1.919792
H	-1.709714	-1.330834	1.015961
H	-1.205439	3.104956	1.035417
H	-2.841049	3.514087	1.560979
H	-1.910364	1.041828	2.277082
H	-4.455937	1.189393	0.529959
H	-3.341178	-1.048626	2.374053
H	-4.748900	-0.046196	2.710363
H	-4.800096	-1.205392	1.380986
H	-1.421749	-1.332477	-2.243084
H	-0.710966	-2.605254	-1.119103
H	-2.922404	-3.137889	-0.246959
C	-4.083206	-1.811879	-1.570417
H	-4.658157	-2.637943	-2.013032
H	-4.721326	-1.378242	-0.792524
H	-3.900664	-1.063154	-2.344828
Au	0.595443	-0.338094	0.008659
C	2.626610	0.031163	0.006028
N	3.339649	0.774562	-0.881878
N	3.542737	-0.406444	0.910621
C	4.680586	0.799466	-0.537163
C	2.792769	1.462093	-2.050389
C	4.808254	0.055848	0.591641
C	3.259843	-1.252545	2.069614
H	5.415572	1.335665	-1.117573
H	2.966939	2.538251	-1.966054
H	1.720794	1.270602	-2.094691
H	3.267197	1.085101	-2.960448
H	5.676155	-0.182051	1.187230
H	3.547522	-0.733987	2.988113
H	2.190956	-1.463879	2.092757
H	3.814627	-2.191344	1.990069

TS($13n_{3a}$)
E = -870.361955368 a.u.

C	2.960241	2.700510	0.455099
C	2.430126	1.368722	1.041493
C	2.540567	0.324899	-0.079284
C	1.542337	-0.756302	-0.212184
C	2.693091	2.611916	-1.062207
C	2.787075	1.130846	-1.390750
C	3.892368	0.304288	-0.804170
C	4.422450	-0.893646	-1.569030
C	2.462974	-2.401198	0.691103
C	1.372431	-2.156175	1.483688
C	1.412308	-1.448822	2.802122
H	2.480632	3.569967	0.914423
H	4.033459	2.801882	0.647167
H	1.373527	1.466974	1.321339
H	2.980782	1.082555	1.945202
H	1.683773	-1.365744	-1.104614
H	1.685162	2.971662	-1.304500
H	3.400685	3.211870	-1.646685
H	2.347572	0.775930	-2.321000
H	4.677064	0.855093	-0.286054
H	3.633359	-1.442447	-2.094846
H	5.138163	-0.558044	-2.327659
H	2.431521	-3.152939	-0.089921
H	2.350907	-0.913791	2.960649
H	1.318456	-2.210989	3.588339
H	0.573172	-0.757991	2.921211
H	4.949477	-1.597883	-0.915224

H	3.440482	-2.016890	0.959843
H	0.443949	-2.668800	1.244385
Au	-0.513434	-0.325815	-0.060693
C	-2.518821	0.165814	-0.107925
N	-3.158837	1.137431	0.596369
N	-3.485455	-0.398979	-0.880215
C	-4.503650	1.178373	0.268638
C	-2.537992	2.031807	1.571914
C	-4.709054	0.210885	-0.661455
C	-3.287221	-1.493197	-1.830139
H	-5.186483	1.881401	0.720404
H	-3.005167	1.897855	2.551398
H	-2.652484	3.070875	1.251461
H	-1.477643	1.788985	1.639060
H	-5.605780	-0.093408	-1.179018
H	-3.510814	-1.152454	-2.844772
H	-2.247152	-1.814741	-1.777540
H	-3.940692	-2.330996	-1.572841

TS($13n_{4a}$)
E = -870.361912838 a.u.

C	2.898764	-2.568170	-1.196342
C	2.427859	-1.112532	-1.434493
C	2.547499	-0.392238	-0.084051
C	1.591128	0.670533	0.273068
C	2.584095	-2.854707	0.287169
C	2.724374	-1.510865	0.985554
C	3.876211	-0.609934	0.648797
C	4.421312	0.333864	1.704052
C	2.653032	2.431139	-0.361711
C	1.620887	2.288031	-1.245414
H	2.407032	-3.274043	-1.872056
H	3.974035	-2.658267	-1.381732
H	1.374390	-1.098707	-1.742154
H	3.007475	-0.621511	-2.227092
H	1.792683	1.139141	1.238951
H	1.554499	-3.215224	0.405244
H	3.246351	-3.615882	0.716479
H	2.272126	-1.383593	1.967219
H	4.657591	-1.045499	0.026377
H	3.635590	0.758365	2.338882
H	5.106393	-0.209479	2.364134
H	2.594681	3.161219	0.441844
H	4.986410	1.163034	1.263100
H	3.609352	1.950037	-0.518167
C	0.421638	3.188466	-1.271912
H	0.629585	3.997468	-1.987388
H	-0.479649	2.673988	-1.612763
H	0.228297	3.645995	-0.297528
H	1.762820	1.634085	-2.102830
Au	-0.463749	0.293938	0.091599
C	-2.462903	-0.229115	0.097698
N	-3.200042	-0.736938	-0.926489
N	-3.324527	-0.163818	1.148025
C	-4.500929	-0.984443	-0.521421
C	-2.711572	-1.002778	-2.278463
C	-4.578963	-0.623750	0.785133
C	-2.997497	0.313780	2.491278
H	-5.246221	-1.388317	-1.189276
H	-3.304868	-0.441835	-3.005609
H	-2.780573	-2.071762	-2.497981
H	-1.670057	-0.687565	-2.339399
H	-5.405511	-0.652494	1.478379
H	-3.133613	-0.492404	3.217266
H	-1.956968	0.637900	2.501275
H	-3.643331	1.155844	2.754075

$13n_{1a}$·Au(NHC)$^+$
E = -870.398138709 a.u.

C	-2.824380	2.903325	-0.653203
C	-2.936933	1.410493	-1.048636
C	-2.492897	0.621788	0.190603
C	-2.116024	-0.825286	0.058429
C	-1.718848	2.961776	0.426775
C	-1.787750	1.606920	1.118085
C	-3.142274	1.064752	1.504690
C	-3.289521	0.150410	2.706922
C	-2.834397	-1.735322	-0.839368
C	-1.390970	-1.431964	-1.311522
H	-2.604348	3.539766	-1.515179
H	-3.774156	3.257083	-0.239926
H	-2.254342	1.198106	-1.882634
H	-3.948280	1.153847	-1.385739
H	-1.747130	-1.293751	0.967335
H	-0.730550	3.083786	-0.037518
H	-1.857393	3.802143	1.116442
H	-0.940269	1.282827	1.721053
H	-3.990263	1.738067	1.384617
H	-2.383634	-0.432337	2.909362
H	-3.490138	0.747770	3.603217
H	-4.123450	-0.550939	2.585034
H	-3.576335	-1.258380	-1.476218
H	-1.355601	-0.841343	-2.222104
C	-3.169895	-3.154358	-0.428853
H	-4.112592	-3.176140	0.128793
H	-3.281230	-3.800499	-1.305958
H	-2.390191	-3.581240	0.212979
H	-0.801304	-2.351169	-1.319800
Au	0.538994	-0.539891	-0.388994
C	2.402151	0.076415	0.104776
N	3.108853	1.089691	-0.458398
N	3.215916	-0.447361	1.057457
C	4.354119	1.199108	0.137671
C	2.661511	1.942252	-1.560583
C	4.420837	0.234480	1.090728
C	2.892250	-1.561505	1.949488
H	5.073629	1.943524	-0.166749
H	3.264712	1.748247	-2.451582
H	2.756001	2.992456	-1.273800
H	1.616730	1.717953	-1.774808
H	5.208143	-0.023529	1.782165
H	2.830252	-1.208121	2.982305
H	1.932198	-1.981488	1.649936
H	3.663775	-2.331286	1.869865

$13n_{2a}$·Au(NHC)$^+$
E =-870.393933836 a.u.

C	-2.247571	2.842089	-0.779682
C	-2.261159	1.343691	-1.167779
C	-2.403072	0.575377	0.153948
C	-2.028773	-0.883515	0.279084
C	-1.660245	2.891442	0.649546
C	-2.061390	1.560775	1.268863
C	-3.486416	1.091396	1.103139
C	-4.133768	0.208080	2.153394
C	-2.755435	-1.984642	-0.386119
C	-1.347841	-1.740881	-0.960099
H	-1.676097	3.444337	-1.492514
H	-3.266778	3.241421	-0.784490
H	-1.301551	1.072361	-1.631610
H	-3.046088	1.123823	-1.900500
H	-1.639278	-1.155066	1.257970
H	-0.564641	2.962790	0.617415
H	-2.023893	3.755689	1.216772
H	-1.530335	1.214070	2.154797
H	-4.183794	1.801916	0.660886
H	-3.410434	-0.434509	2.667101
H	-4.615474	0.827770	2.917805
H	-4.905756	-0.437143	1.717684
H	-1.361884	-1.312495	-1.958090
H	-0.699988	-2.609453	-0.827898
H	-2.808243	-2.900905	0.199885
C	-3.964006	-1.768300	-1.274287
H	-4.108463	-2.631028	-1.932812
H	-4.865754	-1.657885	-0.662275
H	-3.869532	-0.876754	-1.898352
Au	0.585525	-0.641737	-0.230035
C	2.449560	0.072028	0.087340
N	3.138906	0.939301	-0.697698
N	3.285494	-0.232751	1.112740
C	4.397058	1.172789	-0.168538
C	2.668201	1.522789	-1.954757
C	4.488749	0.437667	0.969166
C	2.991369	-1.135827	2.226289
H	5.105741	1.834421	-0.642335
H	2.839249	2.601719	-1.942318
H	1.600777	1.327066	-2.054446
H	3.200270	1.075324	-2.798763
H	5.291556	0.336480	1.683143
H	3.086539	-0.598261	3.173146
H	1.970891	-1.502761	2.118457
H	3.684155	-1.981292	2.211782

$13n_{3a}$·Au(NHC)$^+$
E = -870.387580473 a.u.

C	-2.761810	2.612990	-0.854119
C	-2.597386	1.111323	-1.190947
C	-2.464271	0.398118	0.161276
C	-1.920990	-1.008863	0.265883
C	-2.011746	2.814324	0.482638
C	-2.139492	1.473898	1.192773
C	-3.495485	0.807684	1.216242
C	-3.890006	-0.094251	2.371483
C	-2.652559	-2.159416	-0.354410
C	-1.298998	-2.035608	-0.977601
C	-1.219799	-1.750326	-2.471311
H	-2.378786	3.254288	-1.653659
H	-3.820724	2.863584	-0.737384
H	-1.670959	0.967006	-1.762268
H	-3.422838	0.735912	-1.808652
H	-1.551360	-1.268208	1.257401
H	-0.950000	3.033176	0.303519
H	-2.419418	3.648133	1.065253
H	-1.469791	1.254074	2.023300
H	-4.332566	1.392972	0.837294
H	-3.029532	-0.592105	2.832167
H	-4.375180	0.497494	3.155569
H	-2.851552	-3.026854	0.269887
H	-1.946611	-0.998719	-2.783754
H	-1.462665	-2.682398	-2.997485
H	-0.226599	-1.430853	-2.800106
H	-4.599286	-0.868635	2.056621
H	-3.483525	-1.884861	-1.000940
H	-0.610121	-2.806001	-0.627730
Au	0.470499	-0.576636	-0.110769
C	2.318033	0.215663	0.124026
N	2.882933	1.217362	-0.598430
N	3.257785	-0.148708	1.034023
C	4.165279	1.476091	-0.144504
C	2.261169	1.931073	-1.714348
C	4.400383	0.618411	0.881427
C	3.116436	-1.194093	2.048697
H	4.788589	2.238239	-0.586269
H	2.808107	1.727576	-2.638909
H	2.266578	3.005212	-1.513043
H	1.232028	1.588197	-1.818483
H	5.267968	0.488641	1.509919
H	3.211693	-0.757773	3.046409
H	2.132426	-1.650871	1.944969
H	3.887118	-1.955666	1.904742

$13n_{4a}$·Au(NHC)$^+$
E = -870.389616956 a.u.

C	2.409871	-2.585350	-1.402585
C	2.447990	-1.040261	-1.494885
C	2.399560	-0.541155	-0.044371
C	2.059257	0.904393	0.237930
C	1.656318	-2.902703	-0.089450
C	1.956322	-1.717945	0.818371
C	3.381890	-1.224604	0.908810
C	3.884648	-0.561952	2.178341
C	2.842573	1.956301	-0.473745
C	1.396769	2.055657	-0.855797
H	1.935381	-3.036261	-2.279162
H	3.427742	-2.985437	-1.360712
H	1.557998	-0.677286	-2.029381
H	3.324946	-0.686560	-2.050393
H	1.857320	1.151921	1.277320
H	0.573703	-2.958294	-0.267933
H	1.963543	-3.861984	0.342290
H	1.328631	-1.557296	1.694105
H	4.142387	-1.834712	0.422290

H	3.086167	-0.059067	2.735748
H	4.315276	-1.315916	2.846420
H	3.231086	2.780036	0.121388
H	4.666472	0.177084	1.967273
H	3.531800	1.602895	-1.235780
C	0.691965	3.338279	-0.419978
H	1.136854	4.177430	-0.970109
H	-0.383396	3.336526	-0.619200
H	0.841014	3.530358	0.647844
H	1.196253	1.714830	-1.869668
Au	-0.382102	0.559493	-0.093499
C	-2.237283	-0.217387	0.125643
N	-3.039191	-0.720058	-0.848348
N	-2.950005	-0.331810	1.276048
C	-4.242318	-1.146093	-0.311088
C	-2.710187	-0.818141	-2.270942
C	-4.186607	-0.901557	1.023208
C	-2.517839	0.103916	2.604597
H	-5.020767	-1.581806	-0.918303
H	-3.447065	-0.265447	-2.859291
H	-2.704375	-1.866663	-2.580102
H	-1.722265	-0.387053	-2.431507
H	-4.908172	-1.079615	1.805614
H	-2.604285	-0.726242	3.309957
H	-1.477472	0.423275	2.546506
H	-3.135897	0.939987	2.942923

TS(14_a)
E = -752.451326883 a.u.

C	-4.009461	-0.793606	1.962289
C	-2.657305	-1.190064	1.318999
C	-2.730173	-0.694814	-0.107279
C	-1.670343	-0.011534	-0.867559
C	-4.972734	-0.563021	0.768895
C	-4.051857	-0.308186	-0.398275
C	-2.721316	1.026511	-0.365567
H	-4.380492	-1.550371	2.656681
H	-3.891160	0.134064	2.531976
H	-2.545155	-2.282145	1.242738
H	-1.773649	-0.818866	1.845089
H	-5.567602	-1.458532	0.540231
H	-5.687144	0.250372	0.932044
H	-4.428910	-0.165477	-1.405250
H	-2.582755	1.423232	0.637723
C	-3.227780	2.062026	-1.365369
H	-4.142557	2.549582	-1.016730
H	-2.444067	2.822966	-1.458438
H	-3.399797	1.635770	-2.356047
H	-1.817817	-0.085384	-1.948914
Au	0.343552	0.002410	-0.322403
C	2.360842	0.003978	0.137874
N	3.070043	0.960881	0.794629
N	3.274904	-0.955534	-0.168773
C	4.404829	0.604566	0.895794

Using $[Au(PMe_3)]^+$ as catalyst:
$3a_b$
E = -908.741279234 a.u.

C	2.524389	2.210305	1.320555
C	4.533584	-0.602857	0.289010
C	2.994804	-2.197739	-0.887351
H	5.134590	1.232683	1.383081
H	2.703917	2.271761	2.397404
H	1.451356	2.225918	1.129618
H	2.993932	3.063164	0.822524
H	5.397484	-1.233249	0.144671
H	3.585892	-2.237852	-1.806285
H	3.239390	-3.057041	-0.256919
H	1.934425	-2.221808	-1.138450

14_a
E= -752.462916473 a.u.

C	-3.950197	-1.344268	1.851543
C	-2.565478	-0.767369	1.466944
C	-2.783532	-0.235790	0.054126
C	-1.681500	0.465097	-0.836700
C	-4.633113	-1.660518	0.495002
C	-3.945509	-0.739026	-0.460069
C	-2.536789	1.487797	-0.318653
H	-3.876830	-2.219898	2.500402
H	-4.537602	-0.588167	2.383422
H	-1.795473	-1.548479	1.427153
H	-2.206602	-0.005997	2.166897
H	-4.456519	-2.701060	0.175637
H	-5.721357	-1.528036	0.496645
H	-4.320920	-0.523392	-1.456983
H	-2.347920	1.851900	0.691046
C	-3.495192	2.318335	-1.121893
H	-4.401222	2.574582	-0.565106
H	-2.978868	3.261249	-1.353394
H	-3.762912	1.850576	-2.072857
H	-1.875731	0.269095	-1.894722
Au	0.324538	0.166640	-0.297321
C	2.333008	-0.095206	0.102519
N	3.108317	0.598294	0.978160
N	3.176002	-0.991595	-0.476293
C	4.415285	0.141227	0.947103
C	2.652344	1.685752	1.842089
C	4.457812	-0.859819	0.030985
C	2.808351	-1.967529	-1.501337
H	5.188619	0.562459	1.570842
H	2.817654	1.423608	2.890656
H	1.587338	1.841332	1.670300
H	3.195918	2.604185	1.604313
H	5.275619	-1.481377	-0.299783
H	3.372837	-1.776287	-2.417988
H	3.020069	-2.979184	-1.144860
H	1.742237	-1.870711	-1.706302

C	3.695287	2.091639	0.418113

C	2.398463	1.366604	0.852690
C	2.436352	-0.033814	0.247875
C	1.341771	-0.742372	-0.199899
C	4.123655	1.438766	-0.912687
C	3.757141	-0.027085	-0.830280
C	3.865385	-0.770783	0.398657
P	-2.964355	0.211975	0.043584
Au	-0.638036	-0.259423	-0.082064
C	3.971119	-2.280308	0.422713
H	3.542884	3.167847	0.304114
H	4.479524	1.967790	1.171905
H	1.512499	1.882490	0.468763
H	2.302312	1.322194	1.943413
H	1.579555	-1.706545	-0.655299
H	3.605475	1.889577	-1.765782
H	5.201000	1.540538	-1.097948
H	3.594630	-0.580748	-1.751457
H	4.383875	-0.277721	1.220193
H	3.505298	-2.751672	-0.447379
H	5.031941	-2.554987	0.411507
H	3.524735	-2.696305	1.330761
C	-3.490689	1.653853	-0.970830
H	-4.569286	1.817884	-0.875051
H	-2.961804	2.553140	-0.641654
H	-3.248756	1.476055	-2.022843
C	-4.027129	-1.177569	-0.524879
H	-5.086224	-0.911250	-0.441907
H	-3.799024	-1.417322	-1.567667
H	-3.833266	-2.065855	0.083634
C	-3.553083	0.590742	1.744903
H	-4.630538	0.787115	1.744199
H	-3.344600	-0.255066	2.406725
H	-3.029689	1.469636	2.132811

TS(13n$_{1b}$)
E = -1026.64109633 a.u.

C	-2.658708	-2.804791	1.041054
C	-2.082729	-1.418513	1.420705
C	-2.299498	-0.506861	0.206730
C	-1.317929	0.506332	-0.141499
C	-2.531720	-2.892298	-0.495005
C	-2.677145	-1.463361	-0.992556
C	-3.712755	-0.568077	-0.401752
P	3.058864	-0.289305	-0.106817
Au	0.745885	0.175293	-0.042582
C	-4.325591	0.536131	-1.239768
C	-2.206685	2.666051	0.646585
C	-1.354815	1.961994	1.448282
H	-2.133333	-3.619179	1.547883
H	-3.709036	-2.879424	1.341181
H	-1.004918	-1.488119	1.614180
H	-2.551129	-1.020031	2.329675
H	-1.594230	1.103670	-1.012249
H	-1.547238	-3.277901	-0.786646
H	-3.283290	-3.555105	-0.940604
H	-2.317619	-1.217221	-1.989500
H	-4.433723	-1.048361	0.258879
H	-3.597102	1.028740	-1.893056
H	-5.101303	0.113278	-1.887800
H	-4.805091	1.301110	-0.618906
H	-3.259916	2.395116	0.649997
H	-1.727263	1.278245	2.203006
C	-1.806815	3.804023	-0.231843
H	-2.189830	3.683123	-1.252552
H	-2.255973	4.730268	0.154300
H	-0.721952	3.940470	-0.265490
H	-0.322881	2.280165	1.558694
C	3.965536	0.636715	-1.412417
H	3.864439	1.712859	-1.243152
H	5.028280	0.371883	-1.405484
H	3.544534	0.401391	-2.394339
C	3.442468	-2.058135	-0.435316
H	4.525684	-2.219437	-0.451117
H	2.999053	-2.685080	0.343933
H	3.022444	-2.357171	-1.400204
C	3.958114	0.097956	1.451619
H	5.019687	-0.153780	1.354594
H	3.863645	1.163236	1.682241
H	3.529835	-0.474297	2.279866

TS(13n$_{2b}$)
E = -1026.63760815 a.u.

C	2.525629	2.459219	1.461873
C	2.086839	0.976535	1.508291
C	2.207173	0.439453	0.076901
C	1.256983	-0.549360	-0.422351
C	2.172144	2.936196	0.037460
C	2.333722	1.709499	-0.846014
C	3.507421	0.802859	-0.662924
P	-3.121077	0.174858	0.022059
Au	-0.811845	-0.265272	-0.138557
C	4.035104	0.033012	-1.858510
C	2.559812	-2.613390	0.181907
C	1.264268	-2.395424	0.568049
H	2.036295	3.057001	2.236133
H	3.603215	2.546214	1.636353
H	1.036131	0.898221	1.815873
H	2.679097	0.396275	2.225928
H	1.494251	-0.912304	-1.423908
H	1.132616	3.283187	-0.012518
H	2.806477	3.765648	-0.297777
H	1.851311	1.701805	-1.821184
H	4.295764	1.172236	-0.007927
H	3.237575	-0.295257	-2.533997
H	4.701444	0.677748	-2.441997
H	4.612718	-0.849914	-1.562602
H	1.041529	-2.106278	1.591043
H	0.452529	-2.849678	0.011064
H	2.740152	-3.041414	-0.803857
C	3.756621	-2.319023	1.013348
H	4.338220	-3.243839	1.134282
H	4.423079	-1.601355	0.521050
H	3.492721	-1.941094	2.004009
C	-4.089617	-0.400176	-1.432331
H	-5.150883	-0.160409	-1.305947
H	-3.719432	0.083970	-2.340834
H	-3.978985	-1.482325	-1.548774
C	-3.937649	-0.613241	1.470595

H	-5.005676	-0.371044	1.488924
H	-3.819016	-1.699606	1.418951
H	-3.474855	-0.258775	2.396367
C	-3.523659	1.963098	0.174065
H	-4.607371	2.108660	0.237145
H	-3.055182	2.375221	1.072695
H	-3.140539	2.505152	-0.695532

TS($13n_{3b}$)
E = -1026.63477321 a.u.

C	-2.818588	-2.153962	1.620371
C	-2.233087	-0.721296	1.562748
C	-2.350879	-0.261659	0.102368
C	-1.328812	0.605885	-0.506164
C	-2.600930	-2.741981	0.210581
C	-2.664034	-1.548675	-0.728647
C	-3.723376	-0.506151	-0.540667
P	2.989949	-0.417260	-0.037854
Au	0.723371	0.207808	-0.196027
C	-4.245451	0.262830	-1.739191
C	-2.157611	2.540101	-0.418243
C	-1.076568	2.617192	0.419065
C	-1.138992	2.548783	1.912567
H	-2.347704	-2.757134	2.402022
H	-3.887140	-2.119502	1.856847
H	-1.171345	-0.726934	1.841457
H	-2.748738	-0.051810	2.260667
H	-1.471242	0.771244	-1.573755
H	-1.614136	-3.214882	0.129874
H	-3.346257	-3.505140	-0.043103
H	-2.243746	-1.648441	-1.727567
H	-4.505300	-0.745466	0.179611
H	-3.461498	0.498318	-2.467389
H	-4.996081	-0.339882	-2.262157
H	-2.092218	2.869737	-1.449491
H	-2.105276	2.190262	2.273118
H	-0.988097	3.567009	2.297608
H	-0.341494	1.926497	2.328722
H	-4.730337	1.200511	-1.444931
H	-3.151214	2.354242	-0.026330
H	-0.126187	2.929386	-0.007893
C	3.766038	-0.747595	-1.672870
H	3.723166	0.151447	-2.294729
H	4.812100	-1.046611	-1.547084
H	3.224614	-1.547914	-2.185979
C	4.082838	0.835641	0.751200
H	5.116762	0.475830	0.785881
H	4.050084	1.769195	0.181630
H	3.742349	1.039216	1.770804
C	3.271374	-1.958228	0.927291
H	4.337062	-2.210557	0.944932
H	2.918091	-1.826415	1.954249
H	2.716739	-2.785453	0.474493

TS($13n_{4b}$)
E = -1026.63450998 a.u.

C	2.887834	-2.180828	-1.599169
C	2.296064	-0.750671	-1.598118
C	2.382889	-0.245890	-0.151534
C	1.356379	0.662734	0.374608
C	2.625230	-2.727032	-0.179196
C	2.663948	-1.506687	0.727818
C	3.734656	-0.474994	0.539652
P	-2.925361	-0.535169	0.087265
Au	-0.681428	0.187274	0.141106
C	4.219826	0.326641	1.732518
C	2.238493	2.617697	0.079254
C	1.305381	2.492905	-0.910177
H	2.443025	-2.807988	-2.377041
H	3.963211	-2.149270	-1.802231
H	1.238895	-0.773048	-1.893585
H	2.819981	-0.095146	-2.305749
H	1.530632	0.982492	1.404506
H	1.634341	-3.193930	-0.116276
H	3.358996	-3.484743	0.120330
H	2.214161	-1.575328	1.716461
H	4.538077	-0.741782	-0.146416
H	3.410468	0.597654	2.419790
H	4.938472	-0.269512	2.305501
H	2.029710	3.213022	0.965063
H	4.732239	1.246861	1.429806
H	3.253620	2.265638	-0.047835
C	0.010429	3.247619	-0.938952
H	0.171612	4.162248	-1.528033
H	-0.786324	2.683352	-1.429873
H	-0.317148	3.546655	0.060758
H	1.590720	1.980092	-1.825863
C	-3.744225	-0.478938	1.733639
H	-3.735427	0.545488	2.117627
H	-4.780864	-0.825225	1.662617
H	-3.202308	-1.115559	2.439295
C	-3.133881	-2.272084	-0.482332
H	-4.192377	-2.553317	-0.481617
H	-2.736133	-2.381253	-1.495638
H	-2.584677	-2.948724	0.179088
C	-4.023665	0.449936	-1.013042
H	-5.048080	0.063968	-0.977523
H	-4.027250	1.496908	-0.695419
H	-3.660491	0.400915	-2.043923

$13n_{1b}$·Au(PMe_3)$^+$
E = -1026.67160492 a.u.

C	-2.669209	2.482801	-1.499307
C	-2.689195	0.934845	-1.499658
C	-2.342749	0.518696	-0.064004
C	-1.903656	-0.888308	0.222339
C	-1.674612	2.882753	-0.384547
C	-1.760188	1.747815	0.627978
C	-3.126769	1.247005	1.030102
P	2.840852	0.426540	0.234593
Au	0.781161	-0.527236	-0.168442
C	-3.355637	0.663550	2.412316
C	-2.513413	-2.045936	-0.438918
C	-1.047649	-1.787847	-0.876933
H	-2.389743	2.888303	-2.475865
H	-3.666005	2.874337	-1.273731

H	-1.918110	0.558892	-2.185687
H	-3.651664	0.539487	-1.845433
H	-1.581890	-1.075814	1.243889
H	-0.652341	2.942570	-0.783977
H	-1.909901	3.861535	0.048583
H	-0.965835	1.638937	1.366146
H	-3.980278	1.820271	0.670168
H	-2.454095	0.203515	2.832552
H	-3.660028	1.457358	3.103350
H	-4.150418	-0.091577	2.407702
H	-3.218671	-1.802254	-1.230815
H	-0.964224	-1.469341	-1.911993
C	-2.818935	-3.323628	0.315066
H	-3.801822	-3.255510	0.794107
H	-2.831539	-4.184509	-0.361474
H	-2.075762	-3.514149	1.098100
H	-0.417699	-2.630661	-0.585254
C	3.905249	-0.604627	1.318511
H	4.063476	-1.585838	0.861902
H	4.874951	-0.117012	1.466382
H	3.423415	-0.746279	2.290172
C	2.753046	2.068901	1.050653
H	3.762307	2.463375	1.210866
H	2.190700	2.768209	0.425460
H	2.247057	1.979066	2.016187
C	3.808871	0.688730	-1.303267
H	4.784915	1.125352	-1.065376
H	3.958994	-0.265960	-1.815512
H	3.268761	1.362714	-1.974424

$13n_{2b}\cdot Au(PMe_3)^+$

E = -1026.66741327 a.u.

C	-2.199294	2.381951	-1.589515
C	-2.116284	0.837737	-1.527515
C	-2.255229	0.473609	-0.041742
C	-1.806893	-0.863211	0.501773
C	-1.660355	2.877594	-0.227883
C	-2.000933	1.757875	0.745033
C	-3.392185	1.173246	0.704247
P	2.897428	0.418502	0.142159
Au	0.830117	-0.582033	-0.033525
C	-4.020424	0.595998	1.959044
C	-2.442733	-2.152017	0.163804
C	-1.024974	-1.981829	-0.421837
H	-1.640224	2.787388	-2.438099
H	-3.238304	2.698717	-1.723411
H	-1.128991	0.508858	-1.884104
H	-2.864597	0.367235	-2.175499
H	-1.433612	-0.822199	1.522958
H	-0.570181	3.010808	-0.268705
H	-2.090938	3.842837	0.061487
H	-1.480545	1.715630	1.701497
H	-4.114101	1.683901	0.067970
H	-3.280458	0.164230	2.641543
H	-4.545883	1.384280	2.509305
H	-4.753291	-0.183765	1.720925
H	-1.021422	-1.863325	-1.501452
H	-0.332786	-2.725631	-0.022705
H	-2.464115	-2.867648	0.984020
C	-3.620312	-2.281176	-0.781256
H	-3.697082	-3.309199	-1.149721
H	-4.551147	-2.040948	-0.256029
H	-3.539105	-1.616634	-1.644246
C	3.523159	0.457501	1.867597
H	4.516107	0.919198	1.897490
H	2.841091	1.033365	2.499647
H	3.589510	-0.560173	2.262853
C	4.187351	-0.450186	-0.833155
H	5.152029	0.054890	-0.713809
H	4.279520	-1.485198	-0.491764
H	3.914118	-0.455940	-1.892258
C	2.930206	2.159656	-0.438430
H	3.938939	2.571836	-0.326526
H	2.638888	2.206981	-1.491616
H	2.229340	2.763133	0.145362

$13n_{3b}\cdot Au(PMe_3)^+$

E = -1026.66107715 a.u.

C	2.537493	2.036539	1.782598
C	2.256729	0.526756	1.589548
C	2.300989	0.286563	0.074080
C	1.682901	-0.944601	-0.556557
C	2.017085	2.716105	0.495317
C	2.188103	1.658689	-0.586060
C	3.496703	0.905816	-0.649534
P	-2.747775	0.603564	-0.113144
Au	-0.704117	-0.457884	-0.124940
C	4.012634	0.372405	-1.973000
C	2.328000	-2.294773	-0.408404
C	0.974985	-2.291438	0.216552
C	0.859591	-2.524518	1.714939
H	2.062345	2.426819	2.687534
H	3.611724	2.211831	1.896466
H	1.247474	0.292471	1.956512
H	2.962171	-0.093770	2.155806
H	1.332248	-0.795339	-1.578782
H	0.952315	2.970113	0.595809
H	2.550224	3.647220	0.272469
H	1.644398	1.773787	-1.523515
H	4.295027	1.263531	-0.000086
H	3.205388	0.103318	-2.663089
H	4.621623	1.135033	-2.470759
H	2.479284	-2.882374	-1.310009
H	1.638252	-2.000689	2.271419
H	0.991902	-3.599120	1.893143
H	-0.112119	-2.236243	2.127242
H	4.643532	-0.513001	-1.832494
H	3.161736	-2.331335	0.289656
H	0.230682	-2.816900	-0.383752
C	-3.352539	1.006724	-1.799145
H	-3.459775	0.090359	-2.386614
H	-4.323669	1.509975	-1.739178
H	-2.639083	1.663339	-2.305303
C	-4.079553	-0.393775	0.662915
H	-5.025502	0.157902	0.634353
H	-4.199883	-1.339053	0.126029
H	-3.824749	-0.613723	1.703634
C	-2.728807	2.195573	0.801040

H	-3.720033	2.660677	0.766777
H	-2.451331	2.022610	1.844848
H	-1.998213	2.875546	0.353557

$13n_{4b}$·Au(PMe$_3$)$^+$

E = -1026.66303050 a.u.

C	2.527072	-2.218241	-1.600457
C	2.343747	-0.681616	-1.583462
C	2.283704	-0.290707	-0.100262
C	1.766879	1.075750	0.292973
C	1.869362	-2.727118	-0.295911
C	2.026862	-1.574173	0.686794
C	3.376262	-0.899883	0.778509
P	-2.653368	-0.666692	0.171897
Au	-0.630961	0.414296	-0.025781
C	3.828189	-0.265433	2.081036
C	2.418036	2.266961	-0.336850
C	0.974133	2.193497	-0.718382
H	2.091625	-2.671962	-2.495538
H	3.591646	-2.472044	-1.610832
H	1.389269	-0.417813	-2.062254
H	3.137180	-0.169180	-2.140936
H	1.541020	1.217121	1.347719
H	0.801973	-2.932245	-0.457433
H	2.325370	-3.657386	0.061323
H	1.413677	-1.561184	1.587251
H	4.193345	-1.371525	0.233484
H	2.990439	0.100147	2.685505
H	4.362777	-1.004141	2.688214
H	2.694148	3.089963	0.318667
H	4.510682	0.574557	1.906781
H	3.149851	2.052184	-1.110502
C	0.095414	3.329700	-0.201176
H	0.402141	4.256192	-0.702957
H	-0.971488	3.183331	-0.394856
H	0.230043	3.479585	0.875281
H	0.805109	1.880935	-1.746761
C	-3.340398	-0.584369	1.872410
H	-3.472482	0.459579	2.170761
H	-4.309020	-1.094436	1.912538
H	-2.654126	-1.063440	2.576641
C	-2.588737	-2.452813	-0.248624
H	-3.582305	-2.899499	-0.133280
H	-2.257321	-2.581295	-1.283026
H	-1.885192	-2.969038	0.410567
C	-3.949571	0.041858	-0.918688
H	-4.890574	-0.502897	-0.785476
H	-4.108863	1.096238	-0.675410
H	-3.638227	-0.031244	-1.964676

TS(14_b)

E = -908.724615429 a.u.

C	3.874417	1.906982	0.645157
C	2.510369	1.722587	-0.066501
C	2.524438	0.312155	-0.606901
C	1.431871	-0.670225	-0.570102
C	4.789992	0.798997	0.061728
C	3.824782	-0.219036	-0.493723
C	2.479886	-0.997910	0.542555
P	-2.859449	0.247979	0.175405
Au	-0.571721	-0.199712	-0.188697
H	4.288416	2.906996	0.500454
H	3.752470	1.763461	1.723674
H	2.418151	2.371183	-0.950922
H	1.637812	1.920978	0.562007
H	5.405573	1.168538	-0.770132
H	5.482483	0.371860	0.794195
H	4.166939	-1.089813	-1.042720
H	2.360241	-0.485879	1.494702
C	-3.434269	-0.094619	1.889970
H	-2.879056	0.526380	2.599220
H	-4.504161	0.116938	1.990466
H	-3.253873	-1.145062	2.136953
C	-3.346637	1.994681	-0.139516
H	-4.419657	2.135095	0.029177
H	-2.790527	2.661636	0.526009
H	-3.110017	2.263406	-1.173322
C	-3.980507	-0.744363	-0.894784
H	-3.816606	-1.811087	-0.715439
H	-5.028224	-0.503154	-0.685760
H	-3.768439	-0.536004	-1.947669
C	2.919473	-2.453190	0.685649
H	3.834016	-2.541692	1.278757
H	2.113840	-2.978637	1.211366
H	3.065930	-2.941209	-0.280347
H	1.539494	-1.452724	-1.325866

14_b

E = -908.736309951 a.u.

C	3.850942	2.053285	0.652133
C	2.422476	1.453873	0.655735
C	2.574632	0.162499	-0.138606
C	1.441627	-0.880635	-0.397711
C	4.541766	1.418745	-0.584156
C	3.766992	0.160218	-0.807252
C	2.246385	-1.441143	0.645364
P	-2.829318	0.323395	0.075121
Au	-0.555982	-0.249997	-0.135155
H	3.849272	3.144992	0.618404
H	4.386289	1.753383	1.559256
H	1.707422	2.098602	0.127560
H	2.022571	1.298868	1.663268
H	4.454324	2.055261	-1.480139
H	5.614332	1.233433	-0.452804
H	4.106326	-0.643198	-1.455864
H	2.093494	-1.080597	1.662221
C	-3.660673	-0.448681	1.523367
H	-3.167767	-0.132766	2.447531
H	-4.715769	-0.157447	1.562896
H	-3.593329	-1.538230	1.451405
C	-3.144696	2.126687	0.260403
H	-4.219594	2.322214	0.338468
H	-2.647300	2.501339	1.159920
H	-2.745851	2.664305	-0.604859
C	-3.847002	-0.181449	-1.371784
H	-3.791544	-1.265919	-1.504608

H	-4.893037	0.108702	-1.225532
H	-3.466557	0.296814	-2.279159
C	3.115671	-2.655867	0.525001
H	4.030446	-2.581047	1.119938
H	2.534846	-3.496915	0.932483
H	3.361483	-2.899021	-0.511694

Using $[Au(P(OMe_3)_3)]^+$ as catalyst:

$3b_c$

E = -1134.41340829 a.u.

C	-4.029359	2.206306	-0.287867
C	-2.779481	1.442681	-0.789363
C	-2.876487	0.014395	-0.262659
C	-1.814272	-0.760364	0.148210
C	-4.465261	1.504398	1.015468
C	-4.183072	0.028283	0.847443
C	-4.341335	-0.639672	-0.419203
C	-4.521747	-2.139220	-0.520793
H	-3.819391	3.265435	-0.119329
H	-4.833386	2.163189	-1.029648
H	-1.861220	1.893522	-0.399627
H	-2.707864	1.453336	-1.882827
H	-2.087336	-1.738257	0.550721
H	-3.907687	1.879672	1.880157
H	-5.532102	1.651814	1.230098
H	-4.032314	-0.582593	1.733936
H	-4.851536	-0.078457	-1.201387
H	-4.065189	-2.678289	0.314255
H	-5.594212	-2.363455	-0.504198
H	-4.110767	-2.526616	-1.457741
Au	0.177805	-0.310817	0.067993
P	2.474397	0.194810	0.034055
O	3.249557	0.167044	1.439990
O	2.680758	1.702432	-0.452013
O	3.421930	-0.772707	-0.850475
C	3.479776	-1.063872	2.164771
C	3.973865	2.372201	-0.422964
C	3.060239	-1.168534	-2.193100
H	3.933025	-0.771325	3.111450
H	2.533857	-1.582217	2.354593
H	4.159978	-1.707380	1.602615
H	3.838427	3.294196	-0.986968
H	4.246089	2.591539	0.610587
H	4.736737	1.748169	-0.894308
H	3.776976	-1.936201	-2.484171
H	2.046676	-1.582660	-2.217566
H	3.133503	-0.314826	-2.872598

$TS(13n_{1c})$

E = -1252.31374304 a.u.

C	2.865374	-2.932582	-0.991148
C	2.388223	-1.516510	-1.396382
C	2.670774	-0.599662	-0.199856
C	1.757641	0.477127	0.136142
C	2.733806	-2.982550	0.545989
C	2.983671	-1.559529	1.018616
H	1.593532	-1.389141	-1.353261
C	4.076074	-0.747722	0.411121
C	4.763783	0.327699	1.228422
C	2.770790	2.572886	-0.673890
C	1.879165	1.910622	-1.468052
H	2.282144	-3.716174	-1.482716
H	3.907444	-3.086892	-1.289617
H	1.307690	-1.515593	-1.587462
H	2.881631	-1.168274	-2.312761
H	2.066942	1.067993	0.999849
H	1.724081	-3.289668	0.843975
H	3.436053	-3.689579	1.003977
H	2.642412	-1.270175	2.010424
H	4.761137	-1.287761	-0.241567
H	4.071041	0.881819	1.870991
H	5.508409	-0.135100	1.885465
H	5.294605	1.045237	0.592842
H	3.806281	2.240245	-0.673298
H	2.210712	1.198447	-2.215680
C	2.437275	3.740579	0.192973
H	2.811946	3.607417	1.215279
H	2.940062	4.635359	-0.201149
H	1.362158	3.940317	0.223788
H	0.867657	2.287920	-1.581557
Au	-0.317239	0.236571	0.030962
P	-2.606797	-0.203422	0.120549
O	-3.292300	-0.201234	1.572714
O	-2.872944	-1.693692	-0.390612
O	-3.597697	0.801045	-0.675464
C	-3.447628	1.009738	2.347636
C	-4.169977	-2.347386	-0.283042
C	-3.347328	1.177746	-2.046724
H	-3.828297	0.695314	3.319004
H	-2.482853	1.512175	2.476038
H	-4.161888	1.676816	1.859863
H	-4.093880	-3.249745	-0.888490
H	-4.363135	-2.601225	0.760364
H	-4.958396	-1.697106	-0.669177
H	-4.057278	1.971988	-2.277137
H	-2.324717	1.551352	-2.168173
H	-3.514437	0.325388	-2.711265

$TS(13n_{2c})$

E = -1252.31053314 a.u.

C	-2.771970	2.465431	-1.576042
C	-2.403548	0.963082	-1.566043
C	-2.592004	0.476524	-0.122982
C	-1.702235	-0.532861	0.438635
C	-2.431793	2.968948	-0.158033
C	-2.683740	1.782037	0.757868
C	-3.893183	0.926871	0.565225

C	-4.495581	0.222428	1.765955
C	-3.071077	-2.559719	-0.128162
C	-1.754282	-2.415000	-0.475594
H	-2.233533	3.014128	-2.353864
H	-3.839279	2.598336	-1.782286
H	-1.349275	0.828198	-1.840013
H	-3.001631	0.388703	-2.283640
H	-1.976041	-0.845668	1.447463
H	-1.376534	3.260546	-0.089198
H	-3.029247	3.841156	0.133678
H	-2.231990	1.781372	1.747669
H	-4.640959	1.311760	-0.127220
H	-3.736566	-0.130648	2.472794
H	-5.140468	0.919402	2.312267
H	-5.113764	-0.634927	1.476933
H	-1.484001	-2.181169	-1.501289
H	-0.983580	-2.877912	0.130572
H	-3.304552	-2.935365	0.867719
C	-4.223206	-2.245015	-1.013034
H	-4.859730	-3.136848	-1.097405
H	-4.854817	-1.457959	-0.584237
H	-3.908471	-1.943526	-2.015095
Au	0.374914	-0.318036	0.165904
P	2.644604	0.164247	-0.033341
O	3.216376	1.329329	0.912855
O	2.935138	0.727236	-1.500583
O	3.703432	-1.018364	0.284311
C	3.348618	1.160937	2.343702
C	4.222610	1.284021	-1.892580
C	3.554326	-2.344053	-0.269485
H	3.657316	2.131792	2.730258
H	2.389606	0.875367	2.789051
H	4.108484	0.407644	2.562609
H	4.177623	1.390307	-2.975753
H	4.357770	2.256790	-1.417258
H	5.032186	0.606459	-1.611512
H	4.322449	-2.956011	0.203143
H	2.565129	-2.753767	-0.039002
H	3.709415	-2.324417	-1.351932

TS(13n$_{3c}$)

E = -1252.30826687 a.u.

C	-3.187514	2.239588	-1.502697
C	-2.585823	0.812918	-1.522071
C	-2.751263	0.252458	-0.102529
C	-1.746561	-0.658266	0.472057
C	-3.020471	2.732295	-0.049531
C	-3.101006	1.477026	0.803942
C	-4.145056	0.442874	0.511101
C	-4.693176	-0.411422	1.638346
C	-2.549630	-2.556264	0.205997
C	-1.444727	-2.623089	-0.603400
C	-1.454709	-2.456795	-2.088536
H	-2.699767	2.898811	-2.226569
H	-4.247602	2.210798	-1.774960
H	-1.513970	0.852694	-1.756884
H	-3.062532	0.186838	-2.285261
H	-1.905728	-0.889583	1.524712
H	-2.041508	3.206627	0.094470
H	-3.781052	3.470387	0.231491
H	-2.714145	1.511638	1.820585
H	-4.907287	0.726578	-0.214047
H	-3.926347	-0.689600	2.369694
H	-5.464048	0.146990	2.180725
H	-2.527454	-2.959889	1.212524
H	-2.399475	-2.052348	-2.457438
H	-1.313209	-3.453266	-2.531083
H	-0.626562	-1.833670	-2.438186
H	-5.160043	-1.330595	1.266942
H	-3.527155	-2.343999	-0.212414
H	-0.512534	-2.973448	-0.164891
Au	0.309551	-0.276106	0.190987
P	2.573627	0.233189	-0.036992
O	2.976058	1.398608	-1.067837
O	3.343807	-1.037300	-0.628453
O	3.345679	0.734797	1.293500
C	2.673371	2.788934	-0.809522
C	4.746890	-0.997679	-1.018252
C	3.172535	0.074572	2.567440
H	2.969108	3.330141	-1.707877
H	1.600606	2.924518	-0.634816
H	3.245244	3.142975	0.050926
H	5.029059	-2.033709	-1.201560
H	4.855616	-0.404101	-1.927266
H	5.353086	-0.576759	-0.212755
H	3.613125	0.735920	3.313369
H	2.110048	-0.074522	2.787358
H	3.694098	-0.886595	2.568358

TS(13n$_{4c}$)

E = -1252.30722784 a.u.

C	-3.075232	-2.414383	1.448853
C	-2.600148	-0.943517	1.531911
C	-2.749529	-0.358588	0.121410
C	-1.802897	0.654131	-0.359147
C	-2.792041	-2.847397	-0.005959
C	-2.947445	-1.581130	-0.833807
C	-4.089702	-0.647896	-0.567077
C	-4.650086	0.190386	-1.700429
C	-2.830351	2.501745	0.090590
C	-1.816873	2.433964	1.003759
H	-2.567653	-3.050221	2.179776
H	-4.146065	-2.483878	1.666018
H	-1.539949	-0.901593	1.814211
H	-3.162196	-0.375574	2.284707
H	-2.005639	1.020480	-1.367464
H	-1.766416	-3.222241	-0.110254
H	-3.465053	-3.644018	-0.344640
H	-2.510330	-1.552154	-1.830068
H	-4.859284	-1.016828	0.110525
H	-3.873469	0.547865	-2.385759
H	-5.345037	-0.413995	-2.293527
H	-2.746252	3.144515	-0.782374
H	-5.208200	1.059325	-1.333783
H	-3.797253	2.054316	0.279037
C	-0.596996	3.304201	0.957551
H	-0.792610	4.186123	1.584745
H	0.285946	2.806387	1.365774

H	-0.379677	3.655992	-0.055027
H	-1.983200	1.868021	1.917768
Au	0.258039	0.282640	-0.141379
P	2.503651	-0.343629	-0.139427
O	3.397895	0.116202	-1.391937
O	2.604353	-1.936611	-0.201123
O	3.422615	0.184542	1.086848
C	3.734099	1.501906	-1.630445
C	3.862390	-2.642112	-0.405766
C	2.999730	0.040831	2.460011
H	4.248833	1.523152	-2.590601
H	2.827306	2.113766	-1.686788
H	4.393188	1.868583	-0.840342
H	3.649180	-3.688358	-0.190282
H	4.181124	-2.521419	-1.442173
H	4.627846	-2.262716	0.275206
H	3.707334	0.616175	3.056912
H	1.988791	0.438995	2.600974
H	3.030491	-1.010751	2.758732

$13n_{1c}\cdot Au(P(OMe_3)_3)^+$
E = -1252.34414769 a.u.

C	-2.644528	2.658529	-1.508493
C	-2.858482	1.124846	-1.515525
C	-2.620414	0.670753	-0.069783
C	-2.363856	-0.776703	0.229998
C	-1.653076	2.933136	-0.353092
C	-1.918013	1.819386	0.650801
C	-3.348327	1.488956	1.000704
C	-3.697033	0.935875	2.370556
C	-3.081086	-1.860077	-0.441087
C	-1.580498	-1.788437	-0.846726
H	-2.276809	3.023346	-2.471796
H	-3.593755	3.170977	-1.323187
H	-2.114125	0.653330	-2.171854
H	-3.848742	0.851945	-1.899460
H	-2.078990	-0.996286	1.256199
H	-0.615834	2.865794	-0.706366
H	-1.786008	3.932849	0.075826
H	-1.170038	1.612730	1.415988
H	-4.113395	2.159771	0.611586
H	-2.875463	0.366189	2.819480
H	-3.923311	1.760710	3.055128
H	-4.579669	0.286565	2.333995
H	-3.729240	-1.543949	-1.256172
H	-1.450830	-1.514075	-1.890461
C	-3.556521	-3.087604	0.308307
H	-4.539901	-2.900848	0.753533
H	-3.648308	-3.946525	-0.364529
H	-2.866924	-3.357019	1.116731
H	-1.065222	-2.694263	-0.522906
Au	0.324581	-0.660345	-0.195486
P	2.383859	0.242494	0.194826
O	2.861677	0.341241	1.717645
O	2.370490	1.760605	-0.286807
O	3.627576	-0.525236	-0.479509
C	3.219676	-0.821902	2.505999
C	3.484271	2.675427	-0.051729
C	3.614846	-0.969916	-1.857811
H	3.428994	-0.445467	3.506513
H	2.385182	-1.529493	2.544093
H	4.107204	-1.298092	2.084797
H	3.255216	3.565154	-0.636247
H	3.536760	2.915369	1.011048
H	4.420442	2.227367	-0.391867
H	4.504303	-1.587131	-1.979744
H	2.719172	-1.565506	-2.061487
H	3.659840	-0.110069	-2.531205

$13n_{2c}\cdot Au(P(OMe_3)_3)^+$
E = -1252.33979298 a.u.

C	-2.318753	2.423620	-1.652578
C	-2.426159	0.882031	-1.555995
C	-2.560948	0.569619	-0.058443
C	-2.260620	-0.796052	0.511174
C	-1.684209	2.877830	-0.318106
C	-2.134139	1.831309	0.691138
C	-3.585317	1.416456	0.699957
C	-4.248028	0.944839	1.981182
C	-2.989766	-2.031149	0.176549
C	-1.543932	-2.002678	-0.376337
H	-1.736196	2.736942	-2.523857
H	-3.314350	2.863686	-1.769072
H	-1.501232	0.424241	-1.935945
H	-3.250093	0.497658	-2.167609
H	-1.902985	-0.774613	1.538396
H	-0.588442	2.870305	-0.388465
H	-1.985356	3.894629	-0.041922
H	-1.594089	1.745743	1.633883
H	-4.257385	1.992154	0.064713
H	-3.546953	0.451991	2.663542
H	-4.672122	1.800505	2.518061
H	-5.067393	0.245199	1.777724
H	-1.514346	-1.920969	-1.459579
H	-0.934565	-2.796527	0.058863
H	-3.090508	-2.726557	1.008273
C	-4.149773	-2.086905	-0.796945
H	-4.295203	-3.112188	-1.151996
H	-5.071571	-1.769584	-0.297173
H	-3.999142	-1.443566	-1.666220
Au	0.368402	-0.711133	-0.034064
P	2.416513	0.280051	0.109481
O	2.824333	0.901044	1.524690
O	2.440355	1.535646	-0.869175
O	3.679029	-0.668839	-0.198475
C	3.135232	0.083610	2.681575
C	3.550216	2.484143	-0.914857
C	3.732493	-1.545832	-1.350427
H	3.291144	0.782999	3.501955
H	2.297641	-0.581313	2.915889
H	4.042566	-0.494217	2.495396
H	3.355521	3.113839	-1.781608
H	3.555695	3.078076	0.000028
H	4.497069	1.953248	-1.035013
H	4.617854	-2.165334	-1.211884
H	2.840005	-2.178209	-1.394460
H	3.825475	-0.957252	-2.266702

$13n_{3c}\cdot Au(P(OMe_3)_3)^+$
E = -1252.33282540 a.u.

C	-2.865799	2.178317	-1.633622
C	-2.627262	0.651372	-1.548066
C	-2.660931	0.309394	-0.051293
C	-2.074689	-0.980343	0.486167
C	-2.314407	2.753508	-0.308876
C	-2.504235	1.629537	0.699098
C	-3.832682	0.909846	0.725324
C	-4.349357	0.304733	2.017469
C	-2.776137	-2.293186	0.251576
C	-1.435653	-2.307715	-0.391143
C	-1.339696	-2.431957	-1.903110
H	-2.388609	2.616020	-2.515474
H	-3.935452	2.391768	-1.722719
H	-1.631890	0.411878	-1.947806
H	-3.358956	0.091960	-2.144021
H	-1.715725	-0.918598	1.514856
H	-1.243837	2.985740	-0.401132
H	-2.819592	3.680983	-0.016739
H	-1.951678	1.667380	1.637493
H	-4.626688	1.332286	0.110641
H	-3.541978	-0.029496	2.678609
H	-4.931696	1.049321	2.571200
H	-2.942936	-2.932867	1.114150
H	-2.100088	-1.838004	-2.412518
H	-1.517374	-3.484743	-2.156433
H	-0.359214	-2.155803	-2.302383
H	-5.005965	-0.552670	1.828623
H	-3.621151	-2.241099	-0.431705
H	-0.704692	-2.900289	0.161226
Au	0.304982	-0.566518	0.065351
P	2.415385	0.296444	0.016607
O	2.758643	1.324008	-1.158404
O	3.432159	-0.902790	-0.228893
O	2.868693	1.132558	1.315588
C	2.237662	2.676235	-1.200909
C	4.855781	-0.698693	-0.484900
C	2.658477	0.644420	2.662858
H	2.561544	3.086275	-2.156721
H	1.144214	2.665726	-1.153512
H	2.650885	3.259191	-0.375603
H	5.302778	-1.690100	-0.430648
H	4.985387	-0.271204	-1.479929
H	5.287017	-0.043717	0.275225
H	2.955334	1.457828	3.324016
H	1.602856	0.402576	2.822748
H	3.280767	-0.235121	2.846963

$13n_{4c}\cdot Au(P(OMe_3)_3)^+$
E = -1252.33601771 a.u.

C	-2.534489	2.430997	-1.582400
C	-2.614154	0.884792	-1.565928
C	-2.572876	0.485918	-0.083842
C	-2.266224	-0.941975	0.297442
C	-1.770644	2.821240	-0.295052
C	-2.096327	1.711443	0.695267
C	-3.531398	1.259931	0.824583
C	-4.043671	0.704699	2.140608
C	-3.023726	-2.038505	-0.364120
C	-1.563954	-2.157845	-0.701350
H	-2.047218	2.803846	-2.487975
H	-3.541193	2.860155	-1.572024
H	-1.735980	0.464928	-2.078706
H	-3.502230	0.515441	-2.092795
H	-2.068992	-1.124089	1.351456
H	-0.688151	2.839500	-0.476044
H	-2.057663	3.813892	0.070049
H	-1.470659	1.598127	1.579993
H	-4.278620	1.851084	0.295965
H	-3.256028	0.220410	2.728867
H	-4.445793	1.518267	2.754283
H	-3.422902	-2.826280	0.271374
H	-4.849522	-0.022765	1.988449
H	-3.690845	-1.742592	-1.169105
C	-0.864641	-3.398555	-0.149488
H	-1.292899	-4.283483	-0.637112
H	0.215078	-3.408496	-0.326880
H	-1.033005	-3.503334	0.927585
H	-1.343887	-1.893078	-1.734251
Au	0.195626	-0.586549	-0.065489
P	2.236008	0.403452	0.163375
O	2.819754	0.514179	1.647836
O	2.127987	1.921442	-0.307054
O	3.457901	-0.310263	-0.605643
C	3.254860	-0.642746	2.405721
C	3.218237	2.880286	-0.145992
C	3.363022	-0.741776	-1.984543
H	3.514229	-0.266298	3.394385
H	2.442174	-1.371663	2.488524
H	4.127388	-1.093237	1.928490
H	2.916762	3.757975	-0.715645
H	3.329360	3.125879	0.910924
H	4.147398	2.467969	-0.545267
H	4.277689	-1.298418	-2.185882
H	2.494087	-1.392992	-2.124256
H	3.297634	0.124528	-2.647932

$TS(14_c)$
E = -1134.39799819 a.u.

C	4.191052	-2.001485	-0.724131
C	2.857148	-1.772009	0.029767
C	2.945406	-0.370594	0.585313
C	1.895889	0.658004	0.585219
C	5.169001	-0.942927	-0.150600
C	4.263540	0.108615	0.442527
C	2.932149	0.955029	-0.548155
H	4.566023	-3.020283	-0.607028
H	4.043950	-1.835086	-1.796195
H	2.765629	-2.426777	0.909890
H	1.958867	-1.929419	-0.573695
H	5.787738	-1.350555	0.660850
H	5.861297	-0.536441	-0.894856
H	4.656619	0.955803	0.994370
H	2.765686	0.462321	-1.503407

C	3.426833	2.393492	-0.683793
H	4.329479	2.452258	-1.298396
H	2.631190	2.958651	-1.182824
H	3.617435	2.861677	0.284336
H	2.047510	1.426613	1.347337
Au	-0.122428	0.243272	0.227917
P	-2.380925	-0.232197	-0.110147
O	-3.149883	-1.015110	1.065095
O	-2.552268	-1.223487	-1.354236
O	-3.377236	1.028029	-0.321727
C	-3.378009	-0.409458	2.357925
C	-3.830815	-1.820282	-1.711054
C	-3.038481	2.116177	-1.208513
H	-3.823741	-1.187141	2.977639
H	-2.432140	-0.082193	2.802973
H	-4.064370	0.434841	2.260892
H	-3.680860	-2.272015	-2.691005
H	-4.095750	-2.581243	-0.975221
H	-4.607937	-1.054043	-1.762334
H	-3.774316	2.898551	-1.022553
H	-2.034055	2.496457	-0.993411
H	-3.099760	1.789682	-2.250683

14_c
E = -1134.40930394 a.u.

C	4.154558	-2.127067	-0.800112
C	2.754517	-1.468164	-0.738020
C	2.987680	-0.214245	0.096920
C	1.908119	0.867096	0.424496
C	4.905058	-1.574531	0.440331
C	4.195754	-0.292188	0.733414
C	2.718201	1.423057	-0.618576
H	4.106028	-3.218100	-0.810545
H	4.677910	-1.812495	-1.709274
H	2.028680	-2.101434	-0.210798
H	2.330873	-1.260023	-1.725911
H	4.809118	-2.240962	1.313641
H	5.981760	-1.433453	0.289365
H	4.589425	0.469913	1.400855
H	2.519781	1.112473	-1.643964
C	3.650290	2.588288	-0.475386
H	4.544975	2.491515	-1.097050
H	3.102884	3.472407	-0.834825
H	3.934294	2.778094	0.562752
H	2.102565	1.333345	1.393551
Au	-0.108178	0.309904	0.164619
P	-2.349298	-0.272657	-0.076039
O	-2.907621	-1.462279	0.848560
O	-2.603235	-0.829151	-1.552878
O	-3.441604	0.879997	0.235054
C	-3.050069	-1.315331	2.280333
C	-3.872149	-1.410399	-1.967756
C	-3.302502	2.220315	-0.286897
H	-3.343314	-2.296512	2.652776
H	-2.098647	-1.018733	2.734880
H	-3.824346	-0.578667	2.505688
H	-3.810233	-1.505726	-3.051155
H	-3.992681	-2.390311	-1.503178
H	-4.700375	-0.753443	-1.692018
H	-4.084954	2.811175	0.189078
H	-2.321615	2.636966	-0.035105
H	-3.443665	2.221882	-1.371419

Gold(I)-catalyzed cyclopropanation with (*E*)-hept-1-en-6-yn-1-ylbenzene.

(*E*)-hept-1-en-6-yn-1-ylbenzene
E = -503.718863057 a.u.

C	3.216831	1.470301	-0.129129
C	2.607921	2.508201	-0.239658
H	2.067107	3.421119	-0.342810
C	3.989307	0.230636	-0.012744
H	4.910375	0.346805	-0.600674
H	4.314356	0.100621	1.029827
C	3.271408	-1.056915	-0.482742
H	2.867000	-0.902310	-1.489877
H	4.039454	-1.837086	-0.563584
C	2.157470	-1.583103	0.451215
H	1.916163	-2.610950	0.150711
H	2.569073	-1.646842	1.471252
C	0.893819	-0.767177	0.465370
H	0.985021	0.252330	0.832118
C	-0.297172	-1.227525	0.051584
H	-0.354836	-2.261143	-0.294808
C	-1.574534	-0.497827	0.020926
C	-1.677628	0.886201	0.259493
C	-2.756335	-1.204557	-0.264566
C	-2.912935	1.527249	0.226791
H	-0.781228	1.466636	0.458140
C	-3.994419	-0.563694	-0.298106
H	-2.698133	-2.273516	-0.458026
C	-4.079325	0.806823	-0.049999
H	-2.967333	2.597006	0.412720
H	-4.892028	-1.135615	-0.518980
H	-5.041435	1.311271	-0.076615

Styrene
E = -309.641798753 a.u.

C	0.009076	1.092621	-0.000027
C	-1.362300	1.329980	-0.000006
C	-2.265755	0.262045	0.000018
C	-1.781348	-1.046309	0.000017
C	-0.406621	-1.281740	-0.000003
C	0.515314	-0.220672	-0.000028
H	0.694355	1.935332	-0.000054
H	-1.730400	2.352719	-0.000012
H	-3.335848	0.450818	0.000042
H	-2.472629	-1.885001	0.000038
H	-0.035211	-2.304208	-0.000005

C	1.955060	-0.529580	-0.000024
H	2.186702	-1.594932	-0.000075
C	2.977809	0.335144	0.000040
H	4.004907	-0.016830	0.000034
H	2.840712	1.413167	0.000101

Stilbene

E = -540.698684997 a.u.

C	0.498753	-0.454125	0.000454
H	0.242670	-1.512735	-0.004108
C	-0.498753	0.454125	0.000454
H	-0.242670	1.512735	-0.004107
C	-1.940328	0.186553	0.001287
C	-2.829891	1.277375	-0.033076
C	1.940328	-0.186553	0.001287
C	-2.493925	-1.109270	0.035957
C	-3.872221	-1.299259	0.033520
C	-4.740038	-0.202706	-0.002474
C	-4.210747	1.088133	-0.035460
H	-1.841102	-1.976582	0.067492
H	-4.273988	-2.308879	0.061058
H	-5.815780	-0.355436	-0.003715
H	-4.872845	1.949636	-0.062860
C	2.829891	-1.277375	-0.033076
C	2.493925	1.109270	0.035957
H	1.841102	1.976582	0.067492
C	3.872221	1.299259	0.033521
H	4.273988	2.308879	0.061059
C	4.740038	0.202706	-0.002474
H	5.815780	0.355436	-0.003714
C	4.210747	-1.088133	-0.035459
H	4.872845	-1.949636	-0.062860
H	2.425207	-2.286720	-0.059120
H	-2.425207	2.286720	-0.059120

13p$_1$

E = -813.418342739 a.u.

C	3.520257	-2.311655	-0.856929
C	1.975582	-2.360886	-0.759799
C	1.563053	-1.098435	0.005132
C	0.229752	-1.041638	0.697606
C	3.983181	-1.487031	0.368291
C	2.821311	-0.546721	0.657625
C	2.202431	0.196525	-0.505388
C	-0.997494	-1.759281	0.144470
C	-0.356122	-2.207406	1.446373
H	3.965140	-3.311873	-0.880148
H	3.826194	-1.814025	-1.783822
H	1.666931	-3.246388	-0.188879
H	1.505410	-2.437007	-1.748269
H	0.012122	-0.067734	1.129951
H	4.138884	-2.141728	1.236002
H	4.930971	-0.966308	0.181850
H	2.755293	-0.089646	1.642253
H	2.718171	0.108551	-1.462844
H	-0.802043	-2.412975	-0.702972
H	0.168589	-3.159345	1.444401
H	-0.892883	-2.003351	2.369628
C	1.544251	1.533867	-0.328916
C	0.467389	1.896096	-1.154973
C	1.999464	2.466791	0.612672
C	-0.135961	3.147772	-1.041212
H	0.096660	1.181973	-1.886197
C	1.397518	3.722110	0.729999
H	2.839578	2.211655	1.252939
C	0.327411	4.067011	-0.096063
H	-0.972028	3.403844	-1.686820
H	1.768866	4.430783	1.466088
H	-0.143018	5.042502	-0.004919
C	-2.340488	-1.113116	0.092144
C	-3.177416	-1.347644	-1.009698
C	-2.813421	-0.267162	1.108615
C	-4.440079	-0.760015	-1.097543
H	-2.832752	-2.002340	-1.807334
C	-4.074293	0.322097	1.023531
H	-2.192145	-0.062384	1.976987
C	-4.895606	0.079351	-0.080040
H	-5.067611	-0.960318	-1.962436
H	-4.416209	0.973927	1.823565
H	-5.878434	0.538410	-0.144404

13p$_2$

E = -813.413307608 a.u.

C	0.366356	3.260283	-1.324850
C	1.037731	2.228643	-0.390331
C	-0.102483	1.463524	0.306415
C	0.231475	0.869576	1.651727
C	-1.006173	3.559333	-0.677134
C	-1.357461	2.282827	0.074606
C	-1.205934	0.964272	-0.650465
C	-0.048694	-0.537969	2.110893
C	1.383422	-0.128289	1.877364
H	0.973622	4.162668	-1.451178
H	0.227829	2.836926	-2.326071
H	1.617585	2.743221	0.388088
H	1.732426	1.568300	-0.919080
H	0.183107	1.616991	2.445530
H	-0.921428	4.385924	0.041307
H	-1.763782	3.849664	-1.415706
H	-2.117191	2.338278	0.850559
H	-0.926444	1.031419	-1.701051
H	1.959760	0.084523	2.775845
H	-0.377840	-0.689864	3.135986
H	-0.492500	-1.230037	1.405928
C	-2.121241	-0.193848	-0.410922
C	-2.114555	-1.255154	-1.332758
C	-3.018095	-0.272591	0.667046
C	-2.956204	-2.357533	-1.179855
H	-1.440945	-1.208278	-2.185814
C	-3.860574	-1.373546	0.823565
H	-3.058087	0.528298	1.398552
C	-3.834356	-2.423238	-0.097017
H	-2.928253	-3.161629	-1.910822
H	-4.544095	-1.408144	1.668236
H	-4.493380	-3.278392	0.025739
C	2.228870	-0.695643	0.784129

C	3.620881	-0.517585	0.849696
C	1.710207	-1.409219	-0.308578
C	4.465307	-1.022792	-0.138737
H	4.045447	0.025095	1.691658
C	2.552729	-1.912252	-1.300918
H	0.641097	-1.579186	-0.390071
C	3.933933	-1.722473	-1.223488
H	5.538886	-0.871350	-0.058748
H	2.125794	-2.462792	-2.135713
H	4.587547	-2.119597	-1.995511

13p$_3$
E = -813.418698735 a.u.

C	1.832082	3.623931	-0.171527
C	0.984006	2.809934	0.835844
C	0.879437	1.397315	0.250684
C	-0.218385	0.479310	0.707890
C	1.614361	2.936586	-1.541444
C	1.315355	1.482847	-1.198978
C	2.227408	0.799412	-0.204154
C	-0.857300	0.592654	2.064373
C	-1.667675	0.942505	0.828818
H	1.552747	4.682444	-0.186889
H	2.891183	3.586493	0.106108
H	-0.021932	3.244001	0.911531
H	1.415094	2.824347	1.844548
H	-0.117426	-0.537565	0.336461
H	0.744104	3.367670	-2.053623
H	2.476776	3.058827	-2.208515
H	0.822426	0.872111	-1.950981
H	3.099832	1.369291	0.113932
H	-1.109703	-0.320849	2.596984
H	-0.562905	1.414628	2.711919
H	-1.833093	2.006712	0.674984
C	2.497542	-0.671856	-0.202141
C	3.361645	-1.192890	0.776693
C	1.943723	-1.567959	-1.128959
C	3.655711	-2.553870	0.834096
H	3.807775	-0.515345	1.501523
C	2.232918	-2.933534	-1.072204
H	1.288180	-1.201495	-1.913311
C	3.088895	-3.434057	-0.091133
H	4.329064	-2.927638	1.601380
H	1.790972	-3.604692	-1.804311
H	3.316192	-4.495881	-0.049857
C	-2.796855	0.096998	0.345637
C	-2.822960	-1.297737	0.511718
C	-3.881731	0.700644	-0.308962
C	-3.892650	-2.057222	0.038610
H	-2.000972	-1.800460	1.015374
C	-4.953702	-0.056576	-0.782744
H	-3.883643	1.779805	-0.446728
C	-4.964676	-1.441597	-0.611610
H	-3.888457	-3.135096	0.180408
H	-5.781026	0.438187	-1.285417
H	-5.798086	-2.034527	-0.978563

13p$_4$
E = -813.414988923 a.u.

C	0.360732	3.095618	-1.522224
C	0.995194	2.051497	-0.571135
C	-0.174865	1.392951	0.171308
C	0.025300	0.690021	1.486144
C	-0.974768	3.502429	-0.855840
C	-1.388250	2.277732	-0.051591
C	-1.329603	0.935578	-0.746042
C	1.098085	-0.360874	1.766501
C	1.162088	0.991594	2.435895
H	1.020922	3.952588	-1.691508
H	0.172577	2.650857	-2.505699
H	1.635516	2.561363	0.159289
H	1.626389	1.333731	-1.104590
H	-0.917660	0.461979	1.977057
H	-0.822179	4.345760	-0.169271
H	-1.728000	3.814374	-1.590140
H	-2.114269	2.412536	0.746626
H	-1.090316	0.959429	-1.808289
H	1.933256	1.680740	2.104167
H	0.947221	1.059111	3.499402
H	0.740093	-1.172341	2.400436
C	-2.225479	-0.213733	-0.409305
C	-2.082161	-1.409132	-1.136057
C	-3.217469	-0.168422	0.581935
C	-2.885454	-2.518403	-0.875092
H	-1.329296	-1.461679	-1.919493
C	-4.022174	-1.278497	0.848639
H	-3.377956	0.745486	1.146229
C	-3.859949	-2.459635	0.124163
H	-2.753004	-3.428111	-1.455395
H	-4.784481	-1.213762	1.621060
H	-4.488923	-3.321481	0.329962
C	2.105904	-0.820105	0.755672
C	1.729208	-1.762110	-0.216009
C	3.437376	-0.384235	0.775548
C	2.651453	-2.241136	-1.145836
H	0.700879	-2.114510	-0.239327
C	4.363290	-0.859347	-0.156629
H	3.753621	0.327950	1.532813
C	3.973662	-1.788300	-1.122089
H	2.338705	-2.968502	-1.891028
H	5.391126	-0.506684	-0.122851
H	4.693041	-2.159778	-1.847181

Using [Au(PMe$_3$)]$^+$ as catalyst:

3b
E = -1100.47912389 a.u.

C	2.061418	3.612889	0.721845
C	0.867453	2.641103	0.622742
C	1.348703	1.432499	-0.171617

C	0.655001	0.308693	-0.489592
C	2.940518	3.283062	-0.499782
C	2.795376	1.767648	-0.716522
C	3.242676	0.880295	0.332534
P	-3.633465	-0.543609	0.148903
Au	-1.333721	-0.061232	-0.173556
H	1.748072	4.660120	0.727393
H	2.615942	3.450080	1.653297
H	0.045091	3.094580	0.054009
H	0.459452	2.359132	1.598336
H	1.230405	-0.475592	-0.987815
H	2.558339	3.786021	-1.394643
H	3.986170	3.580876	-0.375153
H	2.973169	1.424354	-1.733527
H	3.249201	1.285020	1.342127
C	-4.742763	0.914260	-0.034180
H	-5.789200	0.628090	0.116613
H	-4.472262	1.679575	0.699406
H	-4.629700	1.341908	-1.034857
C	-4.306348	-1.785299	-1.031606
H	-5.368352	-1.969543	-0.837164
H	-4.188023	-1.422983	-2.057125
H	-3.755909	-2.725703	-0.933830
C	-4.037422	-1.223699	1.811415
H	-5.109234	-1.433445	1.893412
H	-3.477966	-2.148837	1.978820
H	-3.753420	-0.504935	2.585787
C	3.742189	-0.462890	0.197604
C	4.037704	-1.190916	1.375192
C	4.001166	-1.062216	-1.058420
C	4.570198	-2.470713	1.300955
H	3.845756	-0.736373	2.343612
C	4.531221	-2.344414	-1.126052
H	3.804731	-0.518170	-1.976386
C	4.814421	-3.049937	0.050001
H	4.797583	-3.019113	2.209581
H	4.734181	-2.795451	-2.092287
H	5.232803	-4.050393	-0.009288

TS(13p$_1$)

E = -1410.11971697 a.u.

C	-0.947658	-4.389167	0.760453
C	-0.519411	-2.997618	1.285406
C	-1.163916	-1.966318	0.356428
C	-0.543410	-0.709197	0.057775
C	-1.198833	-4.195874	-0.751100
C	-1.691342	-2.764960	-0.908748
C	-2.684418	-2.230099	0.046617
P	3.820969	-0.055103	-0.318421
Au	1.495051	-0.375729	-0.028745
C	-1.663758	1.466274	1.287541
C	-0.978568	0.511789	1.987059
H	-0.190305	-5.153295	0.956416
H	-1.862824	-4.724879	1.259422
H	0.569307	-2.878118	1.229206
H	-0.806683	-2.845609	2.333222
H	-1.141204	-0.078419	-0.601396
H	-0.269964	-4.315505	-1.321132
H	-1.922430	-4.915432	-1.152586
H	-1.603276	-2.298989	-1.885590
H	-3.099092	-2.952940	0.747386
H	-2.711810	1.268733	1.071154
H	-1.519484	-0.304852	2.451036
H	0.036129	0.668279	2.335681
C	4.773561	0.181548	1.239150
H	4.643874	-0.688588	1.889496
H	5.839505	0.311187	1.023356
H	4.407381	1.065627	1.769581
C	4.248865	1.407936	-1.349811
H	5.334716	1.499721	-1.460570
H	3.794819	1.307314	-2.340090
H	3.857350	2.317092	-0.884116
C	4.652761	-1.467865	-1.154801
H	5.722781	-1.268947	-1.277701
H	4.523969	-2.378033	-0.561511
H	4.203937	-1.631703	-2.138964
C	-1.141043	2.711854	0.749164
C	-3.642243	-1.126755	-0.267425
C	-4.571816	-0.755394	0.720163
C	-3.674662	-0.453376	-1.497741
C	-5.494930	0.264192	0.492089
H	-4.576756	-1.280934	1.672592
C	-4.597615	0.570324	-1.727967
H	-2.998909	-0.738456	-2.298861
C	-5.507968	0.935483	-0.734536
H	-6.210262	0.527250	1.266048
H	-4.614491	1.069051	-2.692974
H	-6.233574	1.722223	-0.919370
C	-1.943615	3.445829	-0.148725
H	-2.923968	3.060345	-0.417113
C	0.124527	3.229404	1.100456
H	0.743336	2.704142	1.821765
C	0.569244	4.432148	0.562885
H	1.535732	4.831916	0.856536
C	-1.492347	4.646105	-0.691912
H	-2.121768	5.199587	-1.382243
C	-0.235245	5.141617	-0.337704
H	0.113415	6.084115	-0.749813

TS(13p$_2$)

E = -1410.11481088 a.u.

C	-1.148037	0.113245	3.493055
C	-0.756920	0.631972	2.088855
C	-1.032113	-0.515119	1.109133
C	-0.232547	-0.712549	-0.086399
C	-0.955084	-1.417318	3.429283
C	-1.238853	-1.801950	1.984838
C	-2.420907	-1.219895	1.297882
P	4.151787	-0.040872	-0.288028
Au	1.802251	-0.313447	-0.190327
C	-1.117193	0.283817	-1.709084
C	-0.865953	1.621169	-1.478251
H	-0.547663	0.572943	4.283453
H	-2.192382	0.356197	3.716450
H	0.315913	0.859089	2.048408
H	-1.293481	1.548488	1.823811
H	-0.524498	-1.615015	-0.627309
H	0.078364	-1.691937	3.673423

H	-1.607521	-1.953095	4.129015
H	-0.846871	-2.748921	1.624643
H	-3.086708	-0.631385	1.926631
H	-0.471050	-0.230253	-2.413405
H	-2.118977	-0.120982	-1.605685
H	0.127823	1.983721	-1.740930
C	4.928160	0.429130	1.313565
H	4.707697	-0.330358	2.069580
H	6.014111	0.520809	1.204868
H	4.521299	1.384928	1.656992
C	5.039761	-1.570773	-0.797554
H	6.121566	-1.401647	-0.823736
H	4.820877	-2.377959	-0.092207
H	4.701957	-1.881791	-1.790603
C	4.737013	1.242780	-1.472134
H	5.830814	1.301024	-1.469921
H	4.395104	0.999564	-2.482597
H	4.328216	2.218938	-1.194339
C	-1.739779	2.607454	-0.892194
C	-3.152359	-1.903511	0.186820
C	-4.376008	-1.356506	-0.239723
C	-2.698332	-3.072856	-0.444177
C	-5.109353	-1.941481	-1.271830
H	-4.767470	-0.474777	0.263550
C	-3.428817	-3.657514	-1.481335
H	-1.783864	-3.556475	-0.113463
C	-4.633132	-3.092863	-1.903146
H	-6.056636	-1.504661	-1.575131
H	-3.060099	-4.565847	-1.949472
H	-5.202797	-3.553352	-2.704762
C	-1.223174	3.897451	-0.630615
H	-0.185445	4.112455	-0.873142
C	-3.097231	2.345448	-0.590753
H	-3.521203	1.370949	-0.808435
C	-2.025031	4.885276	-0.070762
H	-1.616980	5.871836	0.125810
C	-3.360979	4.604146	0.232268
H	-3.991559	5.375365	0.664956
C	-3.894223	3.335100	-0.031538
H	-4.936650	3.129622	0.192554

TS(13p$_3$)
E = -1410.11536429 a.u.

C	-1.864951	-1.106124	3.480871
C	-1.143770	-0.170648	2.480958
C	-1.771125	-0.431566	1.110533
C	-1.019520	-0.280713	-0.119105
C	-2.344071	-2.308911	2.638566
C	-2.608962	-1.752496	1.246590
C	-3.340498	-0.468785	1.108332
P	3.196781	-1.607729	-0.535264
Au	0.975693	-0.824595	-0.299050
C	-1.167527	1.726511	-0.775486
C	-0.551566	2.469435	0.206640
H	-1.211452	-1.412367	4.302733
H	-2.719761	-0.596603	3.938084
H	-0.075135	-0.411829	2.422474
H	-1.219505	0.883703	2.777720
H	-1.629376	-0.515864	-0.995201
H	-1.561740	-3.074464	2.571031
H	-3.234178	-2.790072	3.060915
H	-2.620486	-2.450203	0.414349
H	-3.751848	-0.057743	2.029125
H	-0.688979	1.587619	-1.740066
H	-2.251975	1.670265	-0.772516
H	-1.132454	2.675460	1.105000
C	0.801712	2.977340	0.225009
C	-4.145902	-0.094727	-0.094770
C	-4.807903	1.146706	-0.093409
C	-4.287669	-0.920440	-1.221155
C	-5.575228	1.554508	-1.183790
H	-4.729921	1.790649	0.780174
C	-5.052691	-0.511135	-2.315716
H	-3.825014	-1.902783	-1.242928
C	-5.696007	0.727088	-2.303134
H	-6.084713	2.513501	-1.156151
H	-5.156082	-1.169816	-3.173365
H	-6.296593	1.040006	-3.152079
C	3.797531	-1.672246	-2.274397
H	3.760702	-0.672446	-2.717002
H	4.826725	-2.044394	-2.317202
H	3.153920	-2.332203	-2.863652
C	3.452866	-3.315161	0.102417
H	4.496068	-3.625365	-0.020367
H	3.190357	-3.356326	1.163749
H	2.806290	-4.012457	-0.438629
C	4.451231	-0.591355	0.349789
H	5.459930	-0.984249	0.182845
H	4.402502	0.443145	-0.002631
H	4.238429	-0.597177	1.423056
C	1.644490	2.955298	-0.910329
H	1.275553	2.559933	-1.851336
C	1.295016	3.544568	1.421124
H	0.650880	3.581515	2.296001
C	2.587424	4.055042	1.489998
H	2.951532	4.489946	2.415683
C	2.932885	3.470838	-0.840305
C	3.408765	4.018496	0.359496
H	3.564972	3.469875	-1.723627
H	4.412744	4.430561	0.405353

TS(13p$_4$)
E = -1410.11376676 a.u.

C	-0.737209	0.089770	3.546963
C	-0.534362	0.713378	2.145464
C	-0.781505	-0.406424	1.128438
C	-0.047457	-0.485712	-0.112793
C	-0.389025	-1.404403	3.379184
C	-0.767836	-1.754568	1.948869
C	-2.057659	-1.266926	1.390632
P	4.324850	0.253047	-0.372028
Au	1.985344	-0.053794	-0.241487
C	-2.003069	0.963897	-1.573899
C	-0.630588	0.983653	-1.648640
H	-0.119013	0.575541	4.307389
H	-1.776630	0.204431	3.872191
H	0.499260	1.061691	2.023426
H	-1.191396	1.573333	1.978563

H	-0.387732	-1.304081	-0.748476
H	0.686100	-1.573747	3.514382
H	-0.911670	-2.042438	4.102071
H	-0.318874	-2.638944	1.505571
H	-2.727798	-0.789227	2.103047
H	-0.070654	1.852099	-1.320542
H	-0.143396	0.366960	-2.395537
H	-2.518984	0.133824	-2.053903
C	-2.863118	1.925256	-0.914502
C	-2.371440	3.063691	-0.234943
C	-4.261501	1.745797	-0.999867
C	-3.246603	3.971967	0.345991
H	-1.302058	3.238275	-0.167944
C	-5.136519	2.662893	-0.425598
H	-4.649878	0.879154	-1.526821
C	-4.631022	3.774817	0.252809
H	-2.857126	4.842489	0.865251
H	-6.209049	2.514645	-0.506779
H	-5.311125	4.491793	0.703359
C	-2.801567	-1.991197	0.313217
C	-4.131663	-1.616289	0.059283
C	-2.259878	-3.047266	-0.437885
C	-4.888698	-2.258546	-0.920368
H	-4.578612	-0.818103	0.646733
C	-3.012506	-3.684991	-1.426834
H	-1.253911	-3.405742	-0.239842
C	-4.327922	-3.291588	-1.675490
H	-5.920800	-1.961303	-1.085614
H	-2.572351	-4.502485	-1.990828
H	-4.915833	-3.795548	-2.436877
C	5.172215	-1.007391	-1.411044
H	4.779063	-0.971832	-2.431391
H	6.251895	-0.825292	-1.436924
H	4.987293	-2.006753	-1.006121
C	4.842202	1.867519	-1.090614
H	5.934262	1.939578	-1.134683
H	4.437105	1.969272	-2.101848
H	4.454560	2.687997	-0.479414
C	5.186719	0.169939	1.251672
H	6.266114	0.304153	1.123668
H	4.805605	0.951705	1.915404
H	5.000784	-0.801068	1.720149

15_1

E = -1410.13469464 a.u.

C	-0.469834	-4.019659	-1.401060
C	-0.245337	-2.557779	-1.860906
C	0.438300	-1.839838	-0.686241
C	0.275953	-0.355343	-0.555556
C	-0.538959	-3.960607	0.142585
C	0.314347	-2.757845	0.523251
C	1.667849	-2.623595	-0.115385
P	-3.943585	0.770544	0.587889
Au	-1.743879	0.226112	-0.048692
C	2.034920	0.727030	-1.474004
C	0.673837	0.468699	-1.881196
H	-1.372305	-4.453390	-1.841795
H	0.364379	-4.653228	-1.719984
H	-1.208129	-2.065339	-2.053820
H	0.331855	-2.513933	-2.793454
H	0.812650	0.032065	0.319344
H	-1.569420	-3.785784	0.478181
H	-0.198530	-4.890615	0.612087
H	0.176070	-2.323181	1.510677
H	1.973230	-3.452030	-0.752580
H	2.710980	-0.124529	-1.477391
H	0.580446	-0.205487	-2.732910
H	0.062832	1.353184	-2.046346
C	-5.098849	1.021851	-0.823106
H	-5.139247	0.115457	-1.434436
H	-6.106303	1.255334	-0.461859
H	-4.744274	1.844700	-1.450855
C	-4.084732	2.312313	1.582888
H	-5.128801	2.502790	1.853734
H	-3.489338	2.219376	2.495974
H	-3.703727	3.161370	1.007768
C	-4.750110	-0.521205	1.620877
H	-5.768244	-0.220832	1.891183
H	-4.790207	-1.464719	1.068598
H	-4.169508	-0.681077	2.534229
C	2.558480	1.943220	-0.948712
C	2.838400	-1.978038	0.545776
C	4.106519	-2.135599	-0.045159
C	2.759336	-1.242278	1.740250
C	5.250829	-1.585454	0.534204
H	4.197315	-2.720155	-0.958189
C	3.900887	-0.684609	2.318566
H	1.805688	-1.125202	2.246893
C	5.151988	-0.852878	1.720311
H	6.219512	-1.743351	0.067755
H	3.813765	-0.132834	3.250554
H	6.041474	-0.434478	2.182620
C	3.891481	1.948805	-0.457650
H	4.454695	1.020615	-0.448376
C	1.819854	3.157055	-0.935272
H	0.802554	3.179043	-1.311143
C	2.398778	4.321958	-0.456777
H	1.833252	5.248527	-0.453328
C	4.464657	3.121864	0.011949
H	5.485549	3.119311	0.380484
C	3.720203	4.307265	0.014124
H	4.169212	5.225328	0.382180

15_2

E = -1410.12030842 a.u.

C	-0.916299	-0.234426	3.512260
C	-0.659752	0.419034	2.132257
C	-0.886534	-0.680279	1.085684
C	-0.240043	-0.581884	-0.273878
C	-0.602930	-1.735889	3.311453
C	-0.905370	-2.000817	1.842284
C	-2.208844	-1.480633	1.293738
P	4.192368	0.134367	-0.293702
Au	1.832905	-0.160884	-0.280708
C	-1.113921	0.324604	-1.299329
C	-1.031989	1.735284	-1.003580
H	-0.305949	0.216866	4.300477
H	-1.960649	-0.100632	3.814418

H	0.385535	0.747254	2.055173
H	-1.288310	1.306226	1.977689
H	-0.317514	-1.553322	-0.774334
H	0.459590	-1.936832	3.499120
H	-1.178960	-2.377243	3.988516
H	-0.479028	-2.890433	1.384685
H	-2.881900	-1.035837	2.025404
H	-0.600563	0.159796	-2.257829
H	-2.134147	-0.059395	-1.355194
H	-0.032155	2.166033	-1.082146
C	4.923593	0.549420	1.346155
H	4.682883	-0.237748	2.067064
H	6.012132	0.648929	1.275652
H	4.501709	1.490004	1.713013
C	5.119863	-1.364978	-0.829117
H	6.200222	-1.184930	-0.811173
H	4.885665	-2.201082	-0.163337
H	4.819990	-1.642232	-1.844187
C	4.815885	1.463610	-1.408238
H	5.908979	1.523787	-1.371476
H	4.504757	1.259806	-2.437282
H	4.396663	2.428270	-1.106306
C	-2.057117	2.618444	-0.608334
C	-2.959532	-2.129797	0.176866
C	-4.267432	-1.685659	-0.095616
C	-2.443696	-3.164876	-0.620097
C	-5.021494	-2.235250	-1.132593
H	-4.706576	-0.916466	0.537791
C	-3.194737	-3.714253	-1.661810
H	-1.457254	-3.569975	-0.415391
C	-4.483505	-3.249635	-1.927978
H	-6.033437	-1.881343	-1.310907
H	-2.773111	-4.519088	-2.257758
H	-5.067925	-3.683540	-2.733929
C	-1.721522	3.984722	-0.371728
H	-0.688532	4.301517	-0.486649
C	-3.414456	2.204540	-0.459209
H	-3.687440	1.169288	-0.633543
C	-2.696067	4.895624	-0.003637
H	-2.439406	5.934849	0.173516
C	-4.022989	4.463515	0.139555
H	-4.789126	5.177504	0.428574
C	-4.379206	3.123196	-0.086303
H	-5.412582	2.812628	0.028997

15_3

E = -1410.12086871 a.u.

C	-1.652695	-1.062671	3.515213
C	-1.020358	-0.121632	2.460891
C	-1.600798	-0.543790	1.106210
C	-0.902391	-0.220408	-0.177229
C	-1.996491	-2.360008	2.746098
C	-2.257399	-1.905610	1.314962
C	-3.161671	-0.726826	1.115099
P	3.343223	-1.655163	-0.429344
Au	1.135281	-0.795827	-0.276400
C	-1.149160	1.316567	-0.701611
C	-0.815190	2.372053	0.215725
H	-0.980753	-1.244591	4.359310
H	-2.561357	-0.616012	3.933075
H	0.068048	-0.260544	2.425020
H	-1.198709	0.935354	2.706260
H	-1.405822	-0.768691	-0.981430
H	-1.142987	-3.049609	2.750713
H	-2.847516	-2.892766	3.185425
H	-2.198764	-2.650276	0.525462
H	-3.635399	-0.332572	2.013305
H	-0.665014	1.408989	-1.673405
H	-2.245908	1.322671	-0.826235
H	-1.454462	2.465026	1.092458
C	0.256660	3.288989	0.143372
C	-3.988257	-0.498182	-0.105478
C	-4.788253	0.660545	-0.166020
C	-4.028084	-1.380704	-1.198693
C	-5.589141	0.930970	-1.274874
H	-4.794787	1.344552	0.680527
C	-4.826430	-1.109583	-2.310990
H	-3.455109	-2.302811	-1.174587
C	-5.607877	0.046882	-2.356227
H	-6.204782	1.826051	-1.290546
H	-4.847902	-1.812947	-3.138794
H	-6.234374	0.250744	-3.219603
C	4.079329	-1.581686	-2.116715
H	4.137028	-0.541187	-2.450336
H	5.085106	-2.015443	-2.126328
H	3.446238	-2.131712	-2.819373
C	3.456966	-3.433262	0.036622
H	4.483024	-3.802395	-0.066819
H	3.133377	-3.563161	1.073755
H	2.796711	-4.025087	-0.604297
C	4.594470	-0.830675	0.643332
H	5.575156	-1.307267	0.538073
H	4.679577	0.225168	0.369236
H	4.279213	-0.889068	1.689422
C	1.201690	3.283293	-0.923212
H	1.102978	2.561989	-1.726606
C	0.403401	4.253372	1.182668
H	-0.314264	4.262368	1.998526
C	1.441979	5.168909	1.155737
H	1.545669	5.903724	1.947503
C	2.239503	4.199889	-0.938503
C	2.359140	5.142619	0.095193
H	2.955707	4.198922	-1.754105
H	3.170898	5.864056	0.070736

15_4

E = -1410.12696666 a.u.

C	0.417180	-0.805383	3.489873
C	0.455030	-1.370777	2.050275
C	0.662126	-0.167334	1.114655
C	0.149550	-0.253120	-0.295444
C	-0.095045	0.643977	3.339824
C	0.369654	1.075347	1.956805
C	1.795841	0.806289	1.561595
P	-4.363159	0.061027	-0.382369
Au	-2.020004	-0.140592	-0.340984
C	1.837152	-1.149840	-1.596743
C	0.528865	-1.573726	-1.136946

H	-0.213288	-1.406824	4.151573
H	1.420826	-0.809812	3.928277
H	-0.509639	-1.833931	1.799602
H	1.222838	-2.146216	1.946090
H	0.418867	0.639463	-0.870236
H	-1.192097	0.671933	3.373237
H	0.270635	1.302181	4.136532
H	-0.119803	1.930588	1.496051
H	2.434533	0.399006	2.343598
H	0.511157	-2.452231	-0.493216
H	-0.171707	-1.704661	-1.960237
H	1.832780	-0.433611	-2.417112
C	3.117048	-1.489706	-1.086911
C	3.314916	-2.519410	-0.126939
C	4.257832	-0.846108	-1.640167
C	4.595577	-2.881705	0.257103
H	2.460974	-3.039897	0.291040
C	5.536507	-1.223996	-1.260951
H	4.115213	-0.050416	-2.365324
C	5.706336	-2.238327	-0.310447
H	4.741827	-3.673157	0.985361
H	6.401549	-0.732793	-1.694607
H	6.708005	-2.535162	-0.012880
C	2.552806	1.708811	0.642431
C	3.957375	1.672049	0.677759
C	1.947055	2.624890	-0.235059
C	4.727032	2.502600	-0.136019
H	4.451384	0.987310	1.363223
C	2.714533	3.450434	-1.060019
H	0.865830	2.726329	-0.261492
C	4.108217	3.392100	-1.017904
H	5.811289	2.462856	-0.073164
H	2.218795	4.153480	-1.724006
H	4.704259	4.044183	-1.649804
C	-4.981559	1.324315	-1.569253
H	-4.660135	1.069683	-2.583476
H	-6.075480	1.376424	-1.542055
H	-4.569928	2.305209	-1.313787
C	-5.243716	-1.485771	-0.852477
H	-6.327600	-1.327009	-0.858133
H	-4.924205	-1.805698	-1.848663
H	-5.002422	-2.281096	-0.141055
C	-5.104513	0.542824	1.231367
H	-6.193460	0.624413	1.145759
H	-4.860195	-0.205924	1.990639
H	-4.697883	1.506132	1.553057

TS($13p_1$)$_2$

E = -1410.12866523 a.u.

C	-0.312514	-3.967510	-1.353141
C	-0.105216	-2.527158	-1.879113
C	0.556140	-1.746478	-0.730587
C	0.416075	-0.243274	-0.715068
C	-0.441853	-3.826833	0.180983
C	0.380243	-2.590852	0.521748
C	1.758943	-2.473868	-0.081429
P	-3.880477	0.630196	0.665873
Au	-1.716792	0.241885	-0.077045
C	1.690477	0.604725	-1.628503
C	0.333464	0.537914	-2.095364
H	-1.186236	-4.445516	-1.805727
H	0.548904	-4.593657	-1.606350
H	-1.078737	-2.065799	-2.099318
H	0.476349	-2.514778	-2.809781
H	0.668449	0.280338	0.209320
H	-1.488162	-3.655703	0.468110
H	-0.103636	-4.723340	0.712534
H	0.214340	-2.110622	1.483861
H	2.098130	-3.339403	-0.648065
H	2.362581	-0.193025	-1.926671
H	0.098644	-0.145579	-2.904586
H	-0.248248	1.453642	-2.137551
C	-4.062412	2.218981	1.570443
H	-3.787847	3.052814	0.917905
H	-5.097807	2.349480	1.903335
H	-3.401651	2.228186	2.442087
C	-4.489353	-0.658807	1.825245
H	-5.512396	-0.429900	2.142918
H	-4.476873	-1.636886	1.335636
H	-3.842571	-0.703426	2.706317
C	-5.124844	0.693456	-0.684137
H	-6.123841	0.871250	-0.271486
H	-4.877062	1.498458	-1.382049
H	-5.127484	-0.252902	-1.232710
C	2.319238	1.804426	-1.051284
C	3.680624	1.748701	-0.703150
C	1.622158	3.012987	-0.863578
C	4.328291	2.869889	-0.190534
H	4.227968	0.819598	-0.830981
C	2.270308	4.129368	-0.339178
H	0.575915	3.098436	-1.143282
C	3.625207	4.062217	-0.003757
H	5.381612	2.811160	0.066482
H	1.721645	5.057191	-0.205933
H	4.130282	4.936537	0.396170
C	2.895748	-1.786554	0.604683
C	4.195576	-2.005822	0.115921
C	2.748475	-0.965927	1.734084
C	5.307427	-1.429215	0.731279
H	4.337367	-2.655282	-0.745172
C	3.857857	-0.382470	2.348211
H	1.765415	-0.797111	2.166054
C	5.142192	-0.611184	1.851097
H	6.302034	-1.629951	0.342620
H	3.717728	0.241600	3.226476
H	6.005381	-0.167935	2.339044

$13p_1 \cdot (AuPMe_3)^+$

E = -1410.13827632 a.u.

C	-0.068094	2.612147	3.419469
C	0.665015	1.297947	3.054540
C	0.754548	1.291205	1.524365
C	1.043595	0.015751	0.786818
C	-0.956946	2.944099	2.197244
C	-0.217412	2.340562	1.009450
C	1.263301	2.598334	0.888882
P	-3.635895	-0.467458	-0.972747

Au	-1.599233	-0.747529	0.076127
C	1.861604	-1.041481	1.368024
C	0.305536	-1.370910	1.209968
H	-0.646469	2.516120	4.342706
H	0.657018	3.414450	3.588783
H	0.070681	0.437219	3.391216
H	1.643153	1.226756	3.544537
H	1.121140	0.131745	-0.290223
H	-1.939094	2.461604	2.294521
H	-1.132660	4.020628	2.092351
H	-0.769542	2.161564	0.088817
H	1.690650	3.302767	1.602230
H	2.096157	-0.919194	2.423209
H	-0.168225	-1.473925	2.182097
H	0.243185	-2.236260	0.547630
C	-4.029834	-1.832959	-2.135352
H	-4.049276	-2.785465	-1.598084
H	-5.006813	-1.662686	-2.600630
H	-3.265351	-1.889555	-2.915559
C	-3.756737	1.071899	-1.966822
H	-4.740822	1.136232	-2.443664
H	-3.614045	1.944957	-1.323544
H	-2.983118	1.077305	-2.740031
C	-5.042680	-0.402664	0.206155
H	-5.985619	-0.278525	-0.337359
H	-5.083510	-1.327964	0.788011
H	-4.913013	0.436403	0.895669
C	2.838975	-1.880082	0.607558
C	3.304501	-3.067159	1.196185
C	3.316838	-1.516368	-0.658860
C	4.216603	-3.880714	0.527600
H	2.949219	-3.352241	2.184031
C	4.230327	-2.333885	-1.328321
H	3.008880	-0.580110	-1.114746
C	4.678961	-3.517006	-0.740411
H	4.568903	-4.795218	0.995743
H	4.599005	-2.037122	-2.306034
H	5.391956	-4.148912	-1.261835
C	1.966179	2.617959	-0.438564
C	3.345805	2.356247	-0.489520
C	1.304384	2.933044	-1.633345
C	4.038666	2.396259	-1.699409
H	3.879702	2.125733	0.429457
C	1.995634	2.971256	-2.847669
H	0.246447	3.180440	-1.614575
C	3.363535	2.699731	-2.885231
H	5.106444	2.196405	-1.715686
H	1.466180	3.228527	-3.761044
H	3.902826	2.735692	-3.827353

TS(13p$_1$)rot

E = -1410.11762564 a.u.

C	-0.179997	-1.511388	3.526679
C	-0.254013	-0.318468	2.543221
C	-0.454802	-0.922862	1.142088
C	-0.092376	-0.083645	-0.069097
C	0.315352	-2.703927	2.675893
C	-0.170358	-2.390781	1.266534
C	-1.626536	-1.986743	1.104805
P	4.336050	0.590210	-0.490175
Au	1.995493	0.263615	-0.247834
C	-2.366048	1.030505	-0.271142
C	-0.909778	1.221259	-0.092239
H	0.477264	-1.303611	4.376383
H	-1.168762	-1.727703	3.945681
H	0.699897	0.226036	2.534934
H	-1.033153	0.400139	2.830331
H	-0.355891	-0.632307	-0.981358
H	1.412423	-2.745200	2.670124
H	-0.044516	-3.667725	3.053666
H	0.279277	-2.929851	0.435227
H	-2.224299	-2.008384	2.014280
H	-2.670382	0.051740	-0.642451
H	-0.701946	1.875785	0.763573
H	-0.603548	1.823523	-0.974175
C	5.086018	-0.286810	-1.927674
H	4.616518	0.054865	-2.855087
H	6.163973	-0.099457	-1.982230
H	4.914122	-1.363351	-1.834304
C	5.344845	0.027049	0.946402
H	6.411864	0.201325	0.769680
H	5.038943	0.567681	1.847219
H	5.180898	-1.041334	1.116430
C	4.851741	2.343913	-0.728964
H	5.938741	2.420498	-0.840139
H	4.371836	2.751269	-1.623971
H	4.537891	2.942511	0.131529
C	-3.399026	1.965657	-0.103054
C	-4.731770	1.555000	-0.416887
C	-3.176148	3.293500	0.375202
C	-5.790085	2.433688	-0.259921
H	-4.896064	0.542057	-0.774561
C	-4.239513	4.162044	0.522255
H	-2.169515	3.615828	0.619656
C	-5.542550	3.732845	0.205967
H	-6.802632	2.124124	-0.496872
H	-4.077030	5.172547	0.882708
H	-6.372665	4.423216	0.327559
C	-2.434305	-2.349774	-0.092676
C	-3.839972	-2.316001	0.013596
C	-1.887218	-2.735165	-1.330401
C	-4.661101	-2.639968	-1.067043
H	-4.290308	-2.053014	0.968809
C	-2.708053	-3.054493	-2.414833
H	-0.811053	-2.813545	-1.449726
C	-4.097220	-3.005032	-2.292998
H	-5.741338	-2.628233	-0.945339
H	-2.255398	-3.356258	-3.355403
H	-4.732347	-3.264306	-3.134901

TS(13q$_1$)$_1$

E = -1641.16834784 a.u.

C	-0.291790	-3.563259	-2.055671
C	-0.187085	-2.772158	-0.729129
C	-0.796137	-1.385663	-0.998261
C	-0.278166	-0.174611	-0.352426
C	-0.296051	-2.500086	-3.174131
C	-0.936695	-1.271384	-2.548030

C	-2.173517	-1.432100	-1.731912
P	4.131951	0.483593	-0.348525
Au	1.801129	0.131515	-0.250605
C	-1.666836	0.831235	1.324798
C	-0.709099	-0.127724	1.654759
H	0.525249	-4.282040	-2.169478
H	-1.219445	-4.145076	-2.082204
H	0.864219	-2.632289	-0.448042
H	-0.674015	-3.299018	0.094796
H	-0.760895	0.726577	-0.733780
H	0.727090	-2.250121	-3.481870
H	-0.832340	-2.834111	-4.070191
H	-0.755868	-0.308684	-3.017580
H	-2.598705	-2.434128	-1.715863
H	-2.657539	0.488100	1.037795
H	0.230221	0.248135	2.045199
C	4.625715	1.823429	-1.509826
H	4.166359	2.767791	-1.202905
H	5.714472	1.942195	-1.524320
H	4.277941	1.585191	-2.519392
C	5.079502	-0.989787	-0.913380
H	6.151433	-0.769080	-0.957771
H	4.913879	-1.822930	-0.223838
H	4.735528	-1.292240	-1.906960
C	4.921637	0.951873	1.248009
H	5.999255	1.097577	1.116808
H	4.479749	1.880388	1.621550
H	4.756082	0.166508	1.991505
C	-1.482790	2.265040	1.314957
C	-2.565639	3.075050	0.903490
C	-0.286190	2.896402	1.728839
C	-2.457744	4.461377	0.904045
H	-3.488649	2.601396	0.582768
C	-0.181739	4.282056	1.720243
H	0.554045	2.303113	2.074442
C	-1.265342	5.067988	1.309176
H	-3.300534	5.070511	0.591832
H	0.738200	4.756907	2.048307
H	-1.181314	6.150834	1.314413
C	-3.231044	-0.379267	-1.623530
C	-4.401034	-0.680650	-0.902308
C	-3.148442	0.873918	-2.249358
C	-5.444731	0.238924	-0.798482
H	-4.502032	-1.660678	-0.441530
C	-4.193877	1.795552	-2.151509
H	-2.279870	1.131592	-2.847872
C	-5.344454	1.485043	-1.424096
H	-6.342748	-0.024230	-0.246551
H	-4.112558	2.752316	-2.659949
H	-6.162693	2.196678	-1.361242
C	-1.020937	-1.491460	2.150485
C	0.009438	-2.218197	2.768613
C	-0.218487	-3.496014	3.277109
C	-2.297408	-2.072467	2.070674
H	-3.121243	-1.530408	1.617883
C	-2.525591	-3.350540	2.577277
H	-3.519411	-3.784438	2.512808
C	-1.487439	-4.069366	3.177486
H	-1.671001	-5.063419	3.574398
H	0.999386	-1.774748	2.850822
H	0.591099	-4.040650	3.754225

TS($13q_1$)$_2$

E = -1641.17008111 a.u.

C	0.380084	2.761396	2.797161
C	0.239340	2.422461	1.293223
C	-0.582251	1.118443	1.217065
C	-0.382904	0.173105	0.055426
C	0.273377	1.410789	3.537616
C	-0.603121	0.555969	2.634482
C	-1.868588	1.160007	2.087888
P	3.899181	-1.414431	0.344327
Au	1.737330	-0.580125	0.122120
C	-1.727785	0.185054	-1.220631
C	-0.405819	0.658962	-1.501697
H	1.318016	3.283528	3.010076
H	-0.424294	3.432737	3.115583
H	1.227874	2.234886	0.854854
H	-0.202423	3.248903	0.729977
H	-0.649546	-0.869550	0.252726
H	1.261065	0.939283	3.632783
H	-0.133026	1.517373	4.549764
H	-0.586832	-0.522290	2.777776
H	-2.094578	2.165777	2.438329
H	-2.438930	0.883456	-0.794113
H	0.181178	-0.010206	-2.126235
C	3.967709	-3.005348	1.262205
H	3.376076	-3.762280	0.739154
H	5.002561	-3.353990	1.348213
H	3.550403	-2.872460	2.264671
C	5.034891	-0.290983	1.253438
H	6.030132	-0.741017	1.336353
H	5.116386	0.664382	0.726895
H	4.643838	-0.100397	2.257127
C	4.735766	-1.747223	-1.258468
H	5.747059	-2.132866	-1.090015
H	4.163029	-2.482844	-1.830723
H	4.797449	-0.825006	-1.843510
C	-2.283112	-1.087035	-1.696436
C	-3.654811	-1.330704	-1.497066
C	-1.517982	-2.051933	-2.382247
C	-4.246808	-2.494773	-1.980170
H	-4.253984	-0.601392	-0.961265
C	-2.110425	-3.222489	-2.848454
H	-0.459733	-1.891578	-2.566865
C	-3.476717	-3.445871	-2.652851
H	-5.308584	-2.661311	-1.825815
H	-1.509621	-3.956014	-3.378102
H	-3.937545	-4.355302	-3.027145
C	-3.123664	0.375713	1.865149
C	-4.288245	1.076613	1.501747
C	-3.230228	-1.006638	2.079509
C	-5.513980	0.424114	1.363805
H	-4.235545	2.153542	1.355279
C	-4.454303	-1.663662	1.940306
H	-2.362825	-1.580801	2.391866
C	-5.602122	-0.952696	1.585386
H	-6.401238	0.993656	1.101035
H	-4.512158	-2.732547	2.126086

H	-6.556958	-1.462584	1.494906
C	-0.090521	2.094191	-1.826448
C	1.234331	2.441174	-2.126255
C	1.569543	3.747874	-2.475898
C	-1.081369	3.080032	-1.912994
H	-2.121321	2.832055	-1.725059
C	-0.747646	4.390694	-2.260314
H	-1.527944	5.143279	-2.326045
C	0.577451	4.729818	-2.537005
H	0.834166	5.748483	-2.812196
H	2.009934	1.678042	-2.085803
H	2.600616	3.999082	-2.707775